SYMPOSIUM LL

Combinatorial Methods and Informatics in Materials Science

November 28 - December 1, 2005

Chairs

Qi Wang
National Renewable Energy Lab
MS 3212
1617 Cole Blvd.
Golden, CO 80401
303-384-6681

Radislav A. Potyrailo
Combinatorial Chemistry Laboratory
GE Global Research Center
P.O. Box 8
Schenectady, NY 12301
518-387-7370

Michael Fasolka
Polymers Division
National Institute of Standards and Tech
MS 8542
100 Bureau Dr.
Gaithersburg, MD 20899
301-975-6588

Toyohiro Chikyow
Nanomaterial Research Laboratories
National Institute for Material Science
1-2-1 Sengen
Tsukuba, Ibaraki 305-0047 Japan
81-298-59-2746

Ulrich S. Schubert
Macromolecular Chem & Nanoscience Lab
Eindhoven University of Tech
P.O. Box 513
MB Eindhoven, NL-5600 The Netherlands
31-40-247-4083

Anatoli Korkin
Nano & Giga Solutions
1683 E. Spur St.
Mesa, AZ 85296
480-539-4754

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* Invited paper

SESSION LL1: Electronic Materials and Devices I
Chairs: Radislav V. Potyrailo and Qi Wang
Monday Morning, November 28, 2005
Back Bay B (Sheraton)

8:15 AM *LL1.1
Combinatorial Materials Science: Exploring the Wonder World of Complex Materials. Xiao-Dong Xiang, Intematix, Fremont, California.

Looking back to the last 10 years achievement of combinatorial materials science, from the early work on high Tc superconductors as a proof of principle, to the discovery of novel giant magneotoresistive, luminescent and dielectric materials, from the synthesis of polycrystalline discrete materials libraries to the epitaxial growth of continuous materials phase diagrams, from the invention of evanescent microwave probe for electric impedance mapping to the recent invention of spin resonant probe for intrinsic magnetic properties, whence considered unrealistic fantasies are now realities. I will discuss some recent developments and foresee future directions in this field.

8:45 AM *LL1.2
Combinatorial Fabrication and Screening of Organic Light-Emitting Device Arrays. Joseph Shinar, [1]Ames Laboratory - USDOE, Iowa State University, Ames, Iowa; [2]Physics and Astronomy, Iowa State University, Ames, Iowa.

Studies of combinatorial fabrication and screening of organic light-emitting devices (OLEDs) are reviewed. These studies include screening of luminescent materials, electron and hole transport layers, lower-gap emitting guest dopants in small molecular emitters, and electronically doped polymeric anodes. The review focuses on previous studies by the author. These include 2-dimensional arrays of (i) UV/violet OLEDs and (ii) blue-green OLED involving exciplex emission, and 1-dimensional arrays of (iii) blue-to-red OLEDs, (iv) intense white OLEDs, and (v) arrays fabricated to study Foerster energy transfer in guest-host OLEDs. The review demonstrates that combinatorial fabrication of OLEDs has become a powerful tool for screening various OLED materials and configurations, and for studying their basic optoelectronic properties.

9:15 AM *LL1.3
Integrated thin film and device libraries based on conducting wide-gap oxides. Akira Ohtomo[1], Atsushi Tsukazaki[1], Jun Nishimura[1] and Masashi Kawasaki[1,2]; [1]Tohoku University, Institute for Materials Research, Sendai, Japan; [2]Combinatorial Materials Exploration and Technology (COMET), Tsukuba, Japan.

Combinatorial technology is now widely used in the field of inorganic materials research providing an effective solution to conduct rapid screening of materials properties and fast optimization of synthesis parameters [1]. Also, a novel device concept based on oxide heterostructures can be efficiently tested using this approach, where various combinations of materials are integrated in one chip in a parallel fashion. Here we will present two examples to show how combinatorial experimentations can be used to extract the nature and controllability of electronic properties of wide-gap oxide thin films and to develop a novel device. Firstly, we have developed blue light-emitting diodes composed on ZnO pn junction using combinatorial laser molecular-beam epitaxy technique (CLMBE) [2]. In this case, reproducible synthesis of p-type ZnO is established by rapid screening of hundreds of samples grown under different conditions. Additionally, by precise tuning of optimum growth conditions, intrinsic transport properties of ZnO can be studied in high-quality undoped films exhibiting electron mobility higher than that of bulk single crystal. A second area of our focus has been on the electronic states of perovskite titanate based alloys and superlattices, which arises from the valence mismatches between constituting cations [3]. Here what we are interested in is a wide range of electronic conduction emerging at abrupt heterointerfaces as well as in homogeneous alloys consisting of two band insulators. Using CLMBE, we have grown a number of superlattices and alloys, in which the compositions are systematically varied with maintaining global oxygen stoichiometry. One of the extremes is intrinsic electronic conduction in $SrTiO_3$-$LaAlO_3$ alloy system, which is generally expected to serve as high-K dielectric layers. [1] H. Koinuma and I. Takeuchi, *NatureMater.* **3**, 429 (2004). [2] A. Tsukazaki et al. *NatureMater.* **4**, 42 (2005); *Jpn.J.Appl.Phys.* **44**, L643 (2005). [3] A. Ohtomo and H. Y. Hwang, *Nature* **427**, 423 (2004).

9:45 AM LL1.4
Design of a Gradient Annealing Device for the Parallel Thermal Processing of Thin Films. Sigurd Thienhaus[1,2], Alan Savan[1], Robert Hiergeist[1] and Alfred Ludwig[1,2]; [1]Combinatorial Materials Science, caesar, Bonn, Germany; [2]Institute of Materials, Ruhr-University, Bochum, Germany.

This paper discusses the design and use of a gradient annealing device. Generally, such devices can be used for a rapid optimization of thin film materials by simultaneous thermal processing at different temperatures. Here, it is used in order to optimize annealing parameters (temperature, time) for the fabrication of hard magnetic FePt thin films by annealing of nanoscale Fe/Pt multilayer precursor thin films. First results prove the usefulness of the gradient annealing device for high-throughput experiments.

10:30 AM *LL1.5
Combinatorial approach to exploration of a novel fluid oxide flux stable in vacuum for material processing. Yuji Matsumoto, [1]Materials and Structures Laboratory, Tokyo Institute of Technology, Yokohama, Kanagawa, Japan; [2]CREST Japan Science and Technology Agency, Kawaguchi, Saitama, Japan.

A flux, which is often used in bulk process is an admixture characterized by its fluid behavior, thereby to promote crystal growth by lowering a growth temperature and suppressing a formation of impurity phases. If we are to expect the same benefit from the application of flux to vacuum process such as vapor phase epitaxy, as is called flux-mediated epitaxy, we must find out a new fluid flux stabilized even in the vacuum condition at a high temperature. In this talk, we will concentrate on combinatorial discovery of a novel flux for vapor phase epitaxy of ferroelectric $Bi_4Ti_3O_{12}$ (BIT) film. BiOx, which is a well-known flux for the growth of BIT bulk, is likely to evaporate in vacuum at a high temperature, as predicted in bulk phase diagram and thus is no available for vacuum process. We employed combinatorial pulsed laser deposition (PLD) technique for quick screening of the flux stable in vacuum during the BIT growth. We designed flux libraries including a $Bi_{4+}xTi_{3-}xO_d$ ($0 < x < 3$) self-flux and impurity fluxes (V_2O_5, WO_3, CuO, MoO_3, $BiPO_4$ and BaO): (MOx)p($Bi_4Ti_3O_{12}$)q(BiOy)r, where M=V, W, Cu, Mo, BiP, or Ba, p + q +r=1, 0 < p, q, r < 1. This ternary composition spread film was deposited directly on the substrate, and the BIT film was subsequently deposited at a temperature that was expected to melt the flux. Among these flux libraries, we found out that a small amount of CuOx doped in BiOx is very effective to stabilize BiOx even in 6 Torr O_2 at 800^OC, and its fluid behavior was confirmed by in-situ laser microscope observation. As a result, a single crystal BIT film was successfully fabricated by adding this Bi-Cu-Ox flux during the growth. The electrical properties of BIT film were also excellent: the leakage current density was as low as 10^{-7}~10^{-8} A/cm^2, and the remanent polarization was 3μC/cm^2, corresponding to the value of BIT bulk single crystal. The talk will also, time permitting, touch upon other applications of the Bi-Cu-Ox flux for material processing.

11:00 AM *LL1.6
Composition Spread Approaches to the Combinatorial Development of Metal Oxide Thin Films. John D. Perkins[1], Matthew P. Taylor[1,2], Maikel F.A.M. van Hest[1], Charles W. Teplin[1], Jeff L. Alleman[1], Lynn M. Gedvilas[1], Brian M. Keyes[1], Bobby To[1], Dennis W. Readey[2] and David S. Ginley[1]; [1]National Renewable Energy Lab., Golden, Colorado; [2]Colorado School of Mines, Golden, Colorado.

We have employed combinatorial high-throughput approaches to develop improved transparent conducting oxides (TCOs). Two areas of particular interest are TCOs that can be deposited at low temperature and TCOs with high carrier mobilities. Compositionally graded samples ("libraries") are deposited by co-sputtering onto 2"x2" glass substrates. Three to five libraries are generally required to cover the full composition range for a binary tie-line, such as from In_2O_3 to ZnO. After deposition and, in some cases, additional controlled atmosphere annealing, the libraries are characterized by a variety of automated combinatorial mapping tools. At present these include EPMA for metals stoichiometry, 4-pt. probe for sheet resistance, UV/VIS/NIR (200-2000 nm) reflection and transmission, FTIR optical reflection and transmission (1.8 - 25 μm) and x-ray diffraction (XRD) using a large area 2D detector. For selected libraries, smaller samples are cut out for Hall effect measurements to determine the carrier concentration and mobility. The benefit of this combinatorial approach is exemplified by our success with In-Zn-O (IZO). In particular, for IZO we find a broad maximum in the conductivity with $\sigma \approx 2500\ \Omega^{-1}$-cm^{-1} for x $\approx$ 0.55 to 0.75 in $Zn_{1-x}In_xO_y$ deposited at 100 °C which, surprisingly, correlates with the composition range found to be amorphous by the XRD mapping. We have also used these combinatorial tools to optimize the growth of oriented crystalline metal oxide template layers on glass substrates for thin film photovoltaics.

11:30 AM *LL1.7
Combinatorial InkJet Mapping of Sheet Resistivities of Nanothick Conducting Polymer Films. Ghassan Jabbour and Yuka Yoshioka; Department of Chemical and Materials Engineering and Flexible Display Center, University of Arizona, Tempe, Tempe, Arizona.

We will present the use of combinatorial inkjet techniques to change in a unique fashion the sheet resistivity of nanothick layers of conducting polymers. An update to our previous work along with recent studies on the potential mechanisms behind the observed change in sheet resisitivity will be discussed. Numerous examples and potential applications of this approach will be highlighted.

SESSION LL2: Electronic Materials and Devices II
Chairs: Chris Snively and XiaoDong Xiang
Monday Afternoon, November 28, 2005
Back Bay B (Sheraton)

1:30 PM *LL2.1
Combinatorial Studies of Switching and Solid-Phase Crystallization in Amorphous Silicon. Paul Stradins[1], Howard M Branz[1], Jian Hu[2], Scott Ward[1] and Qi Wang[1]; [1]National Renewable Energy Laboratory, Golden, Colorado; [2]MVSystems, Inc., Golden, Colorado.

We use combinatorial techniques extensively to study switching in memory devices based on disordered Si thin films. Hydrogenated amorphous silicon (a-Si:H) films sandwiched between metallic electrodes switch to a low resistance state when subjected to sufficiently high voltage. Easy-to-manufacture write-once, memory devices can be built based on this phenomenon. The memory element consists of the switch layer (antifuse) and an underlying thin-film diode. An array of such elements is addressed by cross-point contact scheme using the underlying diodes [1]. Because of large statistical variation in switching parameters, understanding the switching mechanism requires extensive, automated measurements on many switching elements. The combinatorial approach speeds up the experiments significantly and has provided a new understanding otherwise obscured in the random event-to-event fluctuations. Namely, the switching time dependences on applied voltage were studied for various film thicknesses, deposition conditions, contact metals and their interface conditions. The thickness dependence was studied on a wedge-shaped a-Si:H film grown in a combinatorial hot-wire chemical vapor deposition system [1]. Different points of the wedge were switched and measured by a touch-contact electrical probe. The probe was mounted on an X-Y-Z automated stage equipped with a digital scope, pulse generator, I-V measurement system, and a video camera. These experiments reveal that both a contact voltage and a bulk critical electric field are necessary to initiate the switching, with the former affected by interface properties [2]. We also applied combinatorial technique to study the solid phase crystallization and epitaxy of a-Si:H using optical microscopy and in-situ reflectance spectroscopy. When the crystallization front growing from the c-Si substrate reaches the wedge-shaped film surface, a change in the optical reflection occurs. This results in a visible phase boundary on the surface moving towards the thicker edge of the film. Thus, the vertical movement of the crystal growth is converted into a horizontal movement of the phase boundary at the surface. The movement of the phase boundary is recorded as video image which is processed in real-time to measure the speed of the solid-phase epitaxial growth [3]. 1. Q. Wang, S. Ward, A. Duda, J. Hu, P. Stradins, R.S. Crandall, H. Branz, APL 85 (2004) 2122. 2. P. Stradins, H. M. Branz, W. B. Jackson, R. S. Crandall, J. Hu, Q. Wang, Mat. Res. Soc. Proc. 808 (2004) 465. 3. P. Stradins, D. Young, H.M. Branz, M. Page, Q. Wang, Mat. Res. Soc. Proc. 862 (2005) A16.1.

2:00 PM *LL2.2
Evaluation of Electric Potential at Metal-Insulator Interface Using Electron Spectroscopy and Kelvin Probe Techniques. Michiko Yoshitake, National Institute for Materials Science, Tsukuba, Japan.

Materials prepared under different conditions are often located in two-dimensional coordinates in combinatorial material processing. Hence, combinatorial methods for material characterization are mostly based on imaging techniques. In other words, any existing imaging technique has potential to be applied as a combinatorial characterization method. The characterization of an interface by electron spectroscopic methods will be a topic of this talk. These methods can be extended to an imaging mode. Electron spectroscopic techniques have been utilized to observe chemical compositions and chemical binding states. The talk will show that they also can work as good tools to evaluate electric properties at interfaces through the analysis of binding energy shifts. In the field of electronic devices, the role of interface has become more and more important. The position of the conduction band minimum and valence band maximum in both materials in contact are key factors to determine contact potential, excitation photon energy of photo devices and so forth. Due to downsizing of devices, electron spectroscopic techniques, whose detection depth is rather shallow, have increasingly proved to be a powerful tool to evaluate interfaces in material research for electron devices. We will demonstrate how X-ray and UV photoelectron spectroscopy (XPS and UPS) combined with Kelvin probe method give useful information about the electric property at metal-insulator and semiconductor-insulator interfaces. Since photoelectron spectroscopic techniques have imaging capability in the order of micrometer range, it will be applied to the combinatorial characterization. The principle of the evaluation and the way of analyzing XPS or UPS spectra for the above purpose will be discussed. The examples of electric potential analysis at interfaces will be given in the systems described below. All the systems were prepared in-situ to avoid contamination at interfaces. 1) amorphous Al2O3 on metals vs. epitaxial Al2O3 on metals binding energy difference due to the interface 2) Al2O3 film thickness dependence in epitaxial Al2O3 on metals binding energy and work function difference due to interface thickness 3) Au, Pd on epitaxial Al2O3 on metals matter of Fermi level matching in metallic film on insulator 4) HfO2 on Hf on SiO2 covered Si binding energy difference due to the interface accompanied with the band bending of Si

3:30 PM *LL2.3
Development of Variable Temperature Scanning Microwave Microscope for High Throughput Materials Screening. Noriaki Okazaki[1], Sohei Okazaki[2], Ryota Takahashi[3], Makoto Murakami[4], Parhat Ahmet[1], Nobuyuki Kakiuchi[5], Hitoshi Furusho[5], Taito Nishino[5], Tomoteru Fukumura[6], Yuji Matsumoto[3], Masashi Kawasaki[6], Toyohiro Chikyow[1], Hideomi Koinuma[7,2] and Tetsuya Hasegawa[2]; [1]Nanomaterials Laboratory, National Institute for Materials Science, Tsukuba, Japan; [2]The University of Tokyo, Tokyo, Japan; [3]Tokyo Institute of Technology, Yokohama, Japan; [4]University of Maryland, College Park, Maryland; [5]Nissan Chemical Industries, Ltd., Funabashi, Japan; [6]Tohoku University, Sendai, Japan; [7]National Institute for Materials Science, Tsukuba, Japan.

Scanning Microwave microscope (SμM) has been attracting much interest as a high-throughput electric-property screening tool in the combinatorial material science and technology. The SμM can evaluate surface local electric properties such as linear/nonlinear dielectric constant, dielectric loss and conductivity, using evanescent microwave emitted from the probe tip attached to the resonator. We developed a SμM by using either a lumped-constant (LC) resonator or a coaxial cavity resonator as a sensor probe. By using the LC resonator probe, we succeeded in mapping out dielectric constant for various composition-spread thin films, such as (Ba,Sr)TiO_3, ternary HfO_2-Y_2O_3-Al_2O_3 and Li(Nb,Ta)O_3 from the measurement of resonance frequency shift. On the other hand, the cavity resonator has higher quality factor and is advantageous in imaging surface conductance and dielectric loss. Recently, we developed a new SμM system designed for low-temperature measurement using a high-Q $\lambda/4$ coaxial cavity resonator. Resonance frequency and Q-value were measured by a network analyzer. Sample temperature was regulated by the combination of liquid-helium flow and a stage heater in the temperature range between 4K and room temperature. We measured a superconducting $Nd_{0.9}Ca_{0.1}Ba_2Cu_3O_7$ (NCBCO) thin film by using the developed SμM. The temperature dependence of Q-value shift ($\Delta(1/Q)$) showed a sharp jump at Tc $\sim$ 76K, being consistent with the dc-resistivity curve measured by the four probe method. Next, the sample was annealed with temperature gradient ranging between 490 and 600°C under the oxygen pressure of 1 Torr in order to induce local oxygen content variation along the temperature-gradient axis. Below the measurement temperature of 60K, the line profiles of $\Delta(1/Q)$ showed a clear stepwise change, corresponding to the phase boundary between the superconducting and the normal-metal states. The results indicate that the present SμM system possesses enough performance for high-throughput electric-property screening at low temperatures.

4:00 PM LL2.4
A Composition-Spread Approach to Generating and Characterizing Optical Amplifier Materials. K. E. Downey[1], A. R. Bhagwat[2], R. B. van Dover[1] and A. L. Gaeta[2]; [1]Materials Science and Engineering, Cornell University, Ithaca, New York; [2]Applied and Engineering Physics, Cornell University, Ithaca, New York.

Optical integration is an attractive approach to reducing the cost of optical functions in data networks while also offering the promise of increasing performance and decreasing size. On-chip amplification is a critical function that requires introduction of new materials. We use a combinatorial composition-spread approach to rapidly identify and evaluate possible amplifier materials. We explore oxide systems with up to four cations using a combination of off-axis and on-axis reactive sputtering. This high-throughput synthesis technique is complemented by rapid optical characterization of the resulting thin films. Compositionally dependent properties such as the lifetime and amplitude of Er^{3+} fluorescence are investigated using a 980 nm pump beam and collection with a time-resolved detector. Promising materials are identified by a figure of merit produced by multiplying the fluorescence lifetime with its amplitude. The composition-spread

technique allows us to determine the maximum Er concentration that can be incorporated before Er-Er interactions quench the transition; we can simultaneously determine the optimum levels of substitutions in the SiO_2 matrix to increase the radiative transition probability and/or decrease Er-Er interactions. Using the composition spread approach, we are able to explore rapidly several mechanisms by which the Er luminescence may be increased. Some of these include damping phonon vibrations, disrupting the symmetry of the Er site in the host material, and adding energy-transfer sensitization agents. We have identified compositions in the Er:Bi-Al-Si-O system that perform significantly better than any composition in the benchmark Er:Ln-Al-Si-O system. We are also able to explore the functionality of amorphous compositions related to a known crystalline amplifier in the Er:Zn-Ge-Si-O system. We will report on the systematic dependence of fluorescence on composition in a range of inorganic oxide systems, with an eye toward identifying the most promising candidates for further development, and understanding the underlying science. We will also report on the robustness of these systems with respect to annealing temperatures.

4:15 PM LL2.5
Combinatorial Optimization of Low Electrical Resistivity Pd-based Thin Film Metallic Glass. Ryusuke Yamauchi[1], Seiichi Hata[2], Junpei Sakurai[2] and Akira Shimokohbe[2]; [1]Mechano-Micro Engineering, Tokyo Institute of Technology, Yokohama, Kanagawa, Japan; [2]Precision and Intelligence Laboratory, Tokyo Institute of Technology, Yokohama, Kanagawa, Japan.

