#### ICTP/UCSB/TWAS MINIWORKSHOP ON 'FRONTIERS IN MATERIALS SCIENCE'' 15 - 18 May 2001

#### <u>P R O G R A M M E (as of 1/05/01)</u>

#### Venue: Main Lecture Hall, ICTP Main Building (Entrance Level)

WEEK	Tuesday		Wednesday		Thursday		Friday
15 - 18	<u>15 May</u>		16 May		17 May		18 May
9:00 - 10:45 Main Bldg. Lobby	REGISTRATION	9:30-10:30	<u>Structural &amp; Inorganic Materials</u> (cont'd): G. Stucky (chair)	9:30-10:30	<u>Conducting Polymers (cont'd)</u> : T. Deming (chair)	9:30-10:30	<u>Theory &amp; Modelling (cont'd):</u> N. Hill (chair)
	<b>&amp;</b> Coffee (and Post-Reg. Admin. at E. Fermi Bldg)	14	<b>A. CHEETHAM:</b> Some Recent Developments in Nanoporous Materials	18	<b>G. BAZAN:</b> Strategies for Tailoring Chromophore-Chromophore Interactions in the Solid State	I 12	<b>J. LANGER:</b> Jamming, Deformation & Fracture in Amorphous Materials
10:45-11:00	<b>OPENING</b> M.A. Virasoro A. Cheetham & C.N.R. Rao	10:30-11:00 <b>C4</b>	<b>O.A.YASSIN:</b> Lattice Effects on some Transport & Magnetic Properties of the Rare Earth Manganites	10:30-11:00 <b>C8</b>	<b>W. BANTIKASSEGN:</b> Photo-Voltaic Properties of a Single Layer Polymer (PTOPT)	10:30-11:00 <b>C11</b>	<b>S.A. MUJAHID:</b> Theoretical Analysis of the Composition of Plates Isothermally Formed in Non-Ferrous Binary Alloys
11:00-12:00	<u>Structural &amp; Inorganic Materials</u> : A. Cheetham (chair)	11:00-11:30	Coffee Break	11:00-11:30	Coffee Break	11:00-11:30	Coffee Break
. I1	<b>F.F. LANGE:</b> Nano-Textured, Super- Hydrophobic Sufaces						
12:00-12:30 C1	S.C. PANG: Sol-Gel-Derived	11:30-12:30 <b>I5</b>	C.N.R. RAO: Nanotubes	11:30-12:30	<u>Theory &amp; Modelling</u> : A.R. Bishop (chair)	11:30-12:30	
	Nanoparticulate Manganese Dioxide Thin Films as Novel Electrode Materials			19	<b>N. HILL:</b> Pushing the Limits of the Electronic Structure Theory; Can we design new Spintronic Materials?	I 13	<b>R. PANDIT</b> : Semiflexible Equilibrium Polymers: A Self- Assembling Molecular Model
12:30-13:00 C2	<b>R. SESHADRI:</b> Solvo-thermal Routes to Capped Oxide & Sclenide Nanoparticles	12:30-13:00 <b>C5</b>	<b>M. PRATO:</b> Functionalization of Carbon Networks: from Fullerenes to Nanorods & Nanotubes	12:30-13:00 <b>C9</b>	<b>Z. MA:</b> The Electrical and Optical Properties for Structural-Disordered Solids	12:30-13:00 C12	<b>M.O.MUNYATI:</b> Deformation Studies in Rubber-Modified Polyester Resin Systems
13:00-15:00	Lunch Break	13:00-15:00	Lunch Break	13:00-15:00	Lunch Break	13:00 - <b>14:00</b>	Lunch Break
15:00-16:00	<u>Structural &amp; Inorganic Materials</u> <u>(cont'd</u> ): F.F. Lange (chair)	15:00-16:00 I6	<u>Structural &amp; Inorganic Materials</u> <u>(cont'd)</u> : G. Bazan (chair)	15:00-16:00	<u>Theory &amp; Modelling (cont'd)</u> : J. Langer (chair)	<b>14:00-</b> 15:00	<u>Biomolecular Materials</u> : C.N.R. Rao (chair)
I2	<b>M. RUELHE:</b> Structural & Chemical Analysis of Materials by Advanced Transmission Electron Microscopy Technique	10	<b>C. G. LEVT:</b> High Temperature Thermally Insulative Coatings	I 10	<b>A.R. BISHOP:</b> Multiscale Structure & Function from Competing Short- and Long-Range Forces	I 14	<b>T. DEMING:</b> Synthesis & Self-Assembly of Block Copolypeptide Materials
16:00-16:30 <b>C3</b>	<b>A. NIAZI</b> : Magnetic Characteristics of an Oxide System, Sr3Cu <sub>1</sub> - <sub>x</sub> Zn <sub>x</sub> IrO <sub>6</sub> , with Competing Interactions & Low Dimensionality	16:00-16:30 <b>C6</b>	<b>A.K.M. AKTHER HOSSAIN:</b> Search for Colossal Magnetoresistance in Screen Printed Manganite Thick Films	16:00-16:30 <b>C10</b>	<b>J.W. SIGNORELLI:</b> Incorporating Polycrystalline Plasticity in a Finite Element Code for Modelling Poly- crystals with Complex Microstructure	15:00-15:30 <b>C13</b>	<b>P. FRIERE:</b> Investigation of Vibrational Properties of Amino Acid Crystals
16:30-17:30 <b>I3</b>	<b>G. STUCKY:</b> Organizing Domains in Composite Materials: Synthesis,	16:45-17:45	<u>Conducting Polymers:</u> T. Deming (chair)	16:30-17:30 <b>I 11</b>	<b>M.P.A. FISHER</b> ; Electronic Exotica in Strongly Correlated Materials	15:45-16:45 <b>I 15</b>	<b>D. MORSE</b> : Silicon Biotechnology: New Routes for Structure-Directing Catalysis
	Structure & Function	17	<b>F. WUDL</b> : Synthesis & Optical Properties of Polar Acenes				of Polysiloxane Synthesis
		17:45-18:15 <b>C7</b>	<b>K.R. TEMSAMANI:</b> The Electro- chemistry of Some Organic Compounds of Biological Importance at Conducting Polymer Modified Gold Electrodes: Analytical Performances Study. Part II: Project of Water Pollutants Detection"	17:30-19:30	POSTER SESSION (Terrace Level)	16:45-17:45 <b>I 16</b>	<b>K. FREED</b> : Phase Behavior and Miscibility of Polymer Blends
		19:00-20:00	BUFFET DINNER (Adriatico)			17:45-18:00	CLOSING - C.N.R. Rao & A. Cheetham

