

SYMPOSIUM A

Amorphous and Nanocrystalline Silicon Science and Technology–2005

March 28 - April 1, 2005

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* Invited paper

TUTORIAL

Thin-Film Silicon Materials & Devices for Large-Area and Flexible Electronics
Monday March 28, 2005
8:30 AM - 4:30 PM
Room 2002 (Moscone West)

Hydrogenated amorphous silicon (a-Si:H), nanocrystalline (nc-Si), and polycrystalline silicon (poly-Si) are the thin-film semiconductors used for large-area electronics. They are applied in backplanes for active matrix liquid-crystal displays (AM-LCDs), in optical scanner and radiation imaging arrays, and in thin-film solar cells.

The tutorial describes silicon film growth and properties, device physics, and applications. State-of-the-art, low-temperature processing will be presented and related to recent work with flexible substrates of organic polymers, steel, and glass. Attention will be given to the connection between material properties and device performance. Existing and emerging applications will be described and discussed.

Instructors:

Sigurd Wagner, Princeton University
Joao Pedro Conde, Instituto Superior Tecnico, Lisbon

SESSION A1: Pioneers in the Use of Photons to Study Films

Chair: Reinhard Carius
Tuesday Morning, March 29, 2005
Room 2002 (Moscone West)

8:30 AM *A1.1

The Electronic Structure of a-Si:H as Measured by Photoelectron Spectroscopy. Lothar Ley, Institut fuer Technische Physik II, Universitaet Erlangen-Nuernberg, Erlangen, Germany.

Photoelectron spectroscopy (PES) is the most direct way to gain information about the density of occupied electronic states in condensed matter. As such it complements in an ideal way optical data and has helped to unravel some of the idiosyncrasies of the electronic structure of amorphous materials. Here I shall present seminal results that were obtained in the 80ties and 90ties on amorphous hydrogenated silicon (a-Si:H) and related amorphous materials. The topics covered include the identification of Si-H and Si-F bonding states deep in the valence band and the accompanying recession of the valence band edge which explains the opening of the fundamental gap with increasing hydrogen or fluorine content. Taking advantage of the surface sensitivity of PES some important results concerning the near surface enrichment in hydrogen on freshly prepared a-Si:H are presented which have helped to understand the growth of a-Si:H. The bulk of the talk, however, will cover information obtained from yield spectroscopy which is a variant of PES that has the advantage to cover up to seven orders of magnitude in the density of states. As such it brings valence and conduction band tails and defects in the reach of photoelectron spectroscopy. With yield it was possible to measure directly the exponential slopes of the valence and conduction band edges as a function of deposition conditions and doping. Also, the energies and concentrations of D^- and D^+ defect states created in response to doping were unambiguously located in the gap of a-Si:H. Thereby it was demonstrated that occupied D^- defect states are always created below the Fermi level E_F and unoccupied D^+ above E_F so as to minimize the electronic energy of the network. This was the birth of the defect pool model that has played a central role in the defect dynamics of a-Si:H ever since. By evaluating yield spectra as a function of boron doping it has been demonstrated that the valence band tail slope is unaffected by boron doping. That is in contrast to the weak bond - dangling bond conversion model and requires a reconsideration of this model for the case of heavy doping.

9:00 AM *A1.2

Photothermal Deflection Spectroscopy: Past, Present and Future. Warren Jackson, Hewlett Packard Labs, Palo Alto, California.

Photothermal deflection spectroscopy (PDS) has provided invaluable information about non-crystalline films, amorphous silicon in particular. Because of the potentially wide applicability of PDS to most thin films including those comprised of novel and exotic materials, it is useful to review the role of photothermal spectroscopy in understanding amorphous silicon along with the wide variety of experiments that have been performed using PDS. PDS has proven to be complementary to such measurements as electron spin resonance, luminescence, deep level transient spectroscopy, reflection and

transmission, and photoconductivity. In conjunction with these and other experimental methods, PDS has provided information about both the identity, energy, and distribution of subgap defects in hydrogenated amorphous silicon. In addition PDS has been used to measure surface optical properties, film quality, nonradiative recombination, mu-tau products, thermal properties, and PDS microscopy when applied to amorphous silicon. Present and future prospects for PDS will also be discussed.

9:30 AM *A1.3

Urbach Edge, Disorder, and Absorption on-set in a-Si:H. George Cody, Aerospace and Mechanical Engineering, Visiting Professor, Rutgers University-Piscataway, Princeton, New Jersey.

The optical properties of amorphous silicon are better known and understood, than any other amorphous semiconductor. Starting in the mid-70's, worldwide interest focused on amorphous silicon as the active component of a variety of thin film optical devices. Optimization of the optical properties, building on the independent band model of Jan Tauc, was the first step toward optimization of the performance of thin film solar cells, and the information derived from the optical properties could be related to the electrical properties of the thin film material as well. The device interest in amorphous silicon gave experimentalists access to thin films of unprecedented uniformity, purity and homogeneity, and the precision of these early experiments led to the discovery of the Urbach edge in amorphous silicon[1], and to new fundamental optical models for the absorption edge of amorphous semiconductors by Hass and Ehrenreich[2], Grein and John[3], and more recently by Fortman[4]. The comparison between amorphous semiconductors and their crystalline counterparts highlights the remarkable successes of the theory, as well as its limitations. A recent analysis of extensive experimental data on the Urbach edge of amorphous silicon by Orapunt and O'Leary[5], concludes that not only does amorphous silicon have an Urbach edge which depends on disorder, but it also has an Urbach focus at 2.20eV, plus or minus 0.06eV, which does not! The discovery that crystalline silicon has an Urbach edge[3, 6] suggests a variety of experiments to understand the similarities and differences between the Urbach edge of direct, and indirect, crystalline semiconductors, and their amorphous counterparts. In this talk we review the concept of a "standard model" for the absorption edge of amorphous silicon. We describe the physics of the model, summarize its experimental status, and suggest current limitations, and opportunities. 1 G. D. Cody, in Hydrogenated Amorphous Silicon, Volume 21B: Optical Properties, J. I. Pankove, Ed., Academic Press, Orlando, 1984, pp. 11-82. 2 K. C. Hass, H. Ehrenreich, Annals of Physics, 164, (1985) 77-102. 3. C. H. Grein, S. John, Physical Review B, 39, (1989) 1140. 4 C. M. Fortman, Physical Review Letters, 81, (1998) 3683-6. 5 F. Orapunt, S. K. O'Leary, Applied Physics Letters, 84, (2004) 523-525. 6 G. D. Cody, Journal of Non-Crystalline Solids, 141, (1992) 3-15.

SESSION A2: Growth I: Large Grains and Epitaxy

Chair: Ruud Schropp
Tuesday Morning, March 29, 2005
Room 2002 (Moscone West)

10:30 AM A2.1

Large-grained Polycrystalline Films for Photovoltaic Devices. Christine Esber Richardson and Harry A. Atwater; Thomas J. Watson Laboratory of Applied Physics, California Institute of Technology, Pasadena, California.

We have investigated the low-temperature epitaxial growth of thin silicon films by hot-wire chemical vapor deposition on large-grained polycrystalline template layers formed by selective nucleation and solid phase epitaxy (SNSPE). Using reflection high energy electron diffraction (RHEED), X-ray diffraction (XRD), Raman Spectroscopy, and transmission electron microscopy (TEM), we have found the ideal conditions for epitaxial growth on templates. Epitaxial films were grown to over 500nm thickness with $R=1$ and substrate temperature of 400 C. Previously we have investigated epitaxial thickness as a function of temperature. Now we see the effect of hydrogen dilution on the critical epitaxial thickness and texture of the film. At each temperature there is an optimal dilution to reach the thickest epitaxial film. We have studied several deposition parameters and offer a slice in phase space of those results by varying pressure, H dilution, and substrate temperature. We have also characterized the structure of these films using AFM to look at the surface texture and light trapping advantage; FTIR to look at the H grain boundary and film incorporation; Raman to look at the crystalline fraction and photoconductive decay to look at the minority carrier lifetimes using a 532 nm laser as the excitation source. No effort was made to passivate the film surfaces. Although nickel is a known lifetime killer even in small concentrations, the lifetimes of films on SNSPE templates are comparable to the lifetimes of films on Si(100). Under

LLI conditions, the minority carrier lifetimes for films on Si(100) range from 5.7 to 7.5 μ s and the minority carrier lifetimes for films on SNSPE templates range from 5.9 to 19.3 μ s. Polycrystalline films grown by HWCVD have been used in the fabrication of 1.5 μ m-thick thin-film transistors with channel mobilities of 4.7 cm²/Vs on glass substrates. Using the Einstein relation, we can determine that, if the mobilities in our films were comparable, the minority carrier diffusion coefficient would be 0.1175 cm²/s. From this value and the minority carrier lifetime of \sim 7 μ s measured by RCPD in a 1.5 μ m thick film on Si(100), we obtain a value for the minority carrier diffusion length of approximately 9 μ m, which is comparable to the thicknesses of the active layers for thin-film photovoltaics (1 to 30 μ m). The minority carrier lifetimes of films on SNSPE templates are comparable, making it possible that the growth of epitaxial films by HWCVD on large-grained SNSPE templates is a viable strategy for the fabrication of thin-film photovoltaics. Preliminary device results will be discussed.

10:45 AM **A2.2**

Suppression of Nucleation during the Aluminum-Induced Layer Exchange Process. Jens Schneider, Juliane Klein, Andrey Sarikov, Martin Muske, Stefan Gall and Walther Fuhs; Hahn-Meitner-Institut, Berlin, Germany.

Thin polycrystalline silicon (poly-Si) layers on foreign substrates prepared at low temperature are interesting for large area electronic devices. To form such poly-Si layers crystallization of amorphous silicon (a-Si) using solid phase crystallization (SPC), metal-induced crystallization (MIC), and laser-induced crystallization has been investigated throughout the last decades. MIC has attracted particular interest due to the large silicon grains obtained. Annealing of an aluminum / a-Si layer stack below the eutectic temperature leads to a layer exchange with a concurrent crystallization of the amorphous silicon. A thin permeable membrane, usually an oxide layer, separating the initial aluminum and a-Si layers determines strongly the dynamics of this aluminum-induced layer exchange (ALILE) process by controlling the mass transport across the Al/Si interface. The suppression of nucleation during annealing is a characteristic feature of the ALILE process. Samples with different oxide layer thickness were annealed in the heating stage of an optical microscope for in-situ observation. The number of Si crystallites was monitored as a function of the annealing time. In general the process can be divided into three phases: A first phase until nucleation starts, a second phase with a specific nucleation rate and a third phase when nucleation is suppressed. We found that depending on the process parameters the duration of these phases varies strongly. For very thin oxide layers nucleation occurred continuously till the end of the process. In contrast to that, for very thick oxide layers the second phase is extremely short (i.e. nucleation takes place almost at once) and further nucleation is suppressed. The suppression of the formation of new nuclei is typical for the ALILE process and allows the preparation of poly-Si films with large grain size. The results are discussed in terms of a model derived from thermodynamic nucleation and crystal growth theory. The mechanism behind the experimentally observed behavior can be understood considering the time dependent Si concentration within the aluminum layer and its importance in the Al-Si phase diagram. Si is supplied by diffusion from the a-Si layer across the oxide layer into the aluminum. When a critical nucleation concentration larger than the saturation concentration is exceeded silicon nucleates within the Al. In the second and third phase of the ALILE process the silicon concentration is reduced within the aluminum layer because nucleation and growth of Si crystallites is fed by Si diffusion from the aluminum towards the crystallites. When the amount of silicon incorporated into the crystallites exceeds the supply from the a-Si phase the overall concentration decreases and nucleation is suppressed.

11:00 AM **A2.3**

Improved Low-temperature Silicon Homoepitaxy by Ta-filament Hot-Wire Chemical Vapor Deposition.

Charles Teplin, Eugene Iwaniczko, Dean H. Levi, Joel Pankow, Kim M. Jones, Qi Wang and Howard M. Branz; NREL, Golden, Colorado.

We find that low-temperature silicon epitaxy on (100) silicon wafers by hot-wire chemical vapor deposition is dramatically improved when a tantalum filament is used in place of a tungsten filament to decompose the pure silane gas precursor. With a 12 nm/min growth rate, we obtain the thickest epitaxial layers with a Ta filament current of 11.5 A and a Si substrate temperature of $370 \pm 20^\circ$ C. After 500 nm of epitaxial growth, less than 1% of the film surface is hydrogenated amorphous silicon (a-Si:H). Transmission electron microscopy shows that at a thickness of 200 nm, these films are still entirely epitaxial c-Si and that micron-scale regions remain epitaxial to at least 1 micron in thickness. Epitaxial thicknesses increase with increasing substrate temperature; pressure and flow-rate dependences are also studied. Real-time spectroscopic ellipsometry is used for routine monitoring of the epitaxial growth and subsequent breakdown into a-Si:H cones, and selected films have been studied with

transmission electron microscopy. We will discuss our data in relationship to the hydrogen supersaturation [J. Thiesen et al., APL 77, 3589 (2000).] and limited adatom mobility [D. J. Eaglesham et al., Phys. Rev. Lett. 65, 1227 (1990) and H. Jorke et al., Phys. Rev. B 40, 2005 (1989).] models for epitaxial breakdown.

11:15 AM **A2.4**

Application of Field-Enhanced Rapid Temperature Annealing to Activation of Doped Polycrystalline Si Thin Films. B. S. So¹, Y. H. You¹, Y. H. Kim¹, J. H. Hwang¹, D. H. Shin², S. R. Ryu², K. Choi³ and Y. C. Kim⁴; ¹Dept. of Materials Sci. & Eng., Hongik University, Seoul, South Korea; ²Viatron Technologies, Seoul, South Korea; ³KICET, Seoul, South Korea; ⁴Korea University of Technology and Education, Chunan, South Korea.

Low temperature polycrystalline Si TFTs have opened a way for the next generation of displays, due to higher mobility of charge carriers, relative to amorphous Si (a-Si) TFTs. The applications of polycrystalline silicon extend from the current liquid crystal displays (LCD) to the next-generation organic light-emitting diode (OLED) displays. In particular, the OLED devices require a strict control in TFT characteristics, with emphasis on crystallization, gate dielectrics, and ion-doping. Especially, ion-doping is performed to provide the source/drains, channel-doping, and lightly-doped drains, followed by ion-activation. The activation is generally obtained by furnace-annealing, excimer laser annealing, rapid temperature processing, etc. A new approach to ion-activation has been studied using rapid thermal annealing combined with alternating magnetic fields. In combination with rapid temperature annealing, the activation processing is investigated in terms of preheating temperature, rapid thermal annealing, alternating magnetic field, operating temperature, and activation energy. Comparative approach has been made on i) furnace activation, ii) excimer laser annealing, and iii) Field-Enhanced RTA. The microstructural features were investigated from microscale to nanoscale range using a variety of microscopy techniques (Optical Microscopy, SEM, FESEM) along with the surface characteristics using AFM and the electrical properties using 4 point-probe resistivity and Hall-effect measurements. The crystallinity and/or damage recovery was evaluated using Raman spectroscopy which incorporates both amorphous and polycrystalline portions. The ramifications of a new approach will be discussed in conjunction with active-matrix TFT for OLED.

11:30 AM **A2.5**

Structural Properties of Laser-Crystallized Polycrystalline SiGe Thin Films. Moshe Weizman¹, Norbert H. Nickel¹, Ina Sieber¹ and Baojie Yan²; ¹Hahn-Meitner-Institut, Berlin, Germany; ²United Solar Systems Corp., Troy, Michigan.

Crystalline silicon-germanium alloys exhibit enhanced optical absorption, lower thermal conductivity and lower processing temperature in comparison to c-Si. Additionally, the production methods of SiGe are perfectly compatible with the well established Si technology. This motivates the recently rising interest in SiGe as a substitute for Si in thin film solar cells, thin film electronic devices, and micro electro mechanical systems (MEMS). The SiGe specimens investigated in this work were fabricated by the following steps. Initially, amorphous silicon-germanium films (a-Si_{1-x}Ge_x:H) were deposited by glow-discharge decomposition of a mixture of disilane, germane, and hydrogen to a thickness of 100 to 255 nm. The Ge content of the resulting samples was determined from elastic recoil detection analysis (ERDA) measurements and varied between 19% and 84%. The amorphous samples were crystallized employing a XeCl excimer laser. Phase segregation in the poly SiGe films was studied by energy dispersive X-ray (EDX) and Raman backscattering measurements. Information on the grain size was obtained using scanning electron microscopy (SEM), and atomic force microscopy (AFM) measurements were used to determine the surface roughness. Energy dispersive X-ray composition measurements of the laser crystallized poly-Si_{1-x}Ge_x with 0.33 < x < 0.7 reveal a significant segregation into Ge rich and poor areas, which deviate by up to 40% from the homogeneous composition of the amorphous starting material. The Raman phonon spectra of those samples exhibits peak splitting that is directly correlated with the segregation. This phase segregation effect becomes more pronounced with increasing laser fluence. When the laser fluence is high enough to completely melt the specimen an unexpected and striking phenomenon is observed, namely coherent self-organization. Under these crystallization conditions Ge rich spikes appear that rise up to 120 nm above the surface and have a well defined distance from each other. For poly-Si_{0.55}Ge_{0.45} the distance between spikes can be varied between 1.2 and 1.6 μ m. This surprising result stands in contradiction to the suggestion that fast cooling, which leads to solidification from a super cooled liquid, should result in the formation of a homogeneous SiGe alloy. A further surprising result is the fact that these samples do not reveal an increase in the average grain size in the transition between partial and complete melting that is well-known in poly-Si as the super lateral

growth crystallization regime.

11:45 AM **A2.6**

Ge Growth on Nanostructured Silicon Surfaces.

Ganesh Vanamu¹, Abhaya K. Datye¹ and Saleem H. Zaidi²;

¹Chemical and Nuclear, University of New Mexico, Albuquerque, New Mexico; ²Gratings, Inc, Albuquerque, New Mexico.

Defect-free Ge heteroepitaxial films grown on Si substrates find many applications including III-V solar cells [1], photodetectors in 1.3-1.5 μm wavelength range [2], and high-mobility electron devices [3]. The growth of thick (\sim few μm s) pseudomorphic heteroepitaxial films on Si substrates beyond critical thickness, h_c , is difficult due to thermal and lattice expansion mismatches. In our earlier work on Ge/SiGe growth on patterned Si substrates, we have demonstrated substantial reduction in defect density as pattern sizes are reduced from μm to nm-scales [4]. Here, we report on extension of this work to 100 % Ge epilayer growth on nanostructured Si surfaces. Silicon nanostructured surfaces were prepared through a combination of interferometric lithography and standard semiconductor processing methods. The quality of Ge layers was examined by SEM, TEM, and HRXRD measurements. The defect density was evaluated through etch pit measurements [4]. Preliminary evaluation shows three orders of magnitude defect density reduction to (less than $10^6/\text{cm}^2$) in comparison with growth on un-patterned substrates. Details of characterization and photoresponse in 1.3-1.5 μm wavelength range will be presented at the conference. REFERENCES 1. S. A. Ringel, J. A. Carlin, C. A. Andre, D. M. Wilt, E. B. Clark, P. Jenkins, D. Scheiman, C. W. Leitz, A. A. Allerman, and E. A. Fitzgerald, Prog. Photovoltaics 10, 417 (2002). 2. G. Masini, L. Colace and G. Assanto, Appl. Phys. Lett., 82, 2524 (2003) 3. J. A. Carlin, S. A. Ringel, E. A. Fitzgerald, M. Bulsara, and B. M. Keyes, Appl. Phys. Lett., 76, 1884 (2000). 4. G. Vanamu, A. K. Datye and S. H. Zaidi, Mat. Res. Soc. Symp. Proc. Vol. 809, 2004, Materials Research Society.

SESSION A3: The Roles of Hydrogen
Chair: Pauls Stradins
Tuesday Afternoon, March 29, 2005
Room 2002 (Moscone West)

1:30 PM **A3.1**

First-Principles Analysis of Growth Precursor Diffusion on Surfaces of Plasma-Deposited Silicon Thin Films.

Tamas Bakos, Mayur S. Valipa and Dimitrios Maroudas; Chemical Engineering, University of Massachusetts, Amherst, Massachusetts.

Hydrogenated amorphous silicon (a-Si:H) thin films are commonly deposited using SiH_4 -containing discharges under conditions where the SiH_3 radical is the dominant deposition precursor. The diffusion of deposition precursors on the growth surface determines the film surface smoothness or roughness and, thus, influences the optical and electronic properties of a-Si:H films used in photovoltaic and optoelectronic device fabrication technologies. In this presentation, we analyze various diffusion pathways of the SiH_3 radical on the hydrogen-terminated crystalline Si(100)-(2x1) surface using first-principles density functional theory (DFT) calculations and compare the obtained pathways and corresponding activation barriers for diffusion with results of molecular-dynamics (MD) simulations of SiH_3 migration on a-Si:H surfaces. Radical hopping mechanisms examined on the Si(100)-(2x1):H surface show that the activation energy barrier for radical surface migration (E_m) can be lowered by local surface relaxations that accompany the hopping of the SiH_3 radical from one surface Si atom to another and result in the breaking or forming of strained Si-Si bonds yielding $E_m \sim 0.45$ eV for radical migration along the surface Si dimer rows. The diffusion barrier is especially low when the SiH_3 radical hops between overcoordinated surface Si atoms in the trough between dimer rows yielding $E_m \sim 0.3$ eV. Analysis of MD simulations yields an average diffusion barrier of approximately 0.2 eV for SiH_3 diffusion on a-Si:H growth surfaces, which is mediated largely by surface overcoordination defects. Our synergistic DFT/MD analysis leads to the conclusion that the observed high smoothness of plasma-deposited a-Si:H films grown at low temperatures is due to the low energy barrier for surface diffusion of SiH_3 radicals that hop predominantly between overcoordinated surface Si atoms.

1:45 PM **A3.2**

The Role of SiH_3 Diffusion in Determining the Surface Smoothness of Plasma-Deposited Amorphous Si Thin Films: An Atomic-Scale Analysis.

Mayur S. Valipa^{1,2}, Tamas Bakos¹, Eray S. Aydil² and Dimitrios Maroudas¹; ¹Chemical Engineering, University of Massachusetts, Amherst, Massachusetts; ²Chemical Engineering, University of California, Santa Barbara, Santa Barbara, California.

Under conditions of low SiH_4 dissociation during the plasma-assisted deposition of hydrogenated amorphous silicon (a-Si:H) thin films, the dominant deposition precursor is the SiH_3 radical. The remarkable smoothness of device-quality a-Si:H films grown under these conditions has been used to conclude that the SiH_3 radical is very mobile and can passivate dangling bonds in surface valleys during diffusion, after adsorbing onto the film. However, the fundamental mechanisms underlying SiH_3 radical migration on a-Si:H film surfaces are not well understood and the corresponding activation barrier for the radical's surface diffusion is still not known. In this presentation, we discuss atomic-scale mechanisms of SiH_3 diffusion on a-Si:H surfaces as derived through a detailed fundamental analysis based on atomistic simulation. Using molecular-dynamics (MD) simulations of impingement of SiH_3 radicals on growth surfaces of smooth a-Si:H films, we studied the diffusion mechanism of the SiH_3 radical over the temperature (T) range $475 \leq T \leq 800$ K. By monitoring structural characteristics, such as the atomic coordination of the SiH_3 radical and of the surface Si atoms to which the radical is bonded during diffusion, we elucidated the operative mechanisms that govern radical transport on a-Si:H surfaces. The mobility of the SiH_3 radical was determined through the evolution of the mean squared displacement of the radical's center of mass, as monitored from the MD trajectory. The average activation barrier for radical diffusion on the a-Si:H surface was found to be 0.16 eV; this low barrier for diffusion is due to the weak adsorption of the radical onto the a-Si:H surface and its migration predominantly through overcoordination defects. In addition, we have carried out analysis of SiH_3 surface migration pathways based on density functional theory (DFT) calculations using crystalline Si surfaces as representative models of atomic bonding at film growth surfaces. The DFT analysis revealed that the SiH_3 surface migration barrier was reduced when the radical was weakly bonded to surface Si atoms that were overcoordinated. Interestingly, our MD simulations indicate that the diffusing SiH_3 radical incorporates into the a-Si:H film only when it transfers an H atom and forms a Si-Si backbond; the transferred H atom can then either be abstracted or diffuse into the bulk a-Si:H film. This H-transfer process is thermally activated and has important implications for the valley filling mechanisms responsible for a-Si:H surface smoothing. The H-transfer process does not require the presence of dangling bonds in surface valleys, but leads to preferential Si incorporation in such valleys of the surface morphology.

2:00 PM **A3.3**

Experimental Evidence for Extended Hydrogen Diffusion in Amorphous Silicon during Light-soaking.

Kail Fatiha^{1,2}, Fellah Samira¹, Hadjadj Aomar² and Roca i Cabarrocas Pere¹; ¹Laboratoire de Physique des Interfaces et des Couches Minces, Ecole Polytechnique, 91128 Palaiseau, French Polynesia; ²Laboratoire d'Analyse des Solides, Surfaces et Interfaces, Unite de Thermique et Analyse Physique, Universite de Reims, 51687 Reims Cedex 2, France.

We have studied hydrogen diffusion induced by light-soaking in p-type amorphous and intrinsic polymorphous silicon films deposited on glass substrates. The glass substrate is used to separate the atmospheric pressure from a secondary vacuum obtained by a turbo molecular pump, the film being on the vacuum side. The effects white, blue, green and red light illumination were studied. Mass spectrometry measurements allow to detect the hydrogen effusing from the silicon thin films when they are exposed to the light from the glass side. This indicates a long range hydrogen motion through the whole film, which ends with a release of hydrogen into the vacuum system. The changes in the film structure induced by the diffusion of hydrogen at room temperature during light soaking are characterized by spectroscopic ellipsometry and hydrogen exodiffusion measurements. In particular, a comparison of the hydrogen exodiffusion spectra of as-deposited and light-soaked samples shows that hydrogen content is reduced by 50 % p-type amorphous silicon and by 30 % in polymorphous silicon, with changes in hydrogen bonding configurations. These results unambiguously demonstrate the long range motion of hydrogen during light soaking.

2:15 PM **A3.4**

Initial Stage Hydrogen Movement in Hot-Wire Deposited SiNx:H during High-Temperature Annealing.

Hanno D. Goldbach¹, Andrea Scarfo¹, Vasco Verlaan¹, Karine van der Werf¹, Wim Arnold Bik¹, Henk Ch. Rieffe², Ingrid G. Romijn², Wim J. Soppe², Arthur W. Weeber² and Ruud E. I. Schropp¹; ¹Utrecht University, Debye Institute - SID, Utrecht, Netherlands; ²ECN, Solar Energy, Petten, Netherlands.

Silicon nitride (SiNx:H) layers were deposited using a high deposition rate Hot-Wire CVD technique (up to 3 nm/s) and their application as passivating antireflection coating on multicrystalline silicon solar cells was investigated. An important aspect is the dependence of the hydrogen release and diffusion during a short annealing treatment at temperatures well above the deposition temperature. Such annealing treatments (firing) are used during contact formation of

multicrystalline solar cells. Screen-printed solar cells with Hot-Wire deposited SiNx:H already have efficiencies in excess of 14 %, close to standard reference cells with SiNx:H deposited by PECVD. A series of SiNx:H layers with Si/N ratio in the range of 0.7-1.45 were first characterized using optical R/T, FTIR and ERD (Elastic Recoil Detection) measurements to determine optical constants n and k , Si-H, N-H and Si-N bond densities, Si-H peak position and H content. The H content measured by ERD is 2 at.-% higher than that derived from Si-H and N-H bond densities measured by FTIR. We contribute the difference between the two methods to the presence of molecular H₂, which can be detected as excess H by ERD compared to FTIR. To obtain more insight in the passivation during firing, which takes place at roughly 800 °C, the samples were annealed at this temperature for different times (30 sec - 10 min). For N-rich films and stoichiometric films the bonded H content, measured with FTIR, shows an increase up to 1 at.-% absolute within the first 60 seconds. At longer annealing times, the bonded H content decreases in line with the expected behavior. We suggest that the increase of the bonded H content within the first minute is due to the presence of H₂ incorporated in the SiNx matrix, which may dissociate at this high temperature. NMR measurements are underway to investigate this suggestion.

2:30 PM A3.5

Hydrogen Bonding in Amorphous and Polycrystalline SiGe Alloys. Norbert H. Nickel¹, Ina Sieber¹, Moshe Weizman¹ and B. Yan²; ¹Hahn-Meitner-Institut Berlin, Berlin, Germany; ²United Solar Ovonic Corporation, Troy, Michigan.

While amorphous silicon-germanium alloys are already successfully being used in triple-junction solar cells, polycrystalline SiGe alloys, among other applications, could be a good substitute for the Si absorber layer. The enhanced absorption of SiGe compared to Si makes it a very promising material. A major drawback of poly-SiGe alloys are localized states in the bandgap. However, they can be efficiently passivated with hydrogen. To optimize the defect passivation information on hydrogen bonding is important. The SiGe specimens investigated in this work were fabricated by the following steps. Initially, amorphous silicon-germanium films (a-Si_{1-x}Ge_x:H) were deposited by glow-discharge decomposition of a mixture of disilane, germane, and hydrogen to a thickness of 100 to 255 nm. The Ge content of the resulting samples was determined from elastic recoil detection analysis (ERDA) measurements and varied between 19 and 84 %. A second series of poly-SiGe alloys were fabricated using an excimer laser. Because of the large hydrogen content of the a-SiGe:H films a step-by-step crystallization process was used to avoid ablation of the layers. The amorphous and polycrystalline SiGe films were characterized using Raman spectroscopy and hydrogen effusion measurements. The Raman spectra of the hydrogen related local vibrational modes show modes at 2000, 2100, and 1880 cm⁻¹ that are attributed to isolated Si-H, clustered (Si-H)_x, and Ge-H, respectively. With increasing Ge content in the alloys the intensity of the silicon related local vibrational modes decreases while the Ge-H related modes dominate the spectrum. Laser crystallization leads to a pronounced decrease of the total H concentration. However, in completely crystallized poly-SiGe H related local vibrational modes were no longer detectable. Therefore, information on H bonding could only be obtained from hydrogen effusion measurements. The H effusion spectra were analyzed to obtain the hydrogen density of states distribution [1]. Amorphous SiGe with a Ge content of about 15 % revealed two peaks in the H DOS located at 0.8 and 1.4 eV below the H transport level. With increasing Ge concentration the peak at 1.4 eV decreases until it disappears at a Ge content of about 60 %. Finally, a-Si₂₀Ge₈₀ reveals only one peak that is located 1 eV below the H transport sites. Laser crystallization alters the H DOS completely. Firstly, H becomes more strongly bound by about 0.3 eV. In addition, the distribution of H binding energies increases independent of the Ge content. Laser crystallization causes a significant amount of H atoms to form complexes with binding energies larger than 2.5 eV. [1] N. H. Nickel and K. Brendel, Appl. Phys. Lett. 82, 3029 (2003).

SESSION A4: Nanostructures

Chair: Harry Atwater

Tuesday Afternoon, March 29, 2005

Room 2002 (Moscone West)

3:15 PM A4.1

Conductance Fluctuations in Amorphous Silicon Nanoparticles. T. James Belich¹, Z. Shen², Charles Blackwell¹, Steve Campbell² and James Kakalios¹; ¹School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota; ²Dept. of Electrical and Computer Engineering, University of Minnesota, Minneapolis, Minnesota.

Measurements of the electronic current fluctuations of free-standing

hydrogenated amorphous silicon nanoparticles are described. The nanoparticles are synthesized by high-density plasma chemical vapor deposition and are deposited onto conducting substrates. An insulating matrix, either silicon oxide or silicon nitride is then grown in order to electrically isolate the particles. Electrical contact is made to the top of each nanoparticle by first etching back the insulating matrix until the tops of the nanoparticles are exposed, and then depositing a conducting electrode. Electronic measurements are performed in this transverse geometry, and underneath a top electrode of area 1mm x 1mm are typically 10,000 nanoparticles in parallel. High-resolution transmission electron microscopy confirms that the silicon in the nanoparticles is amorphous and that they are monodisperse with an average diameter of 150 nm with a standard deviation of approximately 5 nm. The spectral density of the current fluctuations in the a-Si:H nanoparticles is well described by a 1/f frequency dependence for frequency f . As in the case of bulk a-Si:H films measured in a co-planar electrode configuration, the conductance fluctuations in the amorphous silicon nanoparticles are characterized by non-Gaussian statistics. Gaussian statistics describe fluctuations that arise from an ensemble of statistically independent fluctuators, while non-Gaussian statistics reflect the presence of either serial interactions between fluctuators or parallel modulations of the properties of the fluctuators. The variation of the correlation coefficients with frequency octave separation of the noise power fluctuations in bulk a-Si:H films indicates serial interactions between fluctuators. In contrast, the octave separation dependence of the correlation coefficients for the nanoparticles are very well described by an ensemble of fluctuators whose amplitudes are independently modulated in parallel. The transition from serial to parallel kinetics in the nanoparticles provides information on the length scales of interactions between fluctuators in amorphous silicon and of conduction mechanisms in the nanoparticles. This work was partially supported by NSF DMR-0212302, NSF NER-DMI-0403887, NREL/AAD-9-18668-13 and the University of Minnesota.

3:30 PM A4.2

Field Emission Studies of Silicon Nanowires Grown by Vapor-Liquid-Solid (VLS) Technique. Niraj Narasinha Kulkarni¹, Joonho Bae² and Chih-Kang Shih^{2,1}; ¹Materials Science & Engineering, University of Texas at Austin, Austin, Texas; ²Department of Physics, University of Texas at Austin, Austin, Texas.

1-D Nanostructures are ideal candidates for electron field emitters because of their high aspect ratio and small tip radii. They could be potential candidates for use in field emission based flat panel displays (FE-FPDs) and other vacuum microelectronic devices. With this motivation silicon nanowires (NWs) were synthesized and their field emission properties investigated. The Si NWs were grown on n-Si substrates using Vapor-Liquid-Solid technique with either an Au film or colloidal Au nanoparticles acting as the catalyst. The growth of Si NWs is carried out in a tube furnace in the temperature range of 850-950 °C by hydrogen reduction of SiCl₄. The NWs have been structurally characterized by SEM. The average diameter of the nanowires is function of the Au film thickness and the growth yields an average nanowire diameter of 20 nm for an Au film thickness of 6 nm. With colloidal Au nanoparticles as catalyst, the nanowire diameter is determined by the diameter of the colloidal nanoparticle itself and is 20 nm in our case. As a consequence of VLS growth the gold resides at the tip of the Si nanowires, and can be selectively etched away with aqua regia. The effect of etching the Au tip on the field emission properties will be reported. Due to the nature of VLS growth, the Si NWs are most likely to be intrinsic or very lightly doped. Effects of n-type doping on the field emission properties of the Si NWs will be studied and reported. Moreover, the effect of alkali metal coating on the field emission properties will also be carried out and reported. Preliminary measurements on as grown Si NWs indicate that the turn-on field of the Si NWs is in the range of 6.8-14 V/ μ m and the current density is as high as 5 A/cm².

3:45 PM A4.3

High-Yield Synthesis of Luminescent Silicon Quantum Dots in a Continuous Flow Nonthermal Plasma Reactor.

Uwe R. Kortshagen, Lorenzo Mangolini and Elijah Thimsen; Mechanical Engineering, University of Minnesota, Minneapolis, Minnesota.

Crystalline silicon quantum dots are of interest for a variety of applications from solid state lighting, to opto-electronic devices, to use as fluorescent tagging agents. Compared to other quantum dot materials, silicon's appeal lies in its low toxicity, its environmental compatibility, and its compatibility with silicon technology used for microelectronics. A variety of liquid and gas phase synthesis approaches for silicon quantum dots has been demonstrated in the past. While liquid phase approaches usually offer excellent control over the size of silicon particles, they are often hampered by low process yields. Gas phase approaches can provide higher yield, however, they are often afflicted with problems of particle

agglomeration, which can annihilate the desired quantum dot behavior. The use of nonthermal plasmas discussed in this presentation can overcome these two main problems of other synthesis approaches: Plasma synthesis offers the efficiency of direct gas-to-particle conversion common to most gas phase approaches. At the same time it strongly reduces or completely eliminates agglomeration since the particles in the plasma are unipolarly negatively charged. We present a method for the production of silicon nanocrystals using a low-pressure nonthermal plasma. It is based on a continuous flow plasma reactor. The reactor consists of a quartz tube with a ring electrode as RF powered electrode. The discharge is generated in an argon-helium-silane mixture, and the plasma excitation frequency is 27.12 MHz. The discharge is generated at pressures of about 1.5 Torr. Typical flow rates are 40 sccm for argon and 10 sccm for the He/SiH₄ (95:5) mixture. Under these conditions the residence time of particles in the plasma region is small (<5 msec) and an aerosol of very small particles is produced. Transmission Electron Microscopy shows that crystalline particles smaller than 5 nm are obtained. Particles are collected on filters, and after the growth of a native oxide layer they show bright photoluminescence in the red-orange region. Photoluminescence data, excitation scans, and absorption data are presented. Mass spectroscopic measurements show that silane is almost completely converted to particles in our discharge reactor. The estimated production rate of luminescent silicon nanocrystals is a few tens of milligrams per hour. The presented reactor can easily be scaled-up by operating multiple discharge reactors in parallel. The comparatively large yield combined with the fact that very small particles are produced in a single step gas phase process without the need for any post-processing makes this system very promising for the large scale production of silicon quantum dots. This work is supported in part by NSF under MRSEC grant DMR-0212302 and by Innovalight, Inc.

4:00 PM A4.4

Electrodeposition of Nanoscale Germanium and Silicon in Ionic Liquids. Frank Endres, Technical University of Clausthal, Clausthal-Zellerfeld, Germany.

Ionic liquids are a new class of solvents with extraordinary physical properties. They are mostly based on organic cations and inorganic or organic anions and by definition their melting points are below 100 Celsius. These liquids have often negligible vapor pressure, high thermal stability (up to 350 Celsius), high ionic conductivity and wide electrochemical windows of up to 7 Volt. The latter property is very important for the electrodeposition of reactive elements such as Ge, Si, Al, Li and many others. We could show by the help of the in situ Scanning Tunneling Microscope that the initial processes of germanium and silicon electrodeposition can be probed on the nanometer scale. For example, before the bulk phase of germanium forms on Au(111), an underpotential deposition sets in, and ultrathin layers between 100 and 300 pm with clearly metallic behavior grow [1-3]. With subsequent reduction nanocrystallites start growing that show a metal to semiconductor transition in the thickness regime between 1 and 10 nm. With these liquids it is also possible to electrodeposit silicon, and we could show by in situ tunneling spectroscopy that a 100 nm thick silicon film has a band gap of 1.0 ± 0.1 eV, proving that intrinsic semiconducting silicon was electrodeposited [4]. Thin nanoscale layers of silicon can be prepared easily. Such ionic liquids are also well suited to the electrodeposition of nanocrystalline metals and alloys with grain sizes down to 10 nm [5]. [1] F. Endres, S. Zein El Abedin, Phys. Chem. Chem. Phys., 4 (2002) 1640 [2] F. Endres, S. Zein El Abedin, Phys. Chem. Chem. Phys., 4 (2002) 1649 [3] F. Endres, S. Zein El Abedin, Phys. Chem. Chem. Phys., 6 (2004) 892 [4] S. Zein El Abedin, N. Borissenko, F. Endres, Electrochemistry Communications, 6 (2004) 510 [5] F. Endres, M. Bukowski, R. Hempelmann, H. Natter, Angew. Chemie, Int. Ed., 42 (2003) 3428

4:15 PM A4.5

Wiring and Introduction of Single Silicon Nanocrystals into Multi-wall Carbon Nanotubes. Vladimir Svrcek¹, Francois Le Normand², Ovidiu Ersen², Cuong Phan-Huu¹, Dominique Begin¹, Benoist Louis¹, Jean-Claude Muller³ and Marc J. Ledoux¹; ¹LMSPC-ECPM, 25, rue Becquerel, F67087 Strasbourg, France; ²IPCMS, UMR 7504 CNRS, 23 rue du Loess, F67087 Strasbourg, France; ³CNRS-PHASE, 23 rue du Loess, F67087 Strasbourg, France.