Thin film metallic glass (TFMG) is an amorphous alloy that softens in a supercooled liquid region (SCLR), and thus can be readily formed into three-dimensional shapes suitable for microelectromechanical systems (MEMS) applications. Although TFMG with the conventional composition Pd76Cu7Si17 (at.%) have been successfully applied to fabricate out of plane micro actuator, micro variable inductor, micro hollow structure and integrated probes, the electrical resistivity of this TFMG is higher than that of conventional metals. For the wide use of TFMG in MEMS applications, the search of new TFMG having low electrical resistivity is needed. The combinatorial material synthesis is powerful method to search for new materials and optimize material compositions. In this work, new combinatorial material synthesis (the arc-combi) using cathodic arc plasma deposition is employed to search for Pd-Cu-Si TFMG that offers lower electrical resistivity. Continuous compositional spread thin film alloy which is mixed at atomic scale can be fabricated on one substrate by this synthesis. The process of Pd-Cu-Si ternary alloy thin film fabrication can be carried out at high vacuum environment. Film thickness is mainly controlled by pulsed discharge frequency and the condenser capacity. Distribution area of deposited film is adjusted by the permanent magnet under the substrate. Three cathodic arc plasma guns (CAPGs) are placed to provide continuous compositional spread across a substrate in apexes of regular triangle configuration. Pulsed depositions of Pd, Cu, sintered alloy Pd50Si50 (at.%) are sequentially carried out using the CAPGs. The fabricated thin film is separated into 1,089 samples (integrated library) and these samples are evaluated respectively. In order to search for low electrical resistivity composition of Pd-Cu-Si TFMG, some integrated libraries have been fabricated and sequentially evaluated. The phases, the compositions and relative electrical resistivities of samples on the integrated library are measured by X-ray diffractometryiXRDjCEnergy dispersive X-ray fluorescence spectrometer (EDX)Cand four-point probe respectively. The samples on the integrated libraries are too small to identify SCLR by differential scanning calorimeter (DSC) and to measure more accurate value of electrical resistivities by conventional four-point probe system. Therefore the same or near compositions of the lower electrical samples found in the integrated libraries are reproduced by the carousel type R.F. sputtering system. The composition of Pd81Cu5Si14 is finally identified to be lower Pd-Cu-Si TFMG than conventional one. That TFMG electrical resistivity is 60$\mu\Omega$·cm and the SCLR is 60K.The optimum composition for Pd-Cu-Si TFMG in electrical resistivity has been successfully identified through this process. Further work will focus on high-throughput evaluation of SCLR of TFMG on the integrated library.

4:30 PM LL2.6
The luminescent characteristics of $Zn_{2-x}Mn_xSiO_4$ studied by combinatorial techniques. Lih-Ping Wang, Wen-Hsuan Chao, Shu-Huei Wang, Tien-Heng Huang and Ren-Jye Wu; Union Chemical Laboratory, Hsinchu, Taiwan.

The $Zn_{2-x}Mn_xSiO_4$ is a widely used green luminescent material in various fields such as PDP, CRT, fluorescent lamp and thin film electro-luminescence devices. Orange luminance from $Zn_{2-x}Mn_xSiO_4$ is seldom found only was found with successive replacement of zinc by beryllium up to large 10∼20 mol%. In this article, the luminescent characteristics of Zn2-x MnxSiO4 were studied by combinatorial synthesis and characterization techniques. $Zn_{2-x}Mn_xSiO_4$ material libraries were prepared with a continuous-compositional-spread method. Photoluminescence (PL) were characterized by imaging system for parallel screening analysis and automatic PL spectrum measurement for sequential analysis. The composition and structure were characterized respectively by EDAX and XRD in a high-throughput way. The PL emission light varied from orange to green, depending on film structure and composition. The correlation among PL characteristic, film structure and composition and the reason for orange photoluminance from $Zn_{2-x}Mn_xSiO_4$ are also discussed.

4:45 PM LL2.7
Combinatorial synthesis of (Al,Ti)N thin films via pulsed laser deposition. Clara Ji-Hyun Cho[1], V. Siva Kumar G. Kelekanjeri[1], Rosario A Gerhardt[1] and Hideomi Koinuma[2]; [1]Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia; [2]Materials and Structures Laboratory, Tokyo Institute of Technology, Yokohama, Japan.

Aluminum nitride (AlN), a wide band gap semiconductor (Eg = 6.2eV), has potential applications in microelectronics due to its excellent insulating properties and compatibility with silicon [1,2]. More recently, the use of AlN thin films in high electron mobility transistors, light emitting diodes and UV sources is explored by altering the band gap of the material [3]. The present work describes the combinatorial synthesis of (Al,Ti)N thin films via pulsed laser deposition (PLD) technique to obtain desirable compositional spreads and corresponding variations in the electrical properties. Films of AlN, TiN and (Al,Ti)N were deposited on 6H-SiC (0001) substrates held at a temperature of 680°C. Films ranging from 60 nm to 170 nm thick were deposited for durations between 2 and 4.5 hours. . The surface quality of the films examined using an AFM revealed island growth of SiO2 and other growth patterns possibly related to substrate defects. X-ray diffraction studies indicated that the growth of AlN and TiN films occurred with corresponding habit planes of (0001) and (111) parallel to the substrate surface. Compositional investigations conducted using energy dispersive spectroscopy (EDS) and x-ray photoelectron spectroscopy (XPS) showed systematic changes in the Al and Ti composition across the thickness of the compositional spread film. Cross-sectional analysis of (Al,Ti)N films conducted in a high-resolution transmission electron microscope revealed that the films were multi-layered. Several orders of magnitude decrease in the measured resistivity across a 15 micron length (Al,Ti)N film was noted corresponding to a systematic increase in the Ti content. Further optimization of deposition conditions is essential for producing thicker films. In addition, films of the same combinatorial spread will be produced via molecular beam epitaxy (MBE) to serve as a reference in assessing the properties of films deposited via PLD. References 1. Mihaela Tanase, C. Morosanu, V. Dumitru, Laura Tugulea, N. Tomozeiu, CAS Proceedings 1 (1998), 221-224. 2. C.L. Aardahl, J.W. Rogers Jr., K.K. Yun, Y. Ono, D.J. Tweet, S.-T. Hsu, Thin Solid Films, 346 (1999), 174-180. 3. M. Razeghi, M. Henini, Optoelectronic Devices: III-Nitrides, Elsevier Ltd, (2004).

SESSION LL3: Poster Session: Combinatorial Material Science
Chairs: Alfred Ludwig and Joseph Shinar
Monday Evening, November 28, 2005
8:00 PM
Exhibition Hall D (Hynes)

***LL3.1**
Inkjet Printing of Functional Polymer and Nanoparticle Libraries for Combinatorial Studies. Emine Tekin, Elisabeth Holder, Veronica Marin and Ulrich S. Schubert; Laboratory of Macromolecular Chemistry and Nano Science (SMN), Eindhoven University of Technology, Eindhoven, Netherlands.

The aim of the project is the incorporation of inkjet printing into a combinatorial workflow, to screen libraries of functional materials and to investigate their properties. Defined films of luminescent ruthenium(II)polypyridyl-poly(methyl methacrylate) (PMMA) and iridium(III)polypyridyl-polystyrene (PS) copolymers could be deposited by inkjet printing resulting in libraries with gradually varied film thickness. The topography of the inkjet printed films was analyzed utilizing an optical profilometer and the absorption and emission spectra were obtained using a parallel UV-Vis and fluorescence plate reader. Currently, the focus is on the optimization and investigation of the printing conditions for MEH-PPV (poly[2-methoxy-5-(2'-ethylhexyloxyl)-1,4-phenylenevinylene]) films and lines, as well as on combinatorial studies of printed libraries of CdTe nanoparticle composites. All described materials are semi-conductive, electroluminescent and very attractive materials for potential applications in optoelectronics.

LL3.2
Probing the Interfacial Adhesion Strength in Compositional Libraries of Epoxy Films. Christopher M. Stafford, Martin Y. M. Chiang, Jae Hyun Kim, Daisuke Kawaguchi and Gareth Royston; Polymers Division, National Institute of Standards and Technology, Gaithersburg, Maryland.

Considerable attention has been devoted to developing high-throughput measurements for characterizing the chemical properties of combinatorial libraries. Less attention has been dedicated to designing high-throughput metrologies for probing the physical or engineering properties of combinatorial libraries. Our research aims to demonstrate and validate successful integration of suitable combinatorial and high-throughput (C&HT) methodologies into new or existing measurement platforms for the physical testing of materials, with an emphasis in the areas of adhesion and mechanical properties. Specifically, this talk will focus on our efforts aimed at developing a measurement platform geared towards C&HT assessment of interfacial adhesion in thermally cured epoxy materials. A critical parameter space to be explored is composition of the epoxy formulation. We are designing an automated mixing and deposition system for the creation of discrete and continuous gradients in composition of a thermally cured epoxy system. Orthogonal gradients in thickness or quench temperature are used to generate a gradient in the applied stress field. By dicing the combinatorial library into a contiguous discrete sample array, the interfacial adhesion strength can be deduced from the critical stress required to debond each film cell from the substrate. These results can be used to predict the adhesion reliability of epoxy formulations as a function of composition and applied stress.

LL3.3
The Computational Materials Design Facility (CMDF): Multi-Paradigm Multi-Scale Simulations of Materials based on Reactive Force Fields (ReaxFF). Markus J. Buehler, Jef Dodson, Adri van Duin and William Goddard; Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

It has always been the dream of computational scientists to predict the properties and behavior of materials by theoretical modeling or computer simulation from a very fundamental, *abinitio* perspective. Within the coming decade, this dream may come true and we will be able to predict macroscopic properties of complex materials throughout hierarchies of scales and paradigms. The key to achieve this is goal is the availability of computational tools that allow straightforward integration of highly complex computational engines for materials simulations. We believe that such paradigm complexity in materials modeling is essential to address important scientific problems, in particular those at the borderlines of different scientific disciplines, as for example interfaces between living and non-living systems in hybrid nano-bio technologies. The development of our new multi-scale multi-paradigm simulation environment, the "Computational Materials Design Facility" (CMDF) is the realization of this vision. The CMDF is capable of simulations of complex materials and de novo materials design at different length and time scales. The method couples quantum mechanical (QM) methods, the first principles ReaxFF reactive force field and empirical all atom force fields (FF), as well as continuum methods. We demonstrate how different modeling paradigms can be seamlessly integrated within a Python scripting layer based on a central data structure "Extended OpenBabel". The CMDF allows integration of distinct monolithic simulation codes and enables development of efficient communication channels between different simulation codes. Particular emphasis of this paper is on coupling reactive force fields (ReaxFF) with empirical potentials (MEAM, EAM, Tersoff) in modeling behavior of materials based on the concept of mixed Hamiltonians. These hybrid techniques, for the first time, allow coupling of complex chemistry and mechanical properties of materials. We exemplify our new methods in studies of surface oxidation of aluminum under applied mechanical strain, crack propagation in corundum under the presence of water, and crack dynamics in a silicon single crystal. We further present applications of our new methods in combining a new reactive force field for proteins ($\text{ReaxFF}_{Protein}$) with classical, non-reactive force fields such as CHARMM, AMBER, DREIDING and UFF in modeling biological systems such as enzymatic reactions.

LL3.4
Materials Design Using an Informatics-Based Approach. Joan T. Muellerleile[1], Kim F. Ferris[2], Dumont M. Jones[3] and Roger W. Hyatt[4]; [1]Polymer Center/Advanced Materials Applications, Battelle Memorial Institute, Columbus, Ohio; [2]Computation and Information Sciences Directorate, Pacific Northwest National Laboratory, Richland, Washington; [3]Proximate Technologies, LLC, Columbus, Ohio; [4]Electronics and Avionics Systems, Battelle Memorial Institute, Columbus, Ohio.

An informatics-based approach to multiply-constrained materials design is outlined, employing the example of coating design for silica fibers. Our approach to the inverse-mapping problem of generating structures from design constraints and QSPRs emphasizes design-rule generation and analysis. As illustrated here, our approach can assist in 1) factoring a larger design problem into tractable components, 2) integrating physical and non-physical requirements (such as cost), 3) identifying information gaps that must be resolved to complete a design, and 4) identifying situations in which a solution consistent with known information is not feasible.

LL3.5
Abstract Withdrawn

LL3.6
Statistical Texture Analysis of Microscopy Images for the Purpose of Surface Characterization. Christine Caragianis Broadbridge[1], Thomas Sadowski[1,2] and J. Daponte[2]; [1]Department of Physics, Southern Connecticut State University, New Haven, Connecticut; [2]Department of Computer Science, Southern Connecticut State University, New Haven, Connecticut.

In a previous study, an examination of the ferroelectric (FE) thin film $SrBi_2Ta_2O_9$ (SBT) revealed a possible correlation between the surface topology and the electronic behavior of the resulting devices [1]. In the earlier study, non-contact atomic force microscopy (nc-AFM) was used to measure surface statistics of the samples including RMS roughness, average grain area, and average grain density. These statistics revealed that the surface structure of SBT thin films is dependent upon annealing temperature. In particular grain size (inversely proportional to grain density) was shown to affect the ferroelectric properties of SBT thin films. Although the methods employed are able to classify the surfaces of a given set of SBT samples, this process becomes labor intensive if multiple images need evaluation. The focus of this study was the use of an image processing technique known as texture analysis to provide a complimentary method for the processing of non-contact AFM data. The analysis of texture was accomplished through a set of gray scale cooccurrence matrices used to provide first and second order statistics about pixel values in the image [2]. Statistics obtained from the previous study were also included in the final analytical model. A stepwise discriminant analysis (DA) was conducted to identify which of the quantitative parameters could best distinguish among the range of annealing temperatures. Of the eight parameters that were identified as contributing to the discrimination of the images, grain density was deemed to be most significant. The parameters obtained from the cooccurrence matrices also corroborated the importance of grain density. Based on the qualitative observation that grain size changes with annealing temperature, it is often chosen to quantitatively describe the surface characteristics of SBT. Thus the results of this study show the potential of texture analysis as a less labor intensive method for the analysis of AFM data, requiring minimal prior knowledge with respect to possible discriminating surface characteristics. [1] Pechkis, D. L. "The Microstructural Characterization of Thin Film Ferroelectrics for Electronic Applications." Honors Thesis, 2001 [2] R.M. Haralick, Proc. of the IEEE, vol. 67, pp. 786-804, 1979

LL3.7
Evaluation of Mo-based Amorphous Alloy Thin Films Exhibiting High Crystallization Temperature. Junpei Sakurai[1], Seiichi Hata[1], Ryusuke Yamauchi[2] and Akira Shimokohbe[1]; [1]Precision and Intelligence Laboratory, Tokyo Insutitute of Technology, Yokohama, Japan; [2]Mechano-Micro Engineering, Tokyo Insutitute of Technology, Yokohama, Japan.

Amorphous alloys are expecting for use as molds of glass optical lens had diffraction grating. Amorphous alloys, such as electroless planted NiP, have been used for injection molding of plastic lens. However, since molding temperature of injection molding for glass is higher than that for plastic, materials for glass molding need to be stable to be used at high temperatures. Thus, amorphous alloys exhibiting high crystallization temperature need to be developed. In order to increase crystallization temperature of the alloy, the melting point needs to rise. Mo-based alloys are expected to exhibit high crystallization temperature, because the melting point of Mo is 2890 K. Moreover, Mo-Zr alloy is expected to tend to become amorphous alloy, because it shows the following conditions; (1) the eutectic reaction takes place at near-equiatomic composition. (2) The mismatching of each atomic size is large. (3) The Gibbs free energy of mixing of each element is negative. In the present study, Mo-Zr amorphous alloys added the third elements were fabricated by a combinatorial materials synthesis using cathodic arc plasma (arc-combi) and sputtering, and their thermal and mechanical characteristics were investigated systematically. Integrated libraries of the Mo-Zr-X (X= Al, Si) alloy system were fabricated at first by arc-combi method. The number of separated micro-samples was 1089 on integrated library. Alloy composition of micro-samples on integrated libraries was determined

by an energy dispersive X-ray fluorescence spectrometer (EDX). The composition region corresponding to an amorphous state was identified by an X-ray diffractmeter (XRD). On the basis of these results, amorphous Mo-Zr-X thin films were fabricated by a carousel-type sputtering system using pure targets for each element. Crystallization temperatures are estimated from the XRD results for specimens annealed at various temperatures for 60 s, because crystallization temperature of all specimens could not be measured by a differential scanning calorimetery (DSC). Mechanical properties were measured by tensile tests, using a thermo-mechanical analyzer (TMA). The integrated library of Mo-Zr-Si alloy system showed that Mo70-50Zr20-40Al10-30 (at%) alloy exhibits amorphous state. While Mo55-50Zr25-40Al10-25 (at%) alloy exhibits amorphous state in the Mo-rich Mo-Zr-Al alloy system. It is found that the range of alloy composition exhibited amorphous state in Mo-Zr-Al alloy was narrower than that in Mo-rich MoZrAl alloy. The results of XRD profiles in the annealed MoZrSi sputter-deposited thin film, crystallization temperature exceeded 1073 K. However, Mo-Zr-Si thin films were so brittle that they could not be subjected to tensile testing. In order to improve toughness of Mo-based alloys, Al rather than Si, were added to Mo-Zr alloy. In Mo-Zr-Al alloy system, crystallization temperature of Mo-Zr-Al- thin films was 973-1073 K. Toughness of Mo-based alloys could be improved slightly by adding Al.

LL3.8
High Throughput Experimentation on Zeolite Membrane Development for the Process Intensification of Organic Chemical Processes. Tomoya Inoue, Yasuhisa Hasegawa, Takako Nagase, Yoshimichi Kiyozumi, Satoshi Hamakawa and Fujio Mizukami; Research Center for Compact Chemical Process, National Institute of Advanced Industrial Science and Technology (AIST), Sendai, Miyagi, Japan.

One of the mission of process chemist is to propose and develop safe and environmentally benign processes for chemicals. Catalysis technology has been successfully applied to petrochemical processes to minimize energy consumption as well as waste production, and we can expect similar story for the development of fine chemical processes. But as the span required for catalyst development suitable for the process has been usually required ten years, while the span for the development of processes for fine chemicals is generally less than three years. This span mismatch has been one of the major reasons why chemical processes for fine chemicals still rely on series of classical organic reactions with producing wastes besides products. We have been succeeded establishing zeolite membrane technology and seeking various kinds of applications, and one of the topics is its application for environmentally benign processes. Recently, we have succeeded developing new type of zeolite membrane to intensify the processes of dehydration related reactions. At first, we applied high throughput screening on water and alcohol adsorption to find out the appropriate zeolite candidate to be formed to membrane - in this case, as we were going to pervaporize water through zeolite membrane, hydrophilic as well as organophobic nature was required. We could choose MER and PHI as candidates as the high throughput screening on the adsorption of water and alcohol indicated. Next, we constructed parallel experimentation for evaluating zeolite membrane in the organic processes, based on parallel batch screening system for organic reactions. We solved various kinds of problems to make the reaction system convenient for pervaporation screenings. In the presentation, we will brief out our effort on this development and show a perspective how to accelerate the membrane refining process via high throughput screening technology.

LL3.9
Crystal Structures and Electrical Properties of Binary-alloy Schottky Contacts on ZnO Fabricated by a Combinatorial Ion Beam Assisted Sputtering. Takahiro Nagata[1,2], Parhat Ahmet[1], Keisaku Yamada[3], Ken Tsutsui[3], Yasuo Wada[3] and Toyohiro Chikyow[1,2]; [1]National Institute for Materials Science (NIMS), Tsukuba, Japan; [2]CREST, Japan Science and Technology Agency (JST), Kawaguchi, Japan; [3]Nano Technology Research Laboratory (NRL), Waseda University, Shinjuku-ku, Japan.

Zinc Oxide (ZnO) is a wide band-gap II-VI semiconductor which has recently been proved to have great potential for use in optical devices. Although those optical devices are mainly based on gallium nitride at the present time, ZnO has remarkable advantages compared to those in GaN, such as higher quantum efficiency, greater resistance to high-energy radiation, and the possibility of wet chemical etching. Among many optical devices using ZnO, the UV region Schottky type photodiode would be the one to exploit most advantages, since it is both light sensitive and structurally simplistic. The heterostructure of ZnO and a metal is the most important part in the Schottky type photodiode, therefore high quality and thermally reliable Schottky contacts are inevitable for these applications. New binary alloy with high Schottky barrier height on ZnO is developed using a combinatorial ion beam assisted deposition system. This system has an Ar gas ion beam gun with 5 kV acceleration energy (Nti, 1403), a target exchange system and a moving mask system. The compositional fraction of the Pt-Ru binary alloy was continuously changed by the composition spread technique. Pt-Ru binary alloy films were deposited on ZnO substrates. Pt-Ru alloy metal film grew on the ZnO epitaxialy, and crystal structures change from Pt-phase (cubic structure) to Ru-phase (hexagonal structure) in the Pt-Ru alloy phase diagram. Schottky barrier heights determined by current-voltage measurements increased with Pt content. Maximum barrier height difference is 137 meV. By the combination of ion beam deposition and combinatorial system, the Schottky barrier heights of Schottky binary alloys have been systematically controlled in response to the compositional fraction of the Pt-Ru binary alloy.

LL3.10
A Calculation Method of Deposition Profiles in Chemical Vapor Deposition Reactors Using Genetic Algorithms for The Automatic Modeling System of Reaction Mechanisms. Takahiro Takahashi and Yoshinori Ema; Dept. of Electrical and Electronic Eng., Shizuoka University, Hamamatsu, Shizuoka, Japan.

An important facet of research and development of chemical vapor deposition processes (CVD) is identification of an appropriate reaction model (reaction mechanism) that shows the reaction routes from source gases to films, both quantitatively and qualitatively. Such a model can indicate potential improvements for the diagnosis of reactor conditions, optimizing reactor designs, scaling up reactors, etc. In order to increase the speed of R&D and decrease the labor requirements, we propose an automatic modeling system of the reaction mechanisms, which we call Evolutionary Analysis for Reaction Systems (EARS). Although we successfully demonstrated the validity of EARS, running EARS requires a huge calculation cost for the repetitions needed in estimating deposition profiles by solving difficult governing equations, such as stiff diffusion-reaction equations. The performance of this calculation process is one of the most important steps in determining the total performance of the system. The huge calculation cost inhibits the applications of the system to various CVD processes in practical time. Therefore, in this study we propose a novel calculation method to reproduce the deposition profiles in various CVD reactors, such as the Macrocavity. Boundary value problems for estimating diffusion-reaction equations by iterations of numerical integrations were changed into problems of finding linear combinations of specific simple functions by genetic algorithms (GA). We have applied the method to calculating conditions for some reaction models and have successfully demonstrated that the method reproduces the deposition profiles with both smaller calculation costs and greater accuracy than the conventional method. In additions, we tried to improve the automatic modeling system by the implementation of the method. We successfully made the system more robust and reliable and substantially expanded the applicable area of the system.

LL3.11
An Autonomous Modeling System of Process Simulators for Film Depositions Using Software Agent Technology. Takahiro Takahashi[1], Masamoto Arakawa[2], Kimito Funatsu[2] and Yoshinori Ema[1]; [1]Dept. of Electrical & Electronic Eng., Faculty of Eng., Shizuoka University, Hamamatsu, Shizuoka, Japan; [2]Dept. of Chem. Sys. Eng., School of Eng., The University of Tokyo, Tokyo, Japan.