# INVITED & CONTRIBUTED <u>TALKS</u>

Structural and Ino	rganic Materials
I1	F.F. LANGE
Cl	S.C. PANG
C2	R. SESHADRI
	M. RUELHE
	A. NIAZI
1 ð	G. SIUCKI
I 4	A. CHEETHAM
<b>C4</b>	O A. YASSIN
I 5	C.N.R. RAO
C5	M. PRATO
I 6	C.G. LEVI
C6	A.K.M. AKTHER HOSSAIN
	F. WUDL
07	K.R. TEMSAMANI
<b>Conducting Polyme</b>	ers
18	G. BAZAN
<b>C8</b>	W. BANTIKASSEGN
Theory & Modellin	Ø
I 9	N. HILL
<b>C9</b>	Z. MA
I 10	A.R. BISHOP
C10	J.W. SIGNORELLI
I 11	M.P.A. FISHER
I 12	J. LANGER
C11	S.A. MUJAHID
I 13	R. PANDIT
C12	M.O. MUNYATI
<b>Biomolecular Mate</b>	erials
I 14	T. DEMING
C13	P. FRIERE
I 15	D. MORSE
1 16	K. FREED



#### Nano-Textured, Super-Hydrophobic Surfaces

## F.F. Lange Materials Department University of California at Santa Barbara

For centuries, eastern religions have recognized the purity of the lotus leaf. Its purity is caused by its super-hydrophobic surface, which allows water drops to form nearly spherical balls that collect water-loving dust particles as they roll off with very little contact resistance. In 1997, biologists Barthlott and Neinhuis [1] showed that small, waxy hills on the lotus leaf produced this super-hydrophobic effect. Tadanaga et al. [2] recognize that the water only wetted the tops of the hills and that air must be trapped in the valleys to relate the wetting angle of the hilly surface, q<sup>\*</sup>, to the wetted area fraction, f, and the wetting angle of a flat surface, q. Bico et al [3] verified this relation by texturing a surface with periodic, micron-size silica features (e.g., wells, plateaus and channels, flat mesas) produced on a substrate with a micro-molding technique. It also has been shown that water droplets bounce on super-hydrophobic surfaces, as well as roll, instead of sliding. We [4] have developed a new method for texturing surfaces with nano-particles. We have shown that nanotextured surface exhibit bazaar phenomena that can be explained with the Laplace equation.