In principle, since bulk silicon is an indirect bandgap semiconductor, it could not be used for optoelectronic applications. However, it has been demonstrated that efficient photoluminescence (PL) can be observed from silicon in the form of quantum dots (wires), i.e., silicon nanocrystals (Si-nc) of sizes less than 5 nm. In that case quantum confinement together with surface state effects start to take place resulting in opening of the bandgap and considerable increase of radiative recombination probability. The most common techniques used for the Si-nc fabrication are silicon ion implantation into silicon dioxide (SiO₂) thin film, annealing of SiO₂/amorphous silicon layers

and chemical vapor deposition. Very often, the problem here is the difficulty in achieving Si-nc concentrations high enough to obtain efficient luminescence and transport properties within the SiO₂ matrix. We have developed an alternative technique for the ex-situ preparation of Si-nc by pulverization of porous silicon layers followed by their implementation into liquid spin on glass (SOG) SiO₂ as basic host matrices where we are able to overcome such problems. We have verified that Si-nc, embedded in SOG, maintains its superior luminescence, transport properties and optical gain. As it is well known, since the first successful synthesis of carbon nanotubes (CNTs), these materials were ever subjected to increased attention from both theoreticians and experimentalists as a unique 1D nano-material. One of the most promising applications is the filling of these CNTs by nanoparticles as a nano-reservoir for the stabilization of these nanoparticles. As has shown our preliminary results, a solution of free floating colloidal prepared Si-nc can be introduced within carbon nanotubes CNTs. The approach for the preparation of Si-nc ex-situ, in principle, offers unique possibilities. For instance we are able to continuously fill CNTs with Si-nc embedded and stabilized in silicon dioxide matrix. In addition, the surface chemistry can be used to effectively alter the properties of the Si-nc including PL brightness, PL maxima position, surface tension and electronic lifetime. In the proposed contribution we will present this innovative and low-cost procedure to wire and introduce Si-nc (2- 5 nm) embedded in liquid by capillary forces, into CNTs with different inner diameters in the range 5 - 40 nm. The Si-nc were formed by electrochemical etching in colloidal suspensions. We will show that we are able to obtain well-separated and wired single Si-nc with conducting multiwall CNTs crucial for real-world applications. Even more, this approach help to localize and manipulate with single Si-nc that offers a unique possibility to fabricate very solid and flexible single Si-nc-based nano-devices and then to study peculiar physical phenomena. The potential of such approach will be discuss in details.

4:30 PM A4.6

Thermal Transport in Nanocrystalline Silicon. Arun Bodapati¹, Pawel Keblinski¹ and Patrick Schelling²; ¹Materials Science, Rensselaer Polytechnic Institute, Troy, New York; ²Physics, University of Central Florida, Orlando, Florida.

Nanocrystalline silicon is an important electronic material with varied applications as light sensors, microchips and solar cells. The performance and reliability of many of these devices are influenced by heat transport characteristics. In this work, we use equilibrium molecular dynamics simulations and fluctuation dissipation relationships to study the effect of grain size on thermal conductivity of nanocrystalline silicon at room temperature. We found that the thermal conductivity decreased linearly with decreasing grain size. Interestingly, the thermal conductivity of model amorphous silicon corresponds to an effective grain size of ~ 1nm, i.e., the length equivalent to the length of two Si-Si bonds. To obtain a more detailed understanding of thermal transport process we performed lattice dynamics calculations on our model structures and compared localization and polarization of vibrations characterizing amorphous and nanocrystalline model silicon structures.

4:45 PM A4.7

Multi-Scale Growth Study of Vacuum Evaporated a-Si Nanostructured Thin Films. Aram Amassian¹, Kate Kaminska², Motofumi Suzuki³, Ludvik Martinu¹ and Kevin Robbie²; ¹Regroupement Quebecois pour les Matériaux de Pointe (RQMP) and Department of Engineering Physics, Ecole Polytechnique de Montreal, Montreal, Quebec, Canada; ²Department of Physics, Queen's University, Kingston, Ontario, Canada; ³Department of Engineering Physics and Mechanics, Graduate School of Engineering, Kyoto University, Kyoto, Japan.

Porous materials with a structure controlled on the nanometer-scale are important in a wide variety of applications, including photonics, electronics and biomaterials. Glancing Angle Deposition (GLAD) allows the fabrication of films with nano-engineered morphology whose properties can be tailored. GLAD is based on thin film deposition by evaporation onto a substrate that is tilted at a high angle, ($\alpha > 75^\circ$), relative to the vapour flux. This geometry leads to an effect called atomic shadowing, which occurs when the vapour flux is prevented from reaching the substrate by previously deposited material. This results in the development of a porous structure forming a 2D array of isolated nanocolumns of material. Atomic shadowing, is scale-invariant and therefore results in the formation of fractal nanostructures, which broaden with height according to a power-law relation. We have investigated the growth of GLAD nanostructures using a combination of in situ spectroscopic ellipsometry (SE) and ex situ atomic force microscopy (AFM) in the sub-nanometer to 10 nm regime, and by in situ SE, ex situ variable angle SE (VASE) and Field-emission Scanning Electron Microscopy (FESEM), in the 10 nm to 0.5 μ m regime. We show that SE allows determination of film thickness, optical properties, birefringence, and

has been found to yield accurate film porosity data. In the ultra-thin regime (0.1 to 10 nm), we have found that the optical behaviour of sub-nanometre GLAD films deposited at 87° from substrate normal is somewhat similar to 0° films, with stark differences starting to appear at nanometre-scale thickness. AFM analysis shows that disk-like island formation occurs in the sub-nanometre range, which leads to nanocolumn formation later on. Both the porosity evolution with thickness, and the scaling of grain size and spacing with film thickness change significantly in the nanometre-range, indicating that surface diffusion plays a dominant role during the initial growth of GLAD nanostructures. For thicker films (10 to 500 nm), we have investigated the effect of geometric shadowing length on nanostructure formation and optical anisotropy and porosity evolution with thickness, by varying vapour flux incidence angle over the range from 0° to 87° . 3D Monte-Carlo simulations of GLAD growth are shown to be capable of predicting the nanostructure of the films.

SESSION A5: Poster Session: Characterization–Nano,
Micro, Poly-crystalline Films
Tuesday Evening, March 29, 2005
8:00 PM
Salons 8-15 (Marriott)

A5.1
Instabilities and Temperature Dependence of Photoelectronic Properties of Microcrystalline Silicon. Rudolf Bruggemann, Institut für Physik, Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany.

We critically assess the determination of the photoelectronic properties of microcrystalline silicon in terms of majority-carrier mobility-lifetime products from steady-state photoconductivity and minority-carrier mobility-lifetime products from the steady-state photocurrent grating experiment. We show how large metastable changes in the dark conductivity upon moderate heat treatment in vacuum to remove adsorbates translate into change in the measured values characterising the photoelectronic properties if excess-carrier measurements in air and after heat treatment are considered. We note that these effects are not related to metastable defect creation and annealing. After establishing a standard heat-treatment procedure prior to photocurrent measurements, we determined the temperature and photogeneration-rate dependence of majority-carrier and minority-carrier mobility-lifetime products in microcrystalline silicon with different degree of crystalline volume fraction. Numerical modelling provides further insight and supports the suggestion of a rather symmetric density-of-states distribution on valence and conduction band tails in microcrystalline silicon.

A5.2
Abstract Withdrawn

A5.3
Microstructural Analysis of Nickel-Mediated Crystallized Poly Silicon by Chemical Etching, AFM, EBSD and HRTEM. Samick Son¹, MyungKyu Park¹, Nari Ahn¹, Ilsang Choi¹, Jinwook Seo² and Jaehak Lee¹; ¹Materials Analysis Team, Corporate R&D Center, Samsung SDI Co, Yongin, Gyeonggi-do, South Korea; ²Tech. Development Team 1, Corporate R&D Center, Samsung SDI Co, Yong In, Gyeonggi-do, South Korea.

Active-matrix organic light-emitting diode (AMOLED) displays fabricated by using low temperature polycrystalline silicon (poly-Si) thin film transistors (TFTs) revealed the possibility of realizing high-quality images with low power consumption. For the crystallization of amorphous silicon (a-Si) in AMOLED fabrication, excimer laser annealing (ELA) method has been widely used because of its reliability without causing any damage to low-cost glass substrates. However, the ELA process that utilizes a line-beam laser, frequently causes line-shape non-uniformity in brightness on AMOLED displays. And also there is a limitation in laser length, which makes it difficult to use ELA for large-size displays. As an alternative crystallization method, metal-induced crystallization (MIC) or metal-induced lateral crystallization (MILC) technique has been developed for the last decade. Recently, an alternative method for silicon crystallization was introduced, which is reducing metal contamination without an additional patterning mask, compared to the conventional MIC or MILC methods. A SiNx capping layer, which plays a role as a barrier for diffusion of metal catalyst for crystallization, is deposited on a-Si films. In this work we investigated the physical properties of Nickel-mediated crystallized poly silicon films used for fabrication of low-temperature polycrystalline silicon (LTPS) thin-film transistors (TFTs) for active-matrix organic light-emitting-diode (AMOLED) display. The grain size is about 10~100 μm . The microstructure such as grain boundary structure, orientation of grains and misorientation between grains was

investigated by Secco etching, atomic force microscope (AFM), electron backscattered diffraction (EBSD) and high resolution transmission electron microscope (HRTEM). The silicon grain grows radial direction from a nucleation site, which is the center of grain. Within a single grain there were several domains with a little different crystallographic orientation. This could be seen in optical microscopy after Secco etching due to a different etching rate according to the crystallographic orientation. We could confirm the low angle boundaries in grain and special high angle boundary between grains by electron-backscattered diffraction. We could confirm the low angle boundary within grain and special high angle boundary between grains. This phenomenon could be explained by the growth mechanism, which is related to the crystal structure of silicon and nickel silicide.

A5.4
Effects of Post Annealing and Material Stability on Undoped and n^+ nc-Si:H Films Deposited at 75°C Using 13.56 MHz PECVD. Czang-Ho Lee, Andrei Sazonov and Arokia Nathan; ECE, University of Waterloo, Waterloo, Ontario, Canada.

Nanocrystalline silicon (nc-Si:H) is a low-cost active layer alternative to polycrystalline silicon (poly-Si) for active matrix thin film transistor (TFT) backplanes for flat panel displays (FPDs). However, this material is highly sensitive to oxygen adsorbed from the atmosphere, which can undermine the long-term device reliability. In this paper, the effects of post-deposition annealing and material stability of undoped and n^+ nc-Si:H films have been investigated. The films were deposited at a very low temperature (75°C) by standard 13.56 MHz plasma enhanced chemical vapor deposition (PECVD) and subsequently annealed at temperatures exceeding the deposition temperature (120–300 $^\circ\text{C}$). Electronic, structural, and chemical composition properties were studied using measurements of electrical conductivity, Raman spectroscopy, X-ray diffraction (XRD), atomic force microscopy (AFM), Fourier transform infrared (FTIR) spectroscopy, and secondary ion mass spectroscopy (SIMS). The as-grown nc-Si:H films showed a high crystallinity of 83 %, an oxygen concentration of 2×10^{18} at./ cm^3 , and a dark conductivity of 10^{-6} S/cm and 1 S/cm in case of undoped and n^+ nc-Si:H films, respectively. The dark conductivity in all films demonstrated high stability against prolonged ambient atmosphere exposure, which can be attributed to low oxygen concentration and stable hydrogen passivated grain boundaries. On the other hand, in undoped nc-Si:H films, the dark conductivity increases by more than one order of magnitude after annealing in ambient atmosphere, followed by a decrease below the as-grown value. Depending on the annealing temperatures, the dark conductivity can drop as low as 10^{-8} S/cm. In n^+ nc-Si:H films, the decrease in the dark conductivity was lower. However, in undoped nc-Si:H films capped by amorphous silicon nitride (a-SiN_x), this was not observed. In all films, no significant change in the film microstructure before and after annealing was detected. However, a small decrease in the hydrogen content accompanied by an increase in the oxygen content was observed in uncapped nc-Si:H films. It was therefore concluded that the dark conductivity is affected by oxygen desorption due to annealing and its absorption from the ambient atmosphere. Detailed experimental results will be presented along with modeling results based on hydrogen effusion-assisted oxygen absorption.

A5.5
Study of Steady State Photoconductivity in Highly Crystallized Doped and Undoped Microcrystalline Si Films. Sanjay Ram^{1,2}, Satyendra Kumar^{1,2}, P. Rocca i Cabarrocas³, R. Vanderhaghen³ and B. Drevillon³; ¹Physics, Indian Institute of Technology, Kanpur, Kanpur, Uttar Pradesh, India; ²Samtel Centre for Display Technologies, Indian Institute of Technology Kanpur, Kanpur-208016, Uttar Pradesh, India; ³Laboratoire de Physique des Interfaces et des Couches Minces (UMR 7647 du CNRS), Ecole Polytechnique, 91128 Palaiseau Cedex, France.

Hydrogenated microcrystalline silicon ($\mu\text{c-Si:H}$) is a promising material for large area opto-electronic devices such as solar cells, sensors and thin film transistors (TFT's) based flat panel displays. Recently, this material has drawn more attention compared with hydrogenated amorphous silicon due to higher conductivity, large carrier mobility and better stability against light induced changes. However, plasma-deposited $\mu\text{c-Si:H}$ is inherently a heterogeneous material consisting of micro and nano size crystallites, amorphous tissues and voids. Understanding carrier transport in such a system is undoubtedly a challenging task. Though there are several reports on the electronic transport in doped $\mu\text{c-Si:H}$, little attention is paid to the carrier transport in undoped $\mu\text{c-Si:H}$. We have obtained fully crystallized dense undoped $\mu\text{c-Si:H}$ films on glass substrates by standard rf glow discharge plasma CVD technique using a mixture of SiF₄, Ar and H₂ at low substrate temperatures ($\sim 200^\circ\text{C}$). Structural properties of the films were well characterized by in-situ spectroscopic ellipsometry, Raman scattering, X-ray diffraction and atomic force

microscopy techniques. This article will basically cover results on the dark and steady state photo conductivity measurements carried out on samples having different thicknesses. For steady state illumination in our photoconductivity measurements on the same sample we used He-Ne red Laser of 15mW output (yields a maximum photo-generation rate of $F = 10^{17} \text{ cm}^{-2} \text{ sec}^{-1}$). Intensity is varied from $8 \times 10^{11} \leq F \leq 10^{17} \text{ cm}^{-2} \text{ sec}^{-1}$ by using neutral density filters. The samples were placed in He cryostat operating in the temperature range of 15 – 325 K. The dependences of photoconductivity (σ_{ph}) on the temperature and the intensity of light were measured in a temperature range 15–325 K. Temperature dependence of photoconductivity data is fitted to standard power law : $\sigma_{ph} \propto F^\gamma$, where the exponent $\gamma = T_0/(T + T_0)$ contains the information on recombination mechanism in the semiconducting material. The variation in γ is found to be $0.5 \leq \gamma \leq 0.9$ for thin samples, and $0.15 \leq \gamma \leq 0.8$ in a thick fully crystallized sample. Mechanisms of carrier transport and recombination governing these temperature and intensity dependences will be discussed in the paper. In order to evaluate the properties like free carrier concentration and mobility in *undoped* $\mu\text{-Si:H}$, Hall effect measurements were also performed in the temperature range 300–450 K.

A5.6

Transport and Meyer-Neldel Rule in Microcrystalline Silicon Films. Steve Reynolds¹, Vladimir Smirnov¹, Friedhelm Finger², Charles Main³ and Reinhard Carius²; ¹EPICentre, University of Abertay Dundee, Dundee, United Kingdom; ²IPV, Forschungszentrum Juelich, Juelich, Germany; ³Dept of Elec Eng and Physics, University of Dundee, Dundee, United Kingdom.

The Meyer-Neldel Rule (MNR) has been observed in microcrystalline silicon thin films where conductivity has been altered by doping or by varying the degree of crystallinity [1]. Although it has been shown that exposure to atmosphere may cause both reversible and irreversible changes in conductivity over a wide range [2], a systematic study of whether these 'aging' states also fit the MNR has hitherto not been carried out. In the present work, changes in dark conductivity, activation energy and conductivity prefactor measured on individual samples due to aging are reported. The data are found to follow the MNR smoothly, and to correlate well with results from a series of samples of varying crystallinity. Our primary motivation for this study is to discover more about reversible and irreversible ageing processes, and how they may affect interpretation of transport measurements [3] and long-term stability of devices such as solar cells [4]. [1] R. Brueggemann, M. Rojahn and M. Roesch, Phys. Stat. Sol. (a) 166, R11 (1998). [2] V. Smirnov, S. Reynolds, C. Main, F. Finger and R. Carius, J. Non-Cryst. Sol. 338-340, 421 (2004). [3] J. Kocka, A. Fejfar, H. Stuchlikova et al, Sol. Energy Mat. Sol. Cells 78, 493 (2003). [4] Q. Wang, K. Wang and D. Han, MRS Symp. Proc. 762, A7.10.1 (2003).

A5.7

Cesium/Xenon Dual Beam Depth Profiling, A New Approach for Semi-Quantitative Depth Profiles with ToF-SIMS: Influence of The Sputtering Parameters On The Cesium Surface Concentration. Jeremy Brison and Laurent Houssiau; University of Namur, Namur, Belgium.

The secondary ion mass spectrometer combined with a time of flight analyzer is well known as a powerful technique for surface analysis and for ultra shallow depth profiles. Unfortunately, the many advantages of the SIMS technique are often shadowed by a major problem: the quantification of the results is not straightforward and sometimes nearly impossible. This inconvenience is caused by a well known phenomenon, the matrix effect, which means that the intensity of the signals depends strongly on the nature of the studied sample and on the primary ions. Using Cs+ ions for sputtering offers a semi-quantitative solution to depth profiling. Specifically, the use of these alkali ions strongly increases negative ion yields, decreases the positive ones and allows the formation of MCs+ and MCs2+ clusters. The study of these clusters has shown their low sensitivity to matrix effect and their applicability to quantitative profiles [1,2]. Recently, Niehuis and Grehl [3] developed a new approach consisting of co-sputtering Xe and Cs in order to control the Cs surface concentration, thus allowing the optimization of elemental and cluster ion yields. In a previous work, we applied that technique on different well-defined samples (e.g. Si, SiO2) and we monitored positive ions as a function of the sputtering beam Cs concentration [4]. First, we observed the decrease of the elemental ions due to the work function lowering, as is predicted by the tunneling model. We then studied the behavior of the MCs+ and the MCs2+ clusters. The MCsn+ yields exhibit a maximum at a given Cs/Xe beam concentration ratio, depending on the studied element M but also on his chemical environment (e.g. Si and SiO2) and on the energy of the Cs beam. Those maximums are a consequence of the competition between the varying surface Cs coverage (direct concentration effect) and the decreasing ionization probability due to that varying Cs. However, at low Cs surface concentration, the Cs ionization probability is close to

1 and the Cs+ signal saturates the detector. In this work, we combined the Cs/Xe co-sputtering with a very low current analysis mode (called burst alignment) in order to measure the Cs+ signal. To perform this analysis, we studied a gold layer deposited on silicon and a bare silicon substrate. We found that in the same way as the MCs+ signal, the Cs+ yield exhibits a maximum at a given Cs/Xe beam concentration ratio, depending on the studied sample. This optimal Cs beam concentration is a few percents higher than the one of the MCs+ signals. References: [1] J. M. Schroeder, H. Gnaaser and H. Oechsner : proc. SIMS IX, New York (1993), 387 [2] Y. Gao, Y. Marie, F. Saldi and H. N. Migeon : proc. SIMS IX, 382 [3] E. Niehuis, T. Grehl : proc. SIMS XII, 49 (2000) [4] J. Brison, L. Houssiau, Appl. Surf. Sci., Vol 231-232C, p 749-753 (2004)

A5.8

Characterization of Silicon Thin Film Deposited by E-beam Evaporator for Flexible Display. In-Hyuk Song, Sang-Myeon Han, Joong-Hyun Park and Min-Koo Han; School of Electrical Engineering, Seoul National University, Seoul, South Korea.

Polycrystalline silicon thin film transistor (poly-Si TFTs) fabricated at low temperature under 200oC may be a promising for flexible substrate application. Unlike the TFT process on glass substrate, the maximum process temperature should be less than 200oC in order to avoid thermal damage on flexible substrate. Recently several deposition methods of active layer have been investigated. Amorphous or polycrystalline silicon precursor prepared by conventional plasma enhanced chemical vapor deposition (PECVD) method has been also researched employing laser dehydrogenation. The hydrogen content exceeding 10% is inherently incorporated in precursor silicon film deposited by conventional PECVD when the process temperature is less than 200oC. Step-by-step excimer laser dehydrogenation could be a candidate to decrease the hydrogen content in amorphous silicon film. However this method would be limited by the hydrogen eruption during excimer laser irradiation. On the other hand, the amorphous silicon film deposited by sputtering has been studied due to small amount of hydrogen content in the silicon thin film. However, some amount of sputter source gases such as Ar and He incorporated in silicon film may cause abrupt during the laser annealing process. The purpose of our work is to report silicon thin film deposited by e-beam evaporator at room temperature. Deposition method using evaporator can avoid any gases incorporated in silicon film such as H, He and Ar, so rather simple laser process can be performed comparable to sputtering and chemical vapor deposition. Our experiments show that the silicon film deposited by e-beam evaporator results in polycrystalline structure and high crystallinity. The microstructure of the deposited silicon films were characterized by SEM image, Raman spectroscopy and x-ray diffraction. SEM image shows that the deposited silicon film is nanocrystalline structure. High crystallinity of the deposited silicon film could be verified by Raman spectroscopy. We have also investigated laser crystallization of silicon film deposited by e-beam evaporator. TEM image shows that grain size of the deposited silicon film is increased after laser irradiation. As laser energy density increase, grain size is increased until laser energy density is critical point to abrupt silicon film. X-ray diffraction shows crystallinity of the silicon film as a function of laser energy density. And the results of the x-ray diffraction verify that the orientation of the silicon film after laser irradiation is <311>. The silicon film deposited by e-beam evaporator may be suitable method for flexible display.

SESSION A6: Poster Session: Growth–Large Grains and Epitaxy
Tuesday Evening, March 29, 2005
8:00 PM
Salons 8-15 (Marriott)

A6.1

In and Ex Situ Correlation of Stress to Microstructures during Al-Induced Crystallization of PECVD Amorphous Silicon. Solomon Ray, Yaguang Lian, Derald J. Tucker and Grant Z. Pan; Microfabrication Laboratory, University of California at Los Angeles, Los Angeles, California.

Formation of high quality polycrystalline silicon (c-Si) at temperatures lower than 500 °C is vital for low temperature large area microelectronics. It was recently reported [1] that high quality c-Si can be achieved from Al-induced crystallization (AIC) of amorphous silicon (a-Si) formed by plasma enhanced chemical vapor deposition (PECVD) at a temperature as low as 200 °C for Al on top (AOT) of a-Si or 300 °C for Al on bottom (AOB) of a-Si. The microstructures and quality of the AIC c-Si are closely related to the stress produced during the deposition process. The stress is a function of thickness of both Al and a-Si, order of layers and deposition temperature. In this study, we report in and ex situ correlation of

stress to microstructures during AIC of PECVD a-Si. A number of AOT and AOB films with equal thickness of Al and a-Si from 20 to 200 nm were studied. The Al layer was deposited by E-beam evaporation at room temperature and the a-Si was formed by PECVD at 100 °C. All films were deposited on a 4-inch Si wafer coated with 300 nm PECVD oxide. The chosen AIC temperatures for AOT and AOB were 225 °C and 375 °C, respectively. We found that the stress of AOB films is always higher than that of AOT films and their difference increases with layer thickness. The PECVD oxide possesses a compressive stress of about 200 MPa before AOT and AOB formation. The high stress of AOB films is because of the fact that both upon deposition of a-Si on top of PECVD oxide and upon deposition of a-Si on top of Al the stress increases compressively; both upon deposition of a-Si on top of PECVD oxide and upon deposition of Al on top of a-Si the stress decreases tensilely. The in and ex situ stress measurements indicated that the compressive stress of AOB films decreases dramatically with a kink before both Al and a-Si exchange their position. However, the in and ex situ AIC stress of AOT films decreases slightly with no kinks. From correlation of stress to microstructures we found that the kink of stress from AOB films is related to the bubbles formed due to high stress during AIC. When they break the stress decreases dramatically. The stress of AOT and AOB films significantly affects final AIC c-Si microstructures and quality. The AIC c-Si from AOB is generally porous due to bubbles and hence less suitable for low temperature large area microelectronics than the AIC c-Si from AOT. 1. K. Jenq, S. S. Chang, Y. G. Lian, G. Z. Pan and Y. Rahmat-Samii, *Amorphous and Nanocrystalline Silicon Science and Technology-2004*, Symposium of the Materials Research Society, edited by Gautam Ganguly, Michio Kondo, Eric A. Schiff, Reinhard Carius, and Rana Biswas, in press.

A6.2
Poly-Crystalline Silicon-Germanium Thin Films Prepared by the Multi-Target RF Sputtering System. Toru Ajiki, Isao Nakamura and Masao Isomura; Tokai University, Kanagawa, Japan.

Next generation thin-film solar cells require higher efficiency, lower cost and wider area. However, the conversion efficiency of thin-film solar cells is lower than that of bulk crystalline silicon solar cells in the present situation. Thus, to improve the conversion efficiency of thin film solar cells, multi-junction thin film solar cells are generally investigated to make more efficient use of the sunlight. We have studied poly crystalline silicon-germanium as a bottom cell material of multi-junction solar cells because it is a narrow gap material that has higher sensitivity in the long wavelength region. In this study, poly crystalline SiGe thin films were prepared by the RF sputtering system with two targets, silicon and germanium. In the case of Ar gas RF sputtering, extremely high defect density is observed due to the dangling bonds in grain-boundaries. We could successfully reduce the defect density by using Ar-H₂ mixture gases. The polycrystalline SiGe thin films were prepared on coming 7059 substrates by the RF sputtering system. Composition of Si_{1-x}Ge_x was controlled by RF power applied to Si and Ge targets, respectively. The substrate temperature was 400-500 degrees. The crystallinity of SiGe films was evaluated by the Raman spectroscopy. The composition was measured by XPS. The optical absorption coefficient was calculated by transmission and reflection spectra. The electrical property was evaluated by electric conductivity in the dark and under illumination of AM-1.5 light. When SiGe films with 60-70 % Ge contents were prepared at 400 degree, amorphous SiGe was formed by the Ar gas sputtering but crystallized SiGe could be obtained by the Ar-H₂ mixture gas sputtering. The H₂ introduction into the sputter gases seems to enhance the crystallization of SiGe films. In the wavelength more than 1000 nm, the optical absorption coefficient (α) of the SiGe films was around 10^4 cm^{-1} , and below 10^3 cm^{-1} in the case of the Ar and Ar-H₂ gas sputtering, respectively. The decrease in α shows a decrease in the defect density, that suggests that the H₂ introduction is effective to eliminate the midgap defects. Besides, the dark electric conductivity decreased from $2.07 \times 10^{-2} \text{ S/cm}$ to $1.67 \times 10^{-7} \text{ S/cm}$, due to the H₂ introduction. This also shows the defect elimination, and is consistent with the trend of α . The results suggest that the Ar-H₂ mixture gas sputtering is effective both to reduce the dangling bond defects and to decrease the crystallization temperature of SiGe films. The results shows that the SiGe films have the sufficient potential as a bottom cell material of multi-junction solar cells.

A6.3
Control of the Crystal Orientation in Metal-Induced Lateral Crystallization. Min-Sun Kim, Yeo-Gun Yoon, Young-Su Kim and Seung-Ki Joo; School of Materials Science and Engineering, College of Engineering, Seoul National University, Seoul, South Korea.

There is a need for low temperature crystallization of amorphous Si thin film on glass substrate for integrated TFT-LCD and AMOLED. So, in recent years, many studies on poly-Si TFT have focused either on raising carrier mobility or on lowering the leakage current. Because of that reason, uncontaminated poly-Si was necessary. As a low

temperature annealing method, Metal-Induced Lateral Crystallization (MILC) is a very advantageous method. Using MILC method, we can crystallize the amorphous Si at low temperature (<500 degree) and process cost is very low. However, MILC poly-Si is contaminated by nickel silicide. Therefore, it caused high leakage current and low carrier mobility. To obtain low silicide contamination and defects, poly-Si with unidirectional orientation is necessary. So, we studied the effects of crystal filter on MILC orientation. Also we observed change of MILC microstructure between normal MILC and CF-MILC. A 500-Å-thick amorphous Si thin film was deposited by low pressure chemical vapor deposition (LPCVD) on the glass wafer. After the amorphous Si deposition, the samples were patterned by photolithography method and then a-Si layer was etched by conventional plasma etching with SF₆. When amorphous Si layer was defined, crystal filter was also defined at the same time. The widths of Crystal filter were 1, 2, 4, 6, and 8 μm each. After etching process amorphous Si layer, 100-Å-thick Ni film was deposited by sputtering with an additional photoresist (PR) mask. Then, the Ni film was removed by lift off. By annealing at 550°C, samples were crystallized in vacuum. The orientations of poly-Si grains which was passed crystal filter and not passed crystal filter were observed by electron back scattering diffraction (EBSD: JSM 6500F). And we used normal scanning electron microscope (SEM) to observe microstructure. We could observe that the width of crystal filter was the narrower, CF-MILC was oriented with $\langle 111 \rangle$ direction. Since the selected unidirectional silicide (1st silicide) which was passout through crystal filter would make 2nd silicide to crystallize amorphous silicon region with same 1st silicide direction. Using CF-MILC, we were able to get unidirectional poly Si.

A6.4
Laser Crystallization of Compensated Hydrogenated Amorphous Silicon Thin Films. Rosari Saleh¹, Norbert H. Nickel² and Karsten von Maydel²; ¹Fisika, Fakultas MIPA, Universitas Indonesia, Depok, Indonesia; ²Hahn-Meitner-Institut, Berlin, Germany; ³Hahn-Meitner-Institut, Berlin, Germany.

Compensated hydrogenated amorphous silicon films were crystallized using a step-by-step laser dehydrogenation and crystallization procedure. The influence of laser crystallization on structural change, hydrogen bonding and hydrogen diffusion is investigated employing Raman spectroscopy and hydrogen effusion measurements. The starting material was grown on a quartz substrate by rf-glow discharge decomposition of silane. Partial and complete compensation was achieved by mixing silane with phosphine and diborane. The nominal gas doping was varied up to 2000 ppm for phosphine and diborane. Our results show that in the first step of the laser crystallization procedure a structural transformation takes place. The films exhibit a stratified structure with a poly-Si layer on the top of an amorphous layer. The Raman spectra of completely crystallized heavily doped and compensated poly-Si are distorted. This phenomenon is due to a resonant interaction between optical phonons and direct intraband transitions of electrons or holes in the samples. The structural change is accompanied by a significant change in Si-H bonding and a decrease of the total hydrogen concentration in specimens. The hydrogen bonding is influenced by the presence of dopant. In P-doped poly-Si a considerable amount of hydrogen is accommodated in the clustered phase, while for B-doped samples most of the H atoms are accommodated in isolated Si-H bonds. In specimens where the boron and phosphorous doping is at equal levels, the hydrogen bonding configuration is close to that found for purely P-doped samples. However, when doping levels are different, the majority specimen tends to be incorporated in the film much more efficiently. From hydrogen effusion measurements, the hydrogen density-of-states distribution in fully crystallized poly-Si is derived. Four peaks arise in the H density-of-state distribution that is located at -2.0, -2.2, -2.5 and -2.8 eV for the compensated poly-Si films. The peak observed at E = -2.8 eV is not observed in B-doped samples.

A6.5
Poly-Crystalline Ge Thin Films Prepared by RF Sputtering Method for Thermo-Photo-Voltaic Application. Daisuke Hoshi, Isao Nakamura and Masao Isomura; Tokai University, Kanagawa, Japan.

Thermo-photo-voltaic (TPV) generation from the solar radiation or waste heat is attractive as one of a new energy sources. The TPV system is composed of an emitter of infrared light, a filter selecting proper wavelength and photo-voltaic-cell (PV-cell). In this system, the PV-cell is required to have a narrow gap which has enough sensitivity in the infrared light. Conventionally, InGaAs and GaSb have been investigated, but these materials are expensive and not suitable to prepare in large area. Then, we propose poly crystalline Ge thin film by the RF sputtering method that may realize a low cost process and a large area. In this study, the poly crystalline Ge thin films were prepared on coming 7059 substrates. Ar and Ar-H₂ mixture were used for sputtering gases. Substrate temperatures were changed from 300

to 600 degrees. The electrical and optical properties of the Ge thin films were evaluated by the Hall effect measurement and the optical absorption spectra. In the case of the Ar gas sputtering, the hole mobility of Ge thin film increased with rising substrate temperature, and reached $40 \text{ cm}^2/\text{Vs}$ at 600 degree. This mobility is an unexpected high value nevertheless the poly crystalline thin film contains many defects of its grain boundary. This result suggests a large potential of Ge thin films for the PV-cell. However, 600 degree is not low enough for using of low cost substrates. On the other hand, in the case of Ar-H₂ mixture gas sputtering, the hole mobility of Ge thin films improved to over $50 \text{ cm}^2/\text{Vs}$, even at 500 degree. The absorption coefficients of Ge thin films prepared by Ar gas sputtering showed 10^4 cm^{-1} at around 1500 nm corresponding to the energy gap, which is much higher than that of the single crystal Ge. On the other hand, the absorption coefficients were reduced to similar values to the single crystal Ge by using Ar-H₂ mixture gases. These results indicate that the Ar-H₂ mixture gas sputtering is able to reduce the defect density and improve the electrical properties. It is suggested that the poly crystalline Ge thin films prepared by the RF sputtering method are hopeful to realize a new PV-cell for TPV system.

A6.6

TCAD Modeling of Metal Induced Lateral Crystallization of Amorphous Silicon. Aleksey M. Agapov¹, Valeri V. Kalinin¹, Alexandre M. Myasnikov¹ and Vincent M. C. Poon²; ¹Institute of Semiconductors Physics, Novosibirsk, Russian Federation; ²Hong Kong University of Science and Technology, Hong Kong, Hong Kong.

In our previous publication (A.M.Myasnikov et al., MRS proc., v.715, 2002, A22.11, and v.762, 2003, A17.2) mechanism of nickel diffusion and spreading resistance probe (SRP) measurements for quality control of metal induced lateral crystallization (MILC) of amorphous silicon (a-Si) were studied. Now we present TCAD modeling and explanation of experimental results, which were obtained. A layer of 300 nm a-Si was deposited on silicon substrate oxidized up to 700 nm. Silicon film was ion implanted at a dose 10^{15} cm^{-2} and an energy 40 keV with B⁺, BF₂⁺, P⁺, As⁺ ions. 5 nm thickness nickel island seeds were used with different pattern. Temperature and time of recrystallization was varied from 550°C to 1100°C and from 10 seconds to 20 hours. The sizes of MILC regions were in the range from some microns to 200 μm. Then MILC regions were measured by spreading resistance profiler with the distance between probes 100 μm. The length and the steps of SRP measurement on surface were changed in dependence on the MILC size and carried out perpendicular nickel/MILC regions. We have been found, that SRP method can use for characterization of MILC process of a-Si. It was shown, that dynamic range of SRP data has about 5 orders that makes possible to measure with high accuracy of the samples having MILC regions differ greatly in conduction, crystallinity, and doping. On a basis of SRP data there is possibility to reveal the degree of recrystallization of a-Si in comparison with single crystal and poly-Si, to find the electrical size of MILC regions for different recrystallization, doping, and impurities, to define the nickel effect and the homogeneity of continuous MILC region from different nickel seeds, to obtain the depth and surface distributions of carrier concentration and mobility. ISE TCAD models were implemented for carrier mobility in a-Si and recrystallized layers implanted by boron, phosphorus and arsenic. By using these models the spreading resistance of different layers was found and compared with experimental results. Nickel penetration and distribution in silicon layers were calculated also and the correlation between Nickel penetration and the motion of recrystallization front was found.

A6.7

Electron Field Emission from SiC/Si Heterostructures Formed by Carbon Implantation into Silicon and Etching of the Top Silicon Layer. Yumei Xing, Yuehui Yu and Jihua Zhang; Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai, China.

High-intensity electron field emissions were obtained from SiC/Si heterostructures prepared by carbon implantation into silicon at 700°C and subsequently etching of the top silicon layer. Carbon implantation was performed at 160 keV with a dose of $3.0 \sim 8.0 \times 10^{17} \text{ cm}^{-2}$. Densely distributed sharp tips were easily obtained at the interface of the SiC/Si heterostructure for all samples. The lowest turn-on field of 2.6 V/micron was attributed to the highest implantation dose in this work. Post-implantation annealing at 1250°C in Ar for 5h was used to improve the crystalline quality of SiC layer, while electron field emission from SiC/Si heterostructures got little enhancement. It suggests that 3C-SiC precipitates embedded in silicon at the interface, which have formed during high temperature carbon implantation. Post-annealing put little effect on these 3C-SiC precipitates.

A6.8

Electron Field Emission from Laser Crystallized HWCVD

and PECVD Thin Silicon Films. M. Z. Shaikh, Kevin O'Neill, Saydullah Persheyev and Mervyn J. Rose; Electronic Engineering and Physics Division, University of Dundee, Dundee, United Kingdom.

This paper reports on Laser crystallisation of thin silicon films by excimer laser and Nd:YAG laser interferometry, to produce an electron source for use as a prospective cold cathode field emission device. This results in a new phase of conducting crystallites in an insulating medium, tested through the performance of field emission measurement. We analysed changes in the morphology, electronic and optical properties of silicon films with varying laser energies. Formation of micron-submicron tip structures, the density of these structures and the relative thresholds for field emission under varying conditions were measured. To produce the silicon films, two growth methods have been employed namely PECVD and HWCVD, thus allowing variations in microstructure from completely amorphous silicon by the PECVD to an almost completely microcrystalline structure by using the HWCVD growth method. The silicon films were deposited on glass, silicon wafer n-type <100> and on glass with various backplane metals such as Cr, Mo, Ti, and Ni. Samples with varying deposition parameters such as pressure (30 to 200 mtorr), gas-flow rate (10 to 200 sccm), hydrogen dilution ratio (5 to 70 %) and substrate temperature (150-400 degree Celsius) were grown. Pulsed excimer laser crystallisation (LC) has been performed using various intensities (50 mJ/cm² to 222 mJ/cm²) and Nd:Yag Laser 3 beam interference pattern to produce an array of uniformly spaced microcrystallites. Infrared and UV-visible spectroscopy were applied for monitoring hydrogen and oxygen bonding configurations and optical gap before and after LC respectively. The surface morphology of the Si layers have been characterized using Atomic Force Microscopy (AFM). This shows how the varying intensities of the lasers affect the films. It was found that the laser energy required for crystallization is highly dependent on the supporting material. Also interaction of these metals with the silicon film during the laser annealing process was studied. Increase in surface roughness was seen after laser annealing.

A6.9

GaAs Growth on Micro and Nano Patterned Ge/ Si1-XGeX and Si Surfaces. Ganesh Vanamu¹, Abhaya K. Datye¹, Ralph Dawson² and Saleem H. Zaidi³; ¹Chemical and nuclear, University of New Mexico, Albuquerque, New Mexico; ²Center for High Technology Materials, University of New Mexico, Albuquerque, New Mexico; ³Gratings, Inc., Albuquerque, New Mexico.