The film deposition process, such as Chemical Vapor Deposition (CVD) is one of the most important ultra fine manufacturing processes for semiconductor devices. Although process simulators are very helpful to developing the deposition process, huge calculation costs of the simulators obstruct the their applications to various deposition processes in practical time. In our previous paper, we showed that modeling of the correlations between calculating conditions and calculated results by the simulators radically decreases the calculation costs. However, because modeling the calculation process of the simulators entails many intellectual procedures, modeling presents significant obstacles for researchers. We believe that one very effective approach is making an autonomous system to model the simulators. Therefore, we have developed the autonomous modeling system using software agent technology. The system consists of software agent, generalized application software for modeling and the process simulator for CVD deposition profiles on the substrates with micrometer-sized trenches. The agent makes input data for the simulators and takes output data by operating the simulators autonomously. Then the agent makes a training data set by combining both the input and output data and analyzes the models of the calculation process of the simulators by operating the modeling software. The agent successfully made the good training data and constructed PLS (Partial Least Squares), QPLS (Quadratic PLS) and NN (Neural Networks) models. These models showed both good reproducibility and predictability for deposited profiles on the

substrates with various specifications.

LL3.12
De Novo Design of Inorganic Binding Polypeptides.
Ersin Emre Oren[1], Ram Samudrala[2], Deniz Sahin[1,3], Sevil Dincer[1], Candan Tamerler[3,1] and Mehmet Sarikaya[1,3]; [1]Materials Science and Engineering Department, University of Washington, Seattle, Washington; [2]Department of Microbiology, University of Washington, Seattle, Washington; [3]Molecular Biology and Genetics, Istanbul Technical University, Istanbul, Turkey.

Using bioinformatic sequence alignment methods and scoring matrices (PAM 250 and BLOSUM 62) we generated similarity scores among inorganic-binding peptide sequences selected by directed evolution. Short (7 or 12 amino acids) peptide sequences with specific binding to a large number of inorganic materials can be selected using combinatorial biology techniques, such as cell surface and phage display [1]. Quantifying similarities and differences among amino acid sequences is the first step towards understanding the nature of molecular recognition and will lead to new generation of tailor made molecules with controlled molecular structure and function. Similar to the detection of homology among naturally evolved proteins having similar functions and/or structure, our method establishes sequence correlation among different inorganic-binding polypeptides with similar affinity and surface specificity to metals, ceramics, and semiconductors. For example, using quartz binding peptide sequences we observed higher self-similarity scores among the experimentally characterized strong quartz binders compared to those among weak binders. Based on the high similarity among strong binding sequences, we developed a neural network-type program and generated a new PAM-like scoring matrix, QUARTZ I. Using this matrix and selecting from a pool of 1,000,000 random sequences, we de novo designed binders that have either strong-binding or non-binding affinity for quartz. The approach is extended to de novo design of other peptide sequences selected for various metals and semiconductors. Research is supported by ARO-DURINT Program. [1] M. Sarikaya, C. Tamerler, K. Schulten, A. Jen, and F. Baneyx, (2003) Nature Mater. 2, 577 (2003).

LL3.13
A Computer Modelling Study on Iron Antimony Oxide FeSbO4. Ricardo Grau-Crespo[1,2], Nora de Leeuw[1,2] and Richard Catlow[3,2]; [1]School of Crystallography, Birkbeck College, London, United Kingdom; [2]Chemistry, University College London, London, United Kingdom; [3]Davy Faraday Research Laboratory, The Royal Institution of Great Britain, London, United Kingdom.

FeSbO4 is a material that is commercially used to catalyze the synthesis of acrylonitrile, an intermediate in the production of acrylic plastics and fibres. Experimental studies using diffraction techniques have shown that FeSbO4 has a rutile-like structure, in which the Fe and Sb cations are distributed in the octahedral positions, with no apparent long-range preferential order. The existence of any order in the distribution of cations at a shorter range or in particular directions within the crystal are much more difficult to investigate using experimental methods. In the present work we employ quantum-mechanical computer modelling techniques to study the cation distribution in the material. By comparing the stabilities of all the different cationic configurations in FeSbO4 supercells, we conclude that Fe and Sb cations strongly prefer to alternate along the c direction of the crystal, but there is no definite order in their distribution in the other two directions. We show that the distribution of cations in this manner can explain some of the magnetic properties observed in this material, including two-dimensional antiferromagnetism and spin-glass behaviour. On the other hand, we have investigated the electronic structure of this material. Considering the failure of the traditional DFT approach (LDA or GGA) in the description of the electronic properties of transition metal compounds, we have used two other methods: hybrid functional (B3LYP) calculations, with localized basis-sets using the CRYSTAL code, and GGA+U calculations, within the plane-wave / pseudopotential formalism using VASP. Standard DFT-GGA and Hartree-Fock (HF) calculations are also presented for comparison. Both the fraction of HF-exchange introduced in the Hamiltonian and the Ueff parameter controlling the orbital-dependant correction in the DFT+U method affect critically the calculated strength of the magnetic interactions, and a reasonable agreement with experiment is obtained for B3LYP (20% of HF-exchange) and for GGA+U with Ueff = 4 eV. Both methods also agree well as to the relative position of the electronic bands, showing that FeSbO4 is a p-d charge-transfer semiconductor.

LL3.14
Universal Quantum Parameters for Drug Design: A New SAR Approach. Vitor R. Coluci[1], Scheila F. Braga[1], Paulo V. M. B. Barone[2] and Douglas S. Galvao[1]; [1]Applied Physics, State University of Campinas, Campinas, Sao Paulo, Brazil; [2]Physics Department, Federal University of Juiz de Fora, Juiz de Fora, Minas Gerais, Brazil.

The electronic theory of cancer proposed by the late Alber Szent-Gyorgyi states that carcinogenic processes are related to the history of how life evolved on Earth. This history can be divided into two great eras separated by the appearance of light and oxygen on the atmosphere. In the first phase (called alpha) when life originated in a dark and airless globe covered by dense water vapor, there was no light and no oxygen. This is the period of simple life forms dominated by fermentation processes which do not require sophisticated structures. In the second phase (beta) when light appeared and life began to develop and differentiate, it was possible to build very complex living organisms with sophisticated regulatory mechanisms. In the alpha phase the atmosphere would be strongly reducing dominated by electron donors and the proteins very little reactive. In the beta phase with the oxygen as an efficient electron acceptor, desaturing the energy bands of the proteins more reactive structures are now possible. During cell division some parts of the biochemical machinery have to be dismantled and, in a certain sense, it is like the cell would travel back in time to the alpha state. After the cell division processes are completed the cell would go back to the modern beta state. If, for some reason, the return to the beta state is blocked the cell would continue to divide uncontrollably, which is basically the cancer definition. From this point of view the cancer would be a two-state problem where the cell is locked in the alpha primitive state. If these ideas are correct, and considering that the thermal/energetic window for biochemical processes is very narrow, we could expect that during life evolution molecules of practical use for the living processes would be selected in terms of their electronic structures. Following these ideas we have developed a new SAR methodology, named Electronic Indices Methodology (EIM). The EIM uses only two quantum electronic descriptors, based on the concept of local density of states and critical values for the energy separation involving molecular frontier orbitals. The EIM has been successfully applied to many classes of materials, such as, carninogenics, antitumorals, hormones, etc., always correctly classifying active and inactive compounds with an accuracy of ∼85-90%. EIM outperformed more standard SAR methods such as principal component analysis and neural networks. Although it is not clear yet the origin of the apparent class of universality of the EIM parameters, this methodology might represent a significant advance in the procedures of drug design.

LL3.15
Knowledge Extraction from an Experimental Crystal Structure Database. Kevin Tibbetts[1], Gerbrand Ceder[1] and Dane Morgan[2]; [1]MIT, Cambridge, Massachusetts; [2]University of Wisconsin, Madison, Wisconsin.

Materials scientists, Physicists and Chemists have been determining the crystal structure of materials through experiment for close to one hundred years. Much of this information is collected in large experimental databases. We have used one of these databases to investigate how much quantitative knowledge can be extracted from the experimental crystal structure observations in nature. The dataset consists of 28,000 entries spanning 1520 structure types in binary alloys. Only low temperature and low pressure entries were used. Most of the data is contained in the 200 most frequent structure types and over half of the structure types have only been observed in one alloy system. We show that very strong correlations exist in the data which could be turned into a method for predicting crystal structure from limited data on an alloy system or for verifying the consistency of data. Several data mining approaches can be used to extract useful correlations.

LL3.16
Microstructure and Composition of Au-Sn Eutectic Solder Electroplated from a Single Solution. G. H. Jeong, J. H. Kim, Duhyun Lee and S. J. Suh; Dept. of Advanced Materials Eng., Sungkyunkwan University, Suwon, Kyonggi-do, South Korea.

Gold-tin eutectic solder (Au-20 wt% Sn) has been widely used in optoelectronics and microelectronics industries for integrated chip or die bonding because it has a relatively high melting temperature (280°C), good creep behavior and good corrosion resistance. Conventionally Au-Sn alloys were deposited with two methods, one is the sequential electrodeposition of Au and Sn layers onto Au seed layers and the other is the sequential vapor deposition technique. Au-Sn eutectic solder has been deposited preferentially with the former because it has economic advantage relative to the latter. But the sequential epectrodeposition has disadvantages of post-deposition annealing, process complexity, cross-contamination between two bath, and Sn layer oxidation. Thus, the electroplating of Au-Sn from a single solution has been investigated as an alternative to conventional methods for depositing Au-Sn alloys. In this work, we produced Au-Sn eutectic solder from a single solution and optimized the composition and the microstructure of eutectic and near eutectic Au-Sn alloy for the micro-patterned cathode. The solution used for electroplating of Au-Sn alloy was cyanide-based solutions and

platinum was used as the anode. The cathode area in Si wafers/Ti (10 nm)/Cu (100 nm) was defined by a photoresist mask. The effects of process temperature and current density on deposition composition and microstructure were observed with EDX and SEM. Changing the process temperature from 40 to 70°C at 0.6 A/dm^2, the deposition composition of Au-Sn alloys changed from Au-4.4 wt% Sn to Au-32.5 wt% Sn including the 20wt% Sn eutectic composition and the grain size was increased monotonically. Also changing the current density from 0.4 to 1 A/dm^2 at 65°C, the deposition composition of Au-Sn alloys changed from Au-4.7 wt% Sn to Au-15.7 wt% Sn and the grain size was significantly increased. We could produce eutectic and near eutectic Au-Sn alloy at $\sim$ 0.7 A/dm^2 and 40°C and it has relatively good compositional uniformity and surface roughness. Uniformity of the deposition composition and the thickness was relatively high in case of the patterned cathode and it could be improved by using the systematical pattern. In addition, we especially investigated methods to improve the uniformity of deposition composition and thickness for the case of the micro-pattered cathode and tried to apply for interconnection process.

LL3.17

Automated Atomic Force Microscopy for Polymer Systems.

Daan Wouters[1,2], Bas G. G. Lohmeijer[1], Jolke Perelaer[1,2], Berend-Jan de Gans[1,2], Nico Adams[1,2] and Ulrich S. Schubert[1,2]; [1]Laboratory of Macromolecular Chemistry and Nanoscience, Eindhoven University of Technology, Eindhoven, Netherlands; [2]Dutch Polymer Institute (DPI), Eindhoven, Netherlands.

With the development of combinatorial materials research (CMR) methods for polymer research applications the demand for automated, high throughput characterization methods is increasing. Many characterization methods like NMR, GPC, DSC and UV-Vis are already available of have been modified in the mean time. With the increased attention of CMR towards the development of coating applications the importance of automated surface characterization techniques is increasing. Traditional scanning probe microscopy based techniques are well-suited for the characterization of (block co)polymer systems and blends. AFM can provide not only detailed topological and morphological information, but also properties like melting and crystallization behavior, conductivity, chemical and magnetic properties as well as stiffness and friction images on a local nanometer to micrometer scale. Whereas sample preparation methods such as multi-sector spincoating or inkjet printing can be automated the automation of SPM techniques is only just emerging. Earlier our group has presented the use of automated scanning probe microscopy for conductive carbon black-polymer composite systems. The effect of composition and curing rate on the morphology and conductivity of these composites was studied using an automated AFM approach. Here, we would like to extend the possibilities of automated AFM methods to the evaluation of the morphology and phase separation of a library of 16 diblock copolymers of polystyrene and polyethylene glycol polymers with metallo-supramolecular linkers as well as to the evaluation of PS-PMMA blends. In addition we applied the automated scanning probe microscope to study the growth of a periodic height relief on photo embossed gratings for display applications. When these films consisting of a mixture of monomers, pre-polymers, photoinitiator, and cross-linkers are illuminated through a grating a radical gradient is formed which causes a gradient in monomer concentration. Because of this gradient material flows from the non-illuminated areas towards the illuminated areas resulting in the formation of a periodic height relief. The height and the shape of this relief depend on the composition of the film, the film thickness, width of the period, light dose, temperature, and presence of additives. Large samples are prepared that allow simultaneous systematic variations in composition and processing conditions. Both automated atomic force microscopy and optical interferometry are used to evaluate the height and shape factor of these films. Rapid screening of important variables has been achieved by a combination of design of experiments and automated sample evaluation.

LL3.18

High-throughput Studies on Photochemical Properties of Transition Metal-Doped $SrTiO_3$ Epitaxial Thin Films.

Takeo Ohsawa[1], Hideomi Koinuma[2,3,4] and Yuji Matsumoto[1]; [1]Tokyo Institute of Technology, Yokohama, Japan; [2]The University of Tokyo, Kashiwa, Japan; [3]CREST-JST, Kawaguchi, Japan; [4]National Institute of Materials Science, Tsukuba, Japan.

Photocatalyst based on oxide semiconductor has now been widely used in water splitting, pollutant decomposition and light-induced hydrophilicity. These photochemical properties should be governed by complex factors such as composition, particle size and surface structure. The conventional one-by-one approach to finding a new photocatalyst or elucidating the mechanism of photocatalysis in polycrystalline form is, therefore, a hard task and time-consuming. An epitaxial oxide thin film would be a good model photocatalyst suitable to simplify the problem and it becomes more effective by combining with combinatorial technology, which has had a great impact on material science in recent years to improve drastically the methodology of synthesis and characterization. We have developed a combinatorial laser molecular-beam epitaxy (CLMBE) system, which can provide the following technological advantages: one is a parallel synthesis of high-quality epitaxial oxide thin films to be integrated on one substrate and the other is an atomically controlled growth of the film by $in-situ$ reflection high-energy electron diffraction (RHEED) intensity monitoring. In this paper, we report on high-throughput studies by the use of CLMBE technique on photochemical properties of transition metal (TM)-doped $SrTiO_3$ epitaxial thin films. The TM-doped $SrTiO_3$ thin films (TM: V and Cr) were epitaxially grown on Nb-doped $SrTiO_3$(001) single crystal substrate. Following the optimization of the growth condition to attain the layer-by-layer mode, composition spread ($SrTi_{1-x-y}V_xCr_yO_3$: 0$\leq$x+y$\leq$1, 20nm) and thickness-gradient films (0 to 30nm) of TM-doped $SrTiO_3$ were fabricated by the use of an originally designed slide mask. The photocatalytic activity on the film library was evaluated simultaneously by photo-reduction of Ag particles from $AgNO_3$ aqueous solution. V-doped $SrV_xTi_{1-x}O_3$ film grown on the Nb-doped $SrTiO_3$ was found to be more photoactive than any other compositions. It was, surprisingly, no enhancement of the photoactivity for $SrV_xTi_{1-x}O_3$ film on the non-doped $SrTiO_3$. Further studies of the V-doping effect revealed that the photocatalytic activity greatly depends on the V composition and film thickness: the optimized composition and thickness are x=0.05 and $\sim$10nm, respectively.

LL3.19

Study of the Martensitic Transformation in Shape Memory Thin Films Using a Combinatorial Approach Based on Micromachined Cantilever Beams.

Hyun-Jong Kim[1], Kyu-Hwan Oh[1] and Joost J. Vlassak[2]; [1]School of Materials Science and Engineering, Seoul National University, Seoul, South Korea; [2]Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts.

The combinatorial approach is ideal for evaluating the behavior of functional materials over a wide range of compositions. In a combinatorial study, the analysis of the property of interest is usually the bottleneck and high-throughput analysis techniques are needed are needed to perform the study efficiently. We have developed a technique that enables rapid determination of martensitic trans?formation temperatures and hystereses. The technique is based on the stress-induced deflection of cantilever beams and is applied to FePd-based ferromagnetic shape memory alloys. In this study, FePd films with Pd composition gradients were sputter deposited onto LPCVD SiNx-coated (100) Si wafers in which arrays of 7 x 8 cantilever beams were fabricated using bulk Si micromachining techniques. Each cantilever beam thus corresponds to an FePd alloy of well defined composition. The stress in the FePd films induces a curvature in the cantilever beams that is measured as a function of temperature using an optical system. In order to perform this measurement as quickly as possible, a Multi-Beam Optical Sensor System (M-BOSS) is used in which a single laser beam is split up into an array of 7 x 8 parallel laser beams using a diffraction grating. Each laser beam in this array is then scanned across a cantilever beam, while the reflected beams are captured on a high-resolution digital camera. As the temperature of the substrate is changed, the martensitic transformation of the film induces a significant change in stress that is readily measured using this approach. The transformation parameters are finally determined from the stress-temperature curve for each cantilever beam.

LL3.20

Novel method for determination of optical properties of wedged, rough, and absorbing thin films.

Jonghoon Baek[1], Desiderio Kovar[2], John W. Keto[3] and Michael F. Becker[1]; [1]Electrical and Computer Engineering, Texas Materials Institute, The University of Texas at Austin, Austin, Texas; [2]Mechanical Engineering, Texas Materials Institute, The University of Texas at Austin, Austin, Texas; [3]Physics, Texas Materials Institute, The University of Texas at Austin, Austin, Texas.

Non-uniformity in thickness and roughness of thin films can severely distort their transmission spectra as compared to those of flat, smooth films. Methods that extract properties such as refractive index, thickness, and extinction coefficient of such films can suffer inaccuracies when applied to wedged or rough films. In order to accurately extract optical properties of non-uniform films, we have developed a novel numerical method and efficient constitutive relations that can determine film properties from just the transmission spectrum. This Optimum Parameter Extraction (OPE) method can accommodate transparent or absorbing films with two-dimensional thickness variation and surface roughness that result in significant errors in the values of refractive index and film thickness if not considered. A packing-density model was proposed and used for refractive index to accelerate the fitting routine and to avoid finding

local minima instead of the global minimum. In this model, refractive index has one fitted parameter, the packing density, p. We show that for test cases and for actual PLD (Pulsed Laser Deposition) AlN thin films, properties such as refractive index, extinction coefficient, and film thickness were very accurately determined using our OPE method. These results are compared with two previous techniques to determine properties of thin films, and the accuracy and applicable conditions for all of these methods are discussed.

LL3.21
Characterizing Cell-material Interactions using Orthogonal Variable Gradient Methods. Lori A. Henderson[1], Matthew L. Becker[1], LeeAnn O. Bailey[1], Nathan D. Gallant[1], Jean S. Stephens[1], Joachim Kohn[2] and Eric J. Amis[1]; [1]Polymers Division, National Institute of Standards and Technology, Gaithersburg, Maryland; [2]Department of Chemistry, Rutgers, The State University of New Jersey, Piscataway, New Jersey.

New combinatorial approaches to material synthesis and characterization are affording opportunities to address complex biological hypotheses. These methods include cell biomaterial interactions and cover large variants in the physico-chemical parameter space simultaneously. Surface characteristics such as hydrophobicity, morphology, surface charge, and chemical functionality each play key roles in governing cell adhesion and proliferation. In addition, when mixing two or more individual materials, there are often instances where the new material shows a synergistic "improvement" in one or more of the properties of the material relative to the respective homopolymers. However, the optimization of polymer mixtures is a complicated process. Screening all combinations of materials and processing conditions by traditional methods for the purposes of optimization is impractical. Additional variables, not withstanding new chemical and processing methodologies, continually increase the physical parameter space, making gradient sample fabrication methods very attractive. Orthogonal gradient methods developed in the NIST Combinatorial Materials Center produce well-defined materials that afford simultaneous coverage of multidimensional chemical, composition, and physical property parameter space, and are finding application in the rapid evaluation of biological hypotheses including biocompatibility. Our efforts described herein, have been focused on the characterization of homopolymer and phase-separated blends films possessing gradients in composition and phase-separated domains, developing *invitro* assays for the measurement of inflammation and ECM gene regulation and identifying key physico-chemical parameters which influence the measurable responses. We anticipate these *invitro* methods will provide preliminary assessments of *invivo* material performance and provide the basis from which to explore further material optimization using combinatorial methods.

LL3.22
Structural, Electrical Properties of Polymers and Metal Doped Polymer Thin Films Deposited by Magnetron Sputtering Assisted Pulsed Laser Eposition Technique. Phani Ratna Ayalasomayajula[1] and James E. Kraznowski[1,2]; [1]Physics, CASTI-INFM Regional Laboratory, L'Aquila, Abruzzo, Italy; [2]Mechanical Engineering, University of New Hampshire, Durham, New Hampshire.

Recent years extensive research has been dedicated in the deposition of polymers and metal doped polymers finding applications in various electronic and optical coatings. In the present investigation, various polymer thin films such as polyacrylic, polyether imide, polyethylene, polyimide, polymethyl methacralate, polypropylene and polyvinyl chloride have been deposited from the respective solid source by ablating the 2 inch targets in Ar atmosphere, 10 mTorr pressure at room temperature. Metal (Ag, Al, Cu) doping of the polymers has been carried out by using simultaneous magnetron sputtering of the metal target and ablation of the polymer target at room temperature on silicon (100) and glass substrates. Several sets of experiments with increasing metal content in the polymers has also been conducted. The electrical properties of the metal doped polymers have been measured using four probe sheet resistance method. Structural, and microstructural properties of the individual polymer thin films as well as metal doped polymer thin films have been measured by X-ray diffraction and scanning electron microscopy as well as atomic force microscopy techniques. The stretching and vibrational modes of the C-C, C-O and C-H bands of various polymer thin films has been measured by Fourier Transform Infrared (FTIR) spectroscopy technique. These results are correlated with the degree of crystallinity and grain structure of the films.