- [1] W. Barthlott and C. Neinhuis, "Purity of the Sacred Lotus, or Escape from Contamination in Biological Surfaces," Ann. Botany, 79, 667 (1997).
- [2] K. Tadanaga, N. Katata, and T. Minami, Super-Water-Repellent Al2O3 Coating Films with High Transparency, J. Am. Ceram. Soc. 80 1040-1042 (1997).
- [3] J. Bico, C. Marzolin and D Quéré, "Pearl Drops," Europhysics Lett. 47 [2], 220-6 (1999).
- [4] Rob J. Klein, P. Maarten Biesheuvel, Ben C. Yu, Carl D. Meinhart, and Fred F. Lange, "Producing Super-Hydrophobic Surfaces with Nano-Silica Spheres" to be published

## Sol-Gel-Derived Nanoparticulate Manganese Dioxide Thin Films as Novel Electrode Materials for Electrochemical Capacitors.

## Dr. Pang Suh Cem Faculty of Resource Sciences and Technology Universiti Malaysia Sarawak 94300 Kota Samarahan, Sarawak, Malaysia.

#### Abstract

Most of the commercially available electrochemical capacitors are carbon-based systems which are made primarily of activated carbon with a specific surface area as high as 2,000  $m^2/g^1$ . They are thought to be true electric double layer (EDL) capacitors. Transition metal oxides, most notably ruthenium dioxide (RuO<sub>2</sub>), have been shown to possess high energy storage capacity, with a specific capacitance of over 720  $F/g^2$ . It has been demonstrated that these are not strictly EDL capacitors but function by redox or faradaic charging mechanisms, often known as pseudocapacitance. Unfortunately, both activated carbon and ruthenium dioxide systems have intrinsic and extrinsic limitations in meeting specific demands of a wide range of applications. The cheap activated carbon suffers from the drawback of high internal series resistance (ESR) arising from contact resistant of carbon particles. The cost of RuO<sub>2</sub> is prohibitively high for most device applications. A new generation of electrochemical capacitor systems based on cheaper mixed valence transition-metal oxides, thin-film nickel oxide using the sol-gel process have been reported by *Liu et al*<sup>3</sup>. The specific capacitance of NiO<sub>x</sub>/Ni in 1M LiOH electrolyte was reported to be as high as 265 F/g. Sol-gel-derived CoO<sub>x</sub> amorphous thin films have been

shown to provide capacitance values approaching 300F/g<sup>4</sup>.

While the utility of manganese dioxide in batteries has long been recognized and well established, its potential application as electrode material for electrochemical capacitors has not been extensively studied. Sol-gel-derived nanoparticulate manganese dioxide thin films have been shown to be potential novel electrode materials for electrochemical capacitors<sup>5,6</sup>. Such films are relatively conductive, highly porous, and possess high specific surface area. Being an inorganic oxide composed of multi-valent ions, manganese dioxide possesses such important characteristics as inherent non-stoichiometric character and a low bandgap for fast adsorption and desorption reactions. Materials with such characteristics are expected to exhibit high pseudocapacitance associated with both surface and bulk redox processes. Sol-gel-derived MnO<sub>2</sub> thin films can be prepared easily and cheaply, and are environmentally friendly. Various research studies conducted by *Pang et al.*<sup>5,6</sup> have shown that sol-gel-derived nanoparticulate MnO<sub>2</sub> thin films exhibit performance approaching that of the RuO<sub>2</sub>-based electrochemical

MnO<sub>2</sub> thin films exhibit performance approaching that of the RuO<sub>2</sub>-based electrochemical capacitor systems, but in mild aqueous electrolytes. The effect of voltammetric cycling on the morphology and microstructure on both electrodeposited and sol-gel-derived MnO<sub>2</sub> thin films have been investigated. Further optimization of the electrochemical performance of MnO<sub>2</sub> thin films as electrode materials for electrochemical capacitors is envisaged through microstructural control of the grain size, specific surface area and pore-size distribution. **References:** 

- 1. Tanashashi, A. Yoshida, A. Nishino, Bull. Chem. Soc. Jpn., 63, 2755 (1990).
- 2. J.P. Zheng, T.R. Jow, J. Electrochem. Soc., 142, L6 (1995).
- 3. K.C. Liu, M.A. Anderson, J. Electrochem. Soc., 143, 124 (1996).
- 4. C. Lin, J. A. Ritter, B.N. Popov, J. Electrochem. Soc., 145, 4091 (1998).
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#### Solvothermal routes to capped oxide and selenide nanoparticles.