Growth of high-quality GaAs films on Si and Ge/ Si1-XGeX surfaces is of interest in a number of material systems including optoelectronic integration with Si [1] and III-V solar cells [2]. Material issues such a thermal expansion and lattice constant mismatches make it difficult to grow thick (~ few μms) heteroepitaxial layers on planar Si substrates [3]. Here, we report on the growth of thick GaAs heteroepitaxial layers on micro and nano patterned Si and Ge/Si1-XGeX surfaces. The GaAs layers were grown using MBE (0.5 μm/hr and 570 degrees C). The GaAs layer quality was evaluated through SEM, TEM, HRXRD, and PL measurements. The quality of GaAs growth mimicked Ge/ Si1-XGeX, i.e., highest defect density layers contributed to the poorest quality GaAs films and vice versa. The GaAs films on patterned Si surfaces were comparable in quality to those grown on the lowest (~ $4 \times 10^6 / \text{cm}^2$) defect density Ge/Si1-XGeX substrates. The photoluminescence (PL) measurements at 532-nm excitation showed peaks at ~ 872 nm for GaAs/Ge/Si1-XGeX micro-patterned substrates and at ~ 868.3 nm for nano-patterned surfaces. The full width half maximum (FWHM) of the PL for nano-patterned surfaces is ~ 20nm. The PL peak for GaAs grown on micro-patterned Si substrate was at ~ 871 nm. Details of microstructure characterization and PL response at long wavelength excitation will be reported at the conference. REFERENCES 1. M. E. Groenert, C. W. Leitz, A. J. Pitera, V. Yang, H. Lee, R. J. Ram, and E. A. Fitzgerald, J. Appl. Phys. 93, 362 (2003). 2. S. A. Ringel, J. A. Carlin, C. A. Andre, D. M. Wilt, E. B. Clark, P. Jenkins, D. Scheiman, C. W. Leitz, A. A. Allerman, and E. A. Fitzgerald, Prog. Photovoltaics 10, 417 (2002). 3. R. M. Sieg, J. A. Carlin, J. J. Boeckl, S. A. Ringel, M. T. Currie, S. M. Ting, T. A. Langdo, G. Taraschi, E. A. Fitzgerald, B. M. Keyes, Appl. Phys. 73, 3111 (1998).

SESSION A7: Poster Session: Metastability
Tuesday Evening, March 29, 2005
8:00 PM
Salons 8-15 (Marriott)

A7.1

Light-Intensity Dependence of the Staebler-Wronski Effect in a-Si:H with Various Densities of Defects. Minoru Kumeda¹, Ryohei Sakai¹, Akiharu Morimoto¹ and Tatsuo Shimizu²; ¹Div. Electrical Engineering and Computer Science, Grad. School of Natural Sci. and Tech., Kanazawa Univ., Kanazawa, Japan; ²NITT

The mechanism of the Staebler-Wronski effect in a-Si:H has not yet been clear, despite many efforts for a long time. According to Stutzmann, the density of photocreated dangling bond (DB) obeys the following relation with $r = 2$ in device quality a-Si:H, $N_s(t)^3 - N_s(0)^3 = AG't$. Here, $N_s(t)$ and $N_s(0)$ are the DB densities for illumination-time t and before illumination, respectively. A is a constant, and G is the light intensity. However, the experimental studies to check the light-intensity dependence are less than the illumination-time dependence. Recently, we reported that the value of r becomes smaller with increasing the N content in a-Si:N:H alloy films[1]. A similar trend has been found in a-Si:H with increased DB density. Samples in which the neutral DB density had been increased to $2.6 \times 10^{16} \text{ cm}^{-3}$ (without surface contribution) by annealing at 400 C for 1 h exhibited a small value of $r = 0.90$ compared to the as-deposited samples. Furthermore, samples which had been illuminated with a light intensity of 1 W/cm^2 for 1 h and having the neutral DB density of $3.5 \times 10^{16} \text{ cm}^{-3}$ without surface contribution also showed a small value of $r = 0.99$. We tried to explain the observed results by using rate equations for the densities of DB and floating bonds (FB) based on the FB-mediated photocreation of DB[2]. When the densities of DB and FB before illumination increase, the light-intensity dependence of the DB density for a moderate value of the illumination time becomes weaker, qualitatively consistent with the observed results. The FB density first increases, having a maximum and then a minimum, and then increases gradually toward the saturated value. After the FB density passes the minimum, the light-intensity dependence of the DB density approaches one with $r = 2$. The model of Stutzmann cannot explain the present results, and the mediation such as FB is needed for the photocreation of DB. It is possible that the H-mediated model of Branz can also explain the results. [1] M.Kumeda, M.Shimada, S.Kimura, A.Morimoto and T.Shimizu, Jpn. J. Appl. Phys., 42 (2003) L255. [2] T.Shimizu and M.Kumeda, Jpn. J. Appl. Phys., 38 (1999) L911.

A7.2

Electronic Properties of Improved Amorphous Silicon-Germanium Alloys Deposited by a Low Temperature Hot Wire Chemical Vapor Deposition Process. Shouvik Datta¹, David Cohen¹, Don L. Williamson², Yueqin Xu³ and Harv Mahan³; ¹Physics, University of Oregon, Eugene, Oregon; ²Physics, School of Mines, Golden, Colorado; ³National Renewable Energy Laboratory, Golden, Colorado.

We have established superior electronic properties for a series of seven a-Si_xGe_{1-x}H alloys with Ge fractions of 0, 0.15, 0.29, 0.47, 0.63, 0.81 and 1.0. These alloy samples were deposited onto stainless steel substrates by the hot-wire CVD growth process using a tantalum filament maintained at 1800°C. This filament temperature is lower than the 2000°C temperature previously used with tungsten filaments to deposit most of the previous a-Si_xGe_{1-x}H alloy samples produced by HWCVD at NREL. Substrate temperatures for the current series of samples were in the 200°C to 250°C range, and growth rates varied between 1.4 to 3.2 Angstrom/sec. Tauc gaps were found to lie in the range of 1.65eV for the 15at.% Ge sample to 0.98 eV for the 100% Ge sample. Small angle X-ray scattering (SAXS) measurements were carried out to determine the small scale microstructure of these samples. Unlike the a-Si_xGe_{1-x}H samples examined previously, including those produced by the glow discharge (PECVD) process, these samples exhibited roughly an order of magnitude lower SAXS signals for Ge fractions ranging from 20 to 80at.%. This is particularly surprising given that moderate ion bombardment of the growing film, long thought to be essential for the production of high quality, dense a-Si_xGe_{1-x}H, is almost totally absent in the HWCVD growth process. To determine the electronic properties of these samples we used drive-level capacitance profiling (DLCP) to establish overall deep defect densities, and sub-band-gap spectroscopy (photocurrent and photocapitance) to determine the spectra of defect related optical transitions. Previous higher filament temperature HWCVD a-Si_xGe_{1-x}H produced at NREL with Ge fractions above 20at.% had revealed quite broad Urbach energies (above 55meV) with deep defect densities in the mid 10^{16} cm^{-3} range. In contrast, the current series of samples exhibit Urbach energies as low as 42meV at 29at.% Ge, with defect densities in the low to mid 10^{15} cm^{-3} range. Thus, these HWCVD alloy samples appear to have electronic properties superior to any a-Si_xGe_{1-x}H samples we have previously examined, produced by any growth method. This is particularly noteworthy given that their growth rate is also significantly higher than that typically employed for the best PECVD alloy films. Preliminary studies of light-induced degradation of some of these alloy samples have also been carried out using a red-filtered (610nm) tungsten-halogen light-source. The degradation behavior of these alloy samples lies well within the range of that determined for a-Si_xGe_{1-x}H alloys obtained from other sources.

A8.1

Experimental Study of Silane Plasma Nanoparticle Formation in Amorphous Silicon Thin Films. Siri Thompson², Chris R. Perrey³, Thomas James Belich¹, Charles Blackwell¹, C. Barry Carter³, James Kakalios¹ and Uwe Kortshagen²; ¹Physics, University of Minnesota, Minneapolis, Minnesota; ²Mechanical Engineering, University of Minnesota, Minneapolis, Minnesota; ³Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota.

Plasma deposited hydrogenated amorphous silicon thin films with nanocrystalline silicon inclusions (a/nc-Si:H) have received considerable attention due to reports of an improved resistance to light-induced defect formation. These films are grown using silane heavily diluted with hydrogen and high reactive chamber gas pressures. An important question for film synthesis is whether the silicon nanocrystals are formed within the silane plasma and transported to the growing silicon surface or by solid-state nucleation of the nanocrystals in the film. Silicon cluster formation within an R.F. plasma is known to be sensitive to thermophoretic forces that can direct them towards or away from the silicon thin film's growing surface, depending on the sign of the thermal gradient. In this study we report plasma electronic diagnostics, optical and electrical measurements, TEM image analysis and infra-red absorption spectroscopy of a/nc-Si:H films deposited with and without a temperature gradient between the capacitively-coupled reactor electrodes. The results of these studies are consistent with particle formation occurring within the plasma. We also find that a-Si:H films grown under nominally optimal conditions (no hydrogen dilution, low gas chamber pressure, low RF power) are also sensitive to a thermal gradient across the silane plasma. In a conventional plasma deposition of a-Si:H, the substrate electrode is heated while the R.F. electrode is not, so that any particles formed within the plasma would experience a thermophoretic force away from the growing film surface. When the direction of the thermal gradient during deposition is reversed, so that the R.F. electrode is at a higher temperature than the substrate (grounded) electrode, the resulting a-Si:H films have a higher Si-H₂ content (determined from infra-red absorption measurements) and lower dark conductivity that materials grown in a standard configuration. This work was partially supported by NSF grants: DGE-0114372, NER-DMI-0403887, and DMR-0212302, DOE grant: DE-FG02-00ER54583 and NREL/AAD-9-18668-13 and the University of Minnesota.

A8.2

Transferred to A4.2

A8.3

Study of the Oxidation of Polycrystalline SiGe: Formation of Ge Nanocrystals and their Related Luminescence. Carmelo Prieto¹, Manuel Avella¹, Juan Jimenez¹, Andres Rodriguez², Jesus Sangrador², Tomas Rodriguez² and Andreas Kling^{4,3}; ¹Fisica Materia Condensada, Universidad de Valladolid, Valladolid, Spain; ²Tecnologia Electronica, Universidad Politecnica de Madrid, Madrid, Spain; ³Centro Fisica Nuclear, Universidade da Lisboa, Lisboa, Portugal; ⁴Instituto Tecnologico e Nuclear, Sacavem, Portugal.

The oxidation of polycrystalline SiGe layers deposited by low pressure chemical vapor deposition (LPCVD) allows the obtention of nanocrystalline Ge. The luminescence emission of the layers evolves with the oxidation time. In particular intense violet luminescence (3.1 eV) related to the Ge nanocrystals is observed. The properties of this emission can be controlled by the adequate selection of the oxidation process parameters (time, temperature and atmosphere). Dry and wet oxidation were used to obtain the nanoparticles, showing differences that concern the evolution of the luminescence emission, the composition of the SiGe layer during the oxidation and the composition of the grown oxides. The characterization study was carried out by cathodoluminescence, Fourier transform infrared (FTIR) spectroscopy, Raman spectroscopy and Rutherford backscattering (RBS). SiGe layers (Ge fraction, 0.3) with thicknesses of 35 and 15 nm, were used in each oxidation atmosphere in order to discern the emission of the grown oxide from the emission of the nanoparticles. The correlation between the violet luminescence, the Raman spectra and the FTIR data and the oxidation time allows to establish that the violet luminescence is related to recombination at Ge related oxygen deficient centers located at the interface of the Ge nanocrystals with the oxide matrix. The recombination centers are formed by incomplete oxidation of the outer shell of the Ge nanocrystals formed by the oxidation of the continuous Ge layer segregated from the oxidized SiGe layer. The violet luminescence is not related to quantum confinement inside the

Ge nanocrystals, since the peak wavelength does not shift with the nanocrystal size. However, it reaches its maximum efficiency when the maximum interface area between nanocrystals and the oxide matrix is formed. On the other hand, once the ge is fully oxidized the violet luminescence is fully quenched and two bands in the near infrared spectral range appear. The differences between the two oxidation mechanisms are discussed in terms of the composition of the oxide, the evolution of the poly SiGe layer, the formation of nanocrystals and the luminescence emission.

A8.4
Thermal and Laser Annealing of Si Nanocrystals, Implanted with B and P Ions. Gregory A. Kachurin¹, S. G. Cherkova¹, V. A. Volodin¹, D. V. Marin¹, V. G. Kesler¹, A. K. Gutakovskiy¹, D. I. Tetelbaum² and H. Becker³; ¹Institute of Semiconductor Physics, Novosibirsk, Russian Federation; ²Nizhgorodsky State University, Nizhny Novgorod, Russian Federation; ³Laser Zentrum Hannover, Hannover, Germany.

Because of the great importance of Si for microelectronics, continuous downscaling of the devices and the ability of quantum-size Si nanocrystals to emit strong visible light, the interest in the development of techniques to create and modify Si nanocrystals has increased considerably. Ion implantation is the most commonly used method for modification of the silicon device features. Here we report on the effect of 1013-1016 cm⁻² B and P ions implantation and of subsequent annealing on the light-emitting Si nanocrystals (Si-ncs), formed preliminarily in the thermally grown SiO₂ layers. The post-implantation heat treatments were performed by the 30 min furnace annealing in an inert ambient within the temperatures of 600-1100°C, and by the 20 nsec excimer laser pulses. Photoluminescence (PL), Raman spectroscopy, high-resolution electron microscopy, X-Ray Photoelectron Spectroscopy (XPS), and optical absorption were used for characterizations. The low fluence implantations have shown even individual displacements in Si-ncs quench their PL. Restoration of PL from partly damaged Si-ncs proceeds at annealing less than 1000°C. However the fully amorphized nanoinclusions need 1000-1100°C anneals to be re-crystallized, that is much more than the crystallization temperature of bulk Si. High crystallization temperature of the amorphized Si-ncs is attributed to a counteraction of their shell layers. In the low dose implanted and annealed samples an increased Si-ncs PL has been found and ascribed to the radiation-induced shock crystallization of stressed Si nanoprecipitates. After implantation of the highest B and P doses an enhanced recovery of PL was observed from the impurity concentrations over 0.1 at.%. Raman spectroscopy and HREM show an increased Si-ncs number in such layers. The effect resembles the impurity-enhanced crystallization, known for heavily doped bulk Si. Comparing to the P-doped Si-ncs those ones doped with B were less perfect and needed higher annealing temperatures to be re-crystallized after implantation. The 300 mJ/cm² laser pulses were found to be sufficient for the PL restoration and gave better results than 1100°C furnace annealing of B-doped nanostructures. This fact was ascribed to the short-time melting under laser irradiation. The impurity effects, along with the data obtained by XPS, are considered as an indication B and P atoms do present inside the Si-ncs. However, no evidence of free carrier appearance has been observed and, contrary to some theoretical predictions, the suppression of PL by Auger recombination does not take place. The fact is explained by an increased interaction of carriers with the atom nuclei in Si-ncs due to significant reduction of static dielectric constant in quantum confined systems.

A8.5
Experimental Evidence of Direct Recombination in Nanocrystalline Silicon Quantum Dots. Tae-Youb Kim¹, Nae-Man Park¹, Kyung-Hyun Kim¹, Kwan Sik Cho¹, Gun Yong Sung¹ and Kyoungwan Park²; ¹Future Technology Research Division, Electronics and Telecommunications Research Institute, Daejeon, South Korea; ²Nano Science & Technology, Univ. of Seoul, Seoul, South Korea.

Recently, a great deal of research effort was focused on the low-dimensional structures of indirect-gap materials such as silicon. Although the bulk crystalline silicon exhibit very weak luminescence due to the indirect band-gap in their electronic structures, silicon nanostructures having a quantum confinement effect (QCE) have provided an efficient luminescence at room temperature due to the enhancement of electron-hole radiative recombination rate. Because the mechanism of the efficient photoluminescence (PL) from nanocrystalline silicon (nc-Si) is controversial and not well understood, it is important to clarify theoretically and experimentally the intrinsic optical properties in these quantum-confined structures. Many theoretical researches have shown that, accompanying the reduction in the sizes of nc-Si quantum dots (QDs), the band-gap energy is blueshifted into the short range of visible light and the type of the band-gap transforms from indirect to direct. Nevertheless, the experimental result has not been reported clearly about direct

recombination in the nc-Si QDs having the QCE so far. In this work, we report on the experimental evidence for the QCE in zero-dimensional c-Si structure and the direct recombination in nc-Si QDs. The direct recombination was observed by examining the relation of the nc-Si QD size and the refractive index of the silicon nitride film. The PL peak energy and the refractive index of the films, which have nc-Si QDs were uniformly changed by controlling the size of the nc-Si QDs. The nc-Si QDs were grown in a silicon nitride film by plasma-enhanced chemical vapor deposition. The composition of silicon nitride matrix was confirmed by XPS and FT-IR measurement. This result is positive evidence of direct recombination in nc-Si QDs.

A8.6
Fabrication of One-Dimensional Silicon Nano-Wires Based on Proximity Effects of Electron-beam Lithography. Shu-Fen Hu, National Nano Device Laboratories, Hsinchu, Taiwan.

One-dimensional silicon nanowire structures have been successfully made by using the proximity and accumulation effects of electron-beam (e-beam) lithography. Wire structures are fabricated in a thin poly silicon layer on a silicon substrate with a 400 nm buried SiO₂. Measurements of the current-voltage characteristics at various temperatures from 4 K up to 300 K show significant nonlinearities and single-electron effect behavior. The blockade size is significantly affected by thermal effects, oscillations of the blockade, and the conductivity dependence on the gate potential.

A8.7
Charging Effect of a Nc-Si in a SiO₂ Layer with Respect to the Post-Sharpening Steps using Scanning Capacitance Microscopy. S. H. Jin¹, Y. Khang², J. M. Son¹, E. K. Lee¹, J. M. Kim³, M. K. Choi³, Eunhye Lee², Kyoyeol Lee⁴, Joohyun Lee⁴, Y. S. Kim³ and C. J. Kang¹; ¹Physics, Myongji University, Yongin, Gyeonggi-do, South Korea; ²Devices Lab, Samsung Advanced Institute of Technology, Yongin, Gyeonggi-do, South Korea; ³Electrical Engineering, Myongji University, Yongin, Gyeonggi-do, South Korea; ⁴Materials Lab, Samsung Advanced Institute of Technology, Yongin, Gyeonggi-do, South Korea.

Scanning probe microscopy (SPM) with a conducting tip has been used to characterize the electrical properties of silicon nanocrystals (NCs). The NC samples measured were produced by aerosol techniques and followed by a sharpening oxidation for improving the uniformity of size distribution and isolation. Through the direct injection and removal of charge from the conducting tip, electrical properties were monitored and analyzed with respect to the shape, size and the materials of capping shell of NC. To find out the effect of interface states formed after a sharpening oxidation, we also measured dC/dV-V dependence of a NC with different capping shells and the results were compared with those of 100µm × 100µm MOS capacitor. Temperature dependence of charging and discharging of each NC were also measured and analyzed

A8.8
Formation of Antimony 1D-Nanostructures on Si(5 5 12) Surface. S. M. Shivaprasad¹, Mahesh Kumar¹, Amish G. Joshi¹ and Vinod Kumar Paliwal^{2,1}; ¹Surface Physics & Nanostructures Group, National Physical Laboratory, Dr. K.S. Krishnan Marg, New Delhi, New Delhi, India; ²Department of Physics, Dyal Singh College (University of Delhi), Lodhi Road, New Delhi, New Delhi, India.

Of late, high index Si surfaces like, (5 5 12) are being probed for forming 1D nanostructures in the form of nanowires or chains. The surface topography of Si(5 5 12) presents a single-domain planar reconstruction that is composed of row like structures having nanoscale widths providing a unique template for the growth of 1D nanostructures. In this paper we are reporting the adsorption-desorption studies of Sb onto (2x1) reconstructed surface of Si(5 5 12). Earlier, we have reported [1,2] the adsorption of Sb on low index surfaces (001 & 111), and thus studying its interaction on high indices like (5 5 12) is interesting. The experiments have been performed UHV with in-situ growth and probed by using AES, LEED and EELS studies. The AES uptake curve taken at RT shows the presence of multiple features that may arise due to the presence of row-like surface topography of (5 5 12). Initially, the Sb adsorption takes place in the form of simultaneous multilayers upto 4ML that gives rise to an island type of growth for coverages upto 20ML. During RT growth, LEED studies at submonolayer coverages show that Sb adatoms preferentially occupy the secondary and tertiary rows, which have higher dangling bond density as compared to primary rows that are devoid of any dangling bonds. The LEED pattern of clean Si(5 5 12) surface shows alternate sharp lines and spotted streaks characteristics of the (2x1) reconstruction. In LEED photographs this can be seen as the disappearance of regular LEED spots within the main lines leaving some equal spaced intense spots for submonolayer coverages. It is also observed that for Sb coverages above 1ML, the remaining strong LEED spots along the lines also

weaken. Ultimately for higher coverages (>4ML), we see reflexes of Sb(111)-(1x1). EELS studies at 250eV primary beam energy show that as the adsorption proceeds the plasmon features (bulk, surface and interband transitions) of bulk Sb start appearing above 4ML coverage. However, the bulk Sb features are not complete until a high enough coverage of Sb (~ 20ML) which suggests the existence of the primary rows upto a higher coverage. Annealing studies have also been performed on the RT adsorbed system, to study the residual thermal desorption. Annealing the system to about 790°C results in a new (1x1) superstructure of Sb at a low coverage of about 0.2ML. The anisotropy in the LEED spots suggest an ordered Sb adsorption along (110) and a local disorder in the (665) direction. This is possible in the wider (225) troughs, and thus we suggest the formation of a zig-zag Sb 1D-nanochain of Sb grown on the (5 5 12). This new phase may be the result of various competing kinetic and thermodynamic factors. [1] V. K. Paliwal, A.G.Vedeshwar, S.M. Shivaprasad, Phys. Rev.B66(2002)245404 [2] V. K. Paliwal, S. M. Shivaprasad, Surf. Sci. 561(2004)L207

A8.9

Fabrication of Silicon Nanowire Network in Aluminum Thin Films. Vincent Liu¹, Husam Abu-Safe² and Hameed Naseem²;

¹Electrical Engineering and Computer Sciences, University of California, Berkeley, Berkeley, California; ²Electrical Engineering, University of Arkansas, Fayetteville, Arkansas.

The formation of isolated silicon nanowires and silicon nanowire networks using aluminum thin film is investigated. The formation mechanism of the network mainly depends on the diffusion of silicon in the aluminum thin film. The silicon stops at the film grain boundaries. The continuous accumulations of silicon at these boundaries give rise to a continuous network of silicon nanowires. Characterization of the nanowires has been done using scanning electron microscopy (SEM) and energy dispersive x-ray spectroscopy (EDS). These results are unique in the fact that the nanowires found are grown in a horizontal fashion instead of the more common vertical direction. Most of the nanowires have a diameter of about 60 nm and a length of over 10 gm.

A8.10

Synthesis of Fluorescent Si Nanomaterial Films from Silicate Water Glass Solutions. Munir H. Nayfeh^{1,2} and Laila Abuhassan³;

¹Physics, University of Illinois, Urbana, Illinois; ²Research Division, NanoSi Technologies, Champaign, Illinois; ³Physics, University of Jordan, Amman, Jordan.

We report on a procedure for the synthesis of fluorescent silicon nanomaterial from silicates or water glass solutions. When a positively biased platinum substrate is immersed in a solution of sodium metasilicate salts (Na₂SiO₃) in HF/H₂O₂, a current is drawn and a thin coating is formed on the substrate. Fluorescence spectroscopy and microscopy, Fourier transform infrared spectroscopy (FTIR), and material analysis using x-ray photo spectroscopy (XPS) and Auger electron spectroscopy (AES) show that the film consists of silicon-based red to infrared fluorescent material, dominated by 2.85 and 3.6 nm diameter nanostructures. The films are useful in large-area electronic and optoelectronics applications.

A8.11

Hot-mesh Chemical Vapor Deposition for 3C-SiC Growth on Si and SiO₂. Kanji Yasui, Jyunpei Eto, Yuzuru Narita, Masasuke Takata and Tadashi Akahane; Electrical, Electronic and Information, Nagaoka University of Technology, Nagaoka, Japan.

SiC is a wide bandgap semiconductor expected in the field of electronic devices for high frequency, high power and high temperature applications. Among many polytypes, cubic SiC (3C-SiC) is stable phase at low temperatures and can be grown on Si substrates. Therefore the epitaxial growth of 3C-SiC on Si substrates has been extensively investigated. In the conventional chemical vapor deposition (CVD), however, SiC growth at high temperatures (>1000 deg C) inevitably results in the formation of voids at SiC/Si interface. It is important for the fabrication of high quality SiC/Si system to lower the growth temperature. In addition to the SiC growth on Si substrates, fabrication of the SiC on insulator (SiCOI) structure has been eagerly investigated for the MEMS applications. In our previous studies, 3C-SiC epitaxial films were grown at 900 deg C by triode plasma CVD using organosilicon compounds such as monomethylsilane (MMS) and dimethylsilane (DMS) as source gases, while those were not grown at the low temperature by low pressure (LP) CVD using the same source gases [1]. From the experiments by triode plasma CVD, H radicals generated in the RF plasma was considered to induce desorption of H atoms and excessive methyl-groups from source molecules on the growing film surface. In the plasma CVD process, however, incident of the charged particles such as ions and electrons may degrade the crystal structure during the SiC growth. By catalytic reaction on hot-tungsten (W) wire

surface, H₂ gas can be effectively decomposed and high density of hydrogen radicals can be generated [2]. In this study, the growth of 3C-SiC on Si(100) and on its thermal oxide layer was investigated by hot-mesh (HM) CVD, which utilizes a hot W wire of a mesh structure as a catalyzer. From the X-ray diffraction spectra of SiC films grown by HMCVD using MMS, it was found that 3C-SiC films were epitaxially grown at above 750 deg C, while those grown by LPCVD were amorphous. From the experimental results of SiC growth on SiO₂ layer, polycrystalline SiC films were grown at the substrate temperature above 900 deg C, while <100> oriented SiC films were grown at the substrate temperature of 750 deg C and the mesh temperature of 1400-1600 deg C. Above 900 deg C, H atoms can be thermally desorbed from Si-H and C-H bonds present at the growing film surface. On the other hand, H atoms of C-H bonds cannot be thermally desorbed at 750 deg C. Therefore, the growth of <100> oriented SiC films at 750 deg C is considered to be the result of a reaction between H radicals and precursors on the growing film surface. 1) K. Yasui, K. Asada, T. Maeda, and T. Akahane: Appl. Surf. Sci. 175-176 (2001) 495. 2) A. Masuda, H. Umemoto, and H. Matsumura: IEICE Trans. on Electron., J87-C No.2 (2004) 203 [in Japanese].

SESSION A9: Poster Session: Novel Devices–Sensors,
Diodes, etc.
Tuesday Evening, March 29, 2005
8:00 PM
Salons 8-15 (Marriott)

A9.1

Advances in Amorphous Silicon Integrated Photonics Science and Technology. Gary P. Halada¹, S. Chawda¹, J. A. Mawyin¹, R. J. Tonucci², A. H. Mahan³ and C. M. Fortmann⁴; ¹Department of Materials Science and Engineering, Stony Brook University, Stony Brook, New York; ²Naval Research Laboratory, Washington, District of Columbia; ³National Renewable Energy Laboratory, Golden, Colorado; ⁴Department of Applied Mathematics, Stony Brook University, Stony Brook, New York.

Over the last few years we have been developing a scientific basis for amorphous silicon integrated photonic technology. In this presentation we report: the successful demonstration of a refractive index patterned amorphous silicon waveguide, other technological developments, as well as the ongoing expansion of the scientific basis for this work. The technological significance of this can be appreciated by the ease by which these coatings can be adapted for inexpensive or large area applications or deposited onto any existing electronic integrated circuit to form complex hybrid opto-electronic integrated circuits. Films and refractive index patterned devices have been analyzed using Raman and diamond crystal attenuated total reflectance (ATR) molecular spectroscopy, X-ray photoelectron spectroscopy (XPS), and extended X-ray absorption fine structure (EXAFS) spectroscopy at the National Synchrotron Light Source at Brookhaven National Laboratory. Complementary Raman and EXAFS analysis provided bonding and short range ordering data which provides a basis for ab initio self-consistent field (SCF) and density functional theory (DFT) calculations. These calculations in turn provide predictions of vibrational frequencies which have been compared to experimental data. ATR and XPS analysis provided data on near-surface chemistry and degree of surface oxidation or adsorption of hydrocarbons. This near-surface chemistry does not appear to adversely affect the optical properties of the surfaces. Films deposited at the National Renewable Energy Laboratory are compared to those deposited using a custom-designed system at Stony Brook University.

A9.2

Spectral Sensitivity and Color Selectivity in Multilayer Stacked Devices. Paula Louro¹, Fernandes Miguel¹, Alessandro Fantoni¹, Guilherme Lavareda², Carlos Nunes de Carvalho², Yuriy Vygranenko¹ and Manuela Vieira¹; ¹DEETC, ISEL, Lisbon, Portugal; ²CFM, UTL, Lisbon, Portugal.

Color detection in two terminal silicon based devices is based on the spatially separated absorption of different wavelengths. The discrimination between the different absorption regions becomes complex when three color information is required. In this work an attempt of full color discrimination is presented. The sensitive devices are multilayer stacked structures (p(SiC:H)/i(SiC:H)/n(SiC:H) /p(SiC:H)/i(SiC:H)/n(SiC:H)) sandwiched between two transparent conductive contacts. The thickness and the absorption coefficient of the front p-i-n cell is optimized for blue collection and red transmittance and the thickness of the back one adjusted to achieve full absorption in the green and high collection in the red spectral ranges. Color discrimination is achieved through the modulation of one, two or both cell depletion regions by an applied external voltage. The devices are characterized through the analysis of the

photocurrent and spectral response under different steady state optical bias ($\lambda_L=650\text{ nm}; 550\text{ nm}; 450\text{ nm}; 0<\Phi_L<500\ \mu\text{Wcm}^{-2}$) and applied voltages ($-15\text{ V}\leq V\leq 2\text{ V}$). In order to tune the external applied voltage for full color discrimination and to evaluate the sensors responsivity to different light wavelengths, the photocurrent generated by a modulated red light ($\lambda_S=650\text{ nm}$) is measured under different optical bias. In these measurements the sensor element is illuminated through the back diode with red modulated light and the optical bias applied through the front diode side. Results show that the conversion efficiency to a red modulated light under blue front optical bias is maximized when a 200nm a-SiC:H front absorber is used, and minimized in the red range if the absorber layer of the back diode is around $1\ \mu\text{m}$ thick. In those devices the green photons absorption mainly occurs across the front diode, the n-p defectuous interface and at the front side of the back diode. Under reverse bias and blue irradiation the collection is high since the back diode becomes fully depleted due to its self biasing process. Under red illumination the a-Si:H back absorber acts as a load due to the high light penetration depth of the red photons and the collection is almost inexistent and determined by the dark characteristics of the front diode. In the green spectral range as the reverse bias increases due to the increase of the potential drop across the back diode the collection increases linearly. The effect of the applied voltage on the color selectivity and spectral sensitivity is discussed and supported by a physical model that takes into account the experimental data and the results obtained through a detailed numerical simulation based on the ASCA simulator.

A9.3

Application of SC-Simul for Numerical Modeling of the Opto-Electronic Properties of a-Si:H/c-Si Heterojunction Diodes. Rudolf Bruggemann, Maximilian Rosch, Saioa Tardon and Gottfried H. Bauer; Institut für Physik, Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany.

We present the numerical-modelling programme SC-Simul which is available free of charge. In addition to stationary device modelling, time-dependent experiments can also be treated for which the progress in the time-dependent current, carrier and other distributions within the devices can be inspected. Typical devices that can be modeled are a-Si:H pin diodes and a-Si:H/c-Si heterojunction diodes. The presentation focusses on the latter devices and shows detailed simulation results on current-voltage characteristics, photoluminescence and electroluminescence, for which the influence of interface defects is shown to be strong. We detail the role of an intrinsic a-Si:H buffer layer between the doped a-Si:H layer and c-Si wafer and how its influence on device behavior is also determined by the density of interface defects. Based on these simulation results we shall also comment on the conflicting experimental results in the literature on the benefits of such a buffer layer

A9.4

Two-Dimensional a-Si:H/a-SiC:H n-i-p Sensor Array with ITO/a-SiN_x Antireflection Coating. Yuriy Vygranenko, Jeff Chang and Arokia Nathan; Department of Electrical and Computer Engineering, University of Waterloo, Waterloo, Ontario, Canada.

This paper presents a two-dimensional a-Si:H/a-SiC:H n-i-p photodiode array with switching diode readout, developed specifically for fluorescence-based bio-assays. Both device structure and fabrication processing has enabled enhancement of the external quantum efficiency of the encapsulated device up to 80%, reduction of the photodiode leakage down to $10\ \text{pA/cm}^2$ at -1 V reverse bias, and increase of the rectification current ratio of the switching diodes up to 10^9 . The critical fabrication issues associated with deposition of device-quality materials, tailoring of defects at the i-p interface, device patterning with dry etching, junction passivation, and contact formation, will be discussed. Both sensing and switching diodes were characterized. While the observed dark current in the photodiodes at low reverse bias voltages is primarily due to carrier emission from deep states in the a-Si:H bulk, the leakage in the small switching diodes stems from peripheral defects along junction sidewalls. Optical losses in the photodiodes with ITO/a-SiN_x:H antireflection coating were evaluated using numerical modeling, and the calculated transmission spectra correlated well with the spectral response characteristics. Measurements of the charge transfer time and output linearity demonstrate the efficiency of the single-switching diode readout configuration. The response of the array to optical excitation was also investigated. The observed long term retardation in the signal rise and decay at illumination levels less than $10^{10}\ \text{photons/cm}^2\text{-s}$ can be associated with charge trapping in the undoped layer.

A9.5

Amorphous Silicon Based piip Structure for Color Sensor. Shubin Zhang, Leandro Raniero, Elvira Fortunato, Isabel Ferreira, Hugo Aguas and Rodrigo Martins; Material Science, Faculty of Science and Technology, New University of Lisbon and CEMOP-UNINOVA, Caprica, Portugal.

The optical band gap of hydrogenated amorphous silicon can be modified by adding controlled amounts of carbon or germanium during the deposition. The amorphous silicon based photodetectors can be obtained with sensitivities ranging from the ultraviolet to the infrared. In the last years, bias controlled two- and three-color detectors on stacked a-SiC:H/a-Si:H heterostructures have been extensively investigated. This work deal with the study of the roles of the film thickness and composition on the colour selection of the collection spectrum of glass/ZnO:Ga/p-a-Si1-xCx:H/ a-Si1-xCx:H/a-Si:H/n-a-Si:H/Al photoelectronic detectors produced in a single chamber plasma enhanced chemical vapour deposition (PECVD) system. The cross contamination were minimized by a rotation cover substrate holder system. The devices can detect the blue illumination at small reverse bias and detect red illumination at large reverse bias. The effects of the parameters, especially the film thickness (p-type and intrinsic a-SiC:H, and the intrinsic a-Si:H) and the band gap offset in the a-SiC:H and a-Si:H films on the devices were studied in detail to achieve better detectivity.

A9.6

Hydrogen Content in Silicon Nitride Films Deposited by PECVD and used as Support Layer and Absorber Layer for Uncooled Microbolometers. Roberto Carlos Ambrosio, Alfonso Torres, Andrey Kosarev, Mauro Landa and Adrian Itzmoyotl; Electronics, INAOE, Puebla, Mexico.

We have studied silicon nitride films SiN_x deposited by Low frequency (LF) PECVD technique at the substrate temperature Ts=350°C using silane and nitrogen as stock gases. The film properties including hydrogen bonding and content, nitrogen content, refraction index and etch rate are reported and analyzed. The results show similar physical properties to those in the films obtained at Ts=700°C by LPCVD. The comparative investigation of bonding structures for the samples was achieved, and quantitative results for hydrogen bondings based on FTIR analysis are presented. It was observed that low hydrogen content in the films correlated with low etch rate in 10% buffered HF solution, therefore these films present a material with a good selectivity for etching in respect to others (PSG, Al etc). It makes promising to employ the films in surface micromachining for fabrication of device structures, e.g. microbolometers. Additionally, the Si-N bond at $830\text{-}840\text{ cm}^{-1}$ was analyzed due to the absorption that produced at $12\ \mu\text{m}$, thus these films can be used as absorber layers in uncooled microbolometers.

A9.7

Fabrication and Characteristics of FeSi2-Si Based Infrared Light Emission and Detection Devices. C. F. Chow^{1,3}, S. P. Wong^{1,3}, Y. Gao¹, N. Ke^{1,3}, Q. Li^{2,3}, W. Y. Cheung^{1,3}, M. A. Lourenco⁴ and K. P. Homewood⁴; ¹Electronic Engineering, Chinese University of Hong Kong, Shatin, N.T., Hong Kong; ²Physics, Chinese University of Hong Kong, Shatin, N.T., Hong Kong; ³Materials Science and Technology Research Centre, Chinese University of Hong Kong, Shatin, N.T., Hong Kong; ⁴School of Electronics Engineering, Computer and Mathematics, University of Surrey, Guildford, Surrey, United Kingdom.

Silicon-based optoelectronics has been a topic of increasing research interest in the past decade and there has been significant progress towards a working Si-based light emitting device despite the indirect bandgap nature of Si. For example, electroluminescence (EL) at room temperature was recently reported from Si metal-oxide-semiconductor (MOS) structures [1] and room-temperature emission from beta-FeSi2 LED was also successfully demonstrated [2]. In this work, MOS structures were fabricated on Si with the oxide layer grown by well-controlled rapid thermal oxidation (RTO). The FeSi2 nanocrystals were formed inside the MOS active region by iron implantation using a metal vapor vacuum arc ion source at various conditions. EL properties from these FeSi2-Si MOS structures after various thermal treatments were measured as a function of temperature from 80 to 300K. Our preliminary results showed that clear EL signals were obtained even at room temperature for some of the devices prepared at appropriate processing conditions. Details on the fabrication and thermal treatments of these devices and the dependence of the EL properties on the processing parameters will be presented and discussed. Metal-semiconductor-metal (MSM) photodetector device structures based on the implanted FeSi2-Si system have also been fabricated and their performance as Si-based IR detectors will be reported. This work is partially supported by the Research Grants Council of Hong Kong SAR (ref. no. CUHK 4231/03E), and C.N. Yang Optical Science Fund. [1] M.-J. Chen et al, J. Appl. Phys. 93 (2003) 4253. [2] M.A. Lourenco et al, Nucl. Instr. Meth. B206 (2003) 436.

A9.8

A Comparison of Light Soaking Effects between Porous Silicon and a-Si:H. S. C. Agarwal and N. P. Mandal; Physics, I.I.T.

Kanpur, Kanpur, U.P., India.