LL3.23
Making Combinatorial Libraries of Titanium Based Alloys by Direct Metal Deposition Technique. Natalia Pimenova and Thomas L. Starr; Chemical Engineering Department, University of Louisville, Louisville, Kentucky.

Alpha/beta type titanium based alloys, such as Ti-6Al-4V and Ti-6Al-7Nb, have been used for orthopedic implant materials because of their combination of biocompatibility, corrosion resistance and mechanical properties. However, toxicity of alloying elements as compared to that of bone has been pointed out. In this project, the new type of titanium based alloys composed of non-toxic elements, such as Ti, Al, and Fe with lower modulus of elasticity, greater strength and greater corrosion resistance is designed. Using combinatorial approach the optimal ratio was found relatively easily. Direct metal deposition (DMD) is a novel precise manufacturing process for fabricating metal parts directly from Computer Aided Design (CAD) solid models. The DMD process allows making the combinatorial library of 49 different Ti based alloys in one piece. This combinatorial library dramatically reduces the time and cost of the investigation. The structure, mechanical and electrochemical properties of each new composition were studied using scanning electron microscopy (SEM) with energy-dispersive X-ray fluorescence analyzer, X-ray diffraction method, Rockwell C hardness test/Vickers microhardness test, potentiodynamic polarization method, and chronoamperometry. The link between the structure and the properties was found.

LL3.24
Optical Analysis of Thin Film Combinatorial Libraries. John D. Perkins[1], Brian M. Keyes[1], Charles W. Teplin[1], Maikel F. A. M. van Hest[1], Matthew P. Taylor[1,2], Lynn M. Gedvilas[1], Jeff L. Alleman[1], Matthew S. Dabney[1] and David S. Ginley[1]; [1]National Renewable Energy Lab., Golden, Colorado; [2]Colorado School of Mines, Golden, Colorado.

The combinatorial development of materials depends critically upon the development of appropriate characterization techniques. Since most optical techniques are inherently non-contact, they are amenable to automated position-scanning and hence for mapping applications of spatially varying libraries. At present, we have developed, and are using, optical reflection and transmission mapping over the spectral range of 200 nm to 25 μm. For the UV/VIS/NIR region, a multi-channel fiber-optically-coupled CCD-array-based spectrometer is used for simultaneous reflection and transmission mapping. For the IR, an FTIR spectrometer is used for sequential reflection and transmission maps. Depending upon the type of library being analyzed, the measured spectra can be analyzed for the optical band gap, film thickness, index of refraction, plasma frequency, conductivity, carrier scattering time and color in addition to simple reflectance and transmittance. For example, we have used reflectance spectroscopy based thickness mapping as the foundation for developing a combinatorial etch-rate mapping tool. This, and other examples, taken from our work on metal oxide thin film materials development will be presented.

LL3.25
The Use of Combinatorial Methodologies to Extract Work Functions of Metal Gates on HfO2, and Comparison with Scanning Kelvin Probe Microscopy (SKPM). Kao-shuo Chang[1,2], Martin Green[1], John Suehle[1], Eric Vogel[1], Hao Xiong[1], Monica Edelstein[1], Seong Eun Park[1], Joseph Kopanski[1], Ichiro Takeuchi[2], Jason Hattrick-Simpers[2], Olugbenga Famodu[2], Parhat Ahmet[3], Toyohiro Chikyow[3], Prashant Majhi[4] and Mark Gardner[4]; [1]Materials Science and Engineering, NIST, Gaithersburg, Maryland; [2]Materials Science and Engineering, University of Maryland, College Park, Maryland; [3]National Institute of Materials Science (NIMS), Tsukuba, Japan; [4]Sematech, Austin, Texas.

Metal gate electrodes are indispensable for future CMOS (Complement Metal Oxide Semiconductor) applications since they avoid poly-Si depletion and dopant diffusion effects. However, the selection of metal gates with proper work functions is very tedious, since elemental metals seem not to have appropriate properties, and the determination of work function is not trivial because it is dependent on integration conditions and the underlying dielectrics. Since work function is directly related to the threshold voltage (VT), work function must be properly selected for optimum transistor performance. We use combinatorial methodologies to systematically study all these issues. Many ternary composition spreads ("libraries") were deposited on HfO2 by ion beam evaporation. In this talk, we will use the Nb-W-Pt ternary system as an example, and demonstrate the effectiveness of combinatorial methodology for the exploration of metal gates. Electrical properties such as capacitance (C) and leakage current (I) were measured by a computer controlled autoprobe. We found that devices near the Nb and Pt rich corners were better than W-rich alloys because of smaller interface trap densities and leakage current. The Hauser CVC program was used to extract the flat band voltage (Vfb) by fitting the measured capacitance-voltage (C-V) curves. The relative work functions were then calculated assuming known interface trap densities. Scanning Kelvin probe microscopy (SKPM) was also used to extract the nominal work function, for

comparison. We found a general agreement between the two measured results by normalizing the extracted work function.

LL3.26
The Investigation of the Effects of Polyelectrolyte Attributes on Complex Coacervate Properties using High-Throughput Formulation and Characterization Techniques.
Robert Yeats Lochhead[1] and Lisa R. Huisinga[1]; [1]School of Polymers & High Performance Materials, The University of Southern Mississippi, Hattiesburg, Mississippi; [2]The School of Polymers and High Performance Materials, The University of Southern Mississippi, Hattiesburg, Mississippi.

Polyelectrolyte-surfactant complex coacervates have a wide variety of applications in the formulation and/or production of consumer products. Many real products require coacervates that have been formed in the concentrated polymer-surfactant regime. However, much of the scientific efforts have been directed at the dilute regime. Therefore, there is a need to understand the mechanisms in the semi-dilute and concentrated regimes. Details of polyelectrolyte-surfactant interactions are complex and known to change with slight changes in composition. A complete study of polyelectrolyte-surfactant interaction would require the formulation and investigation of many thousands of compositions. This challenge is amenable to the high throughput screening formulation techniques that have been developed in our research group. Titration of components into 96-well plates, through the use of state-of-the-art robotics, allows rapid formulation of products over a wide compositional range. Rapid examination of these samples using UV-Vis spectrophotometry provides identification of two phase regions and relative amounts of phase separation in those regions. Examination of the samples through cross-polarizers allows rapid screening for samples that exhibit some degree of coherent ordering. Cationic polyelectrolytes of varying architecture, molecular weight, ion charge density, and hydrophobic modification were studied, in conjunction with anionic surfactants, using the above high-throughput methods. The results are shown as phase diagrams that allow rapid investigation of the effect of the aforementioned polymer attributes, as well as micelle structure and charge density, up to and including lyotropic liquid crystal structures. These phase diagrams enable rapid targeting of optimal systems, providing a guide to formulation and scale-up by allowing the formulator to seek regions of unique attributes that could be missed by conventional formulation approaches.

LL3.27
Abstract Withdrawn

LL3.28
Cathodic Arc Plasma Combinatorial Material Synthesis for Composition Search of New Amorphous Alloy.
Seiichi Hata[1], Ryusuke Yamauchi[2], Junpei Sakurai[1] and Akira Shimokohbe[1]; [1]Precision and Intelligence Labratory, Tokyo Institute of Technology, Yokohama, Kanagawa, Japan; [2]Mechano-Micro Engineering, Tokyo Institute of Technology, Yokohama, Kanagawa, Japan.

This paper reports a new combinatorial materials synthesis using cathodic arc plasma deposition (arc-combi), mainly applicable to searches for new amorphous alloys compositions. The arc-combi setup has three cathodic arc plasma guns which are improved for arc-combi. The CAPGs are arranged at the vacuum chamber sidewall. There is a permanent magnet at the bottom in the chamber. A substrate locates above the magnet. The sample group with composition gradient (integrated library) is deposited on the substrate by the CAPGs. Evaporated cathode material in the CAPG is plasmarized and emitted along the cathode axis. Intermittent (pulse-like) deposition of the film is thus performed by the CAPG. The plasma, which contains vapor deposition particles, can be guided by a magnetic filed of the magnet. Owing to points of deposition convergence are distributed for each element, a thin film showing a continuous composition gradient can be produced on the substrate. The arc-combi setup is simple, layout-free and low-power-consumption design. In the present study, the thin film was divided into 1,089 (33x33) samples, each 1x1 mm in size, by a lift-off grid on the substrate. This sample group became the integrated library. The grid was a patterned Cu thin film on photosensitive polyimide with a 6-bit marker, which indicates the address of matrices, on the sides. The integrated library was deposited on the substrate with the grid which was electrically grounded. The grid was re-moved by acetone after deposition. Fabrication of Pd, Cu, and Si thin films was conducted in an attempt to determine the composition with the lowest electrical resistivity among amorphous PdCuSi alloys. A Pd50Si50 (at.%) cathode manufactured by powder sintering was used as a substitute for the Si cathode, which is difficult to use in the present CAPG since Si is a semiconductor. In order to measure the thickness distribution and deposition rate, Pd, Cu and Si (Pd50Si50) films were deposited on the substrate with the grid. Deposition conditions were as follows. Electric discharge intervals: 1 s, condenser capacity: 8,800 uF, number-of-times of electric discharge (pulse): 10,000, and chamber pressure: 1x10e-3 Pa. Each deposition rate per pulse in the thickest region of Pd, Cu, and PdSi film is on the order of the respective atomic diameter, suggesting that deposited particles were piled up discretely. Co-deposition is performed using three CAPGs to fabricate a Pd-Cu-Si alloy. The Pd-Cu-Si thin film could be deposited to a thickness of 200 nm or more near the center of the integrated library. The average composition in the central region (500 um2) of several samples in the center of the integrated library was measured by EDS. The integrated library (sample group) having over 300 different compositions was successfully established.

LL3.29
Combinatorial Materials Exploration for Gate Stack Structures of Metal Gate Electrodes and High-κ Dielectric Films.
Kenji Ohmori[1], P. Ahmet[1], D. Kukuruznyak[1], T. Nagata[1], K. Nakajima[1], K. Yamada[2], K. Shiraishi[3], G. Richter[4], T. Wagner[4], K.-S. Chang[5], M. L. Green[5] and T. Chikyow[1]; [1]Nanomaterials Lab, National Institute for Materials Science, Tsukuba, Japan; [2]Nanotech Center, Waseda University, Tokyo, Japan; [3]Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Japan; [4]Max Planck Institute for Matals Research, Stuttgart, Germany; [5]National Institute of Standards and Technology, Gaithersburg, Maryland.

Hf-based high-κ dielectric films such as HfO2, HfSiO(N), and HfAlO are of intense interest as the most promising candidates for the replacement of the current gate SiO2 and/or SiON films. However, the Hf-based dielectric films have inevitable fixed charges derived from oxygen vacancies, which cause a crucial problem to control the threshold voltage of devices. Therefore, thermal stability of stacked structures is quite important as well as the selection of gate materials which have suitable work functions for both p- and n-MOS FETs in the future device fabrication. For this issue, we have applied a combinatorial method on the exploration of elemental materials and their stacked structures for next generation CMOS devices. We focus on the flatband shift caused by metal/high-κ and high-κ/Si interfaces and propose a way for finding the ideal gate stack structure which thermodynamically stabilizes under a given materials system from the viewpoint of equilibrium phase diagram. A 5-nm-thick Pt-W alloy spread film with a varied composition ratio R of Pt/(Pt+W) was deposited on a HfO2/Si(001) substrate at room temperature by a combinatorial ion beam sputtering system. Using x-ray photoelectron spectroscopy, the work function was measured and gradually changes by 0.8 eV from 5.5 (R = 1, i.e., Pt) to 4.7 eV (R = 0, W). On the other hand, the changes of flatband shift as a function of R (1 ? R ? 0) obtained by capacitance-voltage measurements is 0.24 eV, much smaller than the work function difference. We attribute this to the Fermi level pinning due to traps at the metal/high-κ interface. A mediate layer such as Y2Si2O7 was inserted in a high-κ/Si structure changing the insert position using a combinatorial technique. Significant improvement in the flatband shift by the mediate layer insertion at the high-κ/Si interface is observed and explained well using equilibrium phase diagrams for the stacked structure. Through these studies, we discuss the combinatorial method and its future direction for the exploration of metal gate electrodes and high-κ gate dielectric films. This work is partially supported by JSPS Core to Core Program.

LL3.30
Study of Binary Oxide Material HfO2: SiO_2 for High-k Gate Oxide Material by Combinatorial Material Library Method.
Wen-Hsuan Chao, Shu-Huei Wang, Tien-Heng Huang, Lih-Ping Wang, Ren-Jye Wu and Hung-Chiao Cheng; High-throughput Synthesis and Analysis Laboratory, Union Chemical Laboratories, Industrial Technology Research Institute, Chutung, Hsinchu, Taiwan.

The scaling of SiO_2 gate oxide film has a fundamental limit of 1.5-1.8 nm, below which the leak current becomes a serious problem. Therefore, the substitution of SiO_2 with high-k materials as gate dielectrics becomes more important. The candidates for next generation gate oxides, which are in direct contact with Si channel, must exhibit high dielectric constant to reduce the thickness of the gate insulation film and to improve leakage current problem. Many high-k materials have been studied for the integration with standard CMOS technology. Hafnium silicates (HfO_2:SiO_2 , HSO) recently attract a lot of fundamental and technological interests due to its high dielectric constant and low leakage current. The structure and properties of HSO gate oxides was studied with a combinatorial continuous-compositional-spread method in this research. HSO material libraries was synthesized on a 4-inch wafer at room temperature and 200°C using a custom-built radio-frequency (RF) sputtering system. The electrical properties of HSO material libraries were measured with Metal-Oxide-Semiconductor structure. X-ray diffraction (XRD) and X-ray Photoelectron Spectroscopy (XPS) were used to characterize the structure and compositions of HSO material libraries. The effects of different sputtering conditions on the properties of HSO gate oxides were studied. The dielectrics constants

(ϵr) of HSO material libraries treated with rapid temperature annealing (600°C/1min/N2) were in the range of 5∼25, determined by C-V measurement, and the dielectric constant was observed to increase with increasing HfO_2 content. The I-V curves of HSO material libraries show that the leakage current decreases with the amount of Si in the HSO films. Structural characteristics of HSO films with RTA treatment (1000°C/10sec/N_2) varied from amorphous to crystalline state (tetragonal and monoclinic phase), depending on the composition of material libraries. The correlation among the electrical property, composition and crystal structure of HSO films will be discussed.

LL3.31
Combinatorial Solution, Powder and Thin-Film Preparation System Applied Electrostatic Atomization Technology.
Kenjiro Fujimoto[1,2], Shigeru Ito[1], Takeji Kato[1], Motohiko Sato[1], Satoru Inoue[2] and Mamoru Watanabe[2]; [1]Tokyo University of Science, Noda, Japan; [2]National Institute for Materials Science, Tsukuba, Japan.

The combinatorial synthesis in present materials science uses equipments which are independent for solutions, powders and thin films preparation. If powder and thin film of ternary or multinary compounds are effectively obtained from one apparatus, materials fabrication corresponding to our purpose will be convenient in case of a series of studies about the powder preparation for making reaction phase diagrams, the thin film preparation for characterization and so on. In this study, we have developed new high−throughput material-exploration system 〃M-ist Combi〃 based on combinatorial chemistry and electrostatic spray deposition technology. In this electrostatic spray deposition technology, the materials to be deposited on the grounded hot substrate are atomized by applying a high voltage to the liquid. The deposition range on the substrate is dependent on the applied voltage. With the increase of the applied voltage, the size of atomized droplet reduces, and the deposition range enlarges by the electrostatic repulsion. The 〃M-ist Combi〃 system has modules such as starting materials adjustment, high voltage power supply and atomization positioning robot which are continuously controlled by the computer. Until now, the researches by using the electrostatic spray deposition technology are only to atomize foggy liquid applied high−voltage and deposit thin film on the hot substrate. So, we added the function which controlled the value of the applied voltage to the liquid. In case that the applied voltage is 9−10 kV, the liquid is atomized and deposited as film on the substrate. In case that the applied voltage is 3−4 kV, the liquid becomes small droplet which is bigger than the mist, and then, the powder deposited on the substrate in narrow range in a only few minutes. Furthermore, this system can use as a synthesizer of liquid library, if the voltage is not applied. Therefore, this 〃M-ist Combi〃 system structure can prepare not only thin film but also powder or solution library which has various compounds ratio. In addition, the material screening is accelerated, if this 〃M-ist Combi〃 is combined with high−throughput evaluation apparatus such as X−ray.

LL3.32
Abstract Withdrawn

LL3.33
Development of high-throughput terahertz time-domain spectroscopy system and its application to combinatorial samples.
Makoto Ohtani[1], Yasushi Hirose[1], Taro Hitosugi[1,2], Yutaka Furubayashi[1], Toshihiro Shimada[1,2] and Tetsuya Hasegawa[1,2]; [1]Kanagawa Academy of Science and Technology, Kawasaki, Japan; [2]Department of Chemistry, University of Tokyo, Tokyo, Japan.

The terahertz (THz) waves fall between microwave and infrared radiation of the electromagnetic spectrum. Recently, THz time-domain spectroscopy (TTDS) has received much attention as a powerful method for measuring electrical and optical properties, such as complex refractive index, complex dielectric function and complex electrical conductivity. In addition, this technique enables us to map out the above-mentioned properties in non-contact and non-destructive manners, which is very useful for high-throughput characterizations of combinatorial libraries. Here, we report on the development of a high-throughput terahertz time-domain spectroscopy (CTTDS) system. The CTTDS system allows us to measure a THz spectrum of each pixel within two seconds, which is approximately 300 times shorter than that of conventional TTDS systems. We have applied the CTTDS to transparent conductor Nb:TiO_2 thin films, and found that the THz time-domain waveforms transmitted through the Nb:TiO_2 films strongly depend on Nb concentration.

LL3.34
Abstract Withdrawn

LL3.35
Rapid Optimization of Pentacene Buffer for Rubrene Thin Film Growth by Using Combinatorial MBE.
Masamitsu Haemori[1], Jun Yamaguchi[1], Seiichirou Yaginuma[1], Kenji Itaka[2,3] and Hideomi Koinuma[2,3,4]; [1]Materials and Structures Laboratory, Tokyo Institute of Technology, Yokohama, Japan; [2]Graduate School of Frontier Sciences, The University of Tokyo, Kashiwa, Japan; [3]CREST-JST, Kawaguchi, Japan; [4]NIMS, Tsukuba, Japan.

In these years, organic field effect transistors (OFETs) have received much attention, and OFETs with high mobility are required for broader application. Recently, a rubrene (5,6,11,12-tetraphenylnaphthacene) single crystal FET, which has the highest mobilities in OFET, was reported. This FET showed *p*-type operation and exhibited high intrinsic mobilities of 4.4 and 15.4 $cm^2/V{\cdot}s$ along the *a* and *b* axes, respectively. Rubrene is the well-known compounds as a yellow electroluminescence dopant, however, there is no report of crystalline rubrene thin film. We suspect that the reason why rubrene thin films are hardly crystallized is the bulky structure of rubrene with four phenyl groups in the side chain. We inserted a ultrasmooth pentacene monolayer between a π-conjugated organic thin film and the substrate to promote the migration of the organic molecules because the existence of a weak attractive interaction between pentacene and rubrene molecules is expected. In order to clarify the effect of the pentacene buffer, we used combinatorial mask system to vary the thickness of pentacene from 0 to 1monolayer. After the deposition of thickness-gradient pentacene buffer, the thick rubrene films were deposited on it. AFM image of this film on the less pentacene buffer side shows droplet-like amorphous morphology, while that of thin film on the 1ML-thick pentacene shows flat morphology. By analysis of x-ray diffraction, the rubrene film only on the pentacene buffer showed the *c*-axis orientation. Finally, we fabricated the rubrene film field effect transistors with and without pentacene buffer. The FET only with pentacene buffer exhibited *p*-type operation, of which mobility of this FET was 0.05 $cm^2/V{\cdot}s$. This is first report for the rubrene thin film transistors in the literature.

LL3.36
Modifying La-Mg-Ni Alloy Thin Film Microstructure Using Combinatorial Methods.
Charles H. Olk[1] and Daad Haddad[2,1]; [1]Materials & Processes Lab, General Motors Research Development & Planning, Warren, Michigan; [2]School of Materials Engineering, Purdue University, West Lafayette, Indiana.

We have grown an array of discrete La-Mg-Ni thin films using combinatorial methods to modify the film microstructure by fine-tuning the composition. This method for creation of nanocrystalline/amorphous microstructure is significantly different from the usual energetic mechanical methods. Electron probe microanalysis measurements showed that our films have a wide range of compositions. The structures and surfaces of the different alloy films were studied using X-ray diffraction (XRD) and atomic force microscopy (AFM). XRD measurements revealed that the Mg-rich alloys consist of a main phase of (La, Mg)Ni3 with the hexagonal PuNi3-type structure and minor impurity phases of LaNi5. However, XRD of the La-rich alloys showed the formation of amorphous and nanocrystalline phases. AFM phase images showed different phases corresponding to different nucleation processes for the Mg-rich and La-rich alloys.

LL3.37
Development of a Modular Platform for High-throughput Formulation of Highly Viscous Fluids
Torsten Zech[1], Gunilla Bohner[1], Alexander Cross[1], Ringo Fodisch[1], Frank Gullich[1], Ralf Nossek[1], Thomas Schrapel[1], Uwe Vietz[1], Guidl Desie[2], Erik Van gell[2], Johan Paul[3]; [1]hte Aktiengesellschaft, Heidelberg, Germany; [2]Agfa-Gevaert N.V., Mortsel, Belgium; [3]Flamac vzw, Zwijnaarde, Belgium.