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## ABSTRACT

Recently Alivisatos and coworkers [1] have described a facile and rather general route to the preparation of capped metal oxide nanoparticles in organic amine solvents through the thermal decomposition of cupferron complexes. These authors use trioctylamine as a solvent, and have been able to prepare amine-capped nanoparticles of single metal-component oxides. We have recently extended this non-hydrolytic route to prepare a number of unary [TiO2, ZrO2, SnO2, Mn3O4, gamma-Fe2O3], binary [MFe2O4 (M=Co, Ni, Zn) and pseudo-ternary [(Co-Zn)Fe2O4] oxides by starting with a mixture of cupferron complexes instead of single complexes. An important advancement is that we perform these reaction in closed stainless steel bombs using inexpensive solvents but under solvothermal conditions. This obviates the need for the use of expensive and toxic amine or phosphine oxide solvents and lends itself to significant scale-up. Our preparations yield stable sub-10 nm particles that are superparamagnetic (in the cases of magnetic oxides) at the room temperature.

Perhaps the most widely used route to semiconducting chalcogenide (quantum dot) nanoparticles is the one exemplified by Bawendi and coworkers [2] where an organocadmium precursor is reacted in a high temperature solvent such as trioctyl phosphine oxide with a chalcogen source. Inert conditions are required to carry out such reactions and the organocadmium precursors used are expensive, toxic and flammable. We have recently proposed a significantly simpler route [3] that employs solvothermal conditions with toluene as the solvent. The cadmium source is the relatively safe stearate and H2Se required for the reaction is generated in-situ through the aromatization of tetralin to naphthalene by Se. In the presence of dodecanethiol as a capping agent, this route yields relatively monodisperse nanoparticles [3.00(16) nm diameter] albeit in the zinc blende structure. Once again, significant scale-up is possible.

#### **References:**

- 1. J. Rockenberger. E. C. Scher, A. P. Alivisatos,
- J. Am. Chem. Soc. 121 (1999) 11595.
- 2. C. B. Murray, D. J. Norris, M. G. Bawendi, J. Am. Chem. Soc., 115 (1993) 8706.
- 3. U. K. Gautam, M. Rajamathi, F. Meldrum, P. Morgan, R. Seshadri,
  - J. Chem. Soc. Chem. Communn. (2001) in press.

## Structural and Chemical Analysis of Materials by Advanced Transmission Electron Microscopy Technique

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#### Abstract

A correlation between the microstructure and properties of a material requires microstructural characterization. Firstly, it is important to identify the different phases of the material. This can be done by X-ray diffraction studies and transmission electron microscopy (TEM), selected area diffraction (SAD) studies, and electron spectroscopic imaging (ESI). For materials with high symmetry, the structure factors can be determined from energy-filtered convergent beam electron diffraction (CBED) investigations.

Most important is, however, the analysis of defects in the material. There exist different ways of analyzing crystal defects by TEM. Conventional TEM allows the qualitative and quantitative analysis of dislocations, dislocation loops, voids, precipitates. Some information can also be obtained on the structure of internal interfaces.

Advanced TEM techniques will be described which can be applied for the analysis of internal interfaces. Quantitative high-resolution TEM (QHRTEM) allows the quantitative determination of the positions of columns of atoms (ions) adjacent to the interface. By analytical electron microscopy (AEM) the composition of the interfaces can be determined with high spatial resolution and an excellent limit of detectability. Details of electron energy-loss spectroscopy (EELS) studies reveal information on electron bonding, coordination and neighboring atoms. Electron loss near-edge structures (ELNES) contain this information.

The different techniques are applied to different problems in materials science.

## Magnetic characteristics of an oxide system, $Sr_3Cu_{1-x}Zn_xIrO_6$ , with competing interactions and low dimensionality

Asad Niazi<sup>†</sup>, E.V. Sampathkumaran<sup>†</sup>, P.L. Paulose<sup>†</sup>,

D. Eckert<sup>‡</sup>, A. Handstein<sup>‡</sup>, K.-H. Mueller<sup>‡</sup>

†Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai-5, India. ‡IFW Dresden, PO Box 270116, D-01171 Dresden, Germany.