Porous silicon (PS) samples are prepared by the electrochemical etching of boron doped crystalline silicon wafers. Micro-Raman shows the presence of nanocrystalline Si and a-Si:H. The as prepared PS samples show a PL peak at 760 nm when excited by a Argon Ion laser. In air, exposure to visible light (LS) decreases PL and increases ESR monotonically as the exposure time increases. On the other hand, an increase in PL is observed after LS of short durations, when the sample is in vacuum. This is accompanied by a decrease in ESR. Longer exposures, however, show an increase in PL and an increase in ESR. These changes cannot be erased by exposure to sub band gap light, but annealing reverses the original state. This shows that LS causes photo structural changes in PS. These effects are similar to the well known Staebler Wronski (SWE) effect observed in a-Si:H. However, when we exposed our PS samples to the cycles of moisture and LS, we found that the final state depends on the order in which LS and moisture exposure are performed. This is contrary to the result in a-Si:H and might mean that whereas the SWE in a-Si:H is a bulk effect, the photostructural changes in PS are at the surface. We have made attempts to make PS stable by applying a thin layer of a polymer. Several polymers (Polystyrene, PMMA, di-chloro di-methyl Silane (DDMS) and Sylgard etc.) have been tried. We find that polystyrene and PMMA arrest the photo-induced degradation of PS up to the maximum duration tested (300hrs). However, PS samples coated with DDMS and Sylgard continue to degrade upon LS. FTIR shows appearance of new bonding configurations at the PS/polymer interface. These may be responsible for the improved stability of PS after polymer coating, by making stronger bonds. The changes at the interface after LS in the DDMS and Sylgard coated PS, which show degradation, will be compared with those found in the PMMA and polystyrene coated samples and the factors responsible for the stability of PL will be examined. It is interesting to note that although Polystyrene coated PS is stable, such a coating on a-Si:H does not remove the SWE, although it makes it somewhat smaller. This and other differences between the degradation of a-Si:H and PS layers will be discussed.

A9.9

Effect of Post-Oxidation of Silicon Nanocrystals as a Floating Gate of Nonvolatile Memory. Jung Min Kim¹, Min Ki Choi¹, Y.

Khang², E. K. Lee³, Eun Hye Lee², Kyo Yeol Lee², Joo Hyun Lee², C. J. Kang³ and Y. S. Kim¹; ¹Electrical Engineering, Myongji University, Yongin, Gyeonggi-Do, South Korea; ²Devices Lab, Samsung Advanced Institute of Technology, Suwon, Gyeonggi-Do, South Korea; ³Physics, Myongji University, Yongin, Gyeonggi-Do, South Korea.

In this work, electrical properties of Si nanocrystals (NCs) were analyzed with respect to the post-oxidation; shell formation of NCs. The Si nanocrystal samples produced by pyrolysis and laser ablation methods were followed by sharpening oxidation steps. In this steps Si NCs are capped with a thin oxide or nitride layer of 1~2nm thickness for isolation and the size control. It also affects the interface states of NCs, resulting in the change of electrical properties. To find out this effect, conventional C-V, I-V measurements were done on a MOS capacitor structure. And the results were analyzed for the size, density, shell materials and shell thickness of NCs. We also present localized property of a Si nanocrystal observed by scanning probe microscopy (SPM).

SESSION A10: Growth II: Microcrystalline Films
Chair: Michio Kondo

Wednesday Morning, March 30, 2005
Room 2002 (Moscone West)

8:30 AM A10.1

Room Temperature Deposition of Nanocrystalline Si Thin Films. Radhika Chandrasekhar Mani and Eray S. Aydil; Chemical Engineering, University of California Santa Barbara, Santa Barbara, California.

Hydrogenated nanocrystalline silicon (nc-Si:H) has tremendous potential for various applications in solar cells, thin film transistors (TFTs) for flat panel displays, single-electron transistors and memory devices, and Si-based light emitting diodes. Low temperature (<100 °C) deposition of nc-Si:H thin films is desirable for manufacturing devices on flexible and inexpensive substrates (e.g. plastic). Plasma enhanced chemical vapor deposition (PECVD) presents an affordable synthesis method for large-area deposition of nc-Si:H thin films. We demonstrate the deposition of thin films containing nanocrystals of silicon using an inductively coupled plasma source and SiH₄ diluted in H₂ at room temperature on silicon and GaAs substrates. In situ surface and film diagnostic techniques, such as attenuated total internal reflection - Fourier transform infrared spectroscopy (ATR-FTIR) and spectroscopic ellipsometry (SE), were used to probe the surface and bulk silicon hydrides species (SiH_x) and to determine

the thickness of the growing film, respectively. The change in the substrate temperature was carefully monitored using the infrared radiation transmission through the ATR crystal in order to eliminate the possibility that nanocrystal formation is due to plasma heating. The deposited films were characterized using ex-situ techniques such as Raman spectroscopy, grazing angle X-ray diffraction (XRD) and Transmission electron microscopy (TEM). Both in situ and ex-situ characterization techniques revealed the presence of 10 nm size crystals in the films deposited at room temperature. Spectroscopic ellipsometry was also used to determine the crystalline fraction in the growing films as a function of H₂-to-SiH₄ ratio in the feed gas and substrate temperature. The in situ ATR-FTIR and SE data are consistent with H-induced ordering of amorphous silicon layers which leads to the nucleation of nanocrystals within the film.

8:45 AM A10.2

Growth and Properties of Nanocrystalline Ge:H Films and Devices. Vikram Dalal² and Xuejun Niu²; ¹Elec. and Comp. Engr., Iowa State University, Ames, Iowa; ²Electrical and Computer Engr., Iowa State University, Ames, Iowa.

Nanocrystalline Ge:H is a potentially important material for solar cells and image sensors. In this talk, we describe the growth and properties of nanocrystalline Ge:H films and devices. The films and devices were grown using a remote ECR plasma discharge. The precursor gases were germane, diluted 10% in hydrogen, and hydrogen. The ratio of hydrogen to germane was systematically varied to study the influence of hydrogen etching. The deposition pressures were low, in the range of 5 mTorr. The deposition temperatures were varied between 150 C and 300 C. The films were measured for their carrier concentration and mobility, using Hall effect measurements as a function of temperature. The films were measured for their structure using x-ray diffraction and Raman spectroscopy. From x-ray diffraction, it was found that the grains had <220> orientation and the grain sizes achieved were unusually large, ranging from 15 nm to as high as 85 nm. All the films showed a sharp Raman peak at 300 cm⁻¹, characteristic of crystalline Ge. It was discovered that as hydrogen etching increased, the grain sizes decreased. Similarly, increasing power decreased the grain size for a given hydrogen dilution and deposition temperature. At very low growth temperatures, the grain size decreased. All the films were n type as grown. The doping varied between 1E16 and 1E17/cm³. Doping could be changed by adding ppm levels of B and P during growth. The mobilities were found to depend upon the grain size, with the largest grains showing Hall mobilities as large as 8 cm²/V-sec. Proof of concept p-i-n junction solar cell devices were made on steel substrates. The devices showed quantum efficiency extending out to 1300 nm. By adding Si to Ge, the open-circuit voltage could be systematically increased.

9:00 AM A10.3

Influence of Pressure and Plasma Potential on High Growth Rate Microcrystalline Silicon Grown by VHF PECVD. Aad Gordijn, Jeroen Francke, Jatindra Kumar Rath and Ruud E. I. Schropp; Debye Institute, SID-Physics of Devices, Utrecht University, Utrecht, Netherlands.

Microcrystalline Silicon ($\mu\text{c-Si}$) based single junction solar cells are deposited by VHF PECVD using a showerhead cathode at high pressures in depletion conditions. At a deposition rate of 1.3 nm/s, a stabilized conversion efficiency of 6.9% is obtained for a single junction solar cell with a $\mu\text{c-Si}$ i-layer of 1 μm thick with a simple Ag back contact. The i-layer is made near the transition from amorphous to crystalline. In order to control the material properties in the growth direction, the hydrogen dilution of silane in the gas phase is graded following different profiles with a parabolic shape. It is observed that the performance of solar cells improves under light soaking conditions at 50 °C (in 400 hrs, the FF improved from 0.67 to 0.70 and the diode quality factor from 1.81 to 1.72), which we attribute to post deposition equilibration of a fast deposited transition material. Upon increasing the deposition rate to 2.5 nm/s, we could still obtain a high efficiency of 7.1% (initial) with a ZnO/Ag back reflector. The performance is generally lower at higher rates due to poorer i-layer quality (higher defect density) due to smaller relaxation times for growth precursors at the growth surface and the higher energy ion bombardment at higher plasma power. High process pressures can be used to reduce the ion energy by decreasing the mean free path. The product of the maximum pressure and the electrode distance at which the plasma can be maintained limits the range of this method. As an alternative method to limit the ion energy, we control the DC self bias voltage using an external power source. In this way the quality of the $\mu\text{c-Si}$ layers and the performance of the solar cells can be further improved.

9:15 AM A10.4

'Seed-Layers' for the Preparation of Hydrogenated Microcrystalline Silicon with Defined Structural Properties on Glass. Christoph Ross, Yaohua Mai, Reinhard Carus and

Friedhelm Finger; Institut fuer Photovoltaik, Forschungszentrum Juelich, Juelich, Germany.

The substrate dependence of the growth of microcrystalline silicon ($\mu\text{c-Si:H}$) generally limits the possibilities of characterization of device-grade material. For example, a deposition process leading to highly efficient absorber layers in a solar cell may produce material with different properties on glass, which is a common substrate for material characterization. This limitation could be overcome if one uses glass coated by a thin 'seed-layer' on which a microstructure similar to that of the absorber layer forms [1]. This presentation will demonstrate the benefits of a thin intrinsic $\mu\text{c-Si:H}$ 'seed-layer'. We comparatively study the properties of $\sim 0.5 \mu\text{m}$ thick absorber-like $\mu\text{c-Si:H}$ layers prepared by plasma-enhanced chemical vapor deposition (PECVD) on bare glass, 'seed-layer' coated glass, and p-type $\mu\text{c-Si:H}$. The hydrogen dilution of the silane source gas is varied in order to cover the full range from highly crystalline to amorphous growth. For 'seed-layers' we use $\sim 9 \text{ nm}$ thick $\mu\text{c-Si:H}$ prepared with high hydrogen dilution in a separate PECVD step. Results from Raman spectroscopy, electrical conductivity measurements, and photothermal deflection spectroscopy (PDS) are presented. While the contribution of the 'seed-layer' to optical absorption and Raman mode excitation can be neglected, the conductivity is corrected for the 'seed-layer' contribution. High hydrogen dilution leads to highly crystalline material for all substrates, where no significant differences in microstructure are detected. On the other hand, major differences occur for a wide range of lower hydrogen dilution including optimum conditions for solar cell preparation as well as the microcrystalline-to-amorphous transition regime. Here, the use of 'seed-layers' turns out to be crucial (1) for achieving a crystalline content higher than of layers on bare glass and close to layers on p-type $\mu\text{c-Si:H}$, (2) for creating a homogeneous structure throughout the layer, and (3) for shifting the position of the microcrystalline-to-amorphous transition towards lower hydrogen dilution. Moreover, the 'seed-layer' is effective for reducing stress as can be seen from film adhesion on flat substrates. Finally, as a consequence of improved homogeneity, artifacts in the PDS spectra, which occur for moderately crystalline material on bare glass, are strongly reduced. Absorption data which are gained in this way are in good agreement with structural data obtained by Raman spectroscopy. It is concluded that 'seed-layers' of the present type significantly improve material characterization for device-grade $\mu\text{c-Si:H}$ films. [1] O. Vetterl, M. Hilsbeck, J. Wolff, R. Carius, F. Finger, Thin Solid Films 427, 46 (2003).

9:30 AM A10.5

Solid Phase Crystallization of Hot-Wire CVD Amorphous Silicon Films. David L. Young, Paul Stradins, Banasri Roy, Eugene Iwaniczko, Bobby To, Bob Reedy, David Ginley, Howard M. Branz and Qi Wang; National Renewable Energy Laboratory, Golden, Colorado.

We measure times for complete solid phase crystallization (SPC) of a-Si:H thin films that vary eight orders of magnitude from a few days to a few ms. The apparent SPC activation energy is approximately 1.6 eV and depends little on film thickness or deposition rate. Hydrogenated amorphous silicon (a-Si:H) films, 1-7 μm thick, were deposited by high deposition rate (10-100 $\text{\AA}/\text{s}$) hot-wire chemical vapor deposition onto various glass, stainless steel and c-Si substrates. We annealed these a-Si:H films over a wide temperature range (500 to 1300 $^{\circ}\text{C}$) using techniques including simple hot-plates and tube furnaces, rapid thermal annealing by a tungsten-halogen lamp, and microwave electromagnetic heating at 2.45 GHz (magnetron) and 110 GHz (gyrotron). We characterize the films' structural properties by x-ray diffraction, scanning electron microscopy, transmission electron microscopy and by optical reflectance in the range of 200 - 1000 nm. Impurity diffusion during annealing is studied by secondary ion mass spectrometry of films and devices.

9:45 AM A10.6

Low Substrate Temperature Deposition of Crystalline SiC using HWCVD. Stefan Klein¹, Reinhard Carius¹, Friedhelm Finger¹ and Lothar Houben², ¹Institut fuer Photovoltaik, Forschungszentrum Juelich, Juelich, Germany; ²Institut fuer Festkoerperforschung, Forschungszentrum Juelich, Juelich, Germany.

Microcrystalline silicon carbide ($\mu\text{c-SiC}$) was prepared at substrate temperatures between 300 $^{\circ}\text{C}$ and 450 $^{\circ}\text{C}$ using Hot Wire Chemical Vapour Deposition (HWCVD). The SiC films were deposited from monomethylsilane (MMS) diluted in hydrogen on glass and crystalline silicon substrates. The influence of the hydrogen dilution, the filament temperature and the deposition pressure on the deposition rate, the structural and the optoelectronic properties were investigated. Infrared and Raman spectroscopy and transmission electron microscopy (TEM) were applied to study the structural properties. Optical absorption measurements by photothermal deflection spectroscopy (PDS) as well as dark and photo-conductivity measurements were used to investigate the optoelectronic properties of

the material. At high hydrogen dilutions material with a high content of crystalline SiC phase is obtained. Crystallites with 20 nm in size were observed by TEM. Transmission electron diffraction shows the typical pattern of tetrahedrally bonded, crystalline SiC. The Raman spectra of such material show narrow peaks at $\approx 795 \text{ cm}^{-1}$ and 965 cm^{-1} , attributed to the TO and LO phonon of SiC. The Raman scattering intensity of Si-Si and C-C bonds, on the other hand, is very low, a crystalline silicon peak was never observed in the Raman spectra. The infrared spectra exhibit a narrow Lorentzian peak near 800 cm^{-1} which originates from the SiC bond. The intensity of this peak suggests a high fraction of SiC bonds in such highly crystalline material. The presence of strong, narrow peaks of SiC in the Raman and IR spectra and only weak Raman scattering signals originating from Si-Si and C-C bonds indicate an ordered lattice site occupation and no clustering of Si or C atoms. However, the nucleation of SiC on glass or crystalline silicon substrates is difficult in this low-temperature deposition regime. The thickness dependence of the material properties was monitored in a thickness series by Raman and infrared spectroscopy and optical absorption measurements. Transmission electron microscopy of cross sectional samples was also applied to study the nucleation of the $\mu\text{c-SiC:H}$ films and their structural properties. An increase of the MMS concentration in the deposition gas results in an increase of the deposition rate and simultaneously in a decrease of the crystallinity, similar as previously described for $\mu\text{c-Si:H}$. The decreasing crystallinity is reflected in the decreasing SiC-Raman peaks, the broadening of the SiC IR-absorption peak, an increasing optical absorption at high energies and the drop of the dark conductivity. Thus, stoichiometric $\mu\text{c-SiC:H}$ could be prepared at a substrate temperature around 300 $^{\circ}\text{C}$ using Hot Wire CVD and hydrogen diluted MMS source gas. Similar to the deposition of microcrystalline silicon the transition from amorphous SiC growth to crystalline SiC growth can be accomplished by decreasing the MMS concentration in the source gas.

SESSION A11: Solar Cells I: Stability
Chair: Christopher Wronski
Wednesday Morning, March 30, 2005
Room 2002 (Moscone West)

10:30 AM *A11.1

Improved Stability of Hydrogenated Amorphous Silicon Solar Cells Fabricated by Triode-Plasma CVD. Hiroshi Sonobe^{1,2}, Aiko Sato², Takashi Fujibayashi², Satoshi Shimizu², Takuya Matsui², Akihisa Matsuda² and Michio Kondo²; ¹Mitsubishi Heavy Industries, Nagasaki, Japan; ²National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan.

In hydrogenated amorphous silicon (a-Si:H), light-induced degradation is considered to correlate with Si-H2 bond density in the film which dominates the structural flexibility of silicon network to cause the bond-breaking. We have developed a deposition method to reduce Si-H2 concentration in the i layer using a triode-plasma chemical vapor deposition method, where a plasma was separated from a film deposition region by a negatively biased mesh electrode [1]. Higher order silane radicals in plasma are responsible for the increase in Si-H2 density in the film, and could be decreased in the region between a mesh and a substrate due to their low diffusion velocity. A stabilized efficiency of 8.1% with degradation ratio of 8% in n-i-p type a-Si:H solar cells has been reported [2]. In this study, we have employed the i layer deposited by a triode system to p-i-n type a-Si:H solar cells. The p-i-n type solar cells were fabricated on a textured SnO₂/glass substrate (ASAHI VU type). By applying triode system, Si-H2 concentration decreased to about one third (from 1.7% for conventional parallel-plate-electrode to 0.6% for a triode configuration), and correspondingly the degradation ratio decreased from 13% to 5% by optimizing the p layer deposition conditions. Further improvement has been developed using a proper hydrogen dilution for the i layer and an antireflection layer between TCO and the p layer. As a result, we have achieved the stabilized efficiency of 9.22% (Jsc=15.9mA/cm², Voc=0.863V, FF=0.672) with degradation ratio of 7.8%. [1] S.Shimizu et al., Proc. of WCPEC-3, Osaka, 2003, p. 1615. [2] S.Shimizu et al., J. Non-Cryst. Solids, 338-340(2004)47-50.

11:00 AM *A11.2

Highly and Rapidly Stabilized Protocrystalline Silicon Multilayer Solar Cell. K. S. Lim and S. Y. Myong; Electrical Engineering and Computer Science, KAIST, Daejeon, South Korea.

We have developed highly and rapidly stabilized protocrystalline silicon (pc-Si:H) multilayer solar cells using a photo-assisted chemical vapor deposition (photo-CVD) technique. In our previous papers, we have reported that the multilayer solar cells show fast initial degradation and stabilization behavior in about 12 h light soaking. In this paper, we report that the multilayer film and solar cell characteristics by employing an amorphous silicon-carbide (a-SiC:H)

double p-layer structure. The solar cell has a structure of glass/SnO₂/undiluted p-a-SiC:H/H₂-diluted p-a-SiC:H/i-pc-Si:H/n- μ c-Si:H/Al. The intrinsic pc-Si:H (i-pc-Si:H) multilayers were prepared by alternate H₂ dilution under continuous ultraviolet (UV) light irradiation using the photo-CVD system. From the Fourier transform infrared (FTIR) and photoluminescence (PL) measurements, we found unique characteristics of the pc-Si:H multilayer absorber, which is different from those of conventional undiluted amorphous silicon (a-Si:H) absorbers. In particular, the pc-Si:H multilayer absorber exhibits a superior light-soaked metastability to the conventional a-Si:H absorbers. In order to improve the pc-Si:H multilayer solar cell performance, we adopted an a-SiC:H double p-layer structure. A lightly boron-doped (1000 ppm) H₂-diluted p-type a-SiC:H (p-a-SiC:H) buffer layer with a high conductivity, low absorption, well-ordered film structure, and slow deposition rate improves the open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), and fill factor (FF) of the solar cells by successfully reducing recombination in the buffer layer and at the undiluted p-a-SiC:H/buffer and buffer/i interfaces. Through a spectroscopic ellipsometry (SE) analysis using the Tauc-Lorentz model, we found a natural hydrogen treatment effect, that is, etching the defective undiluted p-a-SiC:H window layer during the H₂-diluted p-a-SiC:H buffer layer deposition onto the window layer and improving order in the window layer. This is one of the advantages of using the H₂-diluted buffer layer. In addition, the highly conductive buffer layer effectively increases the built-in potential at the p/i interface, diminishing electron back diffusion to the window layer. Thus, we have achieved a high initial efficiency of 10.4 % without using a double back reflector such as ZnO/Ag and also achieved a highly stabilized efficiency of 9.0 % after about 10 h 1-sun (100mW/cm², AM 1.5) light irradiation.

11:30 AM **A11.3**

Correlation between Powder in the Plasma and Stability of High Rate Deposited a-Si:H. Guozhen Yue, Gautam Ganguly, Baojie Yan, Jeffery Yang and Subhendu Guha; United Solar Ovonic Corp., Troy, Michigan.

Improvement of the stability of hydrogenated amorphous silicon (a-Si:H) alloys deposited at high rates is perhaps the most important task for cost reduction of solar cells based on this material. On one hand, correlations between higher silane density (from mass spectroscopy), the concentration of silicon di-hydride bonding in the film and the light soaked (stabilized) solar cell fill factor have suggested that that higher silane radicals arriving at the growth surface are responsible for the development of non-optimum bonding configurations, which are potential metastable defect formation sites [1]. On the other hand, it has been shown that solar cell intrinsic layers incorporating clusters produced in the plasma are more stable than *standard* a-Si:H [2]. Here we report our efforts to ascertain which of these observations is valid in a reactor used to fabricate high efficiency single junction solar cells incorporating high deposition rate (8-10 Å per s) intrinsic layers using modified very high frequency (MVHF) plasma [3]. We have monitored the light scattered at 90° from powder generated in the plasma using a 419nm Ar-laser and a silicon photodiode. This simple, non-invasive technique, allowed us to use the same reactor used to make the solar cells. We first studied the change in the scattering signal as a function of the total gas flow keeping the hydrogen to silane ratio (R) constant. We verified that, as has been reported previously [4], a maximum in the scattered light intensity is observed with increasing flow rate. We then compared the initial performance and the light induced degradation of two sets of single junction cells of similar intrinsic layer thickness as a function of the flow rate. We found that while the initial performance is similar, the stable efficiency was the lowest and the relative degradation the highest at a flow rate where the powder scattered light intensity was maximum. It is reasonable to conclude that there is indeed a correlation between the causes of powder formation and cell degradation as suggested in reference 1 and this is in contradiction with the results in reference 2. We have investigated the effect of changing the deposition temperature and / or adding germane to the gas mixture. These experiments reveal surprising behavior of the powder density with both variables. The behavior can be understood qualitatively by considering the rates of formation (reactions between radicals) and removal (gas flow, temperature gradient) of the powder particulates. We expect to use this formulation to devise the optimum deposition conditions and reactor design for minimizing the effects of powder, and hence improving the stability of devices. [1] R. Hayashi et al., Proc. 2nd World Conf. on PVSEC, Vienna, 1998, p-929 [2] P. Roca i Cabarrocas, MRS Symp. Proc.507 (1998) p-855 [3] J. Yang et al., MRS Symp. Proc.664 (2001) p-A11.3.1 [4] Y. Matsuoka et al., Jpn. J. Appl. Phys. 38 (1999) p-4556

11:45 AM **A11.4**

The Nature of Native and Light Induced Defect States in i-layers of High Quality a-Si:H Solar Cells Derived from Dark Forward-Bias Current-Voltage Characteristics. Jingdong Deng¹,

Matthew L. Albert¹, Joshua M. Pearce², Robert W. Collins³ and Christopher R. Wronski¹; ¹Center for Thin Film Devices, Pennsylvania State University, University Park, Pennsylvania; ²Physics Department, Clarion University of Pennsylvania, Clarion, Pennsylvania; ³Department of Physics and Astronomy, University of Toledo, Toledo, Ohio.

Dark forward bias current, J_D -V, characteristics have been shown to be a new probe for characterizing carrier recombination, identifying the mechanisms limiting solar cell performance, as well as characterizing the defect states in the i-layers of a-Si:H solar cells [1, 2]. From the bias dependence of the differential diode quality factors, $n(V)$, predictions can be made about the nature of the gap state distributions. In this study, the information obtained about the distributions of the gap states directly from the analysis of J_D -V characteristics of the p-i-n solar cells, with optimized p/i interfaces and high quality hydrogen diluted protocrystalline and undiluted i-layers, is presented. The results obtained, in which carrier transport is dominated by bulk recombination, show that there are distinct differences between the two types of i-layers in their distributions of both native and light induced defect states. In the annealed state both types of i-layers have two Gaussian-like distributions in the energy gap: one centered around midgap and the other removed by \sim 0.3 eV away from midgap. The Gaussian-like distributions of the native defects in the undiluted i-layers, however, are quite broad and subsequently cannot be distinguished after the introduction of light induced defects by prolonged degradation. On the other hand, the Gaussian-like distributions in the diluted protocrystalline i-layers can still be identified in the degraded steady state. The new information obtained about the energy distributions of the various gap states has been applied in significantly reducing the currently large uncertainties in the arbitrarily chosen parameters used in numerical modeling. Numerical simulations are presented which show excellent agreement with experimental results obtained not only for the J_D -V but more importantly the $n(V)$ characteristics. Results on the nature of the gap states and their evolution with light induced degradation derived from these simulations are presented and their effects on the performance and stability of high quality a-Si:H solar cells are discussed. [1] J. Deng, J. M. Pearce, V. Vlahos, R. W. Collins, and C. R. Wronski, *Mater. Res. Soc. Symp. Proc.*, **762**, A3.4 (2003) [2] J. Deng, J. M. Pearce, V. Vlahos, R. W. Collins, and C. R. Wronski, *Mater. Res. Soc. Symp. Proc.*, **808**, A8.8 (2004)

SESSION A12: Photonic Devices: Experiment and Theory
Chair: Richard Weisfeld
Wednesday Afternoon, March 30, 2005
Room 2002 (Moscone West)

1:30 PM ***A12.1**

Photonic Band Gap Materials: Engineering the Fundamental Properties of Light. Sajeev John, Physics, University of Toronto, Toronto, Ontario, Canada.

Photonic Band Gap (PBG) materials are artificial, periodic, dielectrics that enable engineering of the most fundamental properties of electromagnetic waves. These properties include the laws of refraction, diffraction, and spontaneous emission of light. Unlike traditional semiconductors that rely on the propagation of electrons through an atomic lattice, PBG materials execute their novel functions through selective trapping or "localization of light" using engineered defects within the dielectric lattice. This is of great practical importance for all-optical communications and information processing. Three dimensional (3D) PBG materials offer a unique opportunity for simultaneously (i) synthesizing micron-scale 3D optical circuits that do not suffer from diffractive losses and (ii) engineering the electromagnetic vacuum density of states in this 3D optical micro-chip. This combined capability opens a new frontier in integrated optics as well as the basic science of radiation-matter interactions. We review recent approaches to micro-fabrication of photonic crystals with a large 3D PBG centered near 1.5 microns. These include direct laser-writing techniques and holographic lithography. We review the concept of a hybrid 2D-3D PBG hetero-structure in which a 2D photonic crystal micro-chip layer is suitably lattice matched and embedded within a 3D PBG material. This microchip layer contains optical wave-guides and optical micro-cavities that enable frequency selective control of spontaneous emission of light from atoms. Unlike traditional wave-guides that confine light in a high refractive index medium using total internal reflection, these air-wave-guides operate using the principle of light localization for confinement of light along a low refractive index path. We demonstrate a nearly universal approach to ultra-dense, three-dimensional, integrated optics in general 3D PBG architectures. These 3D optical circuit paths are constructed using broadband, loss-less, chip-to-chip interconnects between 2D micro-chip layers,

intercalated within the 3D PBG host material. Unlike electronic micro-circuitry, each air-wave-guide path can simultaneously conduct hundreds of wavelength channels of information, throughout the 3D micro-chip. In addition to exhibiting diffraction-less flow of light through micron-scale bends, this optical micro-chip allows the engineering of very large and abrupt changes in the local electromagnetic density of states as a function of frequency. This leads to unprecedented frequency selective control of spontaneous emission, modification of the blackbody radiation spectrum, and some fundamentally new optical functions unattainable in conventional photonics.

2:00 PM *A12.2

Detectors at the Intersection of Photons and Electromagnetic Fields or, Where Einstein Meets Maxwell. Blake Eliasson² and Garret Modde^{1,2}; ¹Electrical & Computer Engineering, University of Colorado, Boulder, Colorado; ²Phiar Corporation, Boulder, Colorado.

For standard visible and near-infrared light detectors, the detection is generally described using photon energies and numbers. For radio frequency waves picked up using an antenna and diode, i.e., a radio receiver, classical electromagnetics is fully adequate to describe the detection. But neither approach works when an antenna and diode are used to detect higher energy radiation in what is generally thought of as the domain of photons. We describe the operation and design of a detector comprising a micro-antenna and an ultra-high-speed metal-insulator tunneling diode. When the photon energy is on the order of or larger than the scale of the diode nonlinearity, we describe the detection using a semiclassical approach. The detector can pick up radiation from gigahertz to infrared (carrier) frequencies, and detect signals at up to terabit/second rates. By incorporating a double-insulator quantum well we provide a highly-nonlinear diode for efficient detection. This crystal radio for photons is a practical, integratable thin-film detector for a wide range of applications from broadband communications, through terahertz imaging, to ultra-high-speed infrared detection.

2:30 PM A12.3

New Light Trapping in Thin Film Solar Cells Using Textured Photonic Crystals. Lirong Zeng, Yasha Yi, Ching-yin Hong, Xiaoman Duan and Lionel C. Kimerling; Materials Science and Engineering, MIT, Cambridge, Massachusetts.

Thin film solar cells are leading candidates for next generation photovoltaic applications due to lower materials costs and simpler device manufacturing technology. However, one crucial problem for thin film solar cells is the short optical path length, which prevents the sufficient absorption of light. In order to improve cell efficiency, it is important to enhance the optical path length, that is, to trap light in the cell. We have successfully developed a new light-trapping scheme applicable to all thin film solar cells by using novel photonic structure on the backside reflector. Our back reflector design combines reflection grating of substrates with distributed Bragg reflector (DBR). It makes incident light strongly bent and reflected almost parallel to the surface of the absorption layer, hence the optical path length can be enhanced by tens of thousands of times, more than two orders of magnitude longer than that obtained by conventional light trapping schemes. Furthermore, it provides extremely high reflectivity with large omnidirectional bandgap over several hundred nanometers in the solar spectrum range. The reflectivity of our Si/Si₃N₄ DBR reaches 99.6%, while that for our Si/SiO₂ DBR is as high as 99.98%, which is significantly higher than that of the best Al reflector (R<98%). Therefore, almost all the incident light with an energy higher than the bandgap of the absorption layer material can be completely absorbed and converted to electron-hole; in turn the quantum efficiency of the solar cells will be enormously enhanced by our new light trapping scheme.

SESSION A13: Metastability
Chair: Rana Biswas
Wednesday Afternoon, March 30, 2005
Room 2002 (Moscone West)

3:15 PM A13.1

Effect of Fermi Level Position in Intrinsic a-Si:H on Evolution of Defect States under Light Exposure. Miro Zeman¹, Vojtech Nadazdy^{1,2}, Rudolf Durny³ and Wim Metselaar²; ¹Delft University of Technology, Delft, Netherlands; ²Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia; ³Slovak University of Technology, Bratislava, Slovakia.

Inherent to hydrogenated amorphous silicon (a-Si:H) are the reversible changes in electronic properties of a-Si:H under light exposure, known today as the Staebler-Wronski effect. It is generally accepted that light soaking leads to the creation of additional dangling-bond defects, which deteriorate the performance of a-Si:H

devices such as solar cells. However, dangling bonds alone are not sufficient to explain changes in solar cell characteristics under light exposure. Recently, the presence of defects other than dangling bonds have been proposed [1-3] that are expected to play a role in the degradation of a-Si:H cells. We present experimental results from charge deep-level transient spectroscopy showing the evolution of the programmed defect-states distributions in intrinsic a-Si:H due to light soaking. This evolution is expected to take place at the p/i and i/n interfaces of the cells. By applying a negative (positive) bias voltage to a metal/insulator/a-Si:H (MIS) structure we are able to move the Fermi level to the valence (conduction) band edge in the a-Si:H layer. By annealing the MIS structure at the freeze-in temperature of a-Si:H, while keeping this structure under bias voltage, a new programmed energy distribution of defect states is obtained. The programmed defect-states distribution at the negative (positive) voltage in the intrinsic a-Si:H layer represents the p-type (n-type) distribution as expected close to the p/i (i/n) interface in the intrinsic layer of the solar cell. We observe that the distributions of these programmed defect states and their following evolution due to light exposure are quite different in comparison to the intrinsic distribution [3]. The defect-state distribution of the intrinsic layer in the bulk of the solar cell is characterized by similar contributions from the positively charged defect states above midgap, Dh, neutral states, Dz, and negatively charged states below midgap, De. In the programmed p-type (n-type) defect-states distribution there is an excess of the Dh (De) states and a small contribution of the De (Dh) states. Light exposure modifies both the p- and n-type distributions, resulting in similar broad distributions of states located at and below midgap, while the states above midgap slightly decrease. This evolution is in contrast with the one of the intrinsic defect-states distribution where a dominant peak of Dz states around midgap accompanied by an elimination of the Dh states is observed. The role of mobile hydrogen in the evolution of p- and n-type distributions under light exposure is discussed. The results give important experimental information about the spatial changes of the defect-states distribution in the pin solar cell. 1. J. Pearce, X. Niu, R. Koval, G. Ganguly, D. Carlson, R.W. Collins, and C.R. Wronski, MRS 2001, A12.3.1. 2. S. Heck and H.M. Branz, Appl. Phys. Lett. 79, 3080 (2001). 3. V. Nadazdy and M. Zeman, Phys. Rev. B 69, 165213 (2004).

3:30 PM A13.2

The Creation and Relaxation Kinetics of Light Induced Defects in a-Si:H Located at Different Energies in the Gap. Matthew Louis Albert¹, Jingdong Deng¹, Xinwei Niu¹, Joshua M. Pearce², Robert W. Collins³ and Christopher R. Wronski¹; ¹Electrical Engineering, The Pennsylvania State University, University Park, Pennsylvania; ²Physics Department, Clarion University of Pennsylvania, Clarion, Pennsylvania; ³Physics Department, University of Toledo, Toledo, Ohio.

Until recently there has been no direct evidence reported for the "fast" and "slow" light induced states in studies on a-Si:H films such as found in the two step experiments carried out on solar cells. An investigation of the nature of these states was carried out in a detailed study on a-Si:H films of the light induced changes, under 1 sun illumination, as well as their subsequent relaxation.[1,2]. This was conducted on both hydrogen diluted, polycrystalline, and undiluted a-Si:H thin films 0.8-1.0 micron thick deposited on 7059 glass with n+ a-Si:H coplanar contacts. In the experiments care was taken to control the sample temperature as well as the intensities of the volume absorbed illumination for adjusting the quasi-fermi level splitting of the photoconductivities used in the characterizing of both the degradation as well as its relaxation. In addition, automation of the experimental procedures enhanced the precision of the measurements and yielded a wide range of results which are highly reproducible. Results are presented for the carrier recombination occurring with different quasi-fermi level splitting from which the relative contributions of states located at different energies in the gap can be identified. In the characterization of the light induced changes, account was taken of a very fast component (< 1 minute) that is present in the photoconductivities which can be attributed to mechanisms other than carrier recombination in the bulk of the films. Distinct differences are found between the changes in the recombination resulting from the states located at mid gap and those closer to the band edge, both during the 1 sun illumination as well as in the subsequent relaxation. The studies of the relaxations, which were investigated for a wide range of 1 sun illumination times, were also extended to include sub-gap absorption. Results are presented in which corresponding changes in the gap states could also be identified. Comparisons are presented between the results obtained with the photoconductivity and those with sub-gap absorption measurements as well as the results on the relaxation of bulk carrier recombination in p-i-n solar cells after 1 sun degradation. New insights obtained in this work into the possible mechanisms of SWE are discussed.

3:45 PM A13.3

Time Evolution of Defect Density in Tritiated Amorphous

Silicon Determined by Transient Capacitance Techniques. Stefan Costea, Nazir P. Kherani and Stefan Zukotynski; Electrical & Computer Engineering, University of Toronto, Toronto, Ontario, Canada.

The increase in the defect density under illumination, the Staebler-Wronski effect, in hydrogenated amorphous silicon (a-Si:H) has been the subject of study for many years. Tritiated amorphous silicon (a-Si:H:T) is prepared by incorporating tritium, a radioactive isotope of hydrogen, into the a-Si:H network. The transmutation of tritium into helium leads to the creation of dangling bonds and the well-defined decay rate of tritium provides a tool for controlled defect creation in the material. Tritiated amorphous silicon samples have been studied using ESR and CPM. These measurements show defect creation dynamics that cannot be explained by the tritium decay process alone [1-3]. Tritiated amorphous silicon films were deposited using the saddle-field deposition system. Tritium atomic concentration in the films was between 0.5% and 1.5%, determined by thermal effusion measurements. Schottky diodes were made by evaporating palladium onto the a-Si:H:T films which had been deposited on n-type crystalline silicon substrates. The junction capacitance of the Schottky devices after annealing showed an increase with time, suggesting an increase in total number of defect states in the gap. Isothermal Capacitance Transient Spectroscopy [4] was used to determine the density of states positioned near the conduction band in the gap. Measurements carried after annealing revealed a peak in the density of states at about 0.6 eV from the conduction band, commonly attributed to positively charged dangling bonds (D^+); the integrated density of states decreased with time. Both time evolutions could be fitted to stretched exponential curves, reaching saturation after about 300 hours. This defect dynamics can be explained by the production of D^+ dangling bonds and their conversion to neutral defects D^0 . This study sheds new light on the mechanisms involved in defect formation in a-Si:H and on the Staebler-Wronski effect. [1] T. Kosterki, N. Kherani, P. Stradins, F. Gaspari, W.T. Shmayda, L. S. Sidhu, and S. Zukotynski, *IEEE Proc.- Circuits Devices Syst.* 150, 274 (2003) [2] J. Whitaker, J. Viner, S. Zukotynski, N. Kherani, E. Johnson, P. C. Taylor, P. Stradins, *Mat. Res. Soc. Symp. Proc. A* 2.4 (Spring 2004) [3] S. Pisana, S. Costea, T. Kosterki, N. P. Kherani, S. Zukotynski and W. T. Shmayda, *Mat. Res. Soc. Proc.: L8.10* (Fall 2004) [4] Y. E. Chen, F. S. Wang, J. W. Tsai, H. C. Cheng, *Jpn. J. Appl. Phys.* 6727, 33 (1994)

4:00 PM **A13.4**

Image and Color Sensitive Detector Based on Double p-i-n a-SiC:H Photodiodes. Manuela Carvalho Vieira¹, Miguel Fernandes¹, Paula Louro¹, Alessandro Fantoni¹, Yuri Vygranenko¹, Guilherme Lavareda² and Carlos Nunes Carvalho²; ¹DEETC, ISEL, Lisbon, Portugal; ²CFM, UTL, Lisbon, Portugal.

A large area optically addressed image and color sensitive detector is presented. The sensor structure is a two terminal multilayered structure based on two stacked sensing/switching p-i-n a-SiC:H diodes and two transparent conductive contacts. The imaging is performed in a write-read simultaneous process: the write exposure, which converts the optical image into a localized packet of charges and the optical read which performs the charge to current conversion by detecting the photocurrent generated by a light beam scanner. In this sensor the charge packets are optically injected either into the p-i-n front sensing photodiode or at the switching one depending on the wavelength of the absorbed radiation. Its confinement inside the illuminated regions promotes a local modulation of the electrical field profile across the p-i-n back switching diode that can be readout through a light scanner without the need of the usual pixel architecture. This approach simplifies the interconnections as only two terminals are necessary. By tailoring of the sensor configuration (layers thickness, absorption coefficient of the absorber layers and junction sequences) and the readout parameters (applied bias and scanner wavelength) this work evaluates the possibility of using this double diode structure as a high-sensitivity optically addressed image and color detection device. The various design parameters and the optical readout process tradeoffs are discussed. The influence on the transfer functions of different a-SiC:H sensing absorbers optimized for red transmittance and blue collection are analyzed. Results show that when a thin (<200 nm) a-SiC:H sensing and a thick (>500 nm) a-Si:H switching absorber are used, the device behaves itself as a filter giving information about the wavelength and the position where the optical image is absorbed. By sampling the absorption region at two bias voltages it is possible to extract separately the RGB integrated information with a good rejection ratio. A readout of 1000 lines per second is achieved allowing continuous and fast image sensing, and color recognition. A transient SPICE model of the three color detector operation will be presented and supported by a 2D numerical simulation.