We present a modular platform for high-throughput formulation of highly viscous fluids and powders that was developed under the scope of the Flamac-hte collaboration. Using weight-based dispensing technologies, liquids and powders can be formulated for a diverse range of applications, such as coatings, inks and catalysts. The platform is designed for a throughput of 48-96 formulations per day, where an individual recipe may easily consist of more than 10 dispense steps (liquids and powders) as well as a number of process steps (stirring at a certain speed for a certain time) with a well-defined sequence. The platform, in its initial state, consists of four individual modules performing the necessary chemical functions, namely a fluid dispensing module, a solid dispensing module, a stirring module and a logistics module (sample storage and barcode reading). These modules are connected by a robotic handling system that performs all transfer tasks of the individual sample vials within the platform. The platform is fully automatically operated by hteControl, hte's advanced process control application, combining proprietary and newly developed equipment as well as commercial

components. Among the major design goals were flexibility and extensibility, as high-throughput experimentation projects tend to vary significantly over time requiring important changes to the initial workflows. Therefore, the platform is flexible with regard to sample size (approximately 5-80 g of formulation) which can be formulated in a broad range of different vials. Additionally, the individual liquid dispense amounts cover four orders of magnitude, i.e. from 50 mg to 50 g, while using the same, newly developed dispense principle. This principle is applicable for low-viscosity liquids such as solvents, highly viscous substances (tested up to 10 Pa s) as well as stirred dispersions. Detailed dispense data, proving accuracy, reproducibility and speed, is presented. Furthermore, the robotic handling system is designed in a way, that the individual modules can be exchanged or re-grouped around the handling system, as well as new modules performing different functions can be added which makes future extensions to the platform possible. The operation of the platform is supported by our data management system myhte, which provides the necessary experimental design features (recipe generation and DoE), workflow integration functions and data analysis capabilities.

SESSION LL4: Polymers and Coatings
Chairs: Eric Amis and Ulrich Schubert
Tuesday Morning, November 29, 2005
Back Bay B (Sheraton)

8:00 AM *LL4.1
High throughput discovery for adhesives and coatings. Didier Benoit, Damian A. Hajduk, Miroslav Petro, Marcelo Piotti, Shaofeng Ran and Steven Zong; Symyx Technologies, Inc., Santa Clara, California.

We describe high throughput instruments and methods for the synthesis of novel resins suitable for adhesives and coatings, the formulation of these resins into model products, and the measurement of numerous chemical and physical properties. Examples of these properties include tack, friction, solvent resistance, durability, and dynamic mechanical response. This talk will survey these capabilities and provide examples of their successful use within industrial discovery programs. One specific application is the development of formulations with adjustable solubilities, active agent release rates, and triggerable consistency changes for personal care applications.

8:30 AM *LL4.2
High-Throughput Preparation and Screening of Polymeric Coatings. Jaime C. Grunlan, [1]Mechanical Engineering, Texas A&M University, College Station, Texas; [2]Polymer Technology Center, Texas A&M University, College Station, Texas; [3]Materials Science and Engineering Program, Texas A&M University, College Station, Texas.

A combinatorial factory for the preparation and screening of polymeric coatings was developed. Coating formulations were prepared and coated using novel combinatorial techniques to obtain libraries of varying composition and thickness. The thickness of each film in a combinatorial array is rapidly determined via visible-light absorbance of optical dyes in conjunction with the Beer-Lambert relationship. These combinatorial libraries were then tested and screened using a variety of custom-made high-throughput methods. Combinatorial screening of oxygen and moisture transmission rate, along with adhesive properties, will be presented here. OTR and MVTR are determined using spectroscopic techniques. For adhesion, a spherical probe adhesive tester is able to generate parameters linked to tack, peel, and shear in one measurement. In addition to describing the testing methodology, benefits and shortcomings of these techniques will be highlighted.

9:00 AM LL4.3
Combinatorial and High-throughput Experimentation in Polymer Science: Recent Advances. Ulrich S. Schubert, Laboratory of Macromolecular Chemistry and Nanoscience, Eindhoven University of Technology and Dutch Polymer Institute, Eindhoven, Netherlands.

Combinatorial and high-throughput technologies and approaches open new avenues for polymer science, both regarding the understanding of structure-property relationships as well as the selected design of new materials and the development of efficient polymerization processes [1]. Therefore, automated synthesizers were successfully utilized to study a variety of polymerizations. This approach was first applied to the living cationic ring opening polymerization (CROP) of 2-oxazoline monomers [2] and to atom-transfer radical polymerization (ATRP) of MMA, followed by RAFT and NMRP experiments and finally ending with anionic polymerizations [3]. For these systems, first the reproducibility and comparability with conventional experiments was proven. Subsequently, new reaction conditions, catalysts and systematical variations in polymer composition have been studied in detail. Furthermore, procedures for automated sampling and sample preparation for online and offline (kinetic) investigations of these polymerization techniques, utilizing GC, GPC and MALDI-TOFMS, were developed in order to gain a better inside into the polymerization processes [2 4]. Moreover, the automation of kinetic studies largely improved the comparability and/or quality of the obtained results. Besides classical thermal heating also microwave-assisted polymerizations were performed [5]. The obtained data were subsequently utilized in order to prepare defined block and random copolymers, star-like architectures and telechelics. These examples can serve as basis for the extension to other polymerization processes, such as e.g. ROMP, polycondensations or olefin polymerizations. In addition, combinatorial methods for defined spot or film preparation utilizing combinatorial spin-coating and ink-jet printing as well as automated methods for the characterization of thin films, such as optical plate reader, nanoindenter or AFM were applied [6]. Finally, a common platform for data-storage and handling was introduced and the combination of Design of Experiments (DoE), data-mining and modeling tools allowed to close the high-throughput experimentation cycle [7]. [1] Recent review: M.A.R. Meier, R. Hoogenboom, U.S. Schubert, Macromol. Rapid Commun. 2004, 25, 21-33. [2] R. Hoogenboom, M.W.M. Fijten, U.S. Schubert, J. Polym. Sci.: Part A: Polym. Chem. 2004, 42, 1830-1840. [3] C. Guerrero-Sanchez, U.S. Schubert, J. Polym. Sci.: Part A: Polym. Chem. 2005, in press. [4] R. Hoogenboom, M.W.M. Fijten, C.H. Abeln, U.S. Schubert, Macromol. Rapid Commun. 2004, 25, 237-242. [5] R. Hoogenboom, F. Wiesbrock, M.A.M. Leenen, M.A.R. Meier, Ulrich S. Schubert, J. Comb. Chem. 2005, 7, 10-13. [6] B.-J. de Gans, P. Duineveld, U.S. Schubert, Adv. Mater. 2004, 16, 203-213; E. Tekin, B.-J. de Gans, L. Xue, U.S. Agarwal, U.S. Schubert. Macromol. Rapid Commun. 2005, 26, 310-314. [7] N. Adams, U.S. Schubert, J. Comb. Chem. 2004, 6, 12-23; N. Adams, U.S. Schubert, QSAR & Comb. Sci. 2005, 42, 58-65.

9:15 AM LL4.4
High Throughput Screening of Marine Coatings using Biological Assays. Bret Chisholm[1,2], Shane Stafslien[1], James Bahr[1], David Christianson[1] and Dean Webster[2]; [1]Center for Nanoscale Science and Engineering, Fargo, North Dakota; [2]Coatings and Polymeric Materials, North Dakota State University, Fargo, North Dakota.

A combinatorial workflow for developing organic surface coatings has been developed. The workflow is uniquely designed to prepare and evaluate marine coatings that prevent biofouling on the hulls of ships. A critical component of the workflow is the high throughput screening of settlement and ease of removal of marine organisms from coating surfaces. Methods have been developed to directly and indirectly quantify settlement and removal of various marine bacteria. In addition, an assay for evaluating settlement and removal of diatoms has been completed. Currently, correlations are being developed between these high throughput bioassays and results from field testing (testing of samples aged in both the Pacific and Atlantic ocean).

9:30 AM LL4.5
High Throughput Characterization of Liquid Crystal - Alignment Layer Interactions Using Planar Array Infrared Spectroscopy. Chris Snively[2,1] and John F. Rabolt[2]; [1]Chemical Engineering, University of Delaware, Newark, Delaware; [2]Materials Science and Engineering, University of Delaware, Newark, Delaware.

The interactions between liquid crystals and alignment layers have historically been probed by a variety of techniques. Of particular interest is the use of infrared spectroscopy due to the ability of obtaining rich chemical information that can give insight into the interactions occurring at the liquid crystal / alignment layer interface. Additional advantages include the ability to study these systems in a realistic sample geometry and the ability to characterize the temporal response over a wide range of scales, from seconds to nanoseconds. The typical approach for these studies has involved the use of step scan time resolved infrared spectroscopy. This technique can simultaneously provide a wide spectral coverage and high temporal resolution. However, it suffers from the necessity to repeat the experiment hundreds of times for the acquisition of a given data set. This requires a highly reproducible sample response. Any changes in response of the sample during the experiment will simply be averaged together and will not be seen. Planar array infrared (PAIR) spectroscopy has been developed as a single-shot approach to the collection of time resolved spectral information. This technique is based upon an infrared spectrograph and a focal plane array detector and is capable of providing spectral coverage over several hundred wavenumbers and temporal resolution down to several hundreds of microseconds. We have applied PAIR as a high throughput tool for the study of the dynamics of liquid crystals in the presence of different types of alignment layers. In a single shot experiment, the dynamic response of several liquid crystal samples can be determined simultaneously. As a proof of principle, we present examples of the dynamics of the nematic liquid crystal 5CB in the presence of a variety of alignment layers, including spin-coated polymer films and dip-coated small molecular films. Results from experiments utilizing

both electric field and shear fields as the perturbation will be presented.

9:45 AM LL4.6
Controlled Radical Polymerization on a Chip. Tao Wu, Ying Mei, Chang Xu and Kathryn L. Beers; NIST, Gaithersburg, Maryland.

Research on chemical reactions in micro-size reactors has attracted wide interests and is a promising field from both academic and industrial perspectives due to potentially better control of reaction conditions, speed, smaller specimen sizes, improved safety, and portability. In our presentation, we demonstrate the successful application of controlled radical polymerization on a chip (CRP chip) to synthesize block copolymers (poly(ethylene oxide-b-hydroxylpropyl methacrylate) (PEO-b-PHPMA) through atom transfer radical polymerization (ATRP). The CRP chip design enables control of polymer relative molecular mass and architecture through flow rates, which govern the polymerization time. Thus by conducting a series of well-controlled copolymerizations, carried out at different pumping rates (i.e., reaction times) with a constant concentration ratio of monomer to initiator, we can produce a block copolymer library with a range of relative molecular masses of the second block. A unique advantage of the CRP chip is that it can be used to execute complex designed experiments. For example, we have used the CRP chip to rapidly measure polymerization kinetics in a new way. Based on the well-known ATRP model, we have derived a relationship between molecular weight and concentration ratio of monomer to initiator. Using this relationship, we are able to study the polymerization kinetics by simply measuring the relative molecular mass of polymer products from a series of experiments having the same reaction time but different initiator concentrations. Compared to the difficulty of preparing batch reactions with a wide range of different concentrations, we show that a CRP chip can quickly produce similar results with this so-called stoichiometric design, in which the stoichiometry of the mixture is adjusted by varying the relative flow rates of each input to change reactant concentrations.

10:30 AM *LL4.7
Microfluidic Technology for High Throughput Polymer Science. Kathryn L. Beers and Eric J. Amis; Polymers Division, NIST, Gaithersburg, Maryland.

Commercially available combinatorial and high throughput fluid handling and measurement capabilities have enabled tremendous progress in product development in the biosciences and the chemical industry; however, the platforms are often costly and time-consuming to implement. The approach adopted by most manufacturers has been to build automated platforms that mimic the development process for a specific material in a narrow application. This greatly increases data acquisition rates, but it is challenging to adapt this system-specific infrastructure to changing R&D needs. In response, our research aims to develop new methods for the manipulation and measurement of complex polymeric fluids, thereby providing flexible and inexpensive alternatives to robotics driven instrumentation. To improve the versatility of high throughput formulations testing, we employ microfluidic technology to build a toolset of complementary library fabrication and test methods. The preparation of devices is fast and modular, allowing for rapid prototype development and increased flexibility. We have demonstrated the use of microfluidic chips for the synthesis, mixing and measurements of a variety of systems. Synthetic techniques include controlled radical polymerization on a chip (CRP chip), and organic phase droplets as polymerization microreactors. Measurement methods include interfacial tension, polymer shrinkage and on-line Raman spectroscopy.

11:00 AM *LL4.8
High Throughput Synthesis And Screening Methods For The Design Of Complex Coating Systems For Marine Applications. Dean Webster[1,2], Bret J Chisholm[2,1], Shane Stafslien[2], James Bahr[2], David Christianson[2], Partha Majumdar[1], Abdullah Ekin[1] and Robert Pieper[1]; [1]Coatings and Polymeric Materials, North Dakota State University, Fargo, North Dakota; [2]Center for Nanoscale Science and Engineering, North Dakota State University, Fargo, North Dakota.

A high throughput workflow has been developed for the rapid synthesis and screening of candidate coatings for ship hulls. New non-toxic ship hull coating systems are needed which either prevent the settlement of marine organisms or permit their easy release. In addition, these coatings need to be mechanically robust, have good adhesion, and be chemically stable under constant water immersion for years. Typical candidate coating systems are comprised of multiple oligomers and crosslinkers, catalysts, solvents, and other additives. Reactive oligomers can also widely vary in composition, functionality and reactivity. Thus, a large number of variables are involved and it is not always clear from first principals what specific composition will lead to a suitable coating system. Libraries of oligomers and coatings having varying composition can be prepared using automated synthesis, formulation, and application systems. Key laboratory screening tests include surface energy and pseudo-barnacle pull-off adhesion, and parallel dynamic mechanical thermal analysis. Stability of the coating surfaces is screened by comparing surface energy and pull-off adhesion before and after water immersion of the coatings. Screening tests where the coatings are also challenged with bacteria, algae, and diatoms have been developed to characterize the adhesion of these organisms to the coatings surfaces.

11:30 AM *LL4.9
Application of HTS to Complex Formulations: Antimicrobials in Latex Systems. Douglas Wicks[1], Alicyn Rhoades[1], John Williamson[2] and Bruhaspathy Miriyala[2]; [1]School of Polymers and High Performance Materials, The University of Southern Mississippi, Hattiesburg, Mississippi; [2]Department of Medicinal Chemistry, The University of Mississippi, Oxford, Mississippi.

The study and application of antimicrobial peptides is a rapidly growing niche field in important areas such as pharmaceutics and medicinal chemistry. As a result, most studies of antimicrobial peptides are completed in environments relevant to in-vivo applications. The use of synthetically derived antimicrobial peptides in applications outside the medical realm is a relatively untapped field, with the impact interaction of these with the ingredients of polymer systems being unknown. Water-based polymer coating systems are attractive targets for microbial invasion because of their inherent material properties. Water-based polymer latex coatings contain a number components which aide in stabilization and coalescence of the polymer particles, such as surfactants and polymeric cellulose-derived molecules, with several types of molecular structures existing for each. Microbes are able to flourish within the water phase of latexes while taking sustenance from these dispersion components, resulting in a loss of system properties commonly recognized as 'spoilage'. This work addresses impactat of formulation variables on conventional biocides and model oligopeptide based ones through use of HT fluoresence measurements. Examples of the ability to detect complex was seen in the observation that the morphology of the surfactant molecules in solution may also have an impact on biocide performance. Surfactant molecules can undergo a wide range of morphological structures, including liquid and solid crystal formation. Within liquid crystal formation surfactant molecules can organize as lamellar and hexagonal structures, just to cite a few examples of morphology changes that can be detected and may have different effects on biocide efficacy.

SESSION LL5: Polymers and Biopolymers
Chairs: Bret Chisholm and Jaime Grunlan
Tuesday Afternoon, November 29, 2005
Back Bay B (Sheraton)

1:30 PM *LL5.1
Thinking Outside the Gradient Box. Eric J. Amis, Michael J. Fasolka, Kathryn L. Beers, Zuzanna Cygan and Sheng Lin-Gibson; Polymers Division, NIST, Gaithersburg, Maryland.

In addition to applications for synthesis, combinatorial methods hold potential for rapid and systematic generation of experimental data over the multi-parameter space typical of materials. At NIST we have applied combinatorial methods for research on polymers using predominately the paradigm of gradients that allow simple and transferable methods of library fabrication to be coupled with high-throughput measurements. While we have shown several examples of this approach to investigations of polymer thin films, biomaterials, polymer blends, and filled polymers, we have also seen that restricting our thinking to gradient approaches can place artificial limitations on parameter space and experimental space. In this talk we will discuss examples that extend the usual definition of gradient approaches. These will include: microreactor droplets, surface polymerization gaps, patterned gradient substrates, and nanobeam mechanical measurements. Applications of these approaches to high-throughput experimentation will be demonstrated.

2:00 PM LL5.2
A Focused Library of Tyrosine-Derived Polycarbonates for the Discovery of Optimal Polymers for Use in Degradable Stents. Aaron Pesnell[1], Durgadas Bolikal[1], Nobert Weber[1], Joan Zeltinger[2], Don Brandom[2] and Joachim Kohn[1]; [1]Chemistry, Rutgers University, Piscataway, New Jersey; [2]REVA Medical, Inc., San Diego, CA, California.

The use of polymer-coated, drug-eluting metal stents has improved the clinical outcome of treating coronary heart disease, but many clinical thought leaders believe that the mechanical support offered by the metal stent may not be necessary for more than the six to nine

months period of vessel healing. Hence, resorbable polymeric stents may provide additional benefits to patients. Currently it is not possible to test this hypothesis as no resorbable polymer stent has yet been commercialized, in part because of the limited availability of degradable polymers specifically engineered for vascular stenting. Tyrosine-derived polycarbonates consisting of desaminotyrosyl-tyrosine alkyl ester (DTR) monomers were employed as a platform technology for the discovery of optimal degradable stent materials. Among the polycarbonates, poly(DTE carbonate), where E = ethyl, has shown exceptional biocompatibility in hard tissue applications. However, its properties were not optimized for vascular applications. Several structural modifications were therefore implemented to allow for radiopacity, tunable degradation rates, enhanced blood compatibility and optimal mechanical properties. Specifically, iodine was covalently bound to the DTE phenolic rings for increased radiopacity, PEG blocks were introduced into the polymer backbone for enhanced bulk and surface properties, and desaminotyrosyl-tyrosine (DT) monomers were incorporated to accelerate polymer degradation. The result was a focused library of polymers represented by the following design formula: $\mathbf{Poly(I_2DTE-co-x\%I_2DT-co-y\%PEG_{2K}carbonate)}$, where x varied from 10 to 20% and y varied from 1 to 4%. This test matrix was used to examine how small changes in the polymer structure affect its utility as a cardiovascular stent material. Polymers were compression molded into thin films and characterized. A one-year in vitro degradation study was conducted to pinpoint formulations that would maintain integrity for at least nine months, analogous to the time needed for vessel healing post stenting. Radiographs of polymer films fabricated into stents by REVA Medical demonstrated radiopacity equivalent to or greater than steel controls when implanted into porcine coronary arteries. Using a quartz crystal microbalance with dissipation monitoring (Q-Sense^{TM}), it was shown that fibrinogen adsorption to the polymer surface, a known marker for hemocompatibility, can be minimized by appropriate modifications of the polymer structure. Tensile testing demonstrated that the polymer mechanical properties were most dependent on the PEG content. Collectively, the data showed that a combinatorial approach is useful in the rapid discovery of optimal materials for use in degradable polymeric stents. This work was supported by NIH SBIR Grant HL075925 to REVA Medical, Inc., NIH Grant NIH Grant EB003057 to Rutgers University, and the New Jersey Center for Biomaterials.

2:15 PM LL5.3
Combinatorial material mechanics: High-throughput polymer synthesis and nanomechanical screening. Catherine A Tweedie[1], Daniel G Anderson[2], Robert Langer[2] and Krystyn J. Van Vliet[1]; [1]Department of Materials Science & Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; [2]Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Combinatorial materials science, an experimental concept developed in the 1960s for alloy development, has resurged via advances in materials synthesis [1]. Application of high-throughput syntheses toward the rapid discovery and optimization of functional materials has required parallel advances in materials characterization [2]. In the context of polymer design for applications ranging from biomaterials to microelectronic insulators, combinatorial approaches can enable systematic, high-throughput surveying of structure-processing-property relationships as a function of composition and operating conditions, in nL to μL volumes [3-5]. Here, we present a high-throughput synthesis / nanomechanical profiling approach capable of accurately screening the mechanical properties of a large, discrete polymer library comprising nL-scale material volumes. Within just a few days, a library of over 1,700 photopolymerizable materials were synthesized and then assayed for mechanical properties using an automated nanomechanical screening system. The approach outlined herein enables the rapid correlation of polymer composition, processing, and structure with mechanical performance metrics. 1. Amis, E. J., Xiang, X. D. & Zhao, J. C. Combinatorial materials science: What's new since Edison? MRS Bulletin 27, 295(2002). 2. Schmatloch, S. & Schubert, U. S. Techniques and instrumentation for combinatorial and high-throughput polymer research: Recent developments. Macromolecular Rapid Communications 25, 69 (2004). 3. Meredith, J. C., Karim, A. & Amis, E. J. Combinatorial methods for investigations in polymer materials science. MRS Bulletin 27, 330 (2002). 4. Stoykovich, M. P., Cao, H. B., Yoshimoto, K., Ocola, L. E. & Nealey, P. F. Deformation of nanoscopic polymer structures in response to well-defined capillary forces. Advanced Materials 15, 1180 (2003). 5. Anderson, D. G., Putnam, D., Lavik, E. B., Mahmood, T. A. & Langer, R. Biomaterial microarrays: rapid, microscale screening of polymer-cell interaction. Biomaterials 26, 4892 (2005).

3:30 PM *LL5.4
Knowledge Discovery Applications in High-Throughput Polymer Characterization. Carson Meredith, Pedro Zapata and Jing Su; School of Chemical & Biomolecular Engineering, Georgia Tech, Atlanta, Georgia.