#### Abstract

1:

The series of oxides of the type,  $A_3A'XO_6$  (A = Sr, Ca, Ba; A' = a magnetic or non-magnetic ion, X = a magnetic ion, ) crystallizing in K<sub>4</sub>CdCl<sub>6</sub>-type rhombohedral symmetry (or its derivatives), are of considerable interest, as these are characterized by the existence of chains of A'-X along c-axis. Here, we report the results of x-ray diffraction, ac and dc magnetization ( $\chi$ ) studies on a solid solution, Sr<sub>3</sub>Cu<sub>1-x</sub>Zn<sub>x</sub>IrO<sub>6</sub>. It has been reported that the Cu and Zn end members order ferro and antiferromagnetically at about 20 and 19 K respectively. We show here that: (i) the structure smoothly varies from monoclinically distorted rhombohedral (C2/c, x = 1) to rhombohedral (R-3c, x = 0); (ii) The ordering temperature  $T_{\circ}$  of the Cu sample is found to be sensitive to preparative conditions and Cu content; it also exhibits a frequency dependence of the peak temperature in the ac  $\chi$  data (in zero dc magnetic field (H)), while an application of H of about 1 kOe washes out this feature. This finding implies that this compound is presumably ferrimagnetic/spin-glass-like in zero field, and the application of H stabilises ferromagnetism. However, there is no such behaviour for the Zn sample, which shows robust, long-range antiferromagnetic order; (ii)Even a small substitution for either end-member (x = .25 and .75) significantly depresses magnetism, with non-monotonic variation of  $T_{\circ}$  upon varying x ( $T_{\circ} \sim 7, 4, 3$  and 7 K for x = .25, .33, .5, .75 respectively); (iii) The plot of inverse susceptibility versus temperature becomes non-linear in the paramagnetic state even for very small replacement of Zn by Cu, indicating variation of magnetic correlation strength (inter/intra-chain) with temperature. Other interesting structural and magnetic features observed in this solid solution will also be presented.

## Organizing Domains in Composite Materials: Synthesis, Structure and Function

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#### Abstract

Patterning and organizing multiple domains by molecular definition over the nano to macro length scales for structure and function provides intriguing challenges and opportunities for the synthetic materials scientist. Of the various length scales, the mesoscale regime has been until recently a "black hole" in materials science. It is at this length scale that bulk and surface properties have comparable weighting, where morphologies may be determined by surface forces instead of internal lattice energies, and where surface dynamics are increasingly integrated into bulk properties. The assembly of 3-d composite mesoscale materials by deposition and patterning techniques is at the limit of the best semiconductor technologies. Since at this length scale the error limits are at the molecular and atomic nanoscale, 3-d assembly approaches based on the cooperative organization of molecular species becomes increasingly attractive. For organic/inorganic host/guest types of materials at a fixed length scale, a binary phase synthesis media which provides the appropriate interface between the molecular species being assembled is a good starting point. Ternary and higher multiphase synthesis media enhance the number of possible spatial permutations and enable "one pot" materials synthesis at multiple length scales. The challenge is to master the kinetics, thermodynamics and processing associated with the competing multi-domain assembly chemistries and the related interfaces. Because 3-d mesostructure inorganic/organic materials are relatively new, their "figure of merit" (FOM) parameters in terms of stability and functional properties are only beginning to be determined. This talk will give a selected overview of "How do you make them?" and "What are they good for?"

## Some Recent Developments in Nanoporous Materials

## Anthony K. Cheetham Materials Research Laboratory, University of California, Santa Barbara, CA 93106.

Nanoporous materials, such as the aluminosilicate zeolites and the openframework aluminum phosphates, find widespread applications in separation processes, ion-exchange, and catalysis [1]. The presentation will review both the history and recent developments in this fast-moving area, including the discovery of nanoporous materials based upon many other types of chemistries, e.g. oxides, halides, nitrides, and open-framework organic-inorganic polymers. We shall then discuss some aspects of our recent work in Santa Barbara on open-framework metal phosphates. There have been two dominant themes. First, we have synthesized a wide range of open-framework tin(II) and antimony(III) phosphates, which contain lone pairs of electrons and offer the possibility of sustaining base-catalyzed reactions [2]. We shall describe the synthesis and architectures of some of these materials and present some preliminary catalysis results. In the second area, we shall describe some recent work on nanoporous nickel phosphates, which exhibit unique catalytic properties [3]. For example, two of the NiPO materials will catalyze shape-selective hydrogenation and dehydrogenation reactions that are not possible with conventional zeolite catalysts [4]. Future developments in this general area will also be discussed.