4:15 PM **A13.5**

Observation of a Hydrogen Doublet Site in High Defect Density As-Grown a-Si:H by ¹H NMR. David Charles Bobela¹,

Tining Su¹, Craig Taylor¹ and Gautam Ganguly²; ¹Physics, University of Utah, Salt Lake City, Utah; ²United Solar Ovonic Corp, Troy, Michigan.

¹H NMR studies of a-Si:H with $\sim 10^{17}$ cm⁻³ defects grown by PECVD with a rate of 5 Å/s, show the existence of a hydrogen doublet for both as-grown and light-soaked samples. The doublet's breadth of ~ 16 kHz corresponds to a pair of hydrogen atoms separated by 2.2 Å. In a previous study by Su et al. [1], a similar doublet (for high quality samples) appears upon light soaking, in densities consistent with densities of optically induced silicon dangling bonds. Su et al. also report the apparent narrowing of this feature for temperatures approaching 20 K. We observe the doublet, in a sample where no intended light-soaking has occurred, over the range of 5 - 20 K. The as-grown sample yields a similar doublet line shape as the light-soaked at 8 K. As-grown T₁ experiments for temperatures within said temperature range show that the doublet component relaxes on the same time scale as hydrogen bonded to silicon component (width ~ 4 kHz) component. Moreover, the doublet line shapes display no narrowing. These results suggest that the doublet is due to SiH₂ for these samples. 1. T. Su, P.C. Taylor, G. Ganguly, and D.E. Carlson, *Phys. Rev. Lett.* 89, 015502 (2002).

4:30 PM **A13.6**

Light-soaking Effects on the Open-circuit Voltage of a-Si:H Solar Cells. Jianjun Liang¹, Eric A. Schiff¹, Subhendu Guha², Baojie Yan² and Jeffrey Yang²; ¹Physics, Syracuse University, Syracuse, New York; ²United Solar Ovonic Corp., Troy, Michigan.

The open-circuit voltage V_{OC} of amorphous silicon (a-Si:H) solar cells measured under intense (solar) illumination generally declines only a few percent under light-soaking. This behavior is remarkable in the context of the much larger relative changes in the photoconductivity and the deep-level density measured in a-Si:H thin films during light-soaking. Since V_{OC} is also a probe of bulk recombination in a-Si:H films (it measures a quasi-Fermi level splitting), it should be consistent with the other measurements, and indeed modeling studies have suggested that even fairly sizable deep level densities need not strongly affect recombination at high intensities (as probed by V_{OC}). In this paper we explore possible reasons for the apparent coincidence that the growth of the deep level density saturates just as it begins to marginally affect V_{OC} . We first present measurements of the kinetics of the decay of the open-circuit voltage at 295 K. In several samples, the long-time decay ΔV_{oc} (between 1 and 200 hours) follows the form $-(kT/e)\ln(t^{1/5})$; the total decay is generally less than $3(kT/e)$ over this time-range. We also present measurements of the temperature-dependence of V_{oc} as light-soaking progresses. We have found a relatively simple model that accounts for the V_{OC} measurements. In the short-time regime (light soaking times less than about 1 hour), the temperature-dependent V_{OC} measurements are consistent with bandtail recombination. While deep-levels are not important to recombination in this regime, we presume that their density grows as $t^{1/3}$. This behavior is expected for the "hydrogen-collision" model due to Branz. In the long-time regime, deep-levels begin to affect photocarrier recombination. A modification of the hydrogen-collision equation that associates deep-level generation with bandtail recombination predicts a deep-level growth-rate of $t^{1/5}$ in this regime, which is consistent with the decay kinetics of V_{OC} . We also compare this prediction with previous work on deep-level kinetics in the "saturation" regime. This model helps account for the fact that the conversion efficiencies of single-junction a-Si:H solar cells decline only moderately (typically 30% or less) during solar illumination before reaching their degraded steady states. If the model is correct, it is an essential component in understanding the exact characteristics of a-Si:H in its degraded state. This research was supported by the Thin Film Photovoltaics Partnership of the National Renewable Energy Laboratory.

4:45 PM **A13.7**

The Effects of Hydrogen Profiling and of Light-Induced Degradation on the Electronic Properties of Hydrogenated Nanocrystalline Silicon. Adam F. Halverson¹, James J. Gutierrez¹, David Cohen¹, Baojie Yan², Jeffrey C. Yang² and Subhendu Guha²; ¹Physics, University of Oregon, Eugene, Oregon; ²United Solar Ovonic Corporation, Troy, Michigan.

The electronic properties of hydrogenated nanocrystalline silicon (nc-Si:H) were studied using drive-level capacitance profiling (DLCP), transient photocapacitance (TPC), and transient photocurrent (TPI) spectroscopies. These measurements were performed both on n-i-p devices (SS/n /i nc-Si:H/p /ITO) as well as a 'sandwich' device structure in which the nc-Si:H layer is sandwiched by two amorphous silicon (a-Si:H) layers (SS/n/i a-Si:H/i nc-Si:H/i a-Si:H/Pd). For both structures, the nc-Si:H layers were deposited using different degrees of hydrogen dilution, and in some samples, hydrogen dilution profiling was employed. Qualitatively similar experimental results were obtained for both types of device structures. First, we found

significant differences in the DLCP profiles for the nc-Si:H layers deposited under constant hydrogen dilution with those deposited using hydrogen profiling. For the former the DLCP density increased in the direction of film growth, exceeding 10^{16}cm^{-3} as one approaches the top surface of the film. This variation is attributed to an increase in crystallite size as the film growth progresses. In contrast, when hydrogen profiling is employed to maintain a smaller crystallite size, the samples exhibited DLCP profiles indicating a maximum value below 10^{16}cm^{-3} within the middle of the film before decreasing again toward the front surface. Second, the TPC measurements reveal spectra that appear quite microcrystalline-like at lower temperatures but more similar to a-Si:H at higher temperatures. We believe that this variation in appearance indicates the mixed-phase nature of the nc-Si:H material studied. Specifically, the photocapacitance spectra for these samples appear more microcrystalline silicon-like when the minority carrier collection is poorer at lower temperatures, but more amorphous silicon-like at higher temperatures when the minority carrier collection is higher in the nanocrystalline component of these nc-Si:H samples. This then suppresses the TPC signal from this component compared to the a-Si:H component. In contrast, because the transient photocurrent signal is only enhanced by the additional minority carrier collection, these spectra appear microcrystalline like at all temperatures. Finally, we have investigated light-induced degradation in these devices after light-soaking for 100 hours with red filtered (610nm) ELH light at 100mW/cm^2 . Such light-soaking is found to cause a dramatic decrease in hole collection, similar to that caused by reducing the measurement temperature of the samples. We believe that this is likely related to the light-induced degradation in performance in these nc-Si:H solar cells. However, the light exposure does not appear to increase the deep defect density (dangling bonds). Possible mechanisms for the observed light-induced degradation in these nc-Si:H films will be discussed.

SESSION A14: In-situ Optical Characterization of
Films I
Chair: Rob Collins
Thursday Morning, March 31, 2005
Room 2002 (Moscone West)

8:30 AM *A14.1

Application of Spectroscopic Ellipsometry and Infrared Spectroscopy for the Real-time Control and Characterization of a-Si:H Growth in a-Si:H/c-Si Heterojunction Solar Cells. Hiroyuki Fujiwara and Michio Kondo; National Institute of Advanced Industrial Science and Technology, Tsukuba-shi, Ibaraki, Japan.

We have performed real-time process control and characterization of hydrogenated amorphous silicon (a-Si:H) growth on crystalline silicon (c-Si) in a-Si:H/c-Si heterojunction solar cells. By applying real-time spectroscopic ellipsometry (SE) [1], thickness control of a-Si:H layers with a precision better than ± 1 has been demonstrated during a-Si:H p-i layer growth on the n-type c-Si substrate by conventional plasma-enhanced chemical vapor deposition. Due to thin layer thicknesses of the a-Si:H p-i layers (5 nm) adopted for the a-Si:H/c-Si heterojunction solar cell, precise real-time thickness control is of significant importance especially for mass production. A heterojunction solar cell fabricated by our process shows a relatively high conversion efficiency of 14.5 % ($V_{oc}=574 \text{ mV}$, $J_{sc}=33.5 \text{ mA/cm}^2$, and $FF=0.756$). In this solar cell, ITO (70 nm) and Al were used for top and rear electrodes, respectively. For the a-Si:H growth, real-time SE revealed (i) island growth of the a-Si:H i-layer on the substrate, (ii) rapid surface roughening during the a-Si:H p-layer growth on the i-layer, and (iii) reduction of H content after the p-layer growth. In order to characterize interface structures, we have further applied real-time infrared attenuated total reflection spectroscopy (ATR). From ATR, we find the formation of a porous interface layer with a large SiH_2 -hydrogen content of 30 at.% at the a-Si:H(i-layer)/c-Si interface, although a-Si:H i-layer has been reported to provide excellent surface passivation on c-Si surface [2]. Furthermore, at the a-Si:H p/i interface, the presence of a transition layer with a thickness of 2 nm was indicated. The above results show that the growth processes of the a-Si:H p-i layers are far more complicated than expected. Based on the SE and ATR results, we discuss the growth processes and structures of a-Si:H in a-Si:H/c-Si heterojunction solar cells. [1] H. Fujiwara, M. Kondo, and A. Matsuda, *Physical Review B* 63 (2001) 115306. [2] M. Taguchi et al., *Prog. Photovolt: Res. Appl.* 8 (2000) 503.

9:00 AM *A14.2

Real-Time Spectroscopic Ellipsometry as an in-situ Probe of the Growth Dynamics of Amorphous and Epitaxial Crystalline Silicon for Photovoltaic Applications. Dean H. Levi, C. W. Teplin, E. Iwaniczko, Y. Yan, Q. Wang, T. H. Wang and H. M. Branz; National Renewable Energy Laboratory, Golden, Colorado.

In-situ real-time spectroscopic ellipsometry (RTSE) is gaining widespread acceptance as a powerful tool for the investigation of the deposition dynamics of myriad types of thin films. R.W. Collins and co-workers have established a broad foundation for these studies with their work using in-situ RTSE to create phase diagrams for amorphous silicon (a-Si) and nano-crystalline silicon (nc-Si) deposited using plasma enhanced chemical vapor deposition (PECVD). Their work takes advantage of the sensitivity of spectroscopic ellipsometry to surface roughness and optical properties, and how these parameters relate to transitions in the growth phase of the material, to provide a microscopic description of the growing material. In this paper we report on our work using in-situ RTSE to study the dynamics of hot-wire chemical vapor deposition (HWCVD) of a-Si and epitaxial crystalline silicon (epi-Si) for photovoltaic applications. We utilize RTSE as both an in-situ diagnostic and post-growth analysis tool for a-Si/crystalline silicon heterojunction (SHJ) solar cells grown by HWCVD. RTSE enables precise thickness control of the 3 to 10 nm thick layers used in these devices, as well as monitoring crystallinity and surface roughness in real time. With the assistance of in-situ RTSE feedback we have achieved a photovoltaic energy conversion efficiency of 17% on an Al-backed p-type float-zone c-Si wafer. Open-circuit voltages above 650 mV indicate excellent passivation of the c-Si surface by the a-Si intrinsic layer. We have found that immediate nucleation and growth of a-Si is crucial to effective surface passivation. Initial growth or nucleation of c-Si or nc-Si produces a rough interface between the c-Si substrate and the a-Si intrinsic layer that contributes to surface recombination. RTSE analysis of crystallinity has been confirmed using high-resolution cross-sectional transmission electron microscopy (TEM). We are also applying in-situ RTSE to study the dynamics of HWCVD growth of epi-Si. The goal of this work is to develop inexpensive methods for growing 10 to 20 um-thick layers of c-Si for solar cell applications. This study presents unique challenges for RTSE, as successful epitaxial growth of c-Si on a c-Si wafer produces no change at all in the RTSE spectra. We have found that by monitoring the pseudo-dielectric function in real time during growth we gain immediate feedback on the breakdown of epi-Si growth. Post-deposition analysis of the RTSE data provides quantitative information on the percent of nc-Si and a-Si versus film thickness. The RTSE analysis has been confirmed by cross sectional TEM. Based on the rapid feedback provided by RTSE we have surpassed the previous HWCVD record of 200 nm of epi-Si growth, achieving a maximum thickness of 500 nm of epi-Si. TEM analysis has shown that micron-sized areas of these films achieve 1000 nm of epi-Si thickness.

9:30 AM *A14.3

Novel in situ and Real Time Optical Probes to Detect (Surface) Defect States of a-Si:H. W. M. M. Kessels, Dept. of Applied Physics, Eindhoven Univ. of Technology, Eindhoven, Netherlands.

In this contribution, an overview will be presented of our efforts to develop novel optical diagnostics for probing a-Si:H defect states present in the bulk and at the surface of a-Si:H films. These diagnostics, applied in situ or real time during film growth, can provide new insight into the a-Si:H film properties as well as into the fundamental surface processes during growth. The first method that will be addressed is spectroscopic second harmonic generation (SHG), which is a surface-sensitive nonlinear optical technique extensively used in c-Si surface science studies. At last year's meeting, we presented the first results obtained on ex situ a-Si:H films and these results illustrated that this technique is potentially very powerful for detecting surface states on a-Si:H such as dangling bonds [1]. This has recently been corroborated by results obtained in situ in an ultrahigh vacuum chamber as well as by results obtained real time during film growth by hot-wire CVD. A resonance peak in the nonlinear susceptibility around a photon energy of $\sim 1.2 \text{ eV}$ has been identified as being generated by Si dangling bonds at the surface as also confirmed by the disappearance of the peak during oxygen dosing. A second resonance peak at $\sim 1.5 \text{ eV}$ is expected to be due to a resonance at twice the photon energy ($\sim 3.0 \text{ eV}$) as concluded from a comparison with the linear susceptibility of a-Si:H. This peak is therefore expected to be generated by strained Si-Si bonds in the surface region. These observations, which will be discussed in detail, are very relevant as both bonds are considered as reactive surface sites for SiH_3 radical adsorption. The second method that will be discussed is cavity ringdown spectroscopy on thin a-Si:H films. It is shown that this method is very powerful for measuring absolute defect-related absorptions at subgap energies without the need for a calibration procedure. This has been illustrated by placing very thin a-Si:H samples (down to 4 nm thickness) in a linear high-finesse optical cavity yielding absorption coefficients in the photon energy range of 0.6-1.8 eV with a very good signal-to-noise ratio [2]. This method can therefore be used for the measurement of dangling bonds in a-Si:H. Currently, the method is being extended for in situ and real time measurements using the evanescent-wave of a total internal reflection at the probe surface. The first results with this so-called folded cavity

design have been obtained and preliminary work on a-Si:H will be presented. [1] W.M.M. Kessels, J.J.H. Gielis, I.M.P. Aarts, C.M. Leewis, and M.C.M. van de Sanden, *Appl. Phys. Lett.* 85, 4049 (2004). [2] I.M.P. Aarts, B. Hoex, A.H.M. Smets, R. Engeln, W.M.M. Kessels, and M.C.M. van de Sanden, *Appl. Phys. Lett.* 84, 3079 (2004).

SESSION A15: Transport and Recombination - Novel Devices

Chair: Eric Schiff
Thursday Morning, March 31, 2005
Room 2002 (Moscone West)

10:30 AM **A15.1**

New Insights into the Recombination Mechanism of Amorphous Silicon. Klaus Lips and Christoph Boehme;

Silizium-Photovoltaik, Hahn-Meitner-Institut, Berlin, Germany.

Since the discovery of photoluminescence (PL) in amorphous Silicon (a-Si:H) in 1974 many experiments have been carried out to identify the underlying recombination mechanisms. With the number of experiments conducted, also the number of models for the explanation of the observations increased. In a-Si:H, a complex interaction of photogenerated excess charge carriers with a high density of localised states in the forbidden gap exists. This results in a wide distribution of distances between photogenerated electron-hole pairs (e-h) and defect states. Between such states, radiative and non-radiative tunnelling as well as excitonic recombination have been proposed to exist but no conclusive evidence has been presented that prove either of these mechanisms. In this presentation, we will revisit this 30 year old problem using a recently developed and very powerful technique, namely pulsed optically detected magnetic resonance (pODMR). Different from standard continuous wave ODMR, the trapped e-h pairs are excited coherently by very short and intensive microwave pulses thereby altering the spin configuration of the recombining e-h pairs on time scales faster than the shortest decoherence time. This then will result in an oscillation of the recombination probability. It is this coherent manipulation of the charge carrier ensemble that enables to extract valuable information about the recombination mechanism such as distance distributions between e-h pairs or recombination rates. The collective spin motion is observed as Rabi oscillations in the PL allowing to identify the different recombination processes by their magnetic field dependence as well as through their characteristic Rabi frequency. In a-Si:H we observe three different Rabi frequencies at 10 K which we identify from their g values to originate from three distinctively different recombination mechanism, namely (i) non-radiative tunnelling of band-tail electrons to neutral dangling bonds (db); (ii) radiative tunneling between dipolar coupled distant e-h pairs trapped at band-tail states which are separated by more than 9 Å; (iii) e-h pairs in close proximity forming a strongly exchange coupled state. We attribute the 9 Å limit below which no dipolar coupled pairs are detected as the localisation length of the exchange coupled e-h pairs. A direct capture process at dangling bonds as observed in microcrystalline silicon and at the c-Si/SiO₂ interface is not observed in a-Si:H at T = 10 K.

10:45 AM **A15.2**

Multiple-Trapping Model with Meyer-Neldel Effect and Field-Dependent Effects: Time-Of-Flight Simulations for a-Si:H. Jesse Maassen¹, Arthur Yelon¹, Louis-Andre Hamel² and

Wen Chao Chen³, ¹Department of Engineering Physics, Ecole Polytechnique de Montreal, Montreal, Quebec, Canada; ²Department of Physics, University of Montreal, Montreal, Quebec, Canada; ³ANIQ R&D Ltd., Montreal, Quebec, Canada.

In the past, various processes have been introduced into the standard multiple-trapping model (MT) to properly reproduce empirical data concerning time-of-flight (TOF) experiments for a-Si:H. Chen et al.[1] incorporated the Meyer-Neldel Effect (MNE) into the MT model, producing good results in the low field regime and a field assisted detrapping model, the diagonal jump model (DJM) [2], giving reasonable results in the high field domain. We have now included both MNE and DJM together in the MT model, assuming exponential band tails of localized states, in the hope of improving agreement with high field experiments without degrading agreement at low field. Monte Carlo simulations show that this combined model (MN-DJM) improves agreement between theory and experiment. Particular attention was paid to general mobility measurements, $\mu(T,F)$, and to $\alpha_1(T,F)$ and $\alpha_2(T,F)$, the dispersion parameters before and after the transit time τ . These results were tested for temperatures ranging from 50K to 350K and for electric fields varying from 20kV/cm to 350kV/cm. We observe that the values of $\alpha_1(T,F)$ and $\alpha_2(T,F)$ improve for all temperatures and that field assisted detrapping describes measurements of $\mu(T,F)$ well for the range of fields mentioned above. The electron distribution function in the localized states, $f(E)$, gives us insight into the behaviour of carriers in deep

traps, which mainly concerns multi-phonon interactions and its effects on transport dynamics. Although this model provides satisfactory results for carrier transport for all temperature and electric field measurements, scarcity of high field experimental data prevents us from more rigorously testing the present model. [1] W.C. Chen, L.A. Hamel and A.Yelon, *J. Non-Cryst. Solids* 220, 254 (1997). [2] W.C. Chen, L.A. Hamel and A.Yelon, *J. Non-Cryst. Solids* 258, 223 (1999).

11:00 AM **A15.3**

Computer Modelling of Non-Equilibrium Multiple-Trapping and Hopping Transport in Amorphous Semiconductors.

Charles Main¹, Joe Marshall², Steve Reynolds³ and Mervyn Rose¹;

¹Division of Electronic Engineering and Physics, University of Dundee, Dundee, United Kingdom; ²University of Wales Swansea, Swansea, United Kingdom; ³University of Abertay Dundee, Dundee, United Kingdom.

In this paper we demonstrate a simple computational procedure for the simulation of non-equilibrium transport in a disordered semiconductor in which both multiple-trapping and hopping processes are occurring simultaneously. The simulation is based on earlier work on hopping transport, which employed a Monte-Carlo method. Using the same model concepts, we now employ a stochastic matrix approach to speed computation, and include also multi-trapping transitions between localised and extended states. We use the simulation to study the relative contributions of extended state conduction (with multi-trapping) and hopping conduction (via localised states) to transient photocurrents, for various distributions of localised gap states, and as a function of temperature. The implications of our findings for the interpretation of transient photocurrents are examined.

11:15 AM **A15.4**

Radiation Hard Amorphous Silicon Particle Sensors.

Nicolas Wyrsh¹, Clement Miazza¹, Sylvain Dunand¹, Arvind Shah¹, Christophe Ballif¹, Matthieu Despeisse², Danielle Moraes² and Pierre Jaron²; ¹IMT, University of Neuchatel, Neuchatel, Switzerland; ²CERN, Geneva, Switzerland.

The future generation of colliders (in the field of high energy physics) will give rise to very challenging demands regarding particle detectors, such as extreme radiation hardness, interconnection density, integration and cost. In this context, vertically-integrated sensors based on the deposition of a thick hydrogenated amorphous silicon (a-Si:H) diode on top of a readout ASIC (Application-Specific Integrated Circuit) are seen as a promising solution. Such vertically-integrated radiation sensors are a particularly interesting example of so-called "thin-film on ASIC" or "TFA" technology. Recently, the authors have successfully developed TFA sensors, aiming at the detection of single charge particles (β particle and protons) at the minimum ionising energy (MIP) [1, 2]. In order to verify the radiation hardness, test sensors consisting of 30 μm thick a-Si:H diodes deposited on glass have been fabricated. These sensors have then been exposed to a 24 GeV proton beam up to fluences in excess of 10^{16} protons/cm². All samples survived the experiment, exhibiting thereby a degradation of the measured signal (in the proton beam) and a subsequent stabilisation at a signal value around 50% of the initial value. No significant change in the dark current of the diodes were observed. In the present paper, the details of the experiments will be discussed and compared to other degradation studies, using low energy proton beams, but also using light illumination. Finally, the potential of a-Si:H for future radiation-hard sensors will be assessed. [1] P. Jaron et al., *Nucl. Instr. and Meth. in Phys. Res.*, A518 (2004) 366. [2] N. Wyrsh et al., *MRS Proc. Vol. 808* (2004) 441.

11:30 AM **A15.5**

Low Temperature Thin-Film Silicon Diodes for Consumer Electronics. Qi Wang¹, Scott Ward¹, Anna Duda¹, Jian Hu⁴, Paul

Stradins¹, Richard Crandall¹, Howard M. Branz¹, Jeffery Frank³, Hao Lou², Craig Perlov², Warren Jackson², Ping Mai² and Carl Taussig²; ¹NREL, Golden, Colorado; ²HP Lab, Palo Alto, California; ³ITFI, Ames, Iowa; ⁴MVsystem, Golden, Colorado.

We have developed high current density thin-film silicon n-i-p diodes for low cost and low temperature two-dimensional diode-logic memory array applications. The diodes are fabricated at temperatures below 250°C on glass, stainless steel, and plastic substrates using hot-wire chemical vapor deposition (CVD). The 0.01-mm² standalone diodes have a forward current-density (J) of near 1 kA/cm² and a rectification ratio over 10⁷ at ± 2 V. The 25 μm^2 array diodes have J > 10 kA/cm² and rectification of 10⁵ at ± 2 V. On plastic substrates, we have also used plasma-enhanced CVD to deposit 10 micron diameter diodes with J \sim 50 kA/cm². We found that the use of microcrystalline silicon ($\mu\text{c-Si}$) i- and n-layers results in higher current-density diodes than with amorphous silicon. Inserting a 30-nm intrinsic Si buffer layer between the i- and p-layers reduces the reverse leakage current in diodes with $\mu\text{c-Si}$ n- and i-layers. Reducing the

diode area increases the forward current density by lowering the voltage drop across the external series resistances. A prototype diode array memory with a 5-micron device was successfully demonstrated by monolithically integrating diodes with a-Si:H filament switching elements. High current density diodes have potential applications in a variety of large area, thin-film electronic devices, in addition to a-Si:H-based memory. This could widen the application of thin-film silicon beyond its present industrial applications as thin-film transistors, solar cells, bolometers and photo-detectors.

11:45 AM A15.6

Effect of the Load Resistance in the Linearity and Sensitivity of Position Sensitive Detectors. Hugo Aguas, Luis Pereira, Leandro Raniero, Elvira Fortunato and Rodrigo Martins; Ciencia dos Materiais, Universidade Nova de Lisboa, Caparica, Portugal.

It is known experimentally by the scientists working in position sensitive detectors (PSD) field, that the linearity and sensitivity of the sensors are dependent on the resistance of the resistive layer, when the sensor is operated in certain conditions where the photolateral voltage of the sensor is measured. Our experimental work, carried on metal - insulator - semiconductor (MIS) PSDs structures, allowed us to determine the optimized value for the load resistance coupled to the sensor that gives the maximum value of sensitivity and linearity. To understand the results achieved with the experimental work, we simulate the sensor response based in its electrical model. This allowed us to determine a model for the sensor linearity and sensitivity, which shows that the linearity and sensitivity depends on the value of the load resistance. This model is valid for PSDs where the resistance of the resistive layer is quite low ($\leq 500 \Omega$), yielding a low output impedance, which means that a load resistance of about 1 k Ω of magnitude must be used to achieve a good compromise between the linearity and the sensitivity. This result was in agreement with the experimental results. The MIS sensor used for the experimental studies was built in a multi-layered structure consisting of Cr / a-Si:H (n+ doped) / a-Si:H (intrinsic) / SiO₂ (passivation layer) / Au, where the active a-Si:H layers were deposited by a Modified Triode Plasma Enhanced Chemical Vapour Deposition (MTPECVD) which allows de deposition of highly electronic grade material with a low defect density of states ($\approx 1 \times 10^{15} \text{ cm}^{-3}$), inferred by CPM. The maximum sensitivity ($\pm 100 \text{ mV}$) was achieved with an optimised structure with an active length of 7 cm yielding linearity better than 98%. It was also observed that the SiO₂ passivation layer plays an important role in the device performance, since it allows the increase of the sensor signal besides allowing the use of large active areas free of pinholes (shortcuts) that damage the device.

SESSION A16: In-situ Optical Characterization of Films II

Chair: Erwin Kessels
Thursday Afternoon, March 31, 2005
Room 2002 (Moscone West)

1:30 PM A16.1

Real Time Monitoring of the Crystallization of Hydrogenated Amorphous Silicon and its Alloys. Paul Stradins, David Young, Yueqin Xu, Howard M. Branz and Qi Wang; National Renewable Energy Laboratory, Golden, Colorado.

Crystallized amorphous silicon thin films on inexpensive substrates may be applied in large area thin-film Si solar cells either as absorbers or as seed layers for subsequent solid- or vapor-phase epitaxy. Precise process control and real-time monitoring are essential to both understanding and engineering these materials. We have developed an optical in-situ monitoring technique that we use to investigate thermally induced crystallization and solid phase epitaxy in hydrogenated amorphous silicon (a-Si:H). We study crystallization of a-Si:H over a wide range of substrates, deposition conditions, film compositions and a-Si:H microstructures. A fiber-optics-based portable spectrometer acquires optical reflectance spectra in-situ from the ultraviolet (UV) to the near infra-red (NIR). This allows us to monitor the crystallization of a-Si:H in real time, at the process temperature. Two main features of the optical spectra help us understand the solid phase crystallization process: UV signatures (3.4 and 4.4 eV) of c-Si that are sensitive to the surface, and the NIR interference fringes that are sensitive to the bulk phase composition. We observe the following stages in solid phase crystallization of a-Si:H films near 600 °C: 1) a rapid H effusion that reduces the optical gap; 2) a latency or nucleation period in which the optical spectrum changes little; 3) the first appearance of the UV signatures of crystalline phase, with simultaneous collapse of the NIR interference fringe pattern; and 4) the increase and saturation of the crystalline-phase UV signature and the crystal Si NIR fringe pattern. Measuring the UV and NIR portion of the spectrum permits us to distinguish between surface and bulk effects. Different seed layers and buffer layers were investigated (e.g., microcrystalline Si, amorphous

silicon nitride), as well as solid-phase epitaxy on poly- and monocrystalline Si. Epitaxy allows us to separate the grain growth and nucleation kinetics and to obtain highly oriented grains. We find that introducing Ge lowers the crystallization temperature of the amorphous layer.

1:45 PM A16.2

Dynamics of the Growth of Microcrystalline Silicon Thin Films from He Diluted SiF₄- and SiH₄- Based PECVD at Low Temperature. Maria Losurdo¹, Maria Michela Giangregorio¹, Pio Capezzuto¹, Giovanni Bruno¹, Laura Urbina², Javier J. Gandia² and Julio Carabe²; ¹Chemistry, INSTM and IMIP-CNR, Bari, Italy; ²CIEMAT, Madrid, Spain.

Microcrystalline, nanocrystalline and protocrystalline silicon thin films are receiving great attention in developing a large-area silicon technology on flexible plastic substrates including optoelectronic devices, thin film transistors and solar cells. Previous studies on the plasma enhanced chemical vapour deposition (PECVD) of the above films using SiH₄-H₂ plasmas put in evidence that the surface temperature and the hydrogen dilution are crucial parameters for the control of film nano- and microstructure. Specifically, for microcrystalline silicon hydrogen dilution >98% and temperature exceeding 180°C are required to obtain dense and ordered microcrystalline films with a crystalline fraction >70%. Furthermore, the existence of a growth dynamics, i.e., an increase of the crystallinity with film thickness and the presence of an amorphous incubation layer limited the possibility of depositing very thin <50 nm fully microcrystalline films on plastics. In this contribution, PECVD from He diluted SiF₄ and SiH₄ is demonstrated to be a valuable process for the deposition of fully microcrystalline (fc>90%) thin films even at low temperature <100°C on plastic substrates and without high H₂ dilution. Peculiarities of the films are the absence of any amorphous incubation layer at the early growth stage, and the complete crystallinity. The effect of the deposition temperature in the range 25°C-240°C, of the substrate (PET, polyimide, glass,...) and of the in-situ substrate pre-treatments on the crystallite nucleation and size is discussed. The existence of a "crystallite induction time" that depends on the substrate pre-treatment and plasma phase is highlighted using real time monitoring by laser reflectance interferometry. The impact of the "crystallite induction time" on the film microstructure and properties is presented. A comparative analysis of the "anatomy" (grain size, orientation, morphology, layered structure,...) of films obtained at <100°C by He-diluted SiF₄ and SiH₄ plasmas is carried out to have a deeper insight into the different role of fluorine and hydrogen atoms in promoting crystallinity at low temperature. Spectroscopic ellipsometry, XRD, and Raman analyses are presented and used to establish a correlation between the growth dynamics and film microstructure.

2:00 PM A16.3

Development of Deposition Phase Diagrams for Thin Film Si_{1-x}Ge_x:H Using Real Time Spectroscopic Ellipsometry. N. J. Podraza¹, G. M. Ferreira², C. R. Wronski² and R. W. Collins¹; ¹Department of Physics and Astronomy, The University of Toledo, Toledo, Ohio; ²Department of Electrical Engineering and Center for Thin Film Devices, The Pennsylvania State University, University Park, Pennsylvania.

In this research, the growth of amorphous silicon-germanium alloys (a Si_{1-x}Ge_x:H) by plasma-enhanced chemical vapor deposition (PECVD) is studied with the motivation to develop deposition phase diagrams for optimization of these materials in photovoltaic applications.¹ The Si_{1-x}Ge_x:H films were deposited on native-oxide/c-Si using rf PECVD and were measured in real time using a rotating-compensator multichannel ellipsometer. Conditions similar to those used for optimum pure a-Si:H were adopted first, including low substrate temperature (T = 200°C), low rf power (0.08 mW/cm²), and low total pressure (<1 Torr). The flow ratio G = [GeH₄]/{[SiH₄]+[GeH₄]} was fixed at G=0.167, leading to a 20°C gap of E_g ~ 1.35 eV. Two significant differences are observed between the phase diagrams of pure Si:H and Si_{1-x}Ge_x:H. First, the a→(a+μc) transition for the series of alloys is shifted to much larger R compared to pure Si:H. Thus, the presence of Ge in the growth process strongly suppresses the H-induced nucleation of microcrystals from the amorphous phase. Second, the a→a roughening transition saturates at a very low bulk layer thickness of 200Å for the alloys, even as the a→(a+μc) transition for thick films is approached and crossed. In contrast for Si:H, the a→a transition increases sharply, exceeding the bulk layer thickness of 4000Å, as the a→(a+μc) transition is approached. This comparison demonstrates that the average diffusion length of precursors on the film surface during growth is significantly reduced for the alloys, likely due to surface defects. Subsequent phase diagrams for Si_{1-x}Ge_x:H obtained at T=260°C, T=290°C, and T=320°C reveal (i) a shift of the a→a transition to higher db, indicating an enhancement in surface diffusion, as well as (ii) a shift in the a→(a+μc) transition to lower R. Although the latter effect is

detrimental for Si:H, it is not for Si_{1-x}Ge_x:H, and the net effect is an improvement in alloy material characteristics at the deposition phase boundary. Additionally, non-standard deposition techniques will be evaluated for potential usefulness in this application. 1. R.W. Collins, A. Ferlauto, G. Ferreira, C. Chen, J. Koh, R. Koval, Y. Lee, J. Pearce, and C. Wronski, "Evolution of microstructure and phase in amorphous, protocrystalline, and microcrystalline silicon studied by real time spectroscopic ellipsometry", *Solar Ener. Mater. Solar Cells* **78**, 143-180 (2003).

2:15 PM **A16.4**

Surface Diffusion Processes during a-Si:H Growth: Temperature Dependent Study of the Surface Roughness Evolution. Johan P. M. Hoegnagels, Erwin W. M. M. Kessels and Richard M. C. M. van de Sanden; Applied Physics, Eindhoven University, Eindhoven, Netherlands.

The growth process of a-Si:H by HWCVD is studied by analyzing the surface roughness evolution during film growth. This analysis, which is the first extensive investigation of the temperature dependence of the surface roughness evolution, is based on the work of Collins and co-workers [1] and gives information on aspects such as initial film growth, surface roughening and smoothening, and surface diffusion mechanisms. Purely amorphous films have therefore been deposited from undiluted silane and at low deposition rates (~8 nm/min) while monitoring the growth by real time spectroscopic ellipsometry for substrate temperatures between 70 and 450 °C. The thickness of the surface roughness is deduced from a two-layer optical and analyzed as a function of the film thickness similar to the analysis performed by Collins et al. [1]. The initial roughness is approximately identical for all substrate temperatures indicating a similar nucleation behavior at the different temperatures. After nucleation and depending on substrate temperature the surface smoothenes during growth for temperatures above 150 °C. The position of the amorphous-to-amorphous roughening transition is observed within the film thickness range of 10-15 nm with the optimum of ~15 nm at ~250 °C. Analysis of the post-initial growth phase by RTSE and ex-situ AFM demonstrates a self-affine growth in good agreement with previous results by, e.g., Smets et al [2]. In general, our results at 250 °C are in excellent agreement with previous work by, e.g., Collins et al. [1] on RF-PECVD deposited a-Si:H. Our temperature dependent studies, however, reveal some new insights in the growth mechanism of a-Si:H. First of all the smoothening rate after nucleation is rather slow and temperature independent. An analysis in the framework of a stochastic growth equation suggests that the usual mono-radical surface diffusion picture of surface smoothening needs to be replaced by a bi-radical picture in which growth only occurs on an active site. This bi-radical picture contains the possibility that both precursor as well as the active site are mobile. Furthermore, the analysis of the stochastic growth equation also suggests a novel interpretation of the post-initial growth phase in which the observed growth exponent beta monotonically decreases from about 0.18 to 0.05. We conjecture that a conserved non-linear term rules the surface smoothening, resulting in a pseudo Edward-Wilkinson scaling behavior in the high temperature limit. [1] R.W. Collins, A.S. Ferlauto, G.M. Ferreira, C. Chen, J. Koh, R.J. Koval, Y. Lee, J.M. Pearce, C.R. Wronski, *Sol. Energy Mater. Sol. Cells* **78** (2003) 143. [2] A.H.M. Smets, W.M.M. Kessels, M.C.M. van de Sanden, *Appl. Phys. Lett.* **82**, 865 (2003).

2:30 PM **A16.5**

Low-to-Medium Energy Ion Bombardment Effects on Interface Formation During Thin Film Growth in Plasma-CVD Environment. Aram Amassian, Patrick Desjardins and Ludvik Martinu; Regroupement Quebecois sur les Materiaux de Pointe (RQMP) and Department of Engineering Physics, Ecole Polytechnique de Montreal, Montreal, Quebec, Canada.

Plasma-enhanced chemical vapor deposition (PECVD) is recognized as a highly versatile and flexible deposition technology. Significant research effort has gone into studying the plasma chemistry and film properties, but many questions remain unanswered, including thin film growth dynamics and interface formation under the influence of plasma irradiation. We demonstrate the capability of in situ real-time spectroscopic ellipsometry (RTSE) to detect and to precisely quantify the modifications of c-Si in O₂ plasma with ion energy ranging from ~0.05 to 0.7 keV. Dynamic Monte-Carlo (DMC) simulations have allowed us to show that these modifications, which include primarily amorphization and oxidation, result from ion implantation and defect generation. Simulations also show evidence of surface swelling and sputtering due to plasma-surface interactions, which occur simultaneously during the initial moments of dielectric thin film growth. In the case of thin film deposition by PECVD, ion bombardment is also responsible for ion-mixing of substrate and film atoms, which results in interface formation. We show excellent agreement between DMC predictions and in situ RTSE characterization. This study has given insight into the PECVD deposition process and the role of ion bombardment in the synthesis

of porous and dense Si₃N₄ for optical coatings by dual-frequency microwave/radiofrequency plasmas.

SESSION A17: Thin Film Transistors

Chair: Joao P. Conde

Thursday Afternoon, March 31, 2005

Room 2002 (Moscone West)

3:15 PM **A17.1**

Low-temperature a-Si:H Thin-film Transistor Backplanes on Flexible Substrates by Digital Lithography. William S. Wong, Rene Lujan, Steven E. Ready, Juergen Daniel and Robert A. Street; Electronic Materials Laboratory, Palo Alto Research Center, Palo Alto, California.

The development of inexpensive high-performance electronics requiring low-temperature device processing would enable low-cost, large-area flexible electronics for applications such as large-area displays, sensors, and evolving technologies such as electric paper. The spatial resolution and small drop volume of jet-printing methods, combined with low-temperature a-Si:H processing, is one approach for integrating a-Si:H thin-film transistors (TFTs) with large-area flexible substrates. A novel digital-lithographic method, in which an electronically generated and digitally aligned etch mask is jet-printed onto a process surface, was used to fabricate a-Si:H TFT arrays. The digital lithographically fabricated arrays had features as small as 30 μm with 5 μm layer-to-layer registration and pixel resolution of 75 dpi over a four-inch diameter wafer. A bottom gate TFT structure was deposited at 170°C using conventional plasma-enhanced chemical vapor deposition. The resulting TFTs, patterned by digital lithography on glass substrates, had on/off ratios of 10⁸ and threshold voltages of 4.5 V with carrier mobility of 0.9 cm²/V·s. These results were comparable to conventionally processed a-Si:H TFTs. Given the ability for high-resolution spatial alignment, the digital lithographic process is ideal for registering multilayer patterns over a large-area flexible substrate, in which localized alignment run out is a problem. The same process was used to make 128×128 pixel matrix addressed TFT arrays having 75 dpi resolution on polyimide and polyethylene naphthalene flexible substrates. The backplanes were then integrated with a-Si:H p-i-n photodiodes to complete an image sensor array fabricated at 170°C. Device performance and stability for low-temperature a-Si:H TFT arrays on flex will be presented and compared to devices created by conventional methods. Pixel design using digital lithographic processing and integration of the flexible TFT array backplane with display media will also be discussed.