Combinatorial and high-throughput experiments, used predominantly in pharmaceutical research, have emerged as a powerful method for materials screening. We present recent advances in the combinatorial design and screening of two classes of complex polymeric materials: (1) impact resistant plastics and (2) biomedical polymers. Formulation of impact modifiers for polymers represents a time-consuming procedure in both industry and research. We present an analysis of the ability to discover optimal formulations using high-throughput mechanical characterization (HTMECH). This talk will focus on nanoparticle-phase modifiers for polyurethanes. In addition, we will discuss the excellent ability to correlate mechanical properties measured with HTMECH to more traditional mechanical assays. Theory and modeling of the biaxial strain used in HTMECH are shown to be useful in interpreting results, ranking impact modifier performance, and extracting mechanical parameters. Designing biomaterial surfaces for applications including tissue engineering, diagnostics, and drug delivery is one of the major challenges facing biomedical engineering. Harnessing pattern recognition of cells on polymer surfaces is a prerequisite for developing successful tissue engineering implants and cell culture surfaces. The essentially infinite number of surface patterns plus the statistical nature of cell responses places a burden on conventional 1-sample-1-measurement methods. We report a comprehensive high-throughput methodology for quantitative discovery of surface descriptors that optimize osteoblast proliferation. The presentation focuses on the recent integration of combinatorial cell-surface experiments with quantitative informatics and data mining techniques.

4:00 PM LL5.5
High Throughput Sample Preparation and Characterization of Polymer Melts. Mary Beth Kossuth, Damian A. Hajduk and Anne F. Xie; Symyx Technologies, Santa Clara, California.

4:30 PM *LL5.6
Combinatorial Compounding. Nico Adams,[1] Ulrich S. Schubert[1], Sergul Acikalin Gulmus[2], Dalil Chenouf[2], Martin Moneke[2], Mattias Rehahn[2], [1]Laboratory of Macromolecular Chemistry and Nanoscience, Eindhoven University of Technology and Dutch Polymer Institute, Eindhoven, The Netherlands; [2]Deutsches Kuststoff Institut (DKI) and Dutch Polymer Institute, Darmstadt, Germany.

The need for fast and low-cost processes for compound development is obvious when"bespoke" products are required in small quantities. In a typical development workflow, many experiments are needed for the systematic study of the effects of additives and their potential synergistic interactions. This is usually accomplished using the one-variable-at-a-time variational principle. However, if the complexity of the formulation is high, the number of experiments that needs to be conducted soon becomes prohibitive. Therefore, new, but potentially more effective additives are not easily introduced. To address this problem, the plastics processing industry is turning to the notion of combinatorics, which has been shown to accelerate RD times both in the pharmaceutical industry as well as in other areas of materials science such as catalysis and polymer chemistry. Using a production size twin screw extrusion line with gravity feeding for a number of additives and fillers, a flame retardant polypropylene for use in cable applications was developed. Properties such as the limiting oxygen index, flame retardancy according to the UL test and mechanical properties were measured and optimized using statistical methods. This contribution highlights the application of combinatorial compounding to produce flame retardant polypropylene and basic principles of combinatorics for materials development in the plastics industry. Early attempts at using high throughput screening techniques for polymeric materials leveraged existing liquid handling technologies for sample preparation. This restricted study to materials which could be formulated as low viscosity solutions, but most investigations of polymer properties are usually done in the absence of solvent. We have developed hardware and software for formulating and processing solid polymers from automated weighing of powders, through compounding and shaping, to analysis. This workflow will be discussed in detail and results from a variety of high-throughput polymer characterization tools will be presented.

4:45 PM LL5.7
Combinatorial Initiated Chemical Vapor Deposition for Antimicrobial Polymer Coatings. Tyler Philip Martin and Karen K. Gleason; Chemical Engineering, MIT, Cambridge, Massachusetts.

Antimicrobial coatings are desired for military, textile and medical applications. The initiated chemical vapor deposition (iCVD) method was selected because it is a solventless, low-temperature process capable of forming very thin conformal layers on complex architectures. For example, finished, dyed fabrics can be easily coated without affecting the color, breathability or flexibility. The iCVD

polymer thin films and coatings are formed in situ on solid substrates via free-radical mechanisms from vapor phase monomers and initiators, and a range of polymeric coatings for diverse applications has been demonstrated. These include fluorocarbon polymers for superhydrophobic materials, organosilicon films for dielectrics and bio-inert coatings, resist materials for lithography, superhydrophilic materials for thin film gels, and pH sensitive films for controlled release. A combinatorial methodology has been developed to both more extensively examine of the deposition window for new materials and more quickly move from the initial material deposition parameter optimization to the application phase of study. The deposition of antimicrobial polymer coatings provides a striking first example of the gains realized by this system. The iCVD deposition parameters for poly(dimethylaminomethylstyrene), the first styrenic polymer successfully deposited by iCVD, was rapidly optimized for deposition rate and structure using the combinatorial system. A maximum deposition rate of 11 nm/min was achieved while maintaining the chemical structure as found by FTIR, compared to the commercially available polymer. Crosslinking was achieved to improve the coating durability, as shown by lack of solubility in aqueous or organic solvents. After the coating deposition was optimized, it was applied to fabrics and proved highly successful in killing E. coli and S. epidermidis, reducing viable bacteria by 99.9999% according to ASTM E2149-01. Direct synthesis from the vapor phase allows for in situ control of film morphology, molecular weight and crosslinking, and the combinatorial system decreases the time required to find the relationship between these interrelated properties. Kinetic examinations of a wide range of vinyl polymerization from the vapor phase now allow us to predict a priori the probability of success with a given monomer and intelligently choose appropriate deposition conditions for optimal processing.

SESSION LL6: Nanomaterials and Catalysts
Chairs: Toyohiro Chikyow and Katharine Dovidenko
Wednesday Morning, November 30, 2005
Back Bay B (Sheraton)

8:00 AM *LL6.1
Combinatorial Catalysis for Hydrogen Production and Purification. Yusuke Yamada, Tomoki Akita, Tetsuo Umegaki, Atsushi Ueda, Hiroshi Shioyama and Tetsuhiko Kobayashi; Ubiquitous Energy Devices, AIST, Ikeda, Osaka, Japan.

Hydrogen production and purification is important technology for the use of polymer electrolyte fuel cells as a power generator of successive generation. The problem of hydrogen is its difficulty in mass storage. High pressure and low temperature are required for keeping liquid hydrogen. Metal hydride and chemical hydride include the problem its reversible hydrogen storage and release. On-site hydrogen production from portable liquid chemicals via reforming reaction is a promising method. Usually hydrogen obtained by reforming reaction contains certain amount of CO which highly deactivates the anode catalyst of PEMFC. Therefore, hydrogen production at low temperature and/or removal of CO with catalysts is important technology for mobile use of fuel cells. Hydrogen can be achieved from various hydrocarbons such as alcohols. MeOH is a promising hydrogen source because its reforming reaction proceeds at relatively low temperature. A problem of MeOH is its high toxicity. Less toxic chemicals which can be converted to hydrogen are dimethyl ether (DME) and EtOH although they require high reaction temperature which leads to high CO concentration in produced hydrogen. In order to reform DME or EtOH at low temperature highly active catalyst using precious metals should be developed. At present, no active catalyst is known for the reforming of DME or EtOH at the temperature lower than 473K. We tested a series of combinatorially designed catalyst for CO shift reaction, MeOH steam reforming, DME steam reforming and EtOH steam reforming reactions. DME and EtOH steam reforming consist of multi-step reactions containing CO shift reaction and MeOH steam reactions. A small modification of the catalyst showing high performance on CO shift or MeOH steam reforming reaction would provide a catalyst suitable for DME or EtOH steam reforming. We found Pd/MnO2 shows high activity for MeOH steam reforming and CO shift reaction after first screening. The combination of Pd/MnO2 with a catalyst suitable for hydrolysis of DME provides a good catalyst for DME steam reforming. Also the combination of Pd/MnO2 with a catalyst suitable for C-H bond activation was tested. Novel catalysts for DME steam reforming and EtOH steam reforming were developed on the basis of fact database for their elemental reaction steps.

8:30 AM *LL6.2
Combinatorial Selection of Metals for Ohmic Contacts to GaN Films and for Catalytic Growth of ZnO Nanowires. Albert V. Davydov[1], William J. Boettinger[1], Daniel Josell[1], Leonid A. Bendersky[1], Richard S. Gates[1], Babak Nikoobakht[2] and Abhishek Motayed[3]; [1]MSEL, NIST, Gaithersburg, Maryland; [2]CSTL, NIST, Gaithersburg, Maryland; [3]Electrical and Computer Engineering Dept., University of Maryland, College Park, Maryland.

GaN and ZnO semiconductor thin films and nanowires (NWs) are finding increased application in opto- and microelectronics. However, performance of GaN and ZnO based devices is still limited by several materials and engineering problems, including difficulties in fabricating NWs with controlled properties and in making reliable electrical contacts to thin film and NW structures. Since the optimization of fabrication/processing schedules requires extensive experimentation, methods of high-throughput testing appear to be appropriate for these problems. Combining such combinatorial approaches with understanding of phase diagrams permits the experimental variables set to be reduced while also providing a system for organizing materials/processing information for future references. This paper demonstrates two applications of this combinatorial/phase-diagram approach: (a) optimizing Ohmic contacts to GaN films and (b) choosing metal catalyst for ZnO NW growth. (a) Optimum composition and processing parameters for realization of high-quality Ohmic contacts to n-GaN thin films were determined using a combinatorial library based on industry-standard Ti/Al/Ti/Au contacts. The library design of metal compositions and processing temperatures was guided using Al-Au-Ti phase diagram so that the contact compositions studied represented several different phase fields. An array of contact elements with varying Ti/Al/Ti/Au thicknesses was deposited on the GaN/sapphire substrate followed by rapid-thermal annealing in the 600-900°C temperature range. Comprehensive structural and electrical characterization of the contact library identified the most Al-rich metallization scheme, annealed at 750°C, as having superior surface morphology and the lowest contact resistivity. Correlation with the phase diagram revealed that these contacts formed a thermally stable two-phase (Al_3Ti and Al_2Au) mixture, which explained the smooth/unchanged morphology of these contacts. (b) ZnO NWs are often grown by the vapor-liquid-solid method that utilizes nano-sized catalytic metal islands as nucleation sites. We conducted a systematic assessment of how Group IB catalytic metals influenced growth parameters, structural and electronic properties of ZnO NWs. An experimental library was designed using the Au-Ag-Cu phase diagram and included five elemental metal and alloy compositions (Au, Ag, AuCu, AgCu, and AgAuCu) and two growth temperatures (850°C and 950°C), with all other processing parameters fixed. The resulting set of ZnO NWs was characterized structurally and spectroscopically. It was found that the NW growth was significantly influenced by the catalytic metal choice: the comprehensive correlation of ZnO structural/spectroscopic data with catalytic metal compositions will be presented in detail. This work demonstrates that high-throughput approach in combination with phase diagram knowledge can provide an efficient means for optimizing semiconductor fabrication and processing.

9:00 AM LL6.3
Combinatorial Flow Studies of Carbon Nanotube Growth Using Microchannel Arrays. Anastasios John Hart and Alexander H. Slocum; Mechanical Engineering, MIT, Cambridge, Massachusetts.

Explorations of nanomaterials growth can benefit tremendously from process controls which match the spatial and temporal dynamics of the growth reactions. For example, a carbon nanotube (CNT) nucleates within micro-milliseconds after carbon reaches the catalyst, yet a typical atmospheric-pressure tube furnace is flushed in no fewer than several seconds, and non-uniformities of gas flows and temperatures limit accuracy of parametric studies. Microreactors have been used for synthesis of chemical compounds [1] and nanocrystals [2], and combinatorial studies have tested nanomaterials growth catalysts [3]. We present a system and methodology for combinatorial flow studies of nanomaterials growth using precisely-fabricated microchannel arrays as reactors, and its application to CVD growth of CNTs. Silicon microchannel arrays are fabricated by potassium hydroxide (KOH) wet etching. By choosing the dimensions of the narrow "entry" region of each microchannel, an arbitrary velocity progression is achieved across the array, enabling dozens of simultaneous isolated flow experiments. Each device has a main array with 45 microchannels, and a secondary array with 4 "high flow" channels, which augment the total flow to facilitate rapid purging. At 4 psi pressure drop, the gas velocity in the microchannels follows a uniform geometric sequence from 0.005-1.0 m/s, and the flow difference between neighboring channels is as low as 1×10^{-5} sccm. A microchannel array is inverted over a second silicon substrate coated with a lithographically-patterned catalyst film, and is clamped in a quartz package which is placed in a tube furnace. Because of a reversible seal, the catalyst pattern is easily removed for characterization, and the microchannel array is cleaned and reused. Gases are drawn into the microchannel array from the tube furnace, enabling precise growth time studies by rapidly reversing the flow through the array, without changing the initial activity of the reactants. The gas chemistry and activity evolve considerably along

slow flows through microchannels, and changes in the CNT products are correlated with open-substrate experiments conducted at different gas compositions. A distinct yield-quality trend occurs as CH_4 decomposes into CH_4/H_2 to grow SWNT films from $Mo/Fe/Al_2O_3$, and a transition from tangled growth to vertically-aligned growth occurs from Fe/Al_2O_3 in C_2H_4/H_2. At flow velocities of approximately 1 m/s, isolated SWNT bundles and self-aligned MWNT strands grow in the flow direction, while CNTs suspended across islands remain anchored perpendicular to the flow due to surface forces. Supplementary figures are at http://pergatory.mit.edu/ajhart/nanotubes_open/ajhartMRSF05_figs.pdf 1. G. Kolb and V. Hessel. Chemical Engineering Journal, 98(1-2):1-38, 2004. 2. E.M. Chan, R.A. Mathies, and A.P. Alivisatos. Nano Letters, 3(2):199-201, 2003. 3. A.M. Cassell, Q. Ye, B.A. Cruden, et al. Nanotechnology, 15(1):9-15, 2004.

9:15 AM LL6.4
Growth of High Fraction of Single Wall Carbon Nanotubes using Both Plasma Enhanced and Thermal CVD within the Same Apparatus. Jeremy J. Jackson, Kevin Johnson and Kalayu G. Belay; Physics, FAMU, Tallahassee, Florida.

Carbon nanotubes (CNTs) were synthesized on Si substrate coated with thin multi-layer metallic catalysts by a system, which was originally designed for plasma assisted chemical vapor deposition (CVD) process. The substrates were coated with a combination of aluminum (Al), iron (Fe), molybdenum (Mo), and cobalt (Co) catalysts. Carbon nanotubes were grown by placing the substrate onto an inductively heated stage with and without using the plasma. The substrate was annealed with Ar and H2 for one hour at atmospheric pressure and the growth temperature. Carbon nanotube growth was initiated by introducing acetylene (C2H2) feedstock at a regulated amount for another hour in both cases. The CNTs were grown as a function of temperature and were analyzed by using Raman and high-resolution scanning electron microscopes respectively. By using the characterization methods, the role of different growth parameters and the plasma have been investigated and optimum conditions for the growth of high fraction of single wall carbon nanotubes were obtained in both environments.

9:30 AM LL6.5
Analysis of the Structural Specificity of ZrO2 Nanoparticles in Pillared Clays by Modeling of the Condensation Process in ZrOCl2*8H2O Solutions. Natalya V. Mezentseva, Vladislav A. Sadykov, Vladimir L. Kuznetsov and Vasiliy I. Avdeev; Boreskov Institute of Catalysis, Novosibirsk, Russian Federation.

Clays pillared by nanosize zirconia particles (Zr PILC) are promising supports and catalysts for different petrochemical processes and selective catalytic reduction of NOx by hydrocarbons in the excess of oxygen. Their performance strongly depends upon the size, shape and structure of nanosized zirconia pillars propping the alumosilicate layers, which are in turn determined by the properties of zirconium hydroxy polycations in pillaring solutions. However, these data are scares, which limit possibilities for molecular design of those systems. In this work, modeling of the tetrameric complexes condensation was carried out using a method of the molecular mechanics (the force field of MM +), a standart semiempirical PM3 method and within the Density Functional Theory approach (DFT). The structure of the neutral Zr4(OH)8(H2O)8(OH)8 complex was used as a basic unit in modeling. In this structure all Zr cations are bound by two bridging hydroxyls and contain two terminal hydroxyls and two terminal water molecules. Stacking of these units could occur forming either bi-dimensional (planar sheets) or three-dimensional (nanorods) structures. According to results of calculations obtained by PM3 method and statistical weights of probable polymerization products the most energetically favourable structure was determined. For structures including two and three tetrameric units, the most stable is the structure corresponding to a distorted loose nanorod, while the least stable is a dense cuboid nanorod structure. Similar trend in stability was obtained for species comprised of three Zr4 units. Hence, in agreement with the GCMC modeling, nanorods formed in pillaring solutions are rather loose structures. Results obtained by the DFT method for the basic tetrameric unit as well as the sheet-like and distorted nanorod-like structures revealed that the basic tetramer has for ~40 kcal/mol lower energy than each distorted tetramer in the nanorods. Among two dimeric structures, the sheet-like is ~56 kcal/mol more stable than the structure of a distorted loose nanorod. Comparison of these results with the experimental data suggests that the exact mode of the tetrameric units condensation is primarily determined not by the strength of Zr-O (OH) bonds but by more subtle effects such as presence of alkaline-earth cations able to coordinate tetrameric units through interaction with terminal/bridging hydroxyls. This agrees with the pronounced effect of the type of these cations on the structure of pillaring species in solutions as well as in clay galleries. Loose nanorods without strong bridging hydroxyls bonds between Zr4 units can be stabilized in solution by Ca or Ba cations. They appear to dissipate into separate tetramers in clay galleries after washing with distilled water which removes those cations. This work is supported by Zamaraev International Charitable Scientific Foundation and Integration Project 8.23 of Presidium RAS.

9:45 AM LL6.6
High-throughput Characterization of Shape Memory Thin Films Using Automated Temperature-dependent Resistivity Measurements. Sigurd Thienhaus[1,3], Christiane Zamponi[2], Ichiro Takeuchi[4] and Alfred Ludwig[1,3]; [1]Combinatorial Materials Science, caesar, Bonn, Germany; [2]Smart Materials, caesar, Bonn, Germany; [3]Institute of Materials, Ruhr-University, Bochum, Germany; [4]Materials Science and Engineering, University of Maryland, College Park, Maryland.

Shape memory alloy (SMA) thin films are used as actuator materials in MEMS due to their unique properties. Binary films with a composition close to Ni50Ti50 are well-established materials, whereas ternaries like NiTiCu, NiTiPd, NiTiHf are less studied. Furthermore new alloys are developed which show a magnetic shape memory effect, e.g. NiMnGa. For the optimization of known SMA thin films and the development of new SMA thin films a fast and reliable characterization technology is needed which yields at least the transformation temperatures (i.e. martensite and austenite start and finish temperatures). In this paper, automated temperature-dependent resistivity measurements (temperature range: -35°C to 250°C) are discussed as a means which yields the thermal hysteresis of the investigated thin films. This paper reports results on monitoring the homogeneity of shape memory film depositions as well as results on the use of this method as a tool for screening for new SMA films by characterization of SMA materials libraries.

10:30 AM LL6.7
Gradient Combinatorial Strategies For Thin Nanomaterials Development And Surface Nanometrology. Michael J. Fasolka, Duangrut Julthongpiput, Wenhua Zhang, Alamgir Karim and Eric J. Amis; Polymers Division, National Institute of Standards and Technology, Gaithersburg, Maryland.

Ultra-thin films of polymers will play a major role in next generation technologies including nano-lithography resists, MEMS* components, and electronics packaging. However, as applications become more complex and demand more tailored materials behavior, the optimization and fine engineering of thin polymer systems can be difficult, time consuming and expensive. We have developed a suite of gradient combinatorial methods aimed towards the more rapid, thorough understanding of thin polymer film materials, and towards accelerating the engineering of these materials. Gradient combinatorial methods involve the fabrication of specimens that gradually and continuously change in one or more properties over space. Our gradients in film thickness, surface energy, temperature, composition, and other governing variables can be used to comprehensively map the effect of these parameters on film behavior and performance. In this presentation, example research studies will be used to illustrate the utility of gradient combinatorial techniques and high-throughput measurement methods for thin film nanotechnology development. Case studies will include the fabrication and use of gradient micropatterns as a high-throughput platform for screening thin film stability and as reference specimens for emerging scanning probe microscopy techniques. The use of gradients methods for block copolymer film engineering will also be discussed. * Micro Electro-Mechanical Systems

10:45 AM LL6.8
Combinatorial Fabrication and Study of Luminescent Nanocrystalline Si Particles Embedded in a SiO2 Matrix. Luis F. Fonseca[1], Oscar Resto[1], S. Zvi Weiss[1] and Joseph Shinar[2]; [1]Physics, University of Puerto Rico, Rio Piedras, Puerto Rico; [2]Physics & Astronomy, Iowa State University, Ames, Iowa.

The combinatorial fabrication of nanocrystalline Si particles embedded in a SiO2 matrix by RF co-sputtering of Si and SiO2 targets is described. The peak of the photoluminescence spectra of the films varies systematically from 760 to 600 nm, consistent with the presumed systematic variation in the size distribution of the embedded Si particles. The correlation between the optical properties of the samples and the formation parameters is also analyzed.

11:00 AM LL6.9
Use of Continuous Composition Spreads to Search for New Fuel Cell Electrocatalysts. Mark David Prochaska[1], Maxim Kostylev[2], Jing Jin[2], John Gregoire[4], David Kim[3], Lin Zhuang[2], Hector Abruna[2], R. Bruce van Dover[3], Francis J. DiSalvo[2] and Dominic Rochefort[5]; [1]Applied and Engineering Physics, Cornell University, Ithaca, New York; [2]Chemistry and Chemical Biology, Cornell University, Ithaca, New York; [3]Materials Science and

Engineering, Cornell University, Ithaca, New York; [4]Physics, Cornell University, Ithaca, New York; [5]Chemistry, University of Montreal, Montreal, Quebec, Canada.