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- B. A. Adair, G. Díaz de Delgado, J. M. Delgado, and A. K. Cheetham, <u>Angew.</u> <u>Chem.</u> 39, 745-747 (2000).
- N. Guillou, Q. Gao, M. Nogues, R. E. Morris, M. Hervieu, G. Férey, and A. K. Cheetham, <u>C. R. Acad. Sciences (Paris)</u> Séries IIc, 387-392 (1999).
- 4. J-S. Chang, S-E. Park, Q. Gao, G. Férey, and A. K. Cheetham, <u>J.C.S. Chem.</u> <u>Comm.</u> 859-860 (2001).

# Lattice effects on some transport and magnetic properties of the rare earth manganites La<sub>0.67-2x</sub>Nd<sub>2x</sub>Ca<sub>0.33-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> La<sub>1-x</sub>Y<sub>x</sub>Sr<sub>2</sub>Mn<sub>2</sub>O<sub>7</sub> manganites

#### Osama Ali Yassin

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Abstract: Understanding the role of the lattice on the so-called "Colossal Magnetoresistance" (CMR) has become of great importance [1]. The coupling between these properties and the lattice disorder is fascinating. We studied the effect of the lattice disorder on the magnetic properties of three dimensional manganites La<sub>0.67-2x</sub>Nd<sub>2x</sub>Ca<sub>0.33-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> (x=0, 0.1, 0.15, 0.2, 0.25 and 0.33). We have also studied this effect on the properties of the two dimensional perovskite LaSr<sub>2</sub>Mn<sub>2</sub>O<sub>7</sub> where the disorder was created at the A-site by replacing La by Y. In the first series the spin waves stiffness constant (D) was determined from the magnetisation data below ~ 100 K. These values when plotted against the variance in the raduis of the A-site ions were found to follow a power law given by  $D = A(\sigma^2)^{\vee}$ , with  $A \approx 11.902$  and  $v \approx 0.31 \pm 0.001$ . This relation suggests that the lattice disorder (represented by ) is the primary cause for the break up of the spin waves and the subsequent disappearance of magnetisation. This relation appears to be universal as it has been found to be applicable to other manganites as well. The analysis of the electrical resistivity data below ~100 K is consistent with the coherent motion of the small polarons which results from the relaxation of a soft optical phonon mode. The Fermi energy  $(E_F)$  calculated from the linear temperature dependence of the thermoelectric power (TEP) below 50 K has been found to decrease with the increase in  $\Box$ . Doping LaSr<sub>2</sub>Mn<sub>2</sub>O<sub>7</sub> with Y resulted in melting of the charge ordered state seen at  $\sim$ 230 K in the parent material. The electrical transport properties above T<sub>MI</sub> of this series also support the ASPH model. The metal-insulator transition seen at 150K in the parent material LaSr<sub>2</sub>Mn<sub>2</sub>O<sub>7</sub> was seen to smear out with increasing content of Y ions.

Currently we are investigating the role of the valence state and the cation size disorder on the density of state of  $La_{1-x}(Ca,Sr)_xMnO_3$  manganites.

## C.N.R. RAO

# Chemistry and Physics of Materials Unit Jawaharlal Nehru Centre for Advanced Scientific Research Jakkur P.O. Bangalore 560 064 India

Carbon nanotubes were discovered soon after the successful laboratory synthesis of fullerenes. Since their discovery in 1991, there has been intensive research activity in the area of carbon nanotubes, not only because of their fascinating structural features and properties but also because of their technological applications. In this presentation, we shall examine some aspects related to the synthesis, structure and characterization of multi-walled and single-walled carbon nanotubes, and the important electronic, mechanical and hydrogen storage properties of the nanotubes. Applications of carbon nanotubes in nanoelectronics are particularly facinating and the disovery of junction nanotubes holds much promise. Nanotubes also exhibit field emission properties suitable for display Similarly, the hydrogen storage properties are indeed most attractive. devices. Doping as well as other chemical manipulations by boron and nitrogen bring about significant changes in the properties of the nanotubes. Carbon nanotubes also serve as useful templates to make other nanostructures. Layered metal chalcogenides form nanotubes providing scope for applications.