3:30 PM **A17.2**

SiNx Stress Control for Overlay Registration in a-Si:H TFTs on Flexible Foil Substrates. I-Chun Cheng, Alex Kattamis, Ke Long, James C. Sturm and Sigurd Wagner; Electrical Engineering, Princeton University, Princeton, New Jersey.

Mechanical stress in hydrogenated amorphous silicon (a-Si:H) thin-film transistors (TFTs) is becoming an important design parameter, especially when the TFTs are made on compliant substrates. Excessive stress always has been avoided to prevent film fracture and peeling. Now attention is turning to the effects of stress on substrate dimensions and thus overlay alignment. The goal is to obtain flat device/substrate composite structures at each photolithographic step, and for the completed circuit. Here we report first, a study of stress and then, the design of stress into TFT layers. We also show that the electrical performance of TFTs does not vary with such designed-in stresses. SiNx films were deposited on 50-micrometer thick Kapton E polyimide over ranges of deposition power and substrate temperature. Three regimes were investigated: built-in stress dominated, thermal stress dominated, and the regime where built-in and thermal stress are comparable. While the built-in stress of SiNx film changes from tensile to compressive as the deposition power increases, the thermal stress measured at room temperature is always compressive for a film deposited at elevated temperature. We find that (a) the crossover deposition power for changing the stress from tensile to compressive decreases as deposition temperature is reduced, (b) the magnitude of the built-in stress increases with film thickness, and (c) thermal stress can be compensated with built-in stress to result in stress-free films. Next we evaluated and compensated stresses in a-Si:H TFTs. Because samples with different, stress-induced, curvatures will flatten to different dimensions, photolithographic misalignment results. The TFTs were fabricated in a non-self-aligned, back-channel-etched geometry on 50-um Kapton E at a maximum process temperature of 150°C. All process steps but the RF power of the SiNx deposition were identical. We varied this power to vary the stress in the SiNx. The sample was carried as a free-standing film through most of the process steps, except in photolithography when it was soft-bonded to glass. We monitored the amount of misalignment between the first and second photolithography levels, i.e., the bottom gate and the source/drain. A

compensating stress can be dialed into the silicon nitride (SiN_x) gate dielectric to keep the substrate size constant. We found that the TFT characteristics did not vary with the stress in the SiN_x gate dielectric. We discuss the flatness requirement, describe the extraction of built-in stress data, demonstrate control of overlay alignment, and show the corresponding TFT characteristics.

3:45 PM **A17.3**

Fabrication of Polycrystalline Silicon Thin Film Transistors (Poly-Si TFTs) in Array Module using Field Aided Lateral Crystallization (FALC) Process. Hyunchul Kim, Hyun-Woong Chang and Duck-Kyun Choi; Ceramic Engineering, Hanyang University, Seoul, South Korea.

For the application of high resolution liquid crystal display (LCD), array of polycrystalline silicon thin film transistors (poly-Si TFTs) were fabricated on a Corning 1737 glass substrate using Ni induced field aided lateral crystallization (FALC) process. In this experiment, Ni, which is the catalyst for metal induced crystallization of amorphous, was deposited only on the source and drain area. Each source and drain was connected by a Mo electrode in order to apply the same electrical field strength for each pattern. After crystallization of amorphous silicon in the channel region, 100-nm-thick SiO₂ and 300-nm-thick Mo films were sequentially formed on the channel as a gate oxide and gate metal, respectively. Finally, poly-Si TFTs were fabricated in the 2-inch array module, using only the thermal process at the peak process temperature of 500°C. The electrical characteristics of poly-Si TFTs were measured by HP 4140B equipment. The electric fields applied through common electrodes connected to source and drain area led the directional crystallization of amorphous silicon from negative electrode side to positive electrode side at 500°C. This directional crystal growth enabled us to remove the metal impurity incorporation, which is the main cause for increased off-state drain leakage current, out of the channel region. Moreover, the applied electric field induced growth of needle-like elongated grains and accelerated the crystal growth rate. As a result, we can increase the carrier mobility because these longish grains reduce the chances of carrier scattering at the poly-Si grain boundary in the channel. Field effect carrier mobility of FALC-processed poly-Si TFTs were estimated to be 200 cm²/Vs at the drain voltage of 0.1V, and off-state drain leakage current at the gate voltage of -10V was approximately on the order of 10⁻¹² A.

4:00 PM **A17.4**

Electrolyte-Gate a-Si:H Thin Film Transistors.

Dina Goncalves^{1,2}, D. M. F. Prazeres², V. Chu¹ and J. P. Conde^{1,3},
¹INESC Microsystems and Nanotechnologies, Lisbon, Portugal;
²Center of Biological and Chemical Engineering, Instituto Superior Tecnico, Lisbon, Portugal; ³Department of Chemical Engineering, Instituto Superior Tecnico, Lisbon, Portugal.

Hydrogenated amorphous silicon (a-Si:H) has been widely used as the active layer of thin film transistors (TFT) for large-area electronic applications such as liquid-crystal displays and imagers. This paper describes the fabrication and characterization of electrolyte-gate a-Si:H TFTs in which the source-drain current is modulated by a voltage applied through a Pt electrode immersed in an aqueous electrolyte solution. The electrolyte solution contacts the TFT dielectric and functions as the gate. We are currently developing electrolyte-gate a-Si:H TFTs in the top-gate configuration for application as biosensors, with the objective of electronically detecting the presence of biomolecules, such as DNA and proteins, immobilized or adsorbed on the surface of the device. We present a new structure based on a top-gate TFT with characteristic width-to-length ratio (W/L) of 5 (W=100 microns, L=20 microns). The substrate is glass. The source and drain contacts are made of Al with a 50 nm n⁺-a-Si:H contact layer. The active layer is 100 nm of intrinsic a-Si:H deposited at 250°C. A silicon nitride layer deposited at 350°C is used as gate dielectric. The main difference between this device and a standard a-Si:H top-gate TFT is that the metal gate of the standard TFT is replaced by an aqueous electrolyte (water with borate buffer) and the gate voltage is applied through a Pt electrode immersed in the liquid. Since the liquid in contact with the device is electrically conductive (resistance is 150 ohm), electrical passivation of the metal source-drain contacts is a crucial issue to avoid undesirable effects such as electrical shorting between the source or drain and the gate or electrochemical reactions (electrolysis). A layer of silicon nitride covering the metal source and drain contacts is used to provide this passivation. Electrolyte-gate top-gate a-Si:H TFTs show qualitatively similar curves to their metal-gate counterparts. The gate-voltage range that can be used depends critically on the quality of the passivation layer. Beyond a certain voltage (between 3 V and 8 V, for the passivation layers developed so far) electrical leakage and electrochemical reactions occur. The best devices fabricated so far, with a working gate voltage range applied between -2.0 to 3.0 V show on/off current ratios of 3 orders of magnitude and a subthreshold slope of 0.5 V/dec. The on/off current ratio and the

mobility are limited in the present devices because the onset of leakage through the passivation layer at 3 V does not allow the device to turn fully on. Electrolyte-gate top-gate a-Si:H TFTs are remarkably stable to gate voltage-bias, showing no shift of the transfer curve upon bias application. Improvements in the device design and in the passivation layer are expected to widen the voltage range available for operation and to optimize the device performances.

4:15 PM **A17.5**

High Electron Mobility (~120 cm²/Vs) PECVD Nanocrystalline Silicon Top-Gate TFTs at 260 °C. Czang-Ho Lee, Andrei Sazonov and Arokia Nathan; ECE, University of Waterloo, Waterloo, Ontario, Canada.

Thin film transistors (TFTs) with high field effect mobility are very attractive for peripheral circuit driver and switching device applications in active-matrix TFT backplanes for flat panel displays (FPDs). Currently, laser annealed polycrystalline silicon (poly-Si) TFTs are being used in such applications. However, the high cost, complex processing, and non-uniformity issues limit its use in large-area high-resolution applications on glass and/or plastic substrates. Hence, the direct deposition of high quality and high mobility Si thin films at low temperatures is a promising alternative. In this work, we deposited high quality undoped nanocrystalline silicon (nc-Si:H) films by conventional large-area radio-frequency (RF) 13.56 MHz plasma enhanced chemical vapor deposition (PECVD) at 260 °C, using 99 % H₂-diluted SiH₄. The nc-Si:H film showed oxygen concentration of 1.5 × 10¹⁷ atoms/cm³ and dark conductivity of ~10⁻⁶ S/cm, while the Raman crystalline volume fraction was over 85 %. The low oxygen concentration and high crystalline volume fraction can be attributed to favourable kinetics associated with energetic atomic hydrogen during the growth process and in the in-situ chemical cleaning of oxygen, along with effective hydrogen passivation of grain boundaries. Top-gate staggered TFTs with 100 nm thick nc-Si:H channel layer and amorphous silicon oxide (a-SiO_x) as the gate dielectric were fabricated. The TFTs showed field effect mobility of ~120 cm²/Vs, threshold voltage of ~2.5 V, ON/OFF current ratio of ~10⁶, and sub-threshold slope of ~0.25 V/dec. To the best of our knowledge, the TFT mobility reported here is the highest achieved to date using state-of-the-art nc-Si:H films prepared by PECVD. These results demonstrate the feasibility of low-temperature and high-speed nc-Si:H TFTs for on-panel circuit integrated using standard PECVD process.

4:30 PM **A17.6**

Investigation of the Effects of X-ray Irradiation of Polycrystalline Silicon, Thin Film Transistors. Yixin Li, Larry E. Antonuk, Hong Du, Youcef El-Mohri, Amit Sawant, Yi Wang, Jin Yamamoto and Qihua Zhao; Department of Radiation Oncology, University of Michigan, Ann Arbor, Michigan.

Excimer-laser-annealed polycrystalline silicon (p-Si) thin-film transistors (TFTs) provide about two orders of magnitude higher mobility than amorphous silicon (a-Si) TFTs. The incorporation of such TFTs into active matrix flat-panel imagers (AMFPs) for x-ray detection makes it possible to improve the signal performance through the creation of more complex pixel circuitry. However, it is important that such TFTs exhibit sufficient tolerance to the effects of ionizing radiation. Accordingly, the properties of a set of 17 individual p-Si TFTs with different aspect ratios were examined as a function of radiation dose. These TFTs are representative of those used in prototype AMFPs incorporating pixel amplifiers recently developed in collaboration with the Palo Alto Research Center. In this study, source-drain current and noise characteristics were measured at dose intervals ranging from 10 to 100 Gy. An examination of room-temperature and elevated-temperature annealing of the resulting radiation effects was also performed. Preliminary analysis of data acquired beyond the lifetime dose of imaging circuits for radiography, fluoroscopy, and mammography indicates that there is no measurable effect upon the mobility of the TFTs. In addition, a measurable but not significant increase (~2 × 10⁻⁴ V/decade/Gy) in the sub-threshold swing was observed. However, the threshold voltage decreased by ~5 × 10⁻³ V/Gy and the transfer characteristic curves shifted toward negative gate voltage. As a result of this shift, under common operational conditions the leakage current of TFTs decreased with increasing dose. Finally, no measurable effect upon either the flicker or the thermal noise component of the TFTs was observed. These initial results are encouraging and suggest that the effects of radiation on p-Si TFTs are relatively small and should not degrade the performance of AMFPs used for radiography, fluoroscopy and mammography. In this presentation, detailed results of the performance of p-Si TFTs as a function of dose up to 1000 Gy (corresponding to the lifetime dose of radiotherapy imagers) will be shown, and mechanisms for the effects of radiation will be discussed.

4:45 PM **A17.7**

Effect of Channel Doping on Low Temperature

Polycrystalline Silicon Thin-Film Transistors. Daechul Choi, Myeong-Seob So, Byoungdeog Choi, Inbok Song and Hokyoon Chung; Corporate Research and Development Center, Samsung SDI, Kyongki, South Korea.

We investigated effects of boron-doped channel on electrical characteristics for low temperature polycrystalline silicon (LTPS) thin film transistor (TFT). We fabricated both intrinsic- and doped-channel n-TFTs and characterized the device performance in view of short channel effect and threshold voltage control that are important aspects especially in the application of system on panel (SOP). For the application of TFTs in SOP, there is a great interest in scaling down of device dimensions to meet the needs of switching speed and low power consumption. As the channel length of the device is scaled down, the drain voltage can lower the barrier height of the channel near the source. Through the investigation of the drain induced barrier lowering (DIBL) effect, the short channel effect was characterized with varying channel length for the intrinsic- and doped- channel TFTs. By channel doping, the DIBL phenomenon begins to appear at shorter gate channel length of about $3\ \mu\text{m}$ or so, compared to intrinsic channel TFT having $6\ \mu\text{m}$ or so. We have confirmed the effectiveness of channel doping to control the threshold voltage. We were able to positively shift the threshold voltage for n-TFT without degrading sub-threshold slope and make sure the switching off at the gate voltage of 0 V. We also found the reduced standard deviation of threshold voltages among the TFTs over the wide range of glass by channel doping.

SESSION A18: Poster Session: Characterization-a-Si:H and Alloys B
Thursday Evening, March 31, 2005
8:00 PM
Salons 8-15 (Marriott)

A18.1
Stark Splitting in Photoluminescence Spectra of Er in a-Si:H. Minoru Kumeda¹, Mitsuo Takahashi¹, Akiharu Morimoto¹ and Tatsuo Shimizu²; ¹Division of Electrical Engineering and Computer Science, Graduate School of Natural Science and Technology, Kanazawa University, Kanazawa, Japan; ²NTT Microsystem Integration Labs., Atsugi, Japan.

The wavelength 1.54 micrometer of the optical transition of Er ions coincides with a minimum loss of silica optical fibers and many works have been done aiming applications to optical devices. Because the optical transition between states with f orbitals is inhibited by symmetry, we need a lower symmetry around the Er ions to obtain mixing of orbitals with different symmetries. a-Si:H films are useful as a host material since the disorder of the amorphous network makes Er ions have the orbitals with different symmetries and the flexibility of amorphous network makes possible a higher amount of Er ions incorporated in the host. Understanding the excitation mechanism for Er ions is important to get a strong emission. The incorporation scheme of Er ions is essential for discussing the excitation mechanism, and should be reflected in the photoluminescence (PL) spectra. We tried to decompose the PL spectra at different temperatures and pursue the change by annealing. Er-doped a-Si:H films were prepared by magnetron sputtering in an atmosphere of Ar and H₂ mixture. The thickness of the films was around 800nm. The content of Er was estimated to be 0.8 at. %. The shape of the Er PL spectra were decomposed into several lines on the photon energy abscissa. At first, the 19K-spectrum was reproduced by adding four Gaussian lines with increasing linewidths. Because at this low temperature only the lowest energy level of ⁴I_{13/2} contributes to the radiative transition, the energy levels in ⁴I_{15/2} which are split by the Stark effect are determined to be located at 5.9 meV, 19.4meV and 36.4meV relative to the lowest energy level of ⁴I_{15/2}. These values are not largely different from those for Er in aluminosilicate glass. This implies the nearest neighbor of Er are oxygens which have been introduced unintentionally in the sample during preparation. Next the spectra observed at higher temperature were decomposed to give the Stark separation between the second lowest level of ⁴I_{13/2} and the lowest level of ⁴I_{13/2} although the number of component lines and ambiguities increased. Annealing makes the PL intensity increase up to 400C and decrease rapidly at 500C. The peak positions of the component lines of PL did not appreciably change by annealing. The PL decrease in 500C-annealed samples is attributed to the loss of the excited carriers to the increased dangling bonds.

A18.2
PECVD Grown Polymorphous Hydrogenated Silicon (pm-Si:H) Studied using Current Transient Spectroscopies in PIN Diodes. Vibha Tripathi¹, Yashowanta N. Mohapatra¹ and Pere Roca i Cabarrocas²; ¹Physics, IIT Kanpur, Kanpur, UP, India;

²LPICM, Ecole Polytechnique, Palaiseau Cedex, France.

Polymorphous Silicon (pm-Si:H) thin films have emerged as alternative to conventional a-Si:H due to their better transport properties and improved stability. These improvements are attributed to the presence of nano-crystalline inclusions in the amorphous matrix when grown under controlled conditions by PECVD. Possible changes in the density of gap states due to the presence of crystallites is of central importance in understanding steady state and dynamic characteristics of devices using these materials. We have studied a-Si:H and pm-Si:H grown by PECVD at different pressures. We monitor the steady state reverse current and their transients in PIN devices fabricated using these materials. The transients are analyzed using isothermal spectroscopic techniques such as Time Analyzed Transient Spectroscopy (TATS), and high resolution Laplace DLTS as a function of temperature. In case of a-Si:H, we obtain expected signature of emission from a broad density of states in the form of stretched exponentials. In contrast the corresponding spectra for pm-Si:H are dominated by nearly exponential fast current decay processes with discrete energies between 0.25 and 0.36 eV from Ec. It is shown that the study of the density of states by dynamic methods such as transient techniques reveal features not accessible to steady state measurements. The origin of multiple discrete traps in presence of disorder is discussed.

A18.3
Characterization of Amorphous Silicon by SIMS. Yupu Li, Shaw Wang and Xue-Feng Lin; Charles Evans & Associates, Sunnyvale, California.

Impurities and dopant profiles in amorphous silicon are important aspects to a-Si(H) solar cell materials and a-Si TFT (Thin Film Transistor) applications. To material engineers, a new challenge is to make more controllable thinner a-Si films for subsequent manufacture into devices. For example, precisely controlling the hydrogen content is key to the functions of a-Si(H) solar cells and a-Si TFT devices. The production of low hydrogen content a-Si is essential for the laser-induced crystallization of a-Si for poly-Si TFT applications. Because of these new manufacturing demands there are also new characterization challenges for SIMS (Secondary Ion Mass Spectrometry) and other material characterization techniques. This presentation will give some examples of SIMS analyses of a-Si thin films, using both O₂ or Cs primary beams on both Cameca magnetic sector and PHI quadrupole SIMS instruments. The various analytical modes used and typical results obtained will be highlighted in the following areas: (1) The analysis of hydrogen in a-Si. This is often done with a combination of SIMS, HFS (Hydrogen Forward Scattering Spectroscopy), and FT-IR (Fourier Transform Infrared Spectroscopy). (2) The analysis of P-doped n+-Si thin layers. This typically requires the use of high mass resolution setting to separate P and (30Si+H) since the H content is so high in a-Si. (3) The analysis of C, N, O, S in a-Si films. (4) The analysis of Li, Na, K, F, Cl in a-Si. These species can be sources of mobile ionic charge at Si-SiO₂ interface and they typically require a lower primary beam energy for profiling thin layers. (5) The analysis of Al, Cr, Fe, Ni, and Cu metallic contaminants in a-Si.

A18.4
A Comprehensive Kinetic Model for Silicon Germanium Wet Oxidation. Mohamed A. Rabie¹, Yaser M. Haddara¹ and Jacques Carette²; ¹Electrical and Computer Engineering, McMaster University, Hamilton, Ontario, Canada; ²Computing and Software, McMaster University, Hamilton, Ontario, Canada.

Thermal oxides play a significant role in device technology. SiO₂ is known to be a good insulator with low trap density and low positive fixed charge. Unlike the high quality oxide resulting from Si oxidation, SiGe oxidation produces a low quality oxide due to several factors: Ge is piled up between the oxide and the substrate [1], there is a high trap density ($\sim 10^{12}/\text{cm}^2\text{eV}$) at the oxidizing interface, and the fixed charge density is high ($\sim 10^{11}\text{-}10^{12}\text{cm}^{-2}$) [2]. To overcome the problems arising from oxidizing SiGe, a sacrificial layer of silicon is deposited over the SiGe alloy and oxidized instead [3]. Addressing the problem in this manner adds processing steps. More significantly, if the deposition and oxidation steps are not properly optimized device performance degrades considerably. What is required is (1) a physically-based model that accurately predicts the kinetics of SiGe oxidation; and (2) an understanding of how the SiGe oxide and interface quality may be improved. Several attempts have been made to model the oxidation of SiGe. However, none of the existing models capture the full range of phenomena reported in the literature for SiGe oxidation. We propose a model based on (1) the simultaneous oxidation of both Si and Ge at different rates (Si oxidizes preferentially); and (2) the replacement of Ge in GeO₂ by Si. The model is parameterized by three reaction rates, by an effective Si-Ge interdiffusivity, and by the solubility and diffusivity of oxidant in the oxide. Whenever values for these parameters are published in the

literature, these values are used. The model succeeds in simulating published results over a wide range of experimental conditions. This model is the first to predict the profile of Ge in the oxide and our results show excellent agreement with experiments. Table 1 shows the extracted reaction rates for a range of experimental conditions showing that all reaction rates increase with temperature and, as expected, that Ge catalyzes both the Si and Ge oxidation reactions. The solubilities of steam and wet O₂ in GeO₂ were found to be $2.2 \times 10^{20} \text{ cm}^{-3}$ and $1.4 \times 10^{20} \text{ cm}^{-3}$ respectively. On the other hand, the value of the solubility of wet O₂ in SiO₂ was obtained from the simulations to be $9.9 \times 10^{18} \text{ cm}^{-3}$ and that of steam is known to be $3.0 \times 10^{19} \text{ cm}^{-3}$. As predicted by previous studies the solubility is significantly higher in case of GeO₂. [1] LeGoues et al., JAP, v65, p1724, 1989. [2] Nayak et al., APL, v57, p369, 1990. [3] Yang et al., Semicon. Sci. and Tech., v16, p972, 2001.

A18.5

AFM Morphology Study of a-Si_{1-y}Ge_y Films Deposited by LF PE CVD from Silane-Germane with Different Dilution.

Liborio Sanchez¹, Andrey Kosarev¹, Alfonso Torres¹, Thomas E. Felter² and Alexander Ilinskii³; ¹Electronics, Inst. Astrophysics, Optics and Electronics, Puebla, Puebla, Mexico; ²Lawrence Livermore National Laboratory, Livermore, California; ³Benemerita Universidad Autonoma de Puebla, Puebla, Puebla, Mexico.

The morphology of a-Si_{1-y}Ge_y films over the entire range of Ge content has been studied by AFM. The films were deposited by Low Frequency (LF) PE CVD at substrate temperature T_s=300°C and discharge frequency f=110 kHz from silane+germane mixture with and without, Ar and H₂ dilution. The films were deposited on silicon and glass (Corning-1737) substrates. AFM images were taken and analyzed for 15x15, 5x5, 2x2 and 1x1 (μm₂) areas. All the images demonstrated "grain" like structure, which was characterized by the standard height deviation R_q, average roughness R_a, height distribution function H(z), mean grain area, area distribution function D(s), mean grain diameter <d> and diameter distribution function F(d). The roughness (R_q, R_a) of the films monotonically increases with Ge content with or w/o H₂ dilution. Films deposited with Ar dilution, on the other hand, are roughest at y=0.6. The films deposited with H₂ dilution showed the lowest values of R_q, R_a and the grain diameters in the range of <d>=30-70 nm.

Acknowledgement. This work is performed in the framework of CIAM-2002 program. The investigations in INAOE are supported by the CONACYT project # 42367. The work of T.Felter was performed under auspices of the U.S.Department of Energy by Lawrence Livermore National Laboratory under contract No.W-7505-Eng-48.

A18.6

Change of the Structure of Nd Doped Amorphous SiN Thin Films After Annealing as Analysed by Electron Microscopy.

Daniel Biggemann¹, Saule Aldabergenova², Horst Strunk² and Leandro Tessler¹; ¹State University of Campinas, Campinas, Brazil; ²Erlangen-Nuernberg University, Erlangen, Germany.

We study the structure of amorphous silicon sub-nitride SiNx (x = 0,43; 0,65; 1,0; 1,15) thin films prepared by RF co-sputtering by means of transmission electron microscopy techniques. As prepared SiNx samples were carefully annealed at different temperatures to enhance the characteristic Nd3+ emission in the infra-red region. The best Nd3+ emitting samples after optimal annealing show the structure of fine dispersed crystalline grains with sizes of 2 -5 nm embedded in an amorphous matrix. Cathodoluminescence measurements (directly in high resolution transmission electron microscope) in optimally annealed samples show broad emission spectra that cover the whole visible region, from 430 to 750 nm. This emission is related to the SiNx matrix and may play an important role in the excitation of the Nd3+ ions.

A18.7

Optical Properties of Amorphous Silicon-Yttrium Films.

Tetyana Vicrobna Semikina¹ and A. N. Shmyryeva²; ¹Teikyo University of Science & Technology, Kitatsuru-gun, Yamanashi-pref., Japan; ²National Technical University of Ukraine, Kiev, Ukraine.

The main technological efforts in technology of amorphous silicon are directed to trap states density decreasing and, as a consequence, to charge carrier mobility, photosensitivity and characteristics stability increasing. The known methods of hydrogen and halogens incorporation to amorphous silicon composition provide some progress, but don't resolve the problem of characteristics degradation of these materials. The goal of our work is deposition of films that have stable electrical characteristics, photosensitivity and optical characteristics fitting for further application in solar cells. In our previous work^{1,2} we demonstrated the results of current-voltage, photoelectrical measurements, reflection and transmission spectrums. The main result was the fact that deposited films didn't show Stebler-Vronskiy effect and had stable electrical characteristics (4 %

of altering) after 2000 hours of testing. It was proved that yttrium changed the structural bonds in amorphous silicon and provided decreasing of energy states density. More over the yttrium concentration enhancement initialises growth of photoactive impurity centres. The highest photosensitivity was of 3x10⁻³ Ohm-1m-1 for films with yttrium content of 12 weight %. The reflective and absorptive spectrums showed the maximum absorption in the spectrum range is less than 0.6 microns and the band gap is of 1.75 eV for the composition with highest photosensitivity. This work presents the new results of atomic force microscope (AFM) and optical investigations (infrared spectrums and ellipsometry) of amorphous silicon alloy with yttrium (a-Si:Y). The amorphous a-Si:Y films were deposited on silicon substrates by electron-beam sputtering of special alloy compositions in vacuum without hydrogen inlet. The reason of hydrogen exclusion is fact that in time hydrogen leaves the film that leads to instability first of all of electric characteristics in time. To fulfil the broken bands yttrium was introduced to technological procedure. In this work we choose yttrium concentration in prepared for sputtering special alloys from 5-25 % because from previous results the samples with yttrium more than 25 % had microcrystalline structure. Also in this work we varied deposition time from 5 to 25 min. From new results of AFM it is obtained that films have amorphous structure with some rare microcrystalline inclusions. For the first time we present the result of ellipsometric analyses. Spectroscopic ellipsometry measurements were performed using a variable angle spectroscopic ellipsometer with a Xe-lamp source, single chamber monochromator, continuously rotating analyser and auto-retarder. The ellipsometric angles and were determined in the spectral range from 0.8 eV to 5 eV at 65deg, 70deg and 75deg angle of incidence.

SESSION A19: Poster Session: Growth-Microcrystalline and Nanocrystalline Films

Thursday Evening, March 31, 2005

8:00 PM

Salons 8-15 (Marriott)

A19.1

Fabrication of Nano-Crystalline Porous Silicon on Si Substrates by a Plasma Enhanced Hydrogenation Technique.

Yaser Abdi^{1,2}, Pouya Hashemi¹, Fatemeh Dehghan Nayeri¹, Ashkan Behnam¹, Shamseddin Mohajerzadeh¹, Javad Koohsorkhi^{1,2}, M. D.

Robertson³ and E. Arzi²; ¹ECE Department, Thin Film Lab, University of Tehran, Tehran, Iran; ²Department of Physics, University of Tehran, Tehran, Iran; ³Department of Physics, Acadia University, Wolfville, Nova Scotia, Canada.

A novel method for fabrication of nano-crystalline silicon films is introduced by using plasma hydrogenation and annealing steps. Using this technique, formation of nano-size grains is achieved by means of hydrogenation of already-deposited silicon layers without a need to ion implantation or wet chemical processing. N-type <100> silicon wafers are used as the substrate. After proper cleaning, a 0.1μm-thick SiO₂ layer is grown by thermal oxidation followed by deposition of a 1000Å silicon layer using e-beam evaporation. The Si deposition was performed at temperature of 250°C and base pressure of 2×10^{-6} Torr. The as-grown samples are amorphous and they are placed in a DC-PECVD reactor for hydrogenation. Several hydrogenation steps were done in base pressure of 3mTorr with power density of 4.5 and 6.5 W/cm² and temperatures ranging from 300°C to 400°C. Each step of hydrogenation has the duration of 15 and 30 mins. This step is followed by an in-situ annealing at a temperature 70°C higher. By successive hydrogenation-annealing steps nano-crystalline porous structures are obtained. It is believed that in the process of hydrogenation, hydrogen radicals replace the dangling bonds of Si atoms in the amorphous structure and when depassivating the previously hydrogenated bonds, they impart energy to silicon atoms, enhancing the chance for nucleation and growth of nano-crystalline sites. The samples are characterized by SEM, TEM and photoluminescence (PL) analyses. The porosity of these structures is confirmed by SEM and small separated spherical grains sizing smaller than 50nm are observed. As indicated by SEM, for a constant plasma power, the samples hydrogenated at higher temperatures have smaller and more isolated grains whereas samples prepared at lower temperatures have a denser distribution of grains. Also by raising the plasma power and at a constant temperature smaller and more closely packed grains are formed. The results of TEM analysis further corroborate the nano-crystalline nature of the annealed Si films with a broad distribution of grain sizes between 3 and 10nm. The electron diffraction pattern also shows concentric rings corresponding to various crystal orientations. The porous Si is also characterized by the PL analysis. The wavelength of the incident light was 254nm. The peak of the PL spectrum varies between 600nm and 650nm for different conditions in experiments which is in the visible light spectrum. The analyses also show that by decreasing the grain size the peak shifts toward smaller wavelengths with a lower peak intensity

in the spectrum. This reduction could be due to an increase in the spread of grains over the sample. By better controlling the annealing condition, a higher density film can be obtained which in turn leads to a higher intensity of emitted light. Patterned structures, realized on such porous samples, confirm the light emission from desired areas. Investigation on possible electro-luminescence is underway.

A19.2

CO₂ Laser Annealing Synthesis of Silicon Nanocrystals Buried in Si-rich SiO₂. Chun-Jung Lin¹, Yu-Lun Chueh², Li-Jen Chou² and Gong-Ru Lin¹, ¹Department of Photonics & Institute of Electro-Optical Engineering, National Chiao Tung University, Hsinchu, Taiwan; ²Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan.

The localized synthesis of 3-8 nm-Si nanocrystals (nc-Si) in Si-rich SiO₂ (SRSO) by CO₂ laser annealing at the power density of below ablation-threshold (5.8×10^3 W/cm²) is demonstrated. The 280 nm-thick SRSO film is prepared by PECVD under a SiH₄-to-N₂O₂ flow ratio of 1:20. Since the SRSO exhibits a high absorption coefficient of up to 0.102 cm^{-1} at wavelength of $10.6 \mu\text{m}$, a direct-writing CO₂ laser annealing system with focusing spot size of 0.2 mm^2 is used to locally anneal the SRSO and precipitate the nc-Si. A thermophysical model reveals the surface temperature of SRSO ranging from 130°C to 1340°C achieved by varying laser power densities from 1.5×10^3 to 6.0×10^3 W/cm². The CO₂ laser-ablation-threshold power density is about 5.8×10^3 W/cm², corresponding to the optimized annealing temperature 1285°C . The CO₂ laser annealing is capable of the precise control on power density and spot size, which benefits from the in-situ and localized annealing temperature control of SRSO film, and also prevents from the eternal damage of the other electronic devices nearby the annealing site. The nc-Si dependent photoluminescence (PL) was observed at 806 nm or longer, whereas the ablation damaged SRSO film exhibits a significant blue PL at 410 nm. The blue PL is contributed by structural defects such as weak oxygen bond [O-O] (410 nm) and neutral oxygen vacancy [O₃≡Si-Si≡O₃] (455 nm), which are greatly enhanced as the laser power increases to 3.0×10^3 W/cm². A PL at 600-620 nm is found as the laser power density enlarges to 4.5×10^3 W/cm², which is mainly attributed to the formation of E'_δ defects prior to the precipitation of nc-Si. At the power density of 6.0×10^3 W/cm², a significant PL at 806 nm with spectral linewidth of 106 nm is observed. The refractive index of the laser-treated SRSO film is increasing from 1.57 to 2.31 as the laser-power density increases from 1.5×10^3 to 6.0×10^3 W/cm² which is mainly due to the increasing density of nc-Si embedded in SRSO. The structure of the CO₂ laser annealed SRSO with buried nc-Si is similar to that treated by conventional furnace annealing process. The highest power of the CO₂ laser as well as the peak surface temperature on SRSO sample is located in the beam spot center since the beam profile of the CO₂ laser is circularly Gaussian distributed. The PL wavelengths at outer area of the laser-treated spot are 600-620 nm since a lower surface temperature only induces a weaker nc-Si precipitating process. The PL at 806 nm is observed near the middle of the illuminated laser spot. High resolution transmission electron microscopy (HRTEM) analysis reveals that the average size of 3-8 nm nc-Si embedded in SRSO film is about 6 nm, which correlates well with the theoretical prediction of a corresponding PL at 806 nm. The TEM estimated square density of the nc-Si in SRSO film under the laser power density of 6.0×10^3 W/cm² is about $1.24 \times 10^{12} \text{ cm}^{-2}$.

A19.3

High Density Plasma Processing of Microcrystalline Si Thin Films. Pooran C. Joshi, Apostolos T. Voutsas and John W. Hartzell; LCD Process Technology Laboratory, Sharp Labs of America, Inc., Camas, Washington.

Microcrystalline silicon (μ -Si) thin films are being actively investigated for TFT and solar cell applications. For large area flat panel display applications, the μ -Si thin films offer the possibility of fabricating TFTs with performance intermediate to those of a-Si and poly-Si TFTs but significantly higher performance-to-cost ratio. A low temperature deposition technique is desired to realize the integration of μ -Si TFTs on plastic or other low temperature substrates. Various thin film deposition techniques are being investigated to address the major issues of deposition rate, processing temperature, and crystallinity of the μ -Si thin films. The main focus of various studies is to fabricate high quality μ -Si thin films by enhancing the plasma and substrate surface reaction kinetics by advanced plasma source and system designs. In the present work, we report on the fabrication of high quality microcrystalline Si thin films by high-density PECVD technique; which is gaining interest in area of thin film processing because of high ion and electron concentration, low plasma potential, and independent control of plasma energy and density. The μ -Si thin films were fabricated on glass substrates using a combination of H₂ and SiH₄ precursors at a temperature of 350°C . The effects of the applied rf power and H₂/SiH₄ ratio on the growth and microstructure of the μ -Si thin films were investigated. The microstructure of the

deposited films was examined by x-ray diffraction, Raman spectroscopy, and TEM techniques. The effects of the film thickness on the microstructure were analyzed in the range of 35-600 nm. The microcrystalline phase was identified by XRD patterns and the crystallite sizes were calculated from the FWHM of the XRD peaks corresponding to various planes. The microcrystalline volume fraction in the as-deposited films was established from the Raman spectra. The surface and cross-sectional morphology of the films were observed by TEM. The typical deposition rate of the μ -Si thin films was greater than $350 \text{ \AA}/\text{min}$ in the H₂/SiH₄ ratio range of 20-100. For a 150-nm-thick film deposited at a H₂/SiH₄ ratio of 20, the typical microcrystalline volume fraction and the average crystallite size corresponding to <111> orientation were 75% and 160 \AA , respectively. The microcrystalline phase formation was further verified by TEM analysis. The observed growth and properties of the μ -Si thin films show the potential of the high-density PECVD technique for the low temperature processing of high quality films with superior control of bulk and interfacial characteristics.

A19.4

Crystallographic Study on Initial Growth Region of μ -Si with Different Preferential Orientations. Yasushi Sobajima, Tsuyoshi Sugano, Takafusa Kitagawa, Toshihiko Toyama and Hiroaki Okamoto; Department of Systems Innovation, Osaka University, Toyonaka, Osaka, Japan.

Microcrystalline silicon (μ -Si) thin films prepared by PECVD have been widely utilized for thin film p-i-n solar cells. In general, the growth of μ -Si is elucidated only by vapor phase growth [1]. In our previous study, however, solid phase structural changes simultaneously occurring with the vapor phase growth were observed in the μ -Si photovoltaic layers by TEM and SAED measurements [2]. In this work, we have investigated crystallographic features in the μ -Si films measured by XRD with an emphasis on those of initial $0.5 \mu\text{m}$ region after the $>2 \mu\text{m}$ thick deposition utilizing the RIE process [3]. The microcrystallinity of the (220) oriented μ -Si being suitable for the photovoltaic layer is discussed in conjunction with that of the randomly oriented μ -Si. The crystalline volume fractions of the both samples were 50-60%. In the case of the (220) oriented μ -Si, the degree of the (220) preferential orientation as well as the grain size in the initial $0.5 \mu\text{m}$ thick region were increased after the $2.5 \mu\text{m}$ thick deposition compared to those of the $0.5 \mu\text{m}$ thick deposited film, which is interpreted as due to the solid phase structural transitions as we have reported [2,3]. Meanwhile, in the initial $0.5 \mu\text{m}$ thick region of random orientation μ -Si, no pronounced difference was monitored between the $2.5 \mu\text{m}$ thick and $0.5 \mu\text{m}$ thick deposited film. In addition, the microcrystallinity was improved with increasing deposition thickness as generally observed. These structural features found in the random orientation μ -Si could be elucidated by the vapor phase model [1]. Therefore, the crystallographic orientation of μ -Si would play a crucial role for the appearance of the solid phase structural transitions. [1] A. Matsuda, et al., JNCS 338-340 (2004)1. [2] T. Toyama, et al., JJAP 42 (2003) L1347. [3] T. Sugano et al., to be presented at 31th IEEE PVSC (2005).

A19.5

Rapid Thermal Annealing Crystallization of a-Si:H Films Deposited by HWCVD. B. Roy², J. Perkins¹, M. Dabney¹, C.

Teplin¹, J. Alleman¹, T. Kaydanova¹, E. Iwaniczko¹, P. Stradins¹, Q. Wang¹, D. Readey², B. To¹, Archie H. Mahan¹, H. Branz¹ and D. S. Ginley¹; ¹NREL, Golden, Colorado; ²Colorado School of Mines, Golden, Colorado.