Recent papers give evidence that some Pt-based ordered intermetallic compounds have lower onset potentials, higher current densities, and better resistance to poisoning than Pt when used as fuel cell electrocatalysts (1, 2). To efficiently search for other binary and ternary intermetallic compounds, we synthesized thin film continuous composition spreads by magnetron cosputtering, producing thousands of compositions on a single substrate. Fluorescent dyes and/or pH-sensitive electrodes were used to identify the location of high-activity electrocatalysts on each sample. We found active compositions for methanol oxidation in Pt-Bi-Pb and two other ternary systems that represent new catalyst candidates. Some of these same regions were also active for ethanol oxidation. Results for other composition spreads will also be presented. (1) E. Casado-Rivera, Z. Gál, A.C.D. Angelo, C. Lind, F.J. DiSalvo, H.D. Abruña, ChemPhysChem 2003, 4, 193-199. (2) E. Casado-Rivera, D.J. Volpe, L. Alden, C. Lind, C. Downie, T. Vázquez-Alvarez, A.C.D. Angelo, F.J. DiSalvo, H.D. Abruña, J. Am. Chem. Soc. 2004, 126(12), 4043-4049.

11:15 AM LL6.10
Frontier Materials on Advanced Nanotechnology.
Kyung M. Choi, Bell Labs, Lucent Technologies, Murray Hill, New Jersey.

Recent developments in nanotechnology have brought us new advances in device fabrications by emerging technologies from physicists, chemists, engineers, biologist, and materials science. There are a lot of challenges for chemists to play an important role in this area since nanotechnology is a part of the chemical domain, which builds up materials at the molecular level. Here we demonstrate a challenge in the development of new materials to achieve high performances in active devices. For a case of technological emergence, we present a new advance in nano-scale resolution soft lithography by developing new stamp materials. Soft lithography has attracted much attention in 'high resolution pattern transfer' by making stamps, molding, and contact-printing with low cost and easy processability, for use particularly in plastic/molecular/organic electronics and microfluidic device fabrications. However, the resolution of soft lithography relies on the mechanical property of stamps, which often result in collapse and mergence due to their low mechanical rigidities. These limitations have motivated this work to develop a new stiff, photocured PDMS stamp material. The molecular modification of PDMS structure results in an excellent stamping performance, which fabricates nano-patterns and structures with high fidelity.

11:30 AM LL6.11
In search of martensites by nanoindentation screening.
Oden L. Warren[1], Arpit Dwivedi[1], Thomas J. Wyrobek[1], Olugbenga O. Famodu[2], Jae Hattrick-Simpers[2] and Ichiro Takeuchi[2]; [1]Hysitron, Inc., Minneapolis, Minnesota; [2]Materials Science & Engineering, University of Maryland, College Park, Maryland.

The combinatorial methodology represents a potentially efficient means for establishing the structure-property relationships of alloy systems exhibiting shape memory and superelastic effects over a portion of their compositional space. Both effects require the existence of a martensitic phase that expresses itself as a rich interplay between composition, structure, temperature, and mechanical stress. Consequently, it is imperative to develop a screening strategy capable of high-throughput phase identification if the goal is to quickly discover and optimize shape memory and superelastic materials. Previous combinatorial searches for martensites invoked microbeam x-ray diffraction and thermal actuation of deposited-upon cantilever arrays; however, the former suffered from low throughput and the latter suffered from poor compositional resolution. Nanoindentation, a technique not normally associated with phase identification, shows considerable promise as a rapid, high-resolution means for narrowing the field of martensite candidates to a small fraction of the alloy library. Here we present results on nanoindentation screening of combinatorial libraries of ternary alloys with the potential for ferromagnetic martensites. Ternary diagrams in terms of elastic modulus, hardness, and other non-conventional figures of merit, such as hysteresis loss factor adapted for nanoindentation, point clearly to the martensitic portion of compositional space when considered as a whole. The conclusions of this nanoindentation screening investigation are consistent with earlier cantilever array results for the same alloy systems.

11:45 AM LL6.12
A Combined High Throughput Experimentation / Design of Experiments Approach for the Study of Heterogeneous Catalysts. Chris Snively[1,2], Jochen Lauterbach[1] and Rohit Vijay[1]; [1]Chemical Engineering, University of Delaware, Newark, Delaware; [2]Materials Science and Engineering, University of Delaware, Newark, Delaware.

Over the past several years, we have developed FTIR imaging as a high throughput analytical technique for the study of heterogeneous catalyzed reactions. This approach is realized by the combination of an FTIR spectrometer, a focal plane array detector, and a sampling accessory tailored to the specific sample geometry. This technique allows the acquisition of infrared spectral information from multiple samples simultaneously with a temporal resolution of less than two seconds. Multivariate factor-based and univariate calibration models were developed to extract quantitative concentration information from highly overlapped IR spectra. With these processing strategies, quantitative information can thus be extracted even when a significant concentration of water vapor is present in the effluent. Even with an effective high throughput experimental methodology, the number of possible experiments needed to completely characterize a given system is still prohibitively large for certain systems. In order to more efficiently explore the vast parameter space typically present in catalytic systems (catalyst identity, catalyst composition, temperature, reactant concentration, etc.) a design of experiments (DoE) approach was utilized. Fractional and full factorial designs were used as screening designs. At this level of experimentation, a linear model was developed relating a performance criterion to the parameters of interest, which allowed the determination of important parameters and the interactions between them. To decrease the number of experiments required in a screening design, a fractional factorial design was used, in which a fraction of the full factorial design was performed. This resulted in a significant decrease in the experimental effort by combining the effects of higher order interactions with lower order interactions. Once the important parameters were identified, a response surface study was completed to refine the model and optimize the catalyst and reaction conditions. Specific examples will be given from studies of nitrogen storage and reduction (NSR) catalysts. This is a particularly complex system both in terms of the catalyst makeup, which typically includes two or more active components, and the product feed, which is typically operated in a transient mode. Examples of both catalyst discovery and catalyst optimization will be presented.

SESSION LL7: Sensors, Materials and Devices
Chairs: Mike Fasolka and Radislav V. Potyrailo
Wednesday Afternoon, November 30, 2005
Back Bay B (Sheraton)

1:30 PM *LL7.1
Gas Sensor Research and Development with a Combinatorial Approach. Mats Eriksson, IFM, Linkoping University, Linkoping, Sweden.

Combinatorial approaches have only recently been applied to study and to develop gas sensors. In this presentation a special attention will be devoted to gas sensitive field-effect devices and in particular to metal-insulator-semiconductor (MIS) capacitors. The properties of the metal layer of such a device are crucial for the gas sensing characteristics. At the metal surface catalytic reactions are occurring and at the metal-insulator interface the actual transduction of chemical information to an electric response takes place. In order to optimize the properties of the metal surface and of the metal-insulator independently, a double metal layer structure is sometimes used. An important parameter of these metal layers is their thickness. To optimize the thickness of both layers, a device with a two-dimensional, continuous variation of the thickness has been produced. One metal layer, on top of the insulator, has a thickness gradient in one dimension. On top of this metal layer the second metal layer is deposited with a thickness gradient in an orthogonal direction to that of the first. The result is a metal layer where every point along the surface has a unique metal thickness combination. In one corner both metals are thin. In the opposite corner both metals are thick. In between these extremes, all possible combinations are available. In order to measure the "local gas response" at different points of the device, a method with a lateral resolution is needed. The method we have used is the Scanning Light Pulse Technique (SLPT). The essential feature of this technique is a focused and intensity modulated light beam that can penetrate the metal and the insulator layers. The light that reaches the semiconductor gives rise to electron-hole pair formation. The electrons and the holes are separated by the electric field in the semiconductor and the concentration of separated electrons and holes depends on the light intensity, the applied voltage across the MIS device and the temperature. Since the light intensity is modulated, a time dependent current is generated in the outer circuit. The size of this current depends on the applied voltage. When hydrogen atoms (produced by the catalytic activity of the metal surface) are trapped at the metal-insulator interface, a shift of the electrical characteristics

occurs. This shift is the gas response of the device and since the light beam is focused, a local gas response is obtained. By scanning the light beam across the surface, a map of the gas response is achieved which can be presented in the form of a "chemical image". Results will be presented that show that this method has the potential to optimize the thickness combination of the metal films in terms of important sensor parameters such as sensitivity, selectivity and stability, using a drastically reduced number of components as compared to working with discrete sensors with constant metal thickness.

2:00 PM LL7.2
Wireless sensor array system for combinatorial screening of sensor materials. William Morris and Radislav Potyrailo; GE Global Research, Niskayuna, New York.

A sensor-array system has been developed for noncontact screening of sensor and other types of materials deposited onto resonant sensors. For demonstration of the applicability of this sensing concept, acoustic-wave devices were coated with candidate sensing films for testing and further connected to small-scale antennas. The readout of the variations in the resonance of the sensors upon exposure to variable environments was performed with a pick-up coil located in proximity to a sensor and connected to a network analyzer. A translation stage was further applied to automatically scan the pick-up coil across multiple sensors. This approach in materials screening provides new opportunities for proximity chemical and mechanical determinations of materials properties without the need for hard-wiring sensors to the readout electronics.

2:15 PM LL7.3
High-Throughput Measurement of Magnetostriction Using MEMS and Composition Spreads. N. C. Woo[1] and R. B. van Dover[2]; [1]Chemistry and Chemical Biology, Cornell University, Ithaca, New York; [2]Materials Science and Engineering, Cornell University, Ithaca, New York.

While measurement of magnetostriction in bulk materials is readily accomplished using a strain gauge, measurement of this quantity for thin films presents a greater challenge, and typically involves measurement of the overall wafer curvature as a function of field, for a film of uniform composition. In order to evaluate magnetostriction locally in a composition-spread sample, we have developed a method using pre-fabricated arrays of cantilever beams on a silicon substrate prepared using MEMS technique. Differential strain of the thin film/cantilever system results in curvature which is detected using an optical (laser/position-sensitive-detector) system. A magnetic field is applied using two orthogonal Helmholtz coils, and the resulting deflection-field curves are used to determine the saturation magnetostriction λs as well as dλ/dH. Composition-spread films are prepared using a three gun on-axis magnetron cosputtering system. The position-dependent composition is inferred using rate calibrations and verified with electron microprobe and Rutherford Backscattering Spectroscopy. Preliminary experiments have measured magnetostrictions in the Ni-Fe-Co system. Our approach can also be used to measure properties of giant magnetostrictive systems, such as TbFe/Fe multilayers, as a function of layer thickness, or could be used to measure the properties of thin film magnetic shape-memory alloys.

3:30 PM *LL7.4
Nanostructured Electronic Nose Microsystem for Rapid Gas Analytical Screening. Joachim Goschnick, Institut fuer Instrumentelle Analytik, Forschungszentrum Karlsruhe, Karlsruhe, Germany.

Integrated chemical condition monitors are prerequisites for intelligent systems to obtain status information for online autonomous response. High gas analytical performance combined with low cost fabrication, low power consumption, high robustness and small size makes an electronic nose microsystem (ENMS) to an appropriate monitor for complex gas ensembles (odors or pollutant cocktails) fingerprinting e.g. process states or environmental conditions. A unique electronic nose microsystem has been developed which withstands even strong mechanical loads and high temperatures. The Karlsruhe Micronose KAMINA is a gas sensor gradient microarray based on a single gas sensitive metal oxide (e.g. SnO2) layer subdivided by parallel electrode strips into 38 or 16 sensor segments. Contrary to conventional arrays with separate sensors much easier fabrication and a higher level of integration is achieved. Gradients of the surface temperature and some nm change in the thickness of a gas permeable SiO2 coating on top of the metal oxide differentiate the segments' sensing properties resulting in gas characteristic conductivity patterns. Based on a 3.5x3mm2 KAMINA chip a battery-operated cylindrical EN module with Φ=32mm was developed fitting into a standard percussion driller soil probe to allow rapid depth-resolved screening for volatile soil pollutants while being robust enough to survive ground penetration by an electric hammer with 1400hits/min. A trampoline-like chip fixation only by the bond wires within the clearance of an alumina card provides extreme mechanical stability and minimum heating power to maintain ca.300°C chip operation temperature. The chip package and the whole electronics are fastened with dampers inside a cladding tube. Test exposures to typical soil pollutants showed mostly excellent detection limits <10mg/m3 at 1 Hz data rate and good discrimination between the pollutants by a stepwise Linear Discriminant Analysis of the signal patterns. The KAMINA equipped percussion driller was tested in sand beds and at several outdoor places without any damage of the KAMINA module. Baking bread rolls release a gas ensemble depending on progress or failures of the process. However, the characteristicity of the oven gas can only be measured within the exhaust gas at its temperature because condensation of components downgrades the quality and reproduceability of the results. To demonstrate the potentials of an ENMS for baking control the oven exhaust pipe was equipped with the described KAMINA chip assembly exploiting its heat resistivity. While the baking gas of ca.200°C was continuously sampled signal patterns were obtained in a characteristic sequence related to the progress of bread roll baking. Even after 60 baking runs the KAMINA chip did not show any fatigue.

4:00 PM *LL7.5
PLD of Semiconductor Compounds, Solid Solutions and Multilayer Structures Based on them for IR Detectors. Arik Aleksanyan and Arsham S. Yeremyan; Dept. of Semiconductor Electronics, Institute of Radiophysics & Electronics of Armenia, Ashtarak, Armenia.

A large number of experimental setups were already developed based on the PLD for high-throughput synthesis of multicomponents with large variation of compositions, combinatorial libraries of electron materials, etc. One of the advantages of PLD is the diversity of reliable technology parameters, which are employed to develop a certain design depending also on the class of synthesized materials and their expected properties. Understanding of physical fundamentals of the growth process is important in defining these parameters and in this work a special attention will be focused on the peculiarities of PLD which are at the starting point of developed approach to experimental design. Here, the peculiarities of laser plasma in PLD process are sketched out, which have substantial role in thin film growth process. 1) The first is associated with the thickness of material layer incoming to the substrate per pulse of evaporating laser. This thickness remains constant in a wide range of radiation intensities. 2) The second peculiarity is related with the growth rate of the film. In order to provide formation of two-dimensional nuclei the flux velocity of atoms incoming to substrate surface must be larger than the rate of their escape from the interaction region due to the diffusion. 3) The third peculiarity is the energy spectrum of particles. Depending on their impact on the substrate surface, particles can be distinguished into two groups: those with energies less than 25 eV, which do not result in defects in substrate, and those with higher energies. The latter dislodge the atoms from the surface layer resulting in vacancy-type defects. The proportion of slow and defect-inducing particles determines the processes accompanying the irradiation of surface by plasma. Reduction of the amount of rapid particles corresponds to the possibility of production of defect-free crystals. In contrast, using only rapid ions causes effective generation of vacancies in near-surface region. Another interesting case is the intermediate regime, when condensation occurs on the surface already irradiated by a dose of rapid ions. The irradiation creates an array of additional centers of crystallization on single-crystalline substrates. This provides the possibility of epitaxial growth of films at comparatively low mobility of adsorbed atoms, The same feature allows the implementation of regime practically excluding interdiffusion of materials. 4) The forth peculiarity is associated with the possibility of laser mixing of materials resulting in new material phases (new compounds, solid solutions, etc.) in a regime of complete interdiffusion of materials. Implementation of these various features will be demonstrated by results of synthesis of photodetector materials and structures, which cover a broad infrared spectral range of sensitivity. Properties of these detectors will be described which determine the class of possible parameters for quality control and optimization.

4:30 PM LL7.6
Focused ion beam microscope as an analytical tool for nanoscale characterization of gradient-formulated polymeric sensor materials. Katharine Dovidenko and Radislav A. Potyrailo; GE Global Research, Niskayuna, New York.

Development of new generation sensor materials based on engineered nanostructures requires adequate characterization tools. Among the key specific requirements for such a characterization tool are nanometer-scale spatial resolution, capability of analysis of sensor materials without altering materials composition, and possibility of performing in-situ nanoscale analysis during exposure of sensor materials to analytes and interferences. Focused ion beam (FIB)

serves as an attractive means to address these and other characterization needs of sensor materials. Our sensor materials contain nanostructures (semiconductor nanocrystals, metal nanoparticles, carbon nanotubes) incorporated into a suitable support (often polymeric) matrix. Such an approach permits development of sensor materials with tailored diversity of their response to species of interest. We take advantage of our earlier developed combinatorial and high-throughput screening expertise to accelerate the development of these sensor materials. By combining these opportunities with FIB characterization, we are able to explore gradient-formulated sensor materials on the previously unavailable level of detail. These materials were made as 30-100 nm diameter Au nanoparticles incorporated in a polymer matrix. The nanoparticles were incorporated to produce concentration gradient in the matrix. The approach generated new knowledge on the effects of immobilized nanostructures at their different levels on the sensor performance.

4:45 PM LL7.7
High-Throughput Screening of Arrays of CdSe Nanocrystal-Formulated Polymeric Coatings for Photoluminescent Sensors. Andrew M. Leach and Radislav A. Potyrailo; Chem/Bio Sensor Laboratory, General Electric Global Research, Niskayuna, New York.

High-throughput screening of arrays of CdSe nanocrystal-formulated polymeric coatings for photoluminescent sensors.

SESSION LL8: Artificial Intelligence: Design
Chairs: James Greer and Anatoli Korkin
Thursday Morning, December 1, 2005
Back Bay B (Sheraton)

8:00 AM *LL8.1
Materials Modeling for Advanced Gate Stacks in CMOS Technology. Alexander A. Demkov, Department of Physics, University of Texas-Austin, Austin, Texas.

The scaling of conventional CMOS and its evolution to non-classical CMOS devices such as Fin-FET brought about the introduction of strained Si configurations to enhance the channel mobility, silicon-on-insulator (SOI) to enhance the reduction of residual parasitics, high-k gate dielectrics to enhance the drive current, metal electrodes to maintain the effective oxide thickness, and many other novel materials related solutions. The industry is pushing the CMOS architecture well beyond the limits thought possible just a few years ago introducing new materials practically in every element of the device: source/drain electrodes, gate dielectrics, gate electrode, channel material (as well as its state and orientation), etc. Modeling and simulation have proven critical both in providing fundamental understanding of the physical mechanisms and processes and in interpreting metrology for nanotechnology nodes. As the size of materials for devices continues to decrease, the impact of interfaces on the measured material properties makes separation of “bulk” and interface properties much more difficult. In addition to merely conceptual difficulties, this presents a practical hurdle for technology computer-aided design (TCAD) a key enabler of advanced technology development. In this talk I will discuss how computational materials methods make the atomistic description of the device “almost possible.” However, since at present these calculations are far from being practical in the development support, an intermediate approach is desirable. I will argue that we may still be able to use traditional tools down to 15 nm provided we have a reliable description of materials systems involved, i.e. ultra-thin multi-material stacks. Conventional TCAD programs can e.g. still describe capacitors for the gate stack development using materials parameters estimated with ab-initio computational materials methods.

8:30 AM LL8.2
Ab Initio Global Optimization of Atomic Cluster Structures Using Parallel Genetic Algorithms. Ofelia Ona[2], Victor E. Bazterra[1,2], Maria C. Caputo[2], Marta B. Ferraro[2] and Julio C. Facelli[1]; [1]Center for High Performance Computing, University of Utah, Salt Lake City, Utah; [2]Departamento de Fisica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Buenos Aires, Argentina.

The study of the structure and physical properties of atomic clusters is an extremely active area of research due to their importance, both in fundamental science and in applied technology. Existing experimental methods for structural determination seldom can obtain the structure of atomic clusters directly. Therefore the calculation, using theoretical structures and comparison with experimental values of their physical and optical properties is the most common way to obtain structural information of atomic clusters. It is universally accepted that DFT (Density Functional Theory) is the preferred method for atomic cluster structure calculations and that other less computationally demanding approximations are used due to the lack of the computing capabilities needed for DFT methods. For medium size atomic cluster only local optimizations of plausible structures have been possible when using DFT methods. Our previous work (Bazterra, V. E., Ona, O., Caputo, M. C., Ferraro, M. B., Fuentealba, P. and Facelli, J. C. (2004) Phys. Rev. A, 69, 053202) shows that local searches can miss important structures with significant lower energy. In this paper, we report the implementation and application of a Parallel Genetic Algorithm (PGA) to predict the structure of medium size atomic cluster of SinH and SinCu using the DFT approximation. We have developed a computational package, named Modified Genetic Algorithm for Crystal and Cluster structures (MGAC). The MGAC package has been implemented in C++ using parallel computing techniques (MPI). The evaluation of the objective function for our PGA, i.e. the local energy minimization using the DFT method is performed using the CPMD (http://www.cpmd.org/) code. Our PGA implementation uses simultaneously two levels of parallelism: at the population level by distributing the evaluation of the fitness function among several groups of processors and at the DFT level using the parallel capabilities build in the CPMD code. The application is driven by an Adaptive Parallel Genetic Algorithm (APGA) designed to make efficient use heterogeneous clusters of computers. The implementation has built in fault tolerant features to be resilient to the failures common in very large computational clusters. In this paper we demonstrate that the method described above exhibit good scalability properties, performing efficiently in more than 200 processors and that it is able to find new cluster structures of SinH and SinCu clusters that were not present in previous searches using local minimization techniques. These new structures are more stable than the previously known structures and in all cases the calculation of their vibrational frequencies shows that they are locally stable minima.

8:45 AM LL8.3
Computational DFT Study of $ZrSiO_4$ Polymorphs: Microelectronic, Nuclear Safety and Geological Implications. Anatoli Korkin[1], Hideyuki Kamisaka[2], Koichi Yamashita[2], Andrey Safonov[3] and Alexander Bagatur'yants[3]; [1]Nano and Giga Solutions, Inc., Gilbert, Arizona; [2]University of Tokyo, Tokyo, Japan; [3]Photochemsitry Center, Moscow, Russian Federation.