The post-deposition crystallization of as-deposited a-Si:H films has the potential to enable scaleable and economic fabrication of polycrystalline Si for solar cells and high performance thin film transistors. Although many different methods are being considered to achieve this goal, rapid thermal annealing (RTA) is particularly promising because it is fast, economical and industrially applicable. Here, we report on application of RTA to thick (1-2 micron) a-Si:H films deposited on glass by HWCVD. A key aspect of the crystallization process is the affect of the initial hydrogen content. RTA experiments were done on both low (1 at.%) and high (8 at.%) hydrogen content a-Si:H films. Optical reflectivity, XRD, SEM and AFM were used to characterize the crystallinity and morphology of the annealed films. Initial experiments were single step (temperature) RTAs of high-H a-Si:H films at temperatures ranging from 650 to 900C with the at-temperature hold time ranging from 720 to about 6 seconds. The ramp to 900C takes 24 seconds. For high-H films annealed at 900C, the crystallite size estimated from XRD increases from ~ 300 to 420 \AA as the hold time is increased from 6 to 90 sec. In addition, using the intensity of the c-Si (111) XRD peak as a metric, complete crystallization can be obtained for high-H films in 6 seconds at 900C and 3.5 minutes at 700C. Further analysis of crystallized high-H films by cross sectional SEM and optical micrographs shows, in some cases, bubble like features which may be formed by extremely rapid hydrogen loss. Preliminary results show

that for the RTA of low-H films, for 6 second 900C anneals, the crystallite size is ~ 400 angstroms compared to 300 angstroms for the high-H content films. Collectively, these results suggest that a two step (temperature) annealing process might improve the crystallite size and reduce the bubble-defect formation. For the high-H films, the first lower-temperature step is intended to evolve hydrogen without causing crystallization. We will compare the crystallite size using the single step and two step process versus the amount of hydrogen evolved during the first anneal. Results will also be reported using a two step process for the low-H films, with the first anneal designed to explore whether nucleation can be initiated before the second anneal takes place. In addition to using a-Si:H films deposited on glass, we will report on selected experiments done with a-Si:H deposited on c-Si to facilitate quantitative tracking of the hydrogen evolution.

A19.6

Dependence of Microcrystalline Silicon Growth on Ion Flux at the Substrate Surface in a Saddle Field PECVD. Erik Johnson, Nazir P. Kherani and Stefan Zukotynski; Electrical & Computer Engineering, University of Toronto, Toronto, Ontario, Canada.

The Saddle-Field Glow Discharge PECVD system emulates RF-like excitation using a semi-transparent anode and a DC power supply. It has been used to deposit high quality amorphous and microcrystalline hydrogenated silicon thin films in the past. The growth of microcrystalline material is particularly sensitive to the conditions under which it is produced. Significant levels of microcrystallinity are only produced under conditions of higher pressure and electrical isolation of the substrate surface from the grounded substrate holder. We present results of a study on the relationship between substrate electrical potential and microcrystalline growth, as quantified by Raman scattering spectroscopy, at growth pressures near the minimum required for microcrystalline growth. A series of films were prepared in the DC Saddle Field Glow Discharge PECVD system at a constant hydrogen dilution level (10% silane in hydrogen) and at pressures between 150 mTorr and 300 mTorr. The substrate electrical bias - which has little effect on the electrical conditions of the plasma by virtue of its remoteness - was varied between 150 V to 250 V for each pressure condition. Under no conditions was this voltage enough to sustain a plasma on its own. It was observed that at the higher growth pressures, applying an external, positive substrate bias promoted microcrystalline growth similar to that on electrically floating substrates. As well, the amount of microcrystallinity increased with increasing substrate bias. At lower pressures, very limited microcrystallinity was observed and no correlation with substrate bias was seen. The minimum substrate bias necessary to achieve microcrystalline growth decreases with increasing pressure. The ion and electron flux to the growth surface under these conditions was also studied. It was observed that the growth conditions that yield microcrystallinity also showed a net negative current to the surface, which increased exponentially with increasing substrate bias. For the non-microcrystalline growth at lower pressures, no such exponential behaviour in the current was observed. The correlation between microcrystallinity, substrate bias, and net substrate current indicates that electrical interaction between the remote plasma and the growth surface strongly influences microcrystalline fraction in the Saddle-Field PECVD.

A19.7

Pit Formation in Amorphous Si Thin Films after High Temperature Thermal Annealing. Tyler Roschuk^{1,2}, Jacek Wojcik^{1,2}, Michael Flynn^{1,2}, Othman Zalloum^{1,2} and Peter Mascher^{1,2}; ¹Engineering Physics, McMaster University, Hamilton, Ontario, Canada; ²Centre for Electrophotonic Materials and Devices, McMaster University, Hamilton, Ontario, Canada.

Thin amorphous silicon (a-Si) films have been deposited using electron cyclotron resonance plasma enhanced chemical vapor deposition (ECR-PECVD). Post-deposition these films have been subjected to thermal annealing at temperatures up to 1200°C for times up to 120 minutes. Annealing at temperatures of 1100°C and higher has been found to cause the formation of a polycrystalline layer within the film through transmission electron microscopy (TEM) images. In addition, scanning electron microscopy (SEM) and atomic force microscopy (AFM) have revealed that the surface of these films become heavily pitted after high temperature annealing. These pits have been observed to show preferential orientation and structure. Further TEM imaging has been used to analyze the formation of this polycrystalline layer and its influence on the observed pit formation. The effects of substrate type and film thickness on pit formation has been analyzed by comparing samples deposited onto $\langle 100 \rangle$ and $\langle 111 \rangle$ oriented Si and oxidized Si substrates with film thicknesses up to 2500 Å. Changes in the film crystallinity have been examined through X-ray diffraction experiments and correlated with the results of TEM imaging. Additionally, the role of the substrate temperature during deposition and its influence on the observed pit formation in these films has been examined. The refractive indices and extinction

coefficients of these films have been determined through the use of spectroscopic ellipsometry and correlated with the processing parameters and structure of the films. Finally, we will discuss the significance of these pits in terms of current research related to Si-based photonics, including applications in optical coatings, waveguides, and Si-based luminescent materials. This work is being supported by Ontario Centres of Excellence (OCE) Inc. and the Ontario Photonics Consortium (OPC).

A19.8

Growth of "New Form" of Poly-Si Thin Films Synthesized by Ceramics Hot-Wire CVD. Abdul Rafik Middy¹, Jian-Jun Liang² and Kartik Ghosh³; ¹Physics, Syracuse University, Syracuse, New York; ²Physics, Syracuse University, Syracuse, New York; ³Physics, Astronomy and Materials Science, Southwest Missouri State University, Springfield, Missouri.

Polycrystalline silicon (poly-Si) thin films synthesized by hot-wire chemical vapor deposition show promise for application of these materials in solar cells and thin film transistors. The special features of hot-wire CVD poly-Si films: high growth rate, textured surface and columnar growth, low process temperature ($\sim 450^\circ\text{C}$), relatively high mobility ($\sim 20 \text{ cm}^2/\text{V}\cdot\text{s}$) [1], low barrier height and nearly ideal intrinsic ($E_a \approx 0.5 \text{ eV}$, carrier concentration $\sim 10^{11} \text{ cm}^{-3}$) character of these films. The room temperature resistivity of these poly-Si films can be varied almost by eight orders of magnitude by in-situ gas phase doping for p-type films. The solar cells performance using these materials in pin structure show high short-circuit current ($J_{sc} \sim 24 \text{ mA}/\text{cm}^2$) for absorber layers with defect density $\sim 10^{17} \text{ cm}^{-3}$ [2], whereas the state-of-the-art $\mu\text{c-Si}$ solar cells produces nearly same amount of current ($\sim 25 \text{ mA}/\text{cm}^2$) with ZnO/Al back reflector and these $\mu\text{c-Si}$ solar cells show light-induced degradation. Clearly, the potential of hot-wire CVD poly-Si thin films solar cells has not yet been achieved in reality. In this work, we report on growth of a new type of poly-Si thin films on glass substrate at low temperature ($\sim 250^\circ\text{C}$) prepared by ceramics hot-wire CVD. For the first time, we introduced "ceramics filament holder" to minimize metallic impurities and a new concept of "confining thermal radiation from the filament" by specially designed the filament holder to reduce substrate temperature by thermally energizing the reacting species. In this new hot-wire CVD equipment, we call it ceramics hot-wire CVD, we developed poly-Si thin films on glass substrate at low temperature ($\sim 250^\circ\text{C}$). We observed for the first time, "pentagonal" and "hexagonal" rings throughout the surface morphology revealed by atomic force microscopy. Consistent with this unusual geometrical pattern on the AFM surface morphology, we observed six transverse optical (TO) mode at 495-500 cm^{-1} , 507 cm^{-1} , 515 cm^{-1} , 517 cm^{-1} , 520 cm^{-1} and 522-523 cm^{-1} respectively, in addition to, TO peak around 370 cm^{-1} . Other than this several TO Raman modes and the presence of "pentagonal" and "hexagonal" rings in the AFM micrograph, we do not have any idea what is the internal structure of these films, a "new form" of poly-Si films? X-ray diffraction also indicates new type of structure of these films. We will discuss the structure and chemical composition of these poly-Si films, combining the observations from SEM, AFM topography, phase image, Raman, XRD and secondary ion mass spectroscopy (SIMS). The electronic properties of these poly-Si films also show surprise, consistent with structural properties. 1. A. R. Middy, J. Guillet, J. Perrin and J. E. Bouree, *Mat. Res. Soc. Symp. Proc. Vol. 420 (1996)* p. 289; 2. J. K. Rath, F. D. Tichelaar, H. Meiling and R. E. I. Schropp, *Mat. Res. Soc. Symp. Proc. Vol. 507 (1998)* p. 879.

A19.9

Nanocrystalline-Si Thin Film Deposited by Inductively Coupled Plasma Chemical Vapor Deposition (ICP-CVD) at 150°C. Sang-Myeon Han, Joong-Hyun Park, Hye-Jin Lee, Kwang-Sub Shin and Min-Koo Han; Seoul National University, Seoul, South Korea.

Nanocrystalline silicon (nc-Si) film thin film transistor (TFT) may be a promising device for various application including flat panel display due to rather simple process compared with poly-Si TFT and better performance compared with a-Si TFT. Conventional plasma enhanced chemical vapor deposition (PECVD) method has been widely reported to deposit nc-Si film. It is known that inductively coupled plasma (ICP) mode can generate high density plasma. ICP-CVD may also provide a certain advantages such as high deposition rate and improved crystallinity over PECVD. The purpose of our work is to report nc-Si film deposited by (ICP-CVD) suitable for low temperature TFTs which can be applied to flexible displays. The flexible displays may have certain merits compared with the present rigid displays. For flexible displays, it is inevitable to limit the process temperature to avoid deforming substrates like plastics. The Si films were deposited at ultra low temperature (below 200°C) and characterized. We deposited nc-Si film by ICP-CVD at 150°C. ICP power was 400W. The process gas was SiH₄ diluted with He as well as H₂. The flow rate of He, H₂ was varied from 20sccm to 60sccm and

that of SiH₄ was 3sccm. The crystalline volume fractions evaluated from the Raman spectrum of the nc-Si film were above 70%. X-ray diffraction (XRD) patterns of the nc-Si films were measured. The Si films deposited by ICP-CVD with He dilution had (311) orientation and the intensity of (311) peak increased as the He dilution ratio increased. In the case of H₂ dilution, (111) and (220) peaks as well as (311) peak were observed. The grain size of 40~50nm was observed by SEM and AFM in the film deposited in the condition of high dilution. Our experimental results show that nc-Si film deposited by ICP-CVD may be suitable for active layer of nc-Si TFTs.

A19.10

Abstract Withdrawn

A19.11

Effects of N₂O Fluence on the PECVD-Grown Si-rich SiO_x with Buried Si Nanocrystals. Chia-Yang Chen¹, Chun-Jung Lin¹, Gong-Ru Lin¹, Hao-Chung Kuo¹, Yu-Lun Chueh², Li-Jen Chou², Chih-Wei Chang³ and Eric Wei-Guang Diao³; ¹Department of Photonics & Institute of Electro-Optical Engineering, National Chiao Tung University, Hsinchu, Taiwan; ²Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan; ³Department of Applied Chemistry and Center for Interdisciplinary Molecular Science, National Chiao Tung University, Hsinchu, Taiwan.

The growth of silicon-rich substoichiometric silicon oxide (SiO_x) with buried Si nanocrystals (nc-Si) by using plasma enhanced chemical vapor deposition (PECVD) with optimized N₂O fluence is demonstrated. The SiO_x with highest excess Si density can be obtained by detuning the fluence ratio of SiH₄ to N₂O. Photoluminescence (PL) analysis reveals an unpredictable result for samples with varying SiH₄ fluence. By changing N₂O fluence from 105 sccm to 130 sccm, strong PL at 550-870 nm has been observed in the post-annealed SiO_x film with dense nanocrystallite Si (nc-Si) clusters. After annealing at 1100°C from 15 to 180 min, a 22-nm redshift in PL is detected. The maximum PL intensity is observed at 761 nm for the 30-min annealed SiO_x film growing at 120-sccm N₂O-fluence. The wavelengths and associated linewidths of PL spectra for samples annealing at different durations are ranging from 735 nm to 761 nm and from 133 nm to 177 nm, respectively. Alternatively, a larger N₂O fluence and a longer annealing time also cause the PL blueshift by 65 nm and redshift by 20 nm, respectively. The blueshift is attributed to shrinkage in the size of nc-Si under the participation of dissolved oxygen atoms from N₂O. The density of precipitated nc-Si reaches its maximum after 30-min annealing. Longer annealing time results in the reduction on both the PL intensity and the size of nc-Si, since the outer surface of nc-Si becomes oxidized by the surround SiO₂ matrix. Besides, different annealing time is required to precipitate nc-Si in the Si-rich SiO_x grown with different N₂O fluences. The bright-field cross-section viewing TEM photograph for the annealed SiO_x film is demonstrated to support the existence of nc-Si. The lattice distance between two (111)-oriented planes of 0.63 nm observed from a Si substrate is employed as a standard ruler to estimate plane-to-plane distance of nc-Si (about 0.19 nm). According to the X-ray diffraction (XRD) data, the oriented planes of nc-Si with diameter ranging from 4.4 to 5.0 nm are determined as (220). The TRPL analysis indicates that the luminescent lifetime lengthens from 20 μs to 52 μs as nc-Si size extends from 4.4 to 5.0 nm, which increases linearly with the size of nc-Si. As the annealing time lengthens from 30 to 120 min, the density of nc-Si is decreased from 8.3×10²²cm⁻³ to 1.2×10²²cm⁻³.

SESSION A20: Poster Session: Growth-a-Si:H and Alloys
Thursday Evening, March 31, 2005
8:00 PM
Salons 8-15 (Marriott)

A20.1

Effect of Ion Bombardment during Expanding Thermal Plasma Deposition on the a-Si:H Material Properties. Arno H. M. Smets¹, Agnes M. H. N. Petit², Vojto Nadazy², Erwin W. M. M. Kessels¹, Rene A. C. M. van Smaaij² and Richard M. C. M. van de Sanden¹; ¹Applied Physics, Eindhoven University of Technology, Eindhoven, Netherlands; ²DIMES-ECTM, Delft University of Technology, Delft, Netherlands.

In the recent years it has been demonstrated that the remote expanding thermal plasma (ETP) is a deposition tool, which has easily access to ultra-high hydrogenated deposition rates for amorphous silicon of up to 100 Å/s. However, preservation of the material quality of a-Si:H material deposited by the ETP technique at high deposition rates, requires higher substrate temperatures. Therefore the incorporation into a pin solar cell where temperatures are limited by the p-layer remains a challenge. Employing an additional ion bombardment by means of an external RF bias under

high growth rate conditions supplies additional energy to the growing film thereby improving the film properties without the necessity to increase the substrate temperature above 250 °C. In this work it is demonstrated that the external rf bias results in the creation of an additional growth flux, a reduction of the void incorporation, smoother surfaces, and an increase in the vacancy density. In general, in absence of external rf substrate bias, the microstructure at certain hydrogen content is fixed for pure ETP a-Si:H growth. However, employing rf substrate bias provides us access to a larger variety of microstructures, i.e. the microstructure of the material can be tuned at constant hydrogen content. The relation of these results to typical ion bombardment enhanced surface processes such as surface diffusion, surface smoothing, Si sputtering and Si displacement are discussed. It is shown that only a moderate rf power is required to improve the opto-electronic performance of the a-Si:H films and to considerably reduce the sub gap absorption related defects. Using this approach the solar-cell performance, utilizing ETP material at high deposition rate and low temperature, has improved.

A20.2

Thin Films of GeC Deposited Using a Unique Hollow Cathode Sputtering Technique. Rodney Joseph Soukup¹, Natale J. Ianno¹, Jason S. Schrader¹ and Vikram L. Dalal²; ¹Electrical Engineering, University of Nebraska, Lincoln, Nebraska; ²Electrical and Computer Engineering, Iowa State University, Ames, Iowa.

Experimental results on thin films of the new material Ge_xC_{1-x}, deposited by a unique dual plasma hollow cathode sputtering technique are presented here. The (Ge, C) system is extremely promising since the addition of C to Ge may reduce the lattice dimensions enough to allow a lattice match to silicon, while increasing the band gap close to that of c-Si. The most important contribution of this work is that it shows that by using non-equilibrium growth conditions using the hollow cathode technique, one can grow Group IV materials which cannot otherwise be grown using normal CVD or MBE processes. The sputtering is accomplished by igniting a plasma of the Ar and H₂ gases which are fed through nozzles, cylindrical tubes 30mm long with 8mm O.D. and 3mm I.D. Initially, the films were deposited onto both silicon and glass substrates. The initial films on the glass substrates had no or very little photo response and after a few depositions it was decided to deposit only onto silicon. The films deposited onto glass were amorphous in nature, but the films deposited onto silicon were quite crystalline. This crystallinity has been characterized with Raman spectroscopy and X-ray diffraction (XRD). A typical Raman spectrum indicated that the pure Ge films were quite crystalline. However, the normal Ge_xC_{1-x} films were not as perfectly crystalline. The indications are that the films are polycrystalline in nature and this has been verified by XRD. Typical samples have peaks at angles which indicate that the 111, 220, and 311 faces are dominant. Auger depth profiling studies of the GeC films have also been made. The incorporation of C into the films is relatively uniform and is on the order of 7 to 8%, higher than any other method at this growth rate, 1.5Å/s. Fourier Transform Infrared Spectroscopy (FTIR) yielded interesting results. The FTIR spectrum over the wave number range of interest was featureless except for a small absorption peak (1110 cm⁻¹) attributable to the SiO₂ at the interface between the Si substrate and the GeC film. This is a desirable result because it means that the hydrogen is not bonding to the film, even though a high density plasma consisting of argon and hydrogen is present in both nozzles, or in some cases, just the Ge nozzle. Prior films of a-SiGe:H had prominent peaks at 1880cm⁻¹ and this indicates a GeH bond. A probable cause of this lack of H bonding in these films is that the substrate temperature in this experiment is considerably higher during deposition than it was during the amorphous Ge deposition. One important factor in achieving useful GeC films for device applications is to get the C to bond interstitially in the Ge crystal. The most recent films have shown a large peak in the FTIR spectra at 530cm⁻¹ which indicates such an interstitial Ge-C bond.

A20.3

Improved Optical Loss Characteristics of PECVD SiON Films using Low Frequency Plasma. Sudipto Naskar^{1,2}, Christopher A. Bower¹, Brian R. Stoner^{1,2} and Jeffrey T. Glass²; ¹MCNC-RDI, RTP, North Carolina; ²Duke University, Durham, North Carolina.

With the continued growth of photonics, silicon oxynitride (SiOxNy) is becoming a popular material for optoelectronic applications owing to its large tunable refractive index. However, with the increase in refractive index, these films tend to show poor optical transmission characteristics since the material tends to become hydrogen rich. In this research effort we have investigated the influence of growth conditions on the loss characteristics of PECVD SiOxNy films. The films are grown at 350 C substrate temperature and 1 Torr pressure with silane (SiH4) and nitrous oxide (N2O) precursor gases. The precursor flow rate and power input to the system are varied as the two primary parameters. It is observed that films grown at 100 kHz

plasma frequency proved to be more transmissive than films grown at 13.56 MHz plasma frequency. Elastic recoil detection analysis results showed the hydrogen content is less in the low frequency films than the high frequency films which is believed to be the reason for the low loss behavior. In this presentation the influence of growth conditions on loss behavior will be discussed with special reference to the effect of hydrogen in the oxynitride film.

A20.4

The Influence of Growth Temperature on the Disorder Within Silicon Films Grown by Molecular Beam Epitaxy. L. Tay², D. J. Lockwood², J.-M. Baribeau², M. Noel³, J. C. Zwinkels³, F. Orapunt¹ and S. K. O'Leary¹; ¹Faculty of Engineering, University of Regina, Regina, Saskatchewan, Canada; ²Institute for Microstructural Sciences, National Research Council, Ottawa, Ontario, Canada; ³Institute for National Measurement Standards, National Research Council, Ottawa, Ontario, Canada.

We study the role that the growth temperature plays in determining the amount of disorder present within silicon films deposited through ultra-high-vacuum molecular beam epitaxy. For the purposes of this study, we have deposited eleven silicon films on quartz substrates for a variety of different growth temperatures, ranging from 98°C to 572°C. Through measurements of the Raman spectrum and the optical absorption spectrum corresponding to each film, we have quantitatively determined how the growth temperature influences the disorder within the deposited silicon films. We find that the disorder decreases as the growth temperature increases, and that there is a particularly dramatic decrease in the disorder as the growth temperature increases beyond 450°C. We suggest that this dramatic increase in order corresponds to a transition in the structural nature of the deposited silicon films, from disordered amorphous silicon to a more ordered form.

A20.5

Low Temperature Growth of Amorphous Silicon Films on Plastic Substrates by Catalytic CVD Technique. Wan-Shick Hong¹, Sunghyun Lee¹, Kyung Eun Lee¹, Chul Lae Cho¹, Seungjin Han¹, Jongman Kiim^{1,2}, Jangyeon Kwon² and Youngsoo Park²; ¹Electronics Engineering, Sejong University, Seoul, South Korea; ²Samsung Advanced Institute of Technology, Yongin-city, Kyunggi-do, South Korea.

Low temperature polycrystalline silicon (LTPS) films are a key component of thin film transistors (TFTs) for driving active matrix organic light emitting displays (AM-OLEDs). Fabricating good quality LTPS films on plastic substrates has been a big challenge, since the overall process temperature is limited to the glass transition temperature of the plastic substrate. Also, a very low content of atomic hydrogen is desired to prevent damage during crystallization. Therefore, a deposition technique that has a high deposition rate, a low hydrogen content and a low process temperature is required for preparing amorphous silicon precursor films on plastic substrates. In this study, amorphous silicon films for application as a precursor for laser-annealed polycrystalline films were deposited by a Catalytic (Hot Wire) CVD technique. The films were successfully deposited on polyethersulfone (PES) substrates held at room temperature. By adopting a custom-designed cooling system, the substrate temperature was suppressed to < 120°C during the process. The chamber pressure and the gas flow rate were chosen as main process parameters, and the deposition rate and the atomic concentration of hydrogen in the films were analyzed. The gas flow rate showed different effects on the deposition rate in the high pressure regime and in the low pressure regime. The hydrogen content varied in rather a complicated way with pressure and flow rate. Also, there exists a certain region of pressure and flow rate, where both the deposition rate and the hydrogen content exhibit abrupt changes. A very high deposition rate (~100 Å/sec) was achieved, and the hydrogen content could be controlled effectively in the range of 0.1 ~ 5 at%. These films are suitable precursor material for the LTPS layer on plastic substrates.

A20.6

Chemical Annealing of Amorphous Silicon and Silicon-Germanium Films and Devices. Vikram Dalal and Nanlin Wang; Elec. and Comp. Engr., Iowa State University, Ames, Iowa.

Chemical annealing, which involves the layer-by-layer growth of a material in a thin layer, followed by annealing in a reactive or non-reactive beam of ions and radicals, has been previously used to change the hydrogen content and electronic and optical properties of a-Si:H. In this paper, we report on a systematic study of chemical annealing in both a-Si:H and a-(Si,Ge):H films and devices. We use both reactive (hydrogen) and non-reactive (helium) ions and radicals for chemical annealing. The films and devices were grown using a remote, low pressure ECR discharge using mixtures of silane, germane and either hydrogen or helium. The thickness of each layer was in the range of 2-3 nm. The total film thicknesses were in the range of 1

micrometer, and of i layers in p-i-n devices, between 0.25 and 0.3 micrometer. The films were characterized using subgap absorption, FTIR spectroscopy, optical spectroscopy, activation energies and electron mobility-lifetime products. p-i-n devices were fabricated on stainless steel substrates, and were characterized using quantum efficiency spectroscopy and capacitance spectroscopy, in addition to the device I-V curves. It was found that hydrogen annealing always increased the bandgap, but did not improve the stability of either films or devices. In contrast, annealing with He decreased the H content and bandgap, and also seemed to improve the stability.

A20.7

Deposition Simulation of Si and SiGe Using a Bond Order Potential. Haydn Wadley and Brian Andrew Gillespie; University of Virginia, Charlottesville, Virginia.

Recently proposed Si-Ge heterostructure devices, such as the spin resonance transistor, require highly precise deposition techniques to realize the devices' complex structure. Molecular dynamics modeling techniques have proven successful in the past at simulating the vapor phase fabrication of metallic magnetoresistive systems (eg. Ni/CoFe/Cu multilayers). This thesis explores extensions of the methodology to semiconductor systems based on Si and Ge. Many interatomic potentials for modeling these semiconductor systems have been proposed. A Bond Order Potential (BOP) developed by David Pettifor et al. at Oxford University, as well as the Stillinger-Weber (SW) and Tersoff potentials, is assessed for modeling the vapor phase growth of Si and SiGe thin films. It is shown that both the SW and BOP potentials predict similar radial distribution functions for amorphous deposition to those seen experimentally. Both the SW and BOP potential also predict crystalline epitaxy under conditions that match experiments that result in crystalline growth.

A20.8

Low-Temperature Deposition of Silicon Oxide Thin Films using Alternating Exposures of SiH₂Cl₂ and O₃/O₂. Chan-Hee Han¹, Min-Ho Chun¹, Sa-Kyun Rha¹, Un-Jung Kim², Sang-Wook Lee², Won-Jun Lee² and Youn-Seoung Lee³; ¹Department of Materials Engineering, Hanbat National University, Daejeon, South Korea; ²Department of Advanced Materials Engineering, Sejong University, Seoul, South Korea; ³Division of Information Communication and Computer Engineering, Hanbat National University, Daejeon, South Korea.

Silicon dioxide (SiO₂) has been one of the most widely used dielectric materials in the Si integrated circuits (ICs). Generally, SiO₂ films have been deposited by low-pressure chemical vapor deposition (LPCVD) method at more than 700 °C in the IC manufacturing processes. However, the high processing temperature of LPCVD process is expected to be an issue in nanoscale ICs in the near future. Atomic layer deposition (ALD) is a promising technique for depositing ultrathin SiO₂ films at lower temperatures in the processing of next-generation ICs. In this study, SiO₂ thin films were deposited on p-type Si (100) substrates by alternating exposures of SiH₂Cl₂ and an O₃(8.6 at%)/O₂ mixture. O₃ was generated by corona discharge inside the delivery line of O₂, and the concentration of O₃ was measured in the reactor. N₂ was used as the purging gas between the pulses of precursors. The deposition of SiO₂ films was investigated as a function of reactant exposures at the deposition temperature ranging from 250 to 450 °C. The growth rate was saturated at approximately 0.25 nm/cycle with the reactant exposures over 5.0 x 10⁹ L [1 L = 10⁻⁶ torr · sec] at 350 °C. The saturation growth rate increased with deposition temperature up to 350 °C, however, decreased with increasing deposition temperature from 350 to 450 °C. The physical and electrical characteristics of ALD SiO₂ films were comparatively studied with the SiO₂ films prepared by thermal oxidation or LPCVD method. The ALD films exhibited comparable composition, wet etching rate and leakage current to the LPCVD films, lowering processing temperature to 350 °C.

SESSION A21: Poster Session: Solar Cells
Thursday Evening, March 31, 2005
8:00 PM
Salons 8-15 (Marriott)

A21.1

Development and Characterization of Transparent Conductive Oxide Materials with Low Indices of Refraction for Application in Amorphous Silicon-Based Solar Cell Technology. Scott J. Jones, Tongyu Liu, David Tsu, Joachim Doehler, Jeff Steele, Rey Capangpangan and Masat Izu; Energy Conversion Devices, Inc., Troy, Michigan.

New types of transparent conductive oxides with low indices of refraction have been developed for use in optical stacks for the

amorphous silicon (a-Si) solar cell and other thin film applications. The alloys are ZnO based with Si and MgF added to reduce the index of the materials through the creation of SiO₂ or MgF₂, with $n=1.3-1.4$, or the addition of voids in the materials. Alloys with 12-14% Si or Mg have indices of refraction at $\lambda=800\text{nm}$ between 1.6 and 1.7. These materials are presently being used in optical stacks to enhance light scattering by Al/multi-layer/ZnO back reflectors in a-Si based solar cells to increase light absorption in the semiconductor layers and increase open circuit currents and boost device efficiencies. In contrast to Ag/ZnO back reflectors which have long term stability issues due to electromigration of Ag, these Al based back reflectors should be stable and usable in manufactured PV products. In this manuscript, structural properties for the materials will be reported as well as the performance of solar cell devices made using these new types of materials.

A21.2

Abstract Withdrawn

A21.3

Effect of P-layer Nanostructure on the Open Circuit Voltage of Amorphous Si:H Solar Cells. Wenhui Du, Xianbo Liao, Xiesen Yang and Xunming Deng; Department of Physics & Astronomy, University of Toledo, Toledo, Ohio.

Amorphous hydrogenated Silicon solar cell (a-Si:H) have high conversion efficiencies when the intrinsic layer is made just prior to the amorphous to amorphous/nanocrystalline (a+nc) mixed phase transition by radio frequency plasma enhanced chemical vapor deposition (RF-PECVD) process. The phenomenon of a-Si:H transition to nc-Si is well known at high H₂ dilution. It is also dependent on substrate temperature, substrate as well as the film thickness. This paper reports that p layers made after the amorphous to a+nc transition shows the best IV property of solar cells. A set of Boron doped a-Si:H p-layers were made with different nc-Si volume fractions. Amorphous silicon with low nc-Si volume fraction p-layers were deposited at low substrate temperature and high power. High nc-Si volume fraction materials were deposited at high substrate temperatures and low power. The nc-Si volume fractions of these layers were determined by Raman spectroscopy. Standard a-Si:H solar cells were made using these p-layers. We found the open circuit voltage increased from 0.97V when p-layer was amorphous but close to the phase transition, to 1.04V when the p-layer had a small nc-Si volume fraction. When the nc-Si volume fraction was increased further the voltage decreased to 0.39V. The explanation is that for small nc-Si volume fraction material nc-Si particle size is about 5nm and quantum size effect produces a bandgap larger than amorphous Si bandgap (1.8eV). The bandgap of p-layer limits its Fermi level position and built-in electric field in the i-layer, therefore, a-Si:H solar cells with small nc-Si volume fraction has a large open circuit voltage. When the nc-Si volume fraction is increased, nc-Si particle size is increased and quantum size effect disappears. The bandgap of p-layer decreases and reduces the open circuit voltage.

A21.4

Material And Device Physics Of Nanocrystalline Si Solar cells. Vikram Dalal, Elec. and Comp. Engr., Iowa State University, Ames, Iowa.

Nanocrystalline Si:H is an increasingly important material for photovoltaic devices. The properties of the devices depend critically upon the physics of the basic material, as well as on the interfaces between the base layer and the front and back junction layers. In this paper, we report on the properties of nanocrystalline Si materials and devices made using different, well controlled techniques. Among these are VHF plasma deposition with varying amounts of hydrogen/silane ratios and varying growth temperatures, use of mixtures of helium and hydrogen instead of hydrogen alone for achieving crystallinity, ECR deposition, also with varying helium/hydrogen ratios, and chemical annealing with helium which can also lead to the formation of a crystalline phase. This last result is unexpected, and it points up the role of controlled ion bombardment in converting an amorphous phase into a crystalline one. We measure systematically the structure using both Raman and x-ray diffraction, electronic properties such as mobility, defect density, carrier lifetimes and diffusion lengths, and device properties for the materials made using the varying deposition conditions described above. From a careful examination of x-ray diffraction, we show that significant stresses exist in these materials, and that the degree of stress varies as a function of grain size and growth temperature. Small grain sizes lead to higher stress values. Both compressive and tensile stress is present in the same material. The shift in the peak position of the Raman spectrum is directly correlated with the stress in the film. The electronic measurements show that the defect density is correlated with the presence of amorphous tissue; the amorphous intergranular tissue seems to passivate the grain boundaries better than H alone and leads to lower defect densities. The presence of helium in the discharge leads to

higher open circuit voltages. The open circuit voltages can also be improved by using appropriate interfacial grading by varying the ratio of helium to hydrogen. We also study whether there is a definite change in absorption coefficients of materials as a function of grain size, and the degree of amorphous to crystalline phases. The measurements are made within a device structure by using quantum efficiency under appropriate conditions. Special device structures are constructed to make sure that QE corresponds to only a single pass of light, thereby avoiding light-trapping effects on the measurement of absorption coefficient.

A21.5

Metal Induced Growth of Poly-Si Solar Cells and Silicide Nanowires by use of Multiple Catalyst Layers. Joondong Kim, Chunhai Ji and Wayne A. Anderson; Electrical Engineering, University at Buffalo, Buffalo, New York.

Polycrystalline Si solar cells have been fabricated by the Metal Induced Growth (MIG) method. Several types of metal (Ni, Co, and mixtures of Co and Ni) were deposited to provide a quality poly-Si solar cell as well as a spontaneous back ohmic contact on the bottom of the grown poly-Si film. A catalyst metal first was thermally deposited on tungsten or a SiO₂ coated Si wafer. Using a D.C. magnetron, a doped Si target was sputtered onto the metal seed layer at a substrate temperature of 550 ~ 650 °C leading to a 2~10 μm poly-Si film by solid phase reaction. The sole use of Ni as a catalyst caused a higher leakage current. The Co-induced poly-Si provided a better performance in open circuit voltage (V_{oc}) while reducing the short circuit current density (J_{sc}). Multiple layers of Co and Ni (Co/Ni/Co or Co/Ni) as catalysts gave better results rather than use of a single metal layer. V_{oc} and J_{sc} improved from 141 mV and 2.71 mA/cm² to 241 mV and 4.78 mA/cm², respectively. The use of a Co coating on the Ni reduced the Ni diffusion into the grown poly-Si resulting in less leakage current. Two poly-Si layers grown by repeating the single step process significantly improved the performance. The surface morphological changes and cross-section have been observed by Scanning Electron Microscopy (SEM). Silicide nanowires (NWs) were also fabricated by the MIG method similar to the MIG-poly Si. X-ray diffraction (XRD) pattern and Auger depth profile have been performed to analyze mechanisms to provide the poly-Si film and single crystalline NWs. Optical reflectance results showed MIG-poly Si to give much lower reflectance than a Si wafer and higher than a MIG-NW grown Si wafer. Optical reflectance at 400 nm was 53.1 % for the bare Si wafer, 29.3 % for the MIG poly Si and 14.08 % for the NW-topped Si wafer. This implies improving the MIG-solar cell performance by topping the Si with a MIG-NW layer.

A21.6

Polyaniline/Amorphous Silicon Heterostructure Solar Cells. Weining Wang and Eric A. Schiff; Physics, Syracuse University, Syracuse, New York.

Hole-transporting, doped polymers are an intriguing alternative to conventional inorganic materials for the p-type layer in amorphous silicon-based *pin* solar cells. In particular, polymers can have larger bandgaps than the inorganic materials usually used as p-layers, such as (boron-doped) microcrystalline silicon and amorphous silicon-carbide. Simple models of devices with wider bandgap p-layers suggests the possibility of improved open-circuit voltages V_{OC} or better conversion of blue light with the use of a polymer p-layer. In the present experiments we have cast doped polyaniline from solution onto the top of an amorphous silicon based n/i structure. The structure was immediately annealed at 100 C. No buffer layer was used. After annealing, a small gold electrode was evaporated onto the polyaniline to serve as a top contact. Current-voltage characteristics of the device under illumination were similar to those in devices with conventional p-layers, indicating both that the polymer layer (about 300 nm thick) was transparent and that series resistance was negligible. The largest open-circuit voltage V_{OC} we have obtained with these devices is 0.78 V, which is at least 0.1 V smaller than expected with conventional inorganic p-layers. V_{OC} also declined more rapidly with intensity than for conventional p-layers. One possible mechanism for this suppression of V_{OC} is the growth of an oxide on the silicon following casting of the polymer layer from solution (and subsequent annealing). Earlier work by Middya [1] using a polymer (PEDOT:PSS) cast onto a-Si:H n/i structures from an aqueous solution achieved open-circuit voltages as large as 0.73 V; these experiments suggested the present experiments with polyaniline, for which the solvent was non-aqueous. We believe that the present work indicates that casting of the polymer from solution is not yielding an acceptable interface, although we cannot presently exclude poor band alignment as an alternative mechanism for the suppression of V_{OC} . This research was supported by the Thin Film Photovoltaics Partnership of the National Renewable Energy Laboratory. 1. National Renewable Energy Laboratory Report SR-520-33164 (December, 2002; <http://www.nrel.gov/docs/fy03osti/33164.pdf>).

A21.7

Ultra-Shallow Junction Formed by Non-Melting Process of Double-Pulsed DPSS Green Laser Annealing. Toshio Kudo, Susumu Sakuragi and Kazunori Yamazaki; R & D Center, Sumitomo Heavy Industries, Ltd., Yokosuka, Kanagawa, Japan.

It has been accepted that general solid-phase (SP) annealing in ultra-shallow junction (USJ) formation cannot activate dopants on time scales $< \mu\text{s}$. In order to investigate the possibility of activation on such short time scales using the diode-pumped solid-state (DPSS) laser annealing system we had developed, we adopted double-pulsed laser irradiation controlling a delay time between two of short green-laser pulses (pulse duration: $\sim 100\text{ns}$), and challenged forming the USJ below 10nm depth in spite of the deep penetration depth (crystal Si: $\sim 1000\text{nm}$) of green lasers. As-implanted samples were prepared as follows: 1) The Ge pre-amorphization implant was performed at an energy of 3keV to a dose of 3×10^{14} ions/cm², and the amorphous layer formed is limited to a depth of 8.3nm from the measurement of ellipsometry. 2) After the pre-amorphization, the B implant was performed at 0.2keV to 5×10^{14} and 1×10^{15} ions/cm². From the result of SIMS analysis at 1×10^{18} at/cm³, the B dopants (5×10^{14} ions/cm²) extend to the depth of 7.9nm into the Si wafer and stay in the amorphous layer (depth: 8.3nm) according to the process design. Post-implantation laser annealing, which the double pulses were irradiated at 1kHz, was performed overlapping a uniform 0.1mmx17mm line beam at an overlap ratio of 90% with scanning a sample stage at a constant velocity. To search a process window of SP activation in the wide range of pulse energy density, a delay time between double pulses as a parameter was changed from 0nsec to 900nsec at intervals of 150nsec. Distinction between solid-phase and liquid-phase activation was judged based on the threshold that surface roughness measured by AFM abruptly increases with the increase of pulse energy density. The threshold point for the B dose of 5×10^{14} ions/cm² is put between 780mJ/cm²x2 and 790mJ/cm²x2 at a delay time of 300nsec. The junction depths are about 9nm in the range less than 780 mJ/cm²x2 and the sheet resistance shows the minimum value of 1.0 k Ω /sq in the same range of pulse energy density. Increasing the B doses from 5×10^{14} to 1×10^{15} ions/cm², the sheet resistance was reduced to 0.65 k Ω /sq at the 300nsec delay time. The increase of the delay time is effective in making the SP process window wider in pulse energy density versus sheet resistance. To overcome the issues of the short annealing time $< \mu\text{s}$ and the deep penetration depth $\sim 1000\text{nm}$, we positively made the most use of double-pulsed laser irradiation of the short pulse $\sim 100\text{ns}$ and the big difference of optical absorption (1:20) between crystal and amorphous Si at a wavelength of green lasers. As a result, the target beyond the 65nm CMOS node, i.e., junction depth below 10nm and sheet resistance below 1k Ω /sq has been accomplished by the non-melting laser annealing.

A21.8

Temperature-Dependent Measurements on a-Si:H Solar Cells. Jianjun Liang¹, Eric A. Schiff¹, Subhendu Guha², Baojie Yan² and Jeffrey Yang²; ¹Physics, Syracuse University, Syracuse, New York; ²United Solar Ovonic Corp., Troy, Michigan.

A conclusive understanding of the as-deposited characteristics of a-Si:H solar cells would be an important advance, albeit one that does not directly address the origins of their degradation. A number of models have been proposed that are capable of accounting satisfactorily for these characteristics at room-temperature. Most of these models would likely be excluded by temperature-dependent measurements, but a satisfactory set of such measurements has not, to the best of our knowledge, been done. To provide measurements that will more rigorously test these models, we prepared a series of a-Si:H single-junction pin solar cells with varying intrinsic layer thickness (200 nm – 800 nm), and did standard room-temperature characterization of the cells under a solar illuminator. To simplify comparison with models, we measured the temperature-dependent characteristics of these cells under intense illumination from a 685 nm laser; illumination at this wavelength is nearly uniformly absorbed throughout the intrinsic layers. The range of temperatures was 230 K – 350 K. We also studied the temperature-dependent characteristics of several light-soaking states. We compared these measurements with the predictions of the "simplest reasonable" model for a-Si:H cells. The model incorporates only bandtail-related trapping and recombination processes for the intrinsic layer, and neglects deep levels altogether; the model parameters were published earlier [1]. Despite its simplicity, this model accounts well for the temperature-dependence and thickness-dependence of the open-circuit voltage and of the power density. These successes suggest that the as-deposited characteristics of the cells under solar illumination do derive primarily from the bandtail properties. However, the measured short-circuit current density declined markedly less with temperature than predicted. We speculate that this discrepancy could be evidence for variation of the bandtail trapping coefficient with trap depth, as

has been proposed previously by Movaghar and Yelon. This research was supported by the Thin Film Photovoltaics Partnership of the National Renewable Energy Laboratory. [1] K. Zhu, *et al.*, in *Amorphous and Nanocrystalline Silicon-Based Films-2003* (MRS Symposium Proc. Vol. 762), 297.

A21.9

Matching of the Amorphous Si Top Solar Cell and Low Temperature Crystallized Si Bottom Solar Cells.

Andrzej Kolodziej and Pawel Krewniak; Department of Electronics, AGH University of Science and Technology, Krakow, Poland.

Proper choice of layer thicknesses and current matching between the series connected top and bottom cell is required for tandem solar cells to obtain optimum energy conversion efficiency. The current matching means that both cells are operating at their maximum power point (MPP) and simultaneously the output current of each cell is the same. The current of the top and bottom cell depends on the thickness of each cell and also on the absorption in successive layers of the tandem structure. In this case we analyze a double terminal (DT) structure instead of the classical tandem cell. Thickness variations of the absorber i layers, degradation effects and spectral changes of the illumination under outdoor conditions lead to a shift of the top and bottom cell operating points. While the $\mu\text{c-Si:H}$ bottom cells are stable or show only little degradation, still considerable degradation is introduced by the a-Si:H top cell. In our case the top cell is a stable filter for changing bottom cells. The deposition of $\mu\text{c-Si:H}$ structure was performed at high pressure and high plasma power of RF PECVD process. However, poly-Si films deposited by the method on ordinary glass or other substrates typically have an average grain size of 10-20 nm. Such a grain structure presents a problem for device performance since it introduces an excessive number of grain boundaries leading to poor cell properties. Therefore poly-Si film was prepared by metal induced low temperature crystallization. The structures of the single amorphous cells, single microcrystalline and polycrystalline cells were studied by Cross-Sectional TEM and X-Ray Analyzing. There were carried out the analyses of FF, V_{oc} and I_{sc} of the structures for various conditions. Finally, we present the parameters for optimal tandem devices.

A21.10

Influence of Hydrogen Plasma on Electrical and Optical Properties of Transparent Conductive Oxides. L. Raniero, I. Ferreira, A. Pimentel, A. Goncalves, S. Zhang, E. Fortunato and R. Martins; Department of Materials Science / CENIMAT, New University of Lisbon and CEMOP-UNINOVA, Caparica, Portugal.

To perform this work the optical and electrical properties of ZnO:Ga, ITO and ZnO:In deposited on glass were studied under different hydrogen plasma time exposition. The electrical and optical properties were respectively studied through conductivity, Hall effect, spectroscopic impedance and UV-VIS-NIR spectroscopy measurements that allow the determine the role of hydrogen plasma on parameters like conductivity, capacitance, Hall mobility, free carrier concentration, sheet resistance, transmittance and optical gap. Apart from that, the performances of such TCO on solar cells based on nanocrystalline silicon will be also studied and presented. The data available show that the electrical properties of solar cells using as back contact ZnO:Ga present the best properties, allowing high current density collection with solar cells with efficiencies exceeding 13%.

SESSION A22: Poster Session: Thin Film Transistors
Thursday Evening, March 31, 2005
8:00 PM
Salons 8-15 (Marriott)

A22.1

Gate Oxide Integrity for Polysilicon Thin-film Transistors: A Comparative Study for ELC, MILC, and SPC Crystallized Active Polysilicon Layer. Byoung D. Choi, Myeong So, Daechul Choi, Inbok Song and Hokyoon Chung; Device Engineering, Samsung, Yongin, South Korea.

Of the several LTPS technologies developed, the ELC technology is most suitable for poly Si TFT manufacturing due to its ability to crystallize silicon films without raising the substrate temperature significantly. However the ELC poly Si have several limitations such as high cost, manufacturing difficulties, and observation of laser scan lines on the finished display products. Because of these limitations, many companies are turning to alternative non-laser crystallization techniques such as MIC, MILC, and SPC. In addition, recently, there is a need for reduction in device feature length and related dimensions for applications such as system-on-panels. For this reason, low temperature polysilicon TFTs have been extensively studied for fabrication of the drivers, digital-to-analog converters (DACs), and

timing controllers.1) Their reliability thus has a direct impact on the product lifetime. One of the most important reliability parameters is gate oxide integrity (GOI), which is the ability of a metal oxide semiconductor (MOS) device to remain operational for many years with the gate voltage applied.2, 3) The breakdown electric field of thermally grown silicon dioxide insulator used in integrated circuits is typically around 10-15MV/cm while that of plasma-enhanced chemical vapor deposited (PECVD) SiO₂ insulator used in low temperature polysilicon TFTs is around 4-10MV/cm.3) The breakdown field of the deposited insulator depends on polysilicon surface roughness, crystal originated pits (COPs), and metallic precipitates as these are responsible for locally high electric fields.2) The low breakdown electric field of insulator deposited using PECVD is also attributed to porous oxides contaminated with metallic or ionic impurities and which also lead to enhanced leakage currents. Here we present an experimental study of the gate oxide breakdown and evaluate its integrity on the three types of poly Si active layers; Excimer laser crystallized (ELC) poly Si, MILC poly Si and SPC poly Si. In this paper, we present the results of PECVD gate oxide (SiO₂) integrity on ELC (excimer laser crystallized), MILC (metal induced lateral crystallized) and SPC (solid phase crystallized) polysilicon films. We observed that gate oxide strength of poly Si TFT strongly depended on the crystallization method for the active silicon layer. In the case of ELC films, asperities on the silicon surface reduce the SiO₂ breakdown field significantly. The metallic contaminants in MILC films are responsible for a deleterious impact on gate oxide integrity. Among the three cases, the SiO₂ breakdown field was the highest for the SPC silicon films. The breakdown fields at the 50% failure points in Weibull plots for the ELC, MILC and SPC cases were 5.1MV/cm, 6.2MV/cm, 8.1MV/cm respectively. We conclude that the roughness and metallic contamination of the poly Si films are the main factors that cause enhanced breakdown of SiO₂ films.

A22.2

Low Temperature Metal-Free Fabrication of Polycrystalline Si and Ge TFT's by PECVD Hydrogenation. Pouya Hashemi¹, Jaber Derakhshandeh¹, Bahman Hekmatshoar¹, Shamseddin Mohajezadeh¹, Yaser Abdi¹ and M. D. Robertson²; ¹ECE Department, Thin Film Lab, University of Tehran, Tehran, Iran; ²Department of Physics, Acadia University, Wolfville, Nova Scotia, Canada.

We report the fabrication of polycrystalline Si and Ge thin film transistors (TFT's) on glass substrate at reduced temperatures. The multi-step PECVD hydrogenation-assisted crystallization method is used to create polycrystalline structures. This method allows crystallization of amorphous Si and Ge films without any metal seed contamination and at a considerably reduced temperature. Using e-beam evaporation, a layer of 1000Å Si (Ge) is deposited on the glass substrate at a temperature of 200°C and a base pressure of 2×10^{-6} torr. The samples are then carried to a conventional RF-PECVD system to perform the multi step metal-seed-free crystallization. Samples are initially treated in RF plasma for 30 minutes in hydrogen ambient. The optimum RF plasma power is 300 W for Si and 150 W for Ge samples. The flow of the hydrogen gas is 50 sccm in both cases. Each step is followed by an annealing treatment of 30 minutes. In total, five successive steps are applied to complete the crystallization process. The temperature of the process is 300 °C for Si and 200 °C for Ge samples and the overall annealing time varies between 3 and 5 hours. The crystallization of the samples is verified by SEM analysis. Both Si and Ge samples have an average grain size of 0.2 μm. We have exploited this crystallization technique to fabricate Si and Ge TFT's. The Ge-based TFT's operate in a depletion mode whereas the Si-based devices work in an inversion mode and their fabrication process is similar. Fabrication process starts with deposition of a 100Å Cr layer on the glass substrate using e-beam evaporation. After patterning the gate metal, a 300Å layer of SiO₂ is deposited followed by a multilayer of 600Å Si/100Å Sb/100Å Ge to form Si TFT's. The active regions and the source and the drain contacts are patterned using standard lithography. The amorphous TFT's are then loaded onto the RF-PECVD system to perform the dopant activation as well as hydrogenation-assisted crystallization processes. The annealing process is performed in the PECVD system at a pressure of 10 mtorr and at a temperature of 300°C for Si-based devices. In the case of Ge-based TFT's no doping incorporation is needed since such devices operate in a depletion mode. The process is followed by a five step plasma hydrogenation-annealing treatment. The current-voltage measurements of the TFT's confirm the transistor behavior with an Ion/Ioff ratio of 4×10^4 and 10^4 for Si and Ge TFT's, respectively. These measurements yield a hole mobility of 80 cm²/V.sec for Ge transistors. The electron mobility for silicon-based devices is expected to be less than 10 cm²/V.sec for Si TFT's. In summary, this technique offers a low temperature, metal-free crystallization method which is quite compatible with standard amorphous silicon fabrication process. Realization of higher performance silicon-based transistors is underway.

A22.3

Abstract Withdrawn

A22.4

Active Pixel TFT Arrays for Digital Fluoroscopy in a-Si:H Technology. Jackson Lai¹, Nader Safavian¹, Arokia Nathan¹ and John A. Rowlands²; ¹Electrical and Computer Engineering Department, University of Waterloo, Waterloo, Ontario, Canada; ²Imaging Research Program, Sunnybrook Health Science Centre, Toronto, Ontario, Canada.

Hydrogenated amorphous silicon (a-Si:H) technology has been extended to digital X-ray diagnostic imaging because of the inherent desired material and technological attributes such as low temperature deposition and high uniformity over large area. Here, major development challenges evolve around dynamic imaging modalities such as fluoroscopy, which demands both high speed readout and signal amplifying capabilities. This paper will report on initial results of a variety of TFT active pixel sensor (APS) structures in a-Si:H technology. The APS circuits each feature unique capabilities such as enhancements in signal gain, TFT V_T shift immunity, and real-time high speed readout. Enhancement in signal gain is achieved through sub-threshold operation of a global shutter TFT that provides a two-fold enhancement in X-ray signal gain compared to a previously reported circuit for real-time imaging [1]. Immunity to TFT V_T shift enables higher device reliability and is accomplished through a two-step reset operation of a 5-TFT APS circuit design. The readout rate of all APS arrays here enables frame-rates of at least 30 frames-per-second (fps), thus allowing real-time X-ray image reproduction. The results of this work demonstrate advancements to present state-of-the-art digital fluoroscopic detectors, to pave the way for better image resolution, and higher safety standards in diagnostic X-ray imaging. [1] K.S. Karim, A. Nathan, IEEE Electron Device Letters, vol. 22, no. 10, pp. 469-471, 2001.

A22.5

The Hysteresis Analysis of Hydrogenated Amorphous Silicon Thin Film Transistors for an Active Matrix Organic Light Emitting Diode. Jae-Hoon Lee, Kwang-Sub Shin, Chi-Heon Kang and Min-Koo Han; Electrical Engineering and Computer Science, Seoul National University, Seoul, South Korea.

Hydrogenated amorphous silicon thin film transistors (a-Si:H TFTs) are widely considered as pixel elements for AMOLED. The stability of a-Si:H TFT in the electrical characteristics is critical. As an a-Si:H TFT exhibits the hysteresis phenomenon due to difference of an interface occupancy, which means the OLED current from high gray to low gray differs that from low gray to high gray in the current driven AMOLED display, the analysis of hysteresis is required to solve the troublesome phenomenon. The purpose of our work is to report a simple experimental method to validate the cause of hysteresis. We have fabricated the a-Si:H TFT of the inverted staggered structure employing the standard process, with W=200μm and L=6μm. Hysteresis in the transfer characteristics (measured at V_{DS}=10V) was observed between forward (V_{GS}=-20V to 20V, gate voltage sweep step=0.2V) and reverse gate voltage sweeps (V_{GS}=20V to -20V). In order to investigate the cause of this phenomenon, we have measured the transfer characteristics for forward-voltage sweeps with different starting gate voltages. The characteristics, measured using HP4156B, were obtained by sweeping the gate voltage in steps of 0.2V. For less positive gate voltages, the transfer characteristics exhibit a parallel shift toward negative direction. The shift in the transfer characteristics depends on the starting gate voltage. Shift in the transfer characteristics was observed for reverse-voltage sweeps with different gate voltages. As the starting gate voltage becomes less positive, the parallel shift toward negative direction in the transfer characteristics was observed. The hysteresis and shift in transfer curves are attributed to differences in an initial Fermi-level at the starting gate voltage. It varies an interface trap occupancy resulting in changes of effective insulator charges. Under channel pinch-off conditions, charge balance equation can be written as (Q_G+Q_I+Q_D)=0, where Q_G is gate charge, Q_I is an insulator charge and Q_D is depletion charge. For less positive starting gate voltage, due to the negative shift of transfer curve, an extra ΔQ_G<0 is required for the same drain current. Under pinch-off conditions, since Q_D is constant, an extra gate charge is the result of an increase in effective insulator charges ΔQ_I>0. For less positive starting gate voltage in the reverse voltage sweeps, since the Fermi-level is further away from the conduction band, fewer acceptor like traps are filled resulting in a ΔQ_I>0. Similarly, since more positively charged donor like traps near the valence band are filled by less positive starting gate voltages, forward voltage sweeps exhibit the negative shift in the transfer curve. Our experimental results show that difference of interface trap occupancy is the cause of hysteresis in the forward and reverse gate voltage sweeps. It is imperative to lower the interface trap occupancy for high quality of AMOLED display.

A22.6

Low Hydrogen Concentration Silicon Nitride as a Gate Dielectric of TFTs for Flexible Display Application.

Joong Hyun Park, Chang Yeon Kim, Kwang Sub Shin and Sang Geun Park; School of Electrical Engineering and Computer Science, Seoul National University, Seoul, South Korea.

Liquid crystal displays (LCDs) using hydrogenated amorphous silicon thin film transistors (a-Si:H TFTs) on flexible plastic substrate is attractive for flexible display. The fabrication temperature on plastic substrate is limited less than ultra low temperature (<180 Celsius). The hydrogenated amorphous silicon nitride (a-SiN_x:H) as a gate dielectric in TFTs has poor characteristics. Especially, hydrogen concentration is strongly influenced on fabrication temperature, and a-SiN_x:H fabricated at 180 Celsius has a high hydrogen concentration. It makes a-SiN_x:H become porous, low density, and weak bonding. The purpose of our work is to obtain a low hydrogen concentration a-SiN_x:H. We used inductive coupled plasma CVD (ICP-CVD) at 180 Celsius, with SiH₄, N₂, He, instead of SiH₄, N₂, NH₃. From FT-IR measurements, we estimated hydrogen concentration in a-SiN_x:H. And we investigated film density in various condition by wet etch rate. We carried out experiments with a various helium dilution. As helium dilution rate increases, film density increases and hydrogen concentration in a-SiN_x:H decreases. Helium dilution increases the release of the hydrogen bonded to silicon atoms because helium gives many excited species, which is dissociates and bonds actively, to reactive gas. Hydrogen atoms are superior to dissociation than bonding due to its light and weak bond strength on ultra low temperature. Film density is closely connected with atom bonding. In our FT-IR data, as the amount of N-H bond peak decreases and Si-H bond peak increases relatively, etch rate increases. In our silicon nitride as a gate dielectric deposited on 180 Celsius, He dilution results in low hydrogen concentration (<15 at. %), high breakdown voltage (>6 MV/cm) and low etch rate (300~400 Angstrom/min). This a-SiN_x:H is useful in TFT fabrication on flexible plastic for high performance.

SESSION A23: Solar Cells II
Chair: Gautam Ganguly
Friday Morning, April 1, 2005
Room 2002 (Moscone West)

8:30 AM *A23.1

Characterization of the Silicon-Based Thin Film Multi-Junction Solar Cells. Yoshihiro Hishikawa, Research Center for Photovoltaics, AIST, Tsukuba, Ibaraki, Japan.

Procedures and technical issues for the characterization of the performance of silicon-based thin film multi-junction devices, such as the a-Si/thin-film c-Si structure, are discussed. Performance of the multi-junction devices is strongly affected by the balance of the photocurrent generated in each component cell. Especially, the total output current tends to be limited by the minimum photocurrent among the component cells, due to the requirement of current continuity. High-fidelity solar simulators, which incorporate Xe lamp(s) and halogen lamps, in order to simulate the AM1.5G standard sunlight, have been employed for characterizing the multi-junction devices. It is shown that they can accurately reproduce the current generated in each component cells and the I-V curve of the devices under the standard sunlight, with simple spectral adjustment procedure, thanks to their basic good spectral fidelity to the standard sunlight. Irradiance dependence of the I-V curve is important for translating the I-V curve for different irradiance conditions. Although the translation is not straightforward for multi-junction devices, experimental results of the present study suggests that it is possible under the spectral conditions where the relative value of the photocurrent among the component cells is constant. Determination of the I-V curves of each component cell, based on the I-V curves of the multi-junction devices, is also discussed.

9:00 AM A23.2

High Efficiency Solar Cells with Intrinsic Microcrystalline Silicon Absorbers Deposited at High Rates by VHF-PECVD. Yaohua Mai^{1,2}, Stefan Klein¹, Reinhard Carius¹, Xinhua Geng² and Friedhelm Finger¹; ¹Institute for Photovoltaic, Forschungszentrum Juelich, Juelich, Germany; ²Institute of Photoelectronics, Nankai University, Tianjin, China.

In this report, we focus on the structural, electrical and optical properties of intrinsic hydrogenated microcrystalline silicon ($\mu\text{c-Si:H}$) material and the properties of corresponding solar cells. The material was prepared using VHF-PECVD working at high-pressure, high-power (hphP), yielding high deposition rate (RD) up to 15 Å/s and at low-pressure, low-power (lpP), yielding RD below 3 Å/s. Different structure phase compositions from highly crystalline to

amorphous were obtained by the variation of the silane concentration. Solar cells with intrinsic layers prepared by both methods were compared. As a result, optimum cells in both hphP and lpP series exhibit high efficiency over 9%. A $\mu\text{c-Si:H}$ single junction p-i-n solar cell with an efficiency of 9.8%, the highest value reported so far, was obtained at a RD of 11 Å/s. Although similar in a number of aspects, the hphP and lpP materials show distinct differences. Raman spectroscopy with different excitation wavelength provides structural information on the top or close to the bottom in the film and solar cells prepared by the two methods. The Raman intensity ratio (ICRS), was used as a semi-quantitative measure for the crystallinity. Both series show similar dark- and photo-conductivities for the same ICRS and high photosensitivities between 200 and 500 at the $\mu\text{c-Si:H}$ to a-Si:H transition, where high efficiency $\mu\text{c-Si:H}$ solar cells were previously found. The optical absorption coefficient was measured by PDS. A low absorption coefficient below the silicon band gap indicates a low defect density and thus a high quality of both materials. With increasing amorphous volume fraction, a higher hydrogen content and lower microstructure factor, determined by FTIR-spectroscopy, were observed. hphP samples show higher hydrogen content but similar microstructure factor R in the transition region, when compared with lpP samples with the same ICRS. The atmospheric gas in-diffusion behaviour was monitored by FTIR measurements after deposition. The lpP material is resistant to post-oxidation. The growing absorption band between 1000-1200 cm⁻¹, due to Si-O bonds, indicates a higher porosity of the hphP material, contradicting to the similar R for both series. In contrast to the remarkable structure development in the growth direction in the films on glass, particularly in the hphP material, the material in the solar cells appears to be very homogeneous. It is proposed that the highly crystalline $\mu\text{c-Si:H}$ p layers facilitate the $\mu\text{c-Si:H}$ growth in solar cells, suppressing thick incubation layer and leading to high FF. Optimum hphP solar cells show no degradation of performance after six months' exposure to air, indicating no detrimental effect from post-oxidation as found in the hphP material on glass. Either the homogeneous growth or the protection by the amorphous n layer and silver back contact is believed to be the reason.

9:15 AM A23.3

Improved Back Reflector for High Efficiency Hydrogenated Amorphous and Nanocrystalline Silicon Based Solar Cells.

Baojie Yan¹, Jessica M. Owens¹, Chun-Sheng Jiang², Jeffrey Yang¹ and Subhendu Guha¹; ¹United Solar Ovonic Corporation, Troy, Michigan; ²National Renewable Energy Laboratory, Golden, Colorado.

Hydrogenated amorphous silicon (a-Si:H) and silicon germanium (a-SiGe:H) alloy based solar cell technology is one of the most attractive photovoltaic technologies due to low cost and large-scale manufacturing abilities. Among the technologies for improving cell performance, light trapping with textured back reflector (BR) is an important method for enhancing short-circuit current density (Jsc) [1]. A textured Ag/ZnO BR was used for achieving 14.6% initial and 13.0% stable efficiencies in an a-Si:H/a-SiGe:H/a-SiGe:H triple-junction structure [2]. Recently, hydrogenated nanocrystalline silicon (nc-Si:H) solar cell has attracted remarkable attention due to its superior long wavelength response and improved stability over a-SiGe:H. However, because of the nature of the nc-Si:H structure, the optimized Ag/ZnO BR used for the a-SiGe:H solar cells may not necessarily be the best choice for the nc-Si:H solar cells. Optimizing the Ag/ZnO BR has the potential to improve the cell efficiency further. In addition, an improved Ag/ZnO BR may result in an improved efficiency for a-Si:H/a-SiGe:H/a-SiGe:H triple-junction cells. In this paper, we present recent results on the optimization of Ag/ZnO BR for both nc-Si:H and a-SiGe:H solar cells. We deposit Ag/ZnO BR on specular stainless steel substrates using a sputtering method. The texture of the Ag and ZnO layers is controlled by deposition parameters. The surface morphology is investigated by atomic-force-microscopy. To characterize the scattering effect from the textured surface, scattered light intensity from a He-Ne laser perpendicular to the sample surface is measured at different angles. Finally, nc-Si:H and a-SiGe:H solar cells are deposited on the BR substrates made under various conditions. For the nc-Si:H solar cells, large micro-features on the Ag/ZnO layer eliminate interference fringes otherwise observed in the quantum efficiency measurement and result in high Jsc. The result is consistent with an enhanced scattering light intensity. For a-SiGe:H, we find that the improved Ag/ZnO BR with large micro-features leads to an enhanced open-circuit voltage and fill factor. We believe that the increase in the micro-feature size reduces the density of the sharp peaks on the BR surface and consequently reduces the back diffusion of photo-generated carriers at the n/i and i/p interfaces. Hence, the cell performance was improved. We also deposited a-Si:H/a-SiGe:H/nc-Si:H triple-junction cells on the optimized Ag/ZnO BR and achieved a high initial active-area efficiency of 14.6%. [1] A. Banerjee and S. Guha, J. Appl. Phys. 69, 1030 (1991). [2] J. Yang, A. Banerjee, and S. Guha, Appl. Phys. Lett. 70, 2975 (1997).

9:30 AM **A23.4**

Bifacial Silicon Heterojunction Solar Cell with Deposited Back Surface Field. Hanno Dietrich Goldbach, Arjen Bink and Ruud E. I. Schropp; Debye SID, University Utrecht, Utrecht, Netherlands.

Silicon heterojunction cells (SHJ) using crystalline silicon wafers and deposited heterojunction thin film emitters are interesting from an economical, technological, and scientific point of view. Modules using such cells (so called HIT cells) are commercially produced by Sanyo using single crystal wafers. Recently reported alternatives still comprise a high-temperature diffused back surface field (BSF). In order to provide a low cost alternative, our goal is to develop SHJ using multicrystalline silicon wafers with both a deposited emitter and a deposited layer at the back, which serves as a BSF and or surface passivation. The present approach truly allows the development of a cheap, low temperature, all-deposited alternative for the HIT cell. We presently made a bifacial silicon heterojunction solar cell, with an emitter consisting of a 7 nm intrinsic a-Si:H layer and a 15 nm n-type uc-Si:H layer. The back surface field is formed by a 15 nm p++ uc-Si:H layer. In order to achieve a functional deposited BSF the thin p++ layer needs to have a higher effective dopant concentration than the substrate (a 375 μm thick p-type FZ wafer 1 Ohmcm) with an activation energy of 0.2 eV. The uc p++ layer has an activation energy of $E_a = 0.04$ eV (for a 100nm thick layer). To detect the operation of the BSF the cell was made bifacial. The cell has an efficiency of 14.8 %, $V_{oc} = 568\text{mV}$ and $J_{sc} = 33.4 \text{ mA/cm}^2$, $R_s = 1.1 \text{ Ohmcm}^2$ and $R_p = 1.3 \text{ kOhmcm}^2$. The cell, illuminated from the back, shows a V_{oc} of 100mV and J_{sc} of 7mA/cm^2 . Reference bifacial cells without BSF illuminated from the back show no cell behavior. These results show evidence for the feasibility of a truly functioning deposited BSF combined with a SHJ with deposited emitter.

9:45 AM **A23.5**

High-Performance Amorphous Silicon Emitter for Crystalline Silicon Solar Cells. Eugene Iwaniczko, Qi Wang, Matthew R. Page, Dean Levi, Yanfa Yan, Howard M. Branz and Tihu Wang; National Renewable Energy Laboratory, Golden, Colorado.

Thin intrinsic and doped n-type hydrogenated amorphous silicon (a-Si:H) double layers are investigated as the emitter layer of crystalline silicon solar cells based on p type wafers. The a-Si:H is deposited by hot-wire chemical vapor deposition from silane gas using Ta or W filaments. Using a substrate temperature below 150°C for the a-Si:H intrinsic layer and conditions that normally promote ledge or /protocrystalline/ Si for the doped n layer, record efficiencies of 17% and 15% are achieved on 1-cm² planar p-type float-zone silicon and Czochralski silicon wafers, respectively. We obtain open-circuit voltages as high as 650 mV and fill factors above 80%, on simple, untextured, ITO / a Si:H / c Si base / Al back-surface-field structures. High performance requires nearly perfect passivation of the c-Si interface by the a Si:H in addition to good a-Si:H electrical conductivity for lateral current collection. We characterize cells by their photovoltaic parameters and study passivation by photoconductive decay minority-carrier lifetime measurements. Real-time spectroscopic ellipsometry (RTSE) and high-resolution transmission electron microscopy are employed to detect phase change and material evolution. We find that the cell performance is best when all crystallinity is avoided in the intrinsic layer. The crystallinity of the deposited layer is found to be very sensitive to the deposition temperature and crystal orientation of the substrate. Deleterious epitaxial growth is promoted by higher substrate temperatures and is more likely on (100) substrates than on (111) substrates. When epitaxy occurs, especially if the epitaxial growth extends beyond the intrinsic layer, open-circuit voltage decreases dramatically to below 600 mV for 1 W-cm Czochralski wafers. The RTSE permits us to control and optimize the a-Si:H layer thicknesses. With a smooth, abrupt, a-Si:H/c-Si interface and a highly conductive doped n-layer, high performance silicon heterojunction solar cells are consistently obtained.

SESSION A24: Characterization of Microcrystalline Silicon

Chair: Sigurd Wagner
Friday Morning, April 1, 2005
Room 2002 (Moscone West)

10:30 AM ***A24.1**

Structure of Microcrystalline Solar Cell Materials: What can we Learn from Electron Microscopy? Martina Luysberg^{1,2} and L. Houben^{1,2}, ¹Forschungszentrum Juelich, Institut of Solid State Research, Juelich, Germany; ²Research Center Juelich, Ernst-Ruska Center for Microscopy and Spectroscopy with Electrons, Juelich, Germany.

Microcrystalline silicon and its group IV alloys are widely explored as

absorber layers in thin film solar cells. Despite the extended research in recent years the fundamental understanding of the relation between macroscopical properties, i.e. electrical and optical properties, and the microstructure is poor. Clearly, the structure of microcrystalline materials consisting of a phase mixture between "amorphous" material, crystalline grains and voids, is too complex to allow for a decisive atomistic description. Is the disordered phase really amorphous? What is the atomic structure of the coherent and heterogeneous grain boundaries? How large is the amorphous volume fraction? Which chemical composition contain the crystallites, if we grow Si-based group IV alloys? These questions (to name only a few), which are relevant to both, the understanding of the microstructure and the performance of a solar cell, are posed on the electron microscopist. To demonstrate the strengths and limitations of transmission electron microscopy on microcrystalline materials, we will discuss different techniques employed to investigate grain sizes and morphologies, crystallographic orientations, amorphous volume fractions and lateral arrangements of crystallites. In particular, we focus on the potential for analyzing the structure of grain boundaries and the amorphous phase in microcrystalline silicon and silicon carbide by the most advanced techniques in atomic resolution imaging in the transmission electron microscope.

11:00 AM **A24.2**

Structural and Electronic Properties of Hydrogenated Nanocrystalline Silicon Films Made with Hydrogen Dilution Profiling Technique. Keda Wang¹, Daxing Han¹, Brittany Huie²,

Jeniffer R. Weinberg-Wolf², Baojei Yan³, Jeff Yang³ and Subhendu Guha³; ¹Physics Department, Boston College, Chestnut Hill, Massachusetts; ²Department of Physics & Astronomy, Department of Physics & Astronomy, Chapel Hill, North Carolina; ³United Solar Ovonic Corporation, Troy, Michigan.

Hydrogenated nanocrystalline silicon (nc-Si:H) has attracted remarkable attention due to the higher long wavelength response and better stability than hydrogenated amorphous silicon alloy. However, post oxygen diffusion for cells with a high crystalline volume fraction (fc) and large grain size degrades the cell performance. So far, the best nc-Si:H solar cells were deposited under conditions close to the nanocrystalline/amorphous transition, where the materials are compact. Even under the condition close to the transition, it is still difficult to obtain thick nc-Si:H cells with good performance due to the increase of fc and grain size that cause high microvoid/microcrack densities. To solve the crystalline evolution problem, a hydrogen dilution profiling technique has been used and proved to be an effective method for improving the cell performance [1]. In this paper, we present recent results of material characterization for the nc-Si:H films made with different hydrogen dilution profilings. Raman spectroscopy with wavelengths of 610 (red), 514 (green), and 480 nm (blue) is used to probe different depths of the materials. The results show that the crystalline peak at 515-520 cm⁻¹ is much larger on the spectrum measured using the green and blue lights than using the red light for the nc-Si:H sample made with a constant hydrogen dilution ratio, indicative of an increase in fc with the film growth. On the other hand, the fc obtained from the deconvolution of the Raman spectra is slightly lower for the excitations with the blue and green lights than with the red light for the sample with a decreasing hydrogen dilution during the deposition. This result confirms that the hydrogen dilution profiling successfully controls the crystalline evolution. Photoluminescence (PL) excited with 632-nm laser also shows distinct signatures in the electronic density of states for the samples made with different hydrogen dilution profilings. First, for a constant hydrogen dilution ratio, the PL spectrum at 80 K shows low energy peak (at 0.8-0.9 eV) domination, which is normally assigned to the recombination due to grain boundaries. The width of the peak increases with increasing hydrogen dilution ratio, associated with increase of the band-tail width. Second, the sample made with hydrogen dilution profiling shows two peaks consisting of an amorphous peak at 1.4 eV and a grain-boundary peak at 0.8-0.9 eV. The amorphous peak reveals that a significant amount of amorphous component exists in the top layer. In addition, the grain-boundary peak becomes narrower than those made with constant hydrogen dilution ratios. Both the Raman and PL results are consistent with the defect density measurement and solar cell performance from other work. [1] B. Yan, et. al., Mater. Res. Soc. Symp. Proc. 808, 575 (2004).

11:15 AM **A24.3**

Microcrystalline and Nanocrystalline Silicon: Simulation of Material Properties. Rana Biswas^{1,3}, Bica Pan² and Venkatesh Selvaraj³; ¹Physics & Astronomy; and Electrical & Computer Engineering, Iowa State University, Ames, Iowa; ²Dept. of Physics, Univ. of Science and Technology of China (USTC), Hefei, China; ³Microelectronics Research Center, Iowa State University, Ames, Iowa.

We have simulated nano-crystalline silicon and microcrystalline silicon structures with varying crystallite volume fractions, using molecular dynamics simulations. The crystallite regions reside in an amorphous

matrix. Both embedding approaches and melt-quenching approaches have been utilized. We find the amorphous matrix is better ordered in nanocrystalline-Si than in the homogenous amorphous silicon networks, consistent with the observed higher stability of H-diluted films and nanocrystalline silicon. We consider crystallite nuclei sizes ranging from sub nm to a few nm in size. There is a critical size above which the crystallites are stable and may grow. In micro-crystalline silicon models we find a relatively uniform H distribution in the amorphous region and a crystal-amorphous phase boundary that is not well-defined. We will discuss calculations on the electronic states at the interfacial boundary region. The vibrational densities of states of nc-Si has been calculated and show the sharp crystallite-derived features typical of Raman measurements. There is a marked density difference between the crystallite and amorphous regions, consistent with measurements. Atomistic mechanisms of grain growth will also be discussed. Supported by NREL.

11:30 AM [A24.4](#)

Doping Dependence of Chlorine Incorporation in SiCl₄ Based Microcrystalline Silicon Films. Wolfhard Beyer, Reinhard Carius and Uwe Zastrow; IPV, Forschungszentrum Juelich, Juelich, Germany.

Recently high electrical conductivities were observed in plasma-grown boron-doped chlorinated microcrystalline Si films [1]. For films deposited at temperatures near 250°C using SiCl₄-H₂-B₂H₆ gas mixtures, conductivities near 300 (Ωcm)⁻¹ were found [2] making this material of interest for application as a p-layer in microcrystalline Si-based thin-film solar cells. Films with high conductivities usually show rather low concentrations of chlorine and hydrogen and, when deposited near the amorphous-microcrystalline transition, reveal little oxidation effects when exposed to ambient. On the other hand, phosphorus-doped and undoped Si:Cl:H were found to have much higher chlorine concentrations and rather rapid oxidation is generally observed. Thus, by variation of rather small B and P dopant concentrations, the incorporation of much higher amounts of Cl and H can be controlled. Here we study the effect of B and P doping (doping range 0.1 to 1 %) on the Cl concentration (and the oxidation) in more detail by investigating films containing both boron and phosphorus. SIMS depth profiling and IR absorption measurements were used for chemical analysis, Raman spectroscopy was employed to characterize crystallinity, and conductivity and thermoelectric power measurements were performed for electrical characterization. The results show that indeed not the presence of B and P, but rather the relative amount ((P-B)/(P+B)), (P and B are the phosphorus and boron concentrations, respectively) determines the Cl concentration, suggesting a Fermi energy dependence. Under our deposition conditions, the highest Cl concentration (near 10 %) is observed for (P-B)/(P+B) ≈ 0.3 while for (P-B)/(P+B) < 0 the Cl concentration never exceeds 2 at%. This was found for a wide range of Raman crystallinities. For the explanation we propose a similar model as has been applied for the modelling of hydrogen surface desorption in doped a-Si:H which has also found to be Fermi level dependent [3]. The model assumes that the rupture energy of silicon-bonded atoms can be decreased by simultaneous electronic transitions which charge the resulting Si dangling bond positive or negative, depending on the Fermi level. The result of a doping dependence of the oxygen takeup in atmosphere suggests, furthermore, that Cl incorporation favors the porosity of the material. 1. Wolfhard Beyer, Bernd Rech, Reinhard Carius, Matthias Albert, Ralf Terasa, Proceedings PV in Europe Conference, Rome, Italy, 7.-11. October 2002 (WIP Munich and ETA Florence, 2002) p. 75 2. Wolfhard Beyer, Reinhard Carius, Michael Lejeune and Uwe Zastrow, MRS Symp. Proc. 808 (2004) 389 3. W. Beyer, J. Herion and H. Wagner, J. Non-Cryst. Solids 114 (1989) 217

11:45 AM [A24.5](#)

Annealing Characteristics of Al-Doped Hydrogenated Microcrystalline Cubic Silicon Carbide Films.

Shinsuke Miyajima¹, Keisuke Haga¹, Akira Yamada² and Makoto Konagai¹; ¹Physical Electronics, Tokyo Institute of Technology, Tokyo, Japan; ²Quantum Nanoelectronics Reserch Center, Tokyo Institute of Technology, Tokyo, Japan.

Crystalline cubic silicon carbide (3C-SiC) is a wide gap material with bandgap of 2.2 eV. Owing to this high bandgap and indirect-bandgap characteristic, optical absorption of this material is very low in the visible light region. In general, monocrystalline and polycrystalline 3C-SiC films are deposited at a high substrate temperature using a thermal chemical vapor deposition, however hydrogenated microcrystalline cubic silicon carbide (uc-3C-SiC:H) films can be deposited on glass substrates below 300 degrees centigrade by a hot wire chemical vapor deposition (HWCVD) technique [1]. Therefore, uc-3C-SiC:H is one of the promising materials for window layer of silicon based thin film solar cells. We have already studied deposition of aluminum (Al) doped uc-3C-SiC:H films by HWCVD, and we found that thermal annealing is required to activate Al acceptors. In order to obtain highly conductive films, we should understand effects of the thermal annealing on the films. However, the effects have not been

clear yet. In this study, we investigated the effects of thermal annealing on the film properties. First, we investigated the effect of annealing temperature on the conductivity of the films. We performed the annealing at 300, 400, 500 and 600 degrees centigrade. Annealing time was changed from 10 to 1e5 sec. The conductivity of as-deposited films was about 1e-8 S/cm. After annealing, the conductivity increased up to about 1e-4 S/cm for annealing at 400, 500 and 600 degrees centigrade. The conductivity increased from 1e-8 to 1e-4 S/cm with increasing the annealing time, and finally the conductivity saturated. The time for the saturation decreased with increasing the annealing temperature. This result indicated that activation of the Al acceptors occurred above 400 degrees centigrade and p-type uc-3C-SiC:H films can be prepared at process temperature above 400 degrees centigrade. Next, we carried out thermal desorption spectroscopy for the Al-doped and undoped uc-3C-SiC:H films. In case of the Al-doped film, hydrogen desorption started from about 400 degrees centigrade. For the undoped film, hydrogen desorption started from about 600 degrees centigrade. This result indicates that hydrogen configuration in the Al-doped film is different from that of the undoped film, and hydrogen plays an important role on the conductivity of the Al-doped uc-3C-SiC:H films. Reference [1] S. Miyajima, A. Yamada, M. Konagai; Jpn. J. Appl. Phys. 43 (2004) L1190