Zirconium silicate has a broad range of existing and potential applications ranging from nuclear safety to microelectronics, protective coating, fuel cells, heterogeneous catalysis and jewelry and other areas. Zircon, an extremely durable and resistant material, is capable to accommodate a large quantity of [radioactive] actinides, which makes it useful as a host material for disposition of nuclear waste. Its structure and stability under irradiation have been investigated in numerous experimental studies. The high optical and mechanical stability of amorphous zirconium silicon oxide films meet the criteria required for the solar control coatings application. Recently Zr and Hf silicates have drawn considerable attention as alternative [to conventional SiO_2] high permittivity (high-k) dielectrics in MOS devices. Besides zircon (group $I4_1/amd$) the only other experimentally known form of ZrSiO4 is reidite, which is similar to scheelite, $CaWO_4$ (group $I4_1/a$) structure. Both zircon and reidite have eight-coordinated zirconium and four-coordinated silicon atoms in their tetragonal unit cells. Using Density Functional Theory (DFT) in generalized gradient approximation (GGA) with plane wave (PW) and numerical atomic orbitals (NAO) basis implemented in VASP and SIESTA codes, respectively, we have revealed eleven new polymorphs of ZrSiO4 within the energy range 1 eV above the most stable zircon. Among the structures, which have higher density than zircon, the low energy fergusonite-like ($YNbO_4$; group C2/c) form is the most promising for experimental verification with its energy and density intermediate between those of zircon and reidite. The new fergusonite-like form has similar bonding pattern as zircon and reidite. Two structures, which have both silicon and zirconium atoms six-fold coordinated, orthorhombic $AlTaO_4$-like (alumotantite) and monoclinic $PbWO_4$-like (respite), are found to have similar energies 0.35 eV above reidite and density intermediate between zircon and reidite. Among the low-density structures, which can be potentially revealed experimentally in the nanocrystalline thin films, the orthorhombic $CaSO_4$-like form has energy similar to reidite but much lower density.

9:00 AM LL8.4
Symmetry-adapted statistics of site-occupation disorder in crystalline solids from supercell models. Ricardo Grau-Crespo[1,2], Said Hamad[3,2], Richard Catlow[3,2] and Nora de Leeuw[1,2]; [1]School of Crystallography, Birkbeck College, London, United Kingdom; [2]Chemistry, University College London, London, United Kingdom; [3]Davy Faraday Research Laboratory, The Royal Institution of Great Britain, London, United Kingdom.

Site-occupation disorder is an ubiquitous phenomenon in solid state chemistry, and one in which computer modeling techniques can

provide valuable insights. The supercell method, that is, the simulation of completely ordered supercells that map onto smaller disordered unit cells, has the drawback of a huge computational cost associated not only with the simulation of many-atom systems, but also with the number of possible configurations which increases dramatically with the cell size. We describe here a method for limiting the configurational space to be explored by using the crystal symmetry of the target lattice, and propose a Boltzmann-type statistics that includes not only the energy of each non-equivalent configuration, but also its multiplicity in the complete configurational space, via an entropic term. A computer code for performing this analysis in systems with arbitrary symmetry and for any supercell size is presented. To provide some examples, the described methodology is applied to the study of the cation distribution in a selected group of materials.

9:15 AM LL8.5
Adsorption of atomic and molecular oxygen on the $SrTiO_3$(001) surfaces: Computer simulations by means of hybrid density functional calculations and ab initio thermodynamics. Sergei Piskunov[1], Eugene A. Kotomin[1], Yuri F. Zhukovskii[1] and Donald E. Ellis[2]; [1]Institute of Solid State Physics, University of Latvia, Riga, Latvia; [2]Department of Physics and Astronomy, Northwestern University, Evanston, Illinois.

The adsorption of gas-phase oxygen at ABO_3 perovskite surfaces is important for high temperature oxygen sensors, in photocatalysis, and fuel cell applications. Ab initio calculations based on density functional theory (DFT) have been used to study the energetics, fully relaxed structure, charge redistribution, and electronic density of states of adsorbed atomic and molecular oxygen on SrO- and TiO_2-terminated $SrTiO_3$(001) surfaces. Exchange-correlation functional applied within DFT contains a "hybrid" of the non-local Hartree-Fock exchange, DFT exchange, and generalized gradient approximation correlation functionals. Such a technique allows us to obtain reliable electronic properties of perfect and defective ABO_3 surfaces. The calculations are performed on periodically repeated systems (two-dimensional slabs) large enough for the adsorbed species to be treated as isolated. We find substantial binding energies of up to 2.3 eV for atomic oxygen adsorption over surface oxygen and of over 2.6 eV at bridge sites on both SrO- and TiO_2-terminated surface. A range of different adsorption sites and orientations for molecular oxygen have been studied but practically in no case does the adsorption energy exceed 1.0 eV. The phase diagram of surface structures in contact with a gaseous oxygen environment is calculated by means of atomistic thermodynamics. Adsorption of the reactants is found to depend significantly on temperature and partial pressures in the gas phase. The relevance of our findings to an understanding of oxygen gas-surface exchange is discussed.

9:30 AM LL8.6
REAlO3 perovskite compounds : Systematic study of phonon instability by first principles calculations. Tetsuya Tohei, Akihide Kuwabara, Tomoyuki Yamamoto, Fumiyasu Oba and Isao Tanaka; Materials Science and Engineering, Kyoto University, Kyoto, Japan.

Recent advances in computational technique enable us to determine full phonon dispersion from first principles. Such first principles method should provide a powerful tool for the systematic investigations of displacive phase transitions, since the structural transitions are often driven by soft phonon modes. Here we report our application of the method to the issue of general behavior of phonon instability in external pressures. Regarding the pressure effect on the structural phase transitions associated with soft phonon modes, an empirical "general rule" has been established [1]. The rule tells that the instability of the cubic perovskite structure decreases for zone center transitions and increases for zone boundary transitions (ZBT) with pressure in general. Very recently, pressure induced rhombohedral to cubic transition of LaAlO3 has been reported for the first time [2]. Since LaAlO3 is a typical of the ZBT compound, if the behavior in the compound can be really verified, the general rule of ZBT need to be reinvestigated. In the present study, we have made a theoretical approach based upon the first principles projector augmented wave (PAW) method. In addition to the conventional static total energy calculations, we have computed phonon states by the direct method. With the method we can perform quantitative analysis of phonon dispersion relations in arbitrary compounds. The present calculations quantitatively well reproduce the experimental observations including the phase transition pressure and the pressure dependence of phonon frequencies, confirming the compound's exceptional behavior for the general rule. We have further performed systematic phonon-state calculations on a series of REAlO3 (RE=rare earth elements) and REGaO3 compounds. We found that the behavior is not peculiar to LaAlO3 but rather ubiquitous among many compounds. REAlO3 (RE = La, Nd, Sm, Gd) and LaGaO3 can be classified in the same group. A good correlation between the tolerance factor and the instability is found among aluminates and gallates. Such information should provide a clue toward new general rule of displacive transitions. The present work demonstrates the strong capability of this type of first principles method for the systematic investigations which are experimentally unattainable. [1] G. A. Samara et al., Phys. Rev. Lett. 35 (1975) 1767, [2] P. Bouvier and J. Kreisel, J. Phys.:Condens. Matter 14 (2002) 3981

10:15 AM *LL8.7
Statistical Estimates of Molecular Correlation Energies. Werner Gyoffry and James Greer; Tyndall National Institute, Cork, Ireland.

Accurate determination of molecular dissociation limits, transition states, spectra, polarizabilities, essentially all molecular properties requires a determination of the electron correlation energy. The electronic correlation energy is formally defined as the difference in energy between the Hartree-Fock approximation and the exact solution to the molecular electronic Hamiltonian within a given basis set. Wave function methods allow for systematic approximations to the correlation energy, but due to their scaling properties, their use is limited to small molecular systems. The configuration interaction (CI) method allows for convergence to the solution of the exact correlation energy problem, but requires diagonalization of matrices whose dimensions increase combinatorially with the number of electrons and basis sets used to approximate the electronic wavefunction. However, of these expansion states, relatively few contribute significantly to molecular energies or to the wavefunction. In this talk, we present a computational method which relies on a Monte Carlo sampling of the CI expansion space, and is used to build statisticals estimates of the correlation energy. By estimating neglected contributions, corrections for the correlation energy may be made- extending application of the method to a larger systems, and allowing estimates for electronic transition energies.

10:45 AM LL8.8
Development of a free volume photopolymerization model for high-throughput conversion analysis. Peter Johnson[1], Chrisotpher N Bowman[1] and Jeffrey W Stansbury[2,1]; [1]Department of Chemical and Biological Engineering, University of Colorado at Boulder, Boulder, Colorado; [2]School of Dentistry, University of Colorado Health Sciences Center, Aurora, Colorado.

A method for high-throughput analysis of photpolymerization conversion has the capability to produce hundreds of data points, each with a distinct composition, temperature and exposure time. Each analyzed sample is varied in two different factors with the third factor at a constant value, yielding two orthogonal gradients that produce double bond conversion as a function of exposure time, composition, and polymerization temperature. Multiple samples with varying factors allow for the entire parameter space to be analyzed within a short period of time. However, gaps will still remain within the parameter space, so determining the conversion between the samples will provide the entire range for study. A kinetic model describing the comonomer photopolymerization would allow for variation of species composition, temperature and exposure time to predict and analyze the parameter space. To provide the type of analysis required, a robust photopolymerization kinetic model including temperature, composition, and free volume factors has been developed for data analysis and prediction of photopolymer conversion. This model then uses post-cure conversion data collected from a high-throughput method to predict kinetic parameters. This model is capable of analyzing a system containing multiple monomers with or without post-cure polymerization. In addition, the model requires a smaller set of data to predict the rest of the parameter space, increasing the speed at which systems are analyzed. Kinetic parameters are predicted from the experimental data and then used to calculate the other regions of the experimental space and yield a more comprehensive analysis of the system. A comparison of model estimates to methacrylate/dimethacrylate and diacrylate/dimethacrylate systems will be shown to elucidate the process and final result. These systems exhibit different conversion profiles due to reactivity and functionality changes, which are explained through the effects incorporated into the model.

11:00 AM LL8.9
Designing Conducting Polymers Using Ant Systems. Gustavo Brunetto, Bruno VC Martins, Fernando Sato, Vitor R. Coluci and Douglas S. Galvao; Applied Physics, State University of Campinas, Campinas, Sao Paulo, Brazil.

Ant Systems are a computational metaphor inspired in real ant colonies. They represent a new and very powerful computational tool to the study of optimization problems. They were first proposed by Marco Dorigo and collaborators as a multi-agent technique to solve difficult combinatorial optimization problems. Real ants exhibit the remarkable ability to quickly locate food and to establish very

efficient food/nest paths. This can be explained in terms of pheromone deposition trails. Ants deposit markers (pheromones) as they walk and when choosing their paths they tend to follow the ones where the presence of the markers are more pronounced. These ideas can serve of basis to build evolutionary based algorithms. Here we show that ant systems can be used to help to design conducting polymers with pre-specified properties. Conducting polymers are a new class of materials presenting new and exciting phenomena, in particular high conductivity. In the last years the possibility of creating new classes of conducting polymers exploring the concept of co-polymerization has attract much attention from experimental and theoretical point of view. As structural disorder is always present in these systems (polymeric alloys) theoretical analysis is very difficult due to the necessity of analyzing a very large number of possible configurations. In this work we present a new ant-based methodology to solve this kind of problem. We show that ant systems can be very effective to determine optimum polymeric alloy compositions. The ant algorithm efficiently probes the vast phase space of solutions. Our results are contrasted against other evolutionary search techniques (such as genetic algorithms) and proved to outperform them under certain conditions.

11:15 AM LL8.10
Predicting crystal structure with a high throughput informatics model. Chris Fischer[1], Dane Morgan[2] and Gerbrand Ceder[1]; [1]Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; [2]Materials Science and Engineering, University of Wisconsin, Madison, Wisconsin.

Crystal structure is a fundamental and widely applicable facet of materials science. Despite significant advances in this field, high quality prediction of crystal structure remains an elusive and difficult task. This talk will discuss a predictive model of crystal structure combining the suggestive power of empirical data and the accuracy of modern electronic structure methods. Our model, utilizing artificial intelligence techniques, encapsulates correlation among crystal structures extracted from a large experimental database in a generic manner. As a consequence of the framework on which correlations are built, our model is not restricted to any particular host lattice, range, or complexity of atomic interaction. Combining empirical correlations with *abinitio* electronic structure methods results in a robust, exhaustive, and highly efficient structure predictor suitable for ground state searches, screening candidate chemical systems, and ferreting out suspected compounds.

SESSION LL9: Artifical Intelligence: Data Management
Chair: Krishna Rajan
Thursday Afternoon, December 1, 2005
Back Bay B (Sheraton)

1:30 PM *LL9.1
Materials Informatics for Combinatorial Chemistry.
Krishna Rajan, Changwon Suh and Michael Stukowski; Materials Science and Engineering, Iowa State University, AMES, Iowa.

Seeking structure-property relationships is an accepted paradigm in materials science, yet these relationships are often not linear and the challenge is to seek patterns among multiple length and time scales. There is rarely a single multiscale theory or experiment which can meaningfully and accurately capture such information. In this presentation we outline a process which can permit one to survey complex, multiscale information in a high throughput, statistically robust and yet physically meaningful manner. The application of such approaches are shown to have a significant impact in materials design and discovery. In this talk we describe how we are using data mining techniques combined with ab-intio, crystallographic and crystal chemistry data to establish a combinatorial chemistry framework for materials design. The informatics infrastructure being established through the NSF International Materials Institute: Combinatorial Sciences and Informatics Collaboratory is also described. NSF Intl. Materials Inst.: Combinatorial Sciences and Materials Informatics Collaboratory (CoSMIC-IMI)

2:00 PM LL9.2
Information-Based Development of New Radiation Detection Materials. Kim F. Ferris[1], Bobbie-Jo Webb-Robertson[1] and Dumont M. Jones[2]; [1]Pacific Northwest National Laboratory, Richland, Washington; [2]Proximate Technology LLC, Columbus, Ohio.

With our current concerns for a secure environment, the development of new radiation detection materials has focused on the capability to characterize potential radiation sources at increasingly tighter detection sensitivity levels. As the initial framework for a materials-informatics approach to radiation detection materials, we have explored structural signatures and patterns consistent with improved energy resolution and efficiency, and our current results are reported here. To build structural signatures for radiation detectors, we employed both supervised and unsupervised learning methods to a candidate scintillator material database derived from the NIST resource (250,000+ inorganic compounds), using raw descriptors developed from readily available or easily computed atomic and molecular properties. These results indicate that practical bounds in the physical properties of the radiation materials will impose significant limits for detector design. The authors gratefully acknowledge financial support from the PNNL Laboratory Directed Research and Development Project. The Pacific Northwest National Laboratory (PNNL) is operated by Battelle Memorial Institute for the US Department of Energy under Contract DE-AC06-76RLO 1830.

2:15 PM *LL9.3
eScience-Driven Discovery and Optimization of Polymeric Materials–Concepts, Examples, Experiences. Nico Adams[1,2] and U. S. Schubert[2]; [1]Dutch Polymer Institute, Eindhoven, Netherlands; [2]Macromolecular Chemistry and Nanoscience, Eindhoven University of Technology, Eindhoven, Netherlands.

The ever widening application of combinatorial and high-throughput methods for the development or optimization of new polymeric materials has triggered the need for sophisticated informatics to deal with the potential data flood and design-based approaches for the development of libraries and screening designs. Particularly the latter requires input from a diverse range of methods, such as statistical experimental design, molecular modeling and QSAR, all of which are "eScience" approaches. The talk will illustrate the fundamental concepts pursued by the Dutch Polymer Institute (DPI) in this area and show results from recently finished or ongoing research projects, in which laboratory experimentation was driven by eScience. Examples include topics such as the optimization of polymer formulations, the design of discovery libraries for new polymeric materials and the rationalization of experimental results, using modeling techniques.

3:15 PM *LL9.4
Pulsed Laser Deposition Process as a Target for Data Mining.
Tsuyoshi Ohnishi[1,2], Takahisa Yamamoto[3], Shinya Meguro[4,2], Hideomi Koinuma[4,5,3] and Mikk Lippmaa[1,2,3]; [1]Institute for Solid State Physics, The University of Tokyo, Kashiwa, Chiba, Japan; [2]Combinatorial Materials Exploration and Technology, Tsukuba, Ibaraki, Japan; [3]Graduate School of Frontier Sciences, University of Tokyo, Kashiwa, Chiba, Japan; [4]National Institute for Materials Science, Tsukuba, Ibaraki, Japan; [5]CREST, Japan Science and Technology Agency, Kawaguchi, Saitama, Japan.

For the growth of high-quality functional oxide thin films, Pulsed Laser Deposition (PLD) is widely used and believed to be one of the best methods. However, the PLD process has a serious problem: lack of repeatability. Accurate reproduction of film growth experiments based on published data is usually very difficult, and even with the same PLD system, it is not easy to obtain perfectly repeatable result over long time periods. The purpose of this study was, first, to locate some of the hidden growth parameters that affect reproducibility with the aid of statistical analysis of the numerous growth parameters and films properties, and second, to control these parameters to consolidate high-quality oxide thin film growth by PLD in a reproducible fashion. As a target material system, $SrTiO_3$ homoepitaxy was chosen in view of multiple interesting properties, such as quantum paraelectricity, large permittivity, metal-to-insulator phase transition at a fairly low electron carrier density (10^{-18} cm^{-3}), superconductivity, etc. Ideally, there is also no lattice mismatch between the film and the substrate, and therefore this system should be studied before attempting heteroepitaxy. In order to standardize growth parameters, especially the laser ablation conditions, a special PLD system was constructed, which enabled us to control the true energy of a KrF excimer at the target surface, beam shape and area on the target, and the target-substrate distance precisely. The real laser energy density and spot area were found to have a significant correlation with the deposition rate as well as the film properties, such as optical absorption, crystallographic constants, microstructure, and dopant activation. By controlling these two parameters accurately, fairly reproducible film growth could be achieved, and defect-free bulk equivalent $SrTiO_3$ films were obtained.

3:45 PM LL9.5
Data Management and Visualization of X-ray Diffraction Spectra From Thin Film Ternary Composition Spreads.
Christian J. Long[1], Ichiro Takeuchi[1], Olugbenga Famodu[1], Makoto Murakami[1], Jason Hattrick-Simpers[1], Gary Rubloff[1], Michael Stukowski[2] and Krishna Rajan[2]; [1]U of MD, College Park, Maryland; [2]Rensselaer Polytechnic Institute, Troy, New York.

We discuss techniques for managing and visualizing x-ray diffraction spectrum data for thin film composition spreads which map large

fractions of ternary compositional phase diagrams. An in-house x-ray microdiffractometer is used to obtain spectra from over 500 different compositions on an individual spread. The MATLAB software is used to quickly organize the data and create various plots from which one can quickly grasp different information regarding structural and phase changes across the composition spreads. Such exercises are valuable in rapidly assessing the overall picture of the structural evolution across phase diagrams before focusing in on specific composition regions for detailed structural analysis. We have also shown that simple linear correlation analysis of the XRD peak information (position, intensity and full width at half max) and physical properties such as magnetization can be used to obtain insight about the physical properties. As a model system, we have looked at the Ni-Mn-Al system whose rich functional phase diagrams include compositions displaying ferromagnetism and reversible martensites depending on atomic ordering.

4:00 PM LL9.6
A Prototyping Study on Building the Dental Materials Data Warehouse. Yong Li, International Metrology Systems, Orange, California.

In this study, the effectiveness of a new data management technique of data warehousing is critically evaluated for integrating dental materials data, in attempt to facilitate efficient informational services including data retrieval and materials selection. A scaled-down version of the dental materials data warehouse (DMDW) is constructed and an English Query application, which allows the end users to formulate the queries in natural English language, is developed on top of the DMDW. The current application supports five types of queries ranging from basic practice of data retrieval to more advanced information analytical service of materials selection. The results demonstrate that the data warehousing technique is of a great potential in storing, processing and managing dental materials data, and will have a tangible impact on research and education in the dental materials community.

4:15 PM LL9.7
On-line Data Management for High-throughput Experimentation. Mikk Lippmaa[1], Shinya Meguro[2], Tsuyoshi Ohnishi[1] and Hideomi Koinuma[2]; [1]Institute for Solid State Physics, Kashiwa, Chiba, Japan; [2]National Institute for Materials Science, Tsukuba, Japan.

Development of new parallel solid state synthesis and characterization equipment has meant that the combinatorial methodology can now be applied to numerous solid state materials science problems. The improved experimental throughput has created new challenges for processing the experimental data, starting with raw data storage and visualization, but also affecting the ways that the experimental results are analyzed, presented, and shared. We present some of the techniques and software that we have developed for on-line storage, sharing, and visualization of data from combinatorial experiments. The system is based on a centralized database and a Web interface that can be accessed from any networked computer. The greatest challenge facing us is the variety of data types and formats that such a system has to support in such a way that data from many different sources, i.e. from synthesis and characterization instruments, could be combined. We discuss the data storage and sharing format issues, proposing a generalized extensible markup language (XML) derivative for this purpose. Our approach is driven by the desire to avoid as much as possible instrument or workflow-specific software and generalize the data access and processing tools. This allows the core part of the software to remain useful even when the experimental needs and procedures change. In particular, in addition to simple visualization, we also attempt to support interactive statistical data analysis tools and ongoing materials structure and property database construction efforts.

4:30 PM LL9.8
Using the Cambridge Structural Database in Materials Science Research. John Walter Liebeschuetz, Applications Group, Cambridge Crystallographic Data Centre, Cambridge, United Kingdom.

The Cambridge Structural Database(1) is the world's repository of validated crystal structure data for organic and metal-organic compounds. From small beginnings 40 years ago, this repository has grown to over 330,000 datasets and aims to be comprehensive for published structures determined by x-ray and neutron diffraction analysis. It represents a treasury of information on molecular geometry and intermolecular interactions. The database is accompanied by a set of software tools and derived databases that allow the user to investigate many aspects of molecular structure, inter- and intramolecular interactions, and crystal packing. The Cambridge Structural Database is already established as an essential component of chemical and crystallographic research in academia. It has also been of significant benefit to discovery researchers in the pharmaceutical industry, where the high quality information on both molecular conformation and non-covalent interactions has been applied to optimising drug-receptor interactions. Because knowledge of molecular interactions is of crucial importance in the design of, for example, synthetic receptors, organic microelectronic materials, catalysts and macromolecular aggregates, the information within the CSD is also potentially valuable to researchers in these fields. This talk will present an overview of the Cambridge Structural Database System and its applications to materials science research will be demonstrated. In particular, we will demonstrate the value of the CSD in overcoming, through better understanding interactions in the solid state, some of the problems of bringing a pharmaceutical clinical candidate to market. 1 F.H.Allen, Acta Cryst., B58, 380-388, 2002