## Functionalization of Carbon Networks: From Fullerenes to Nanorods and Nanotubes

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In recent years, the fullerenes have generated great excitement inside the scientific community, mainly because of their interesting physical and chemical properties. In this field, one of the fast moving disciplines is the "functionalization chemistry". New opportunities arise from the combination of the fullerene properties with those of other classes of materials, such as polymers, electro- or photoactive units, liquid crystals, etc. In most cases, the new derivatives retain the main properties of the original fullerene, and many functionalized fullerenes may find useful applications in the field of materials science and technology.

Our contribution to this field has been the preparation of a variety of fullerene derivatives, mainly generated through the 1,3-dipolar cycloaddition of azomethine ylides to C60. This reaction leads to a class of stable and characterizable compounds, colloquially termed "fulleropyrrolidines". Given the large number of methods used to generate the reactive azomethine ylides, the ready availability of the starting materials, as well as the easy functionalization of the reaction products, a wide range of fulleropyrrolidines have already become available. Applications of the functionalized fullerenes to different fields have included long-range electron-transfer processes in fulleropyrrolidine-containing donor-acceptor dyads for the development of devices employable for electron/energy storage and nonlinear optical properties. In particular, the preparation of transparent thin films containing fullerenes offers the possibility of producing active shields against optical damage, providing protection against high-energy laser light.

In some cases, when appropriate functionalization is provided, fullerenes self-organize in superstructures such as vesicles and nanorods.

Within this contribution, we will review our most recent achievements in the field of fullerene synthesis and applications, including our preliminary efforts in the self-assembly of carbon networks.

### References

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- Prato, M. J. Mater. Chem. 1997, 7, 1097-1109; Prato, M. Top. Curr. Chem. 1999, 199, 173-188.

## HIGH TEMPERATURE THERMALLY INSULATIVE COATINGS

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#### **ABSTRACT**

Engineered coating systems with enhanced high temperature capability and reliability are arguably the most important materials challenge in advanced gas turbine technology. Much of the research emphasis is on thermal barrier coatings (TBCs), which have become essential to extending the temperature capability of metallic components, as well as to the future utilization of ceramics in gas turbines. The presentation will first review some of the characteristics of the problem and the approaches taken to solve it, and then focus on the connection between microstructure and process in the context of desired performance goals. Electron-beam physical vapor deposition (EB-PVD) is often favored for the synthesis of high performance TBCs. The resulting microstructure is columnar, with segmentation at the grain boundaries that enables strain tolerance during thermal cycling, and fine scale porosity within the columns that enhances their thermal resistivity. The development of this characteristic microstructure will be examined, with emphasis on the selection of in-plane and out-of-plane textures, and on the implications for the incorporation of porosity in different length scales. The relative roles of crystallography, surface diffusion and local flux variations due to shadowing will be discussed in the context of experiments where temperature, vapor incidence pattern and substrate characteristics are varied in a controlled manner. Of particular interest is the effect of substrate rotation on the evolution of morphology vis-à-vis deposition on stationary substrates. Additional insight on the interplay between the vapor flux and the surface morphology is provided from continuum and ballistic deposition models.

## Search for Colossal Magnetoresistance in Screen Printed Manganite Thick Films

## A. K. M. Akther Hossain Department of Physics Bangladesh University of Engineering & Technology, Dhaka 1000, Bangladesh

## Abstract

Thick films of La0.67Ca0.33MnO3 and La0.63Y0.07Cao.30MnO3 were fabricated on (100) oriented single crystal LaAlO3 (LAO), (100) oriented yttria stabilised zirconia (YSZ) and on polycrystalline Al2O3 by a screen printing technique. The films of La0.67Ca0.33MnO3 were sintered at 1200, 1300 and 1400C, in air, oxygen and nitrogen atmospheres to explore the optimum annealing conditions of manganite thick films. The films of La0.63Y0.07Cao.30MnO3 were sintered at 1200C in air and oxygen atmosphere. Magnetic and DC resistance properties were measured on all films. So called colossal magnetoresistance (CMR) behaviour was found to occur for films on all substrates under certain preparation conditions. The salient features of the CMR observed in these thick films are following:

- (i) MR is not limited to a small temperature window near the metal-insulator transition (M-I) at Tp1. The MR peak is very broad and for some films a temperature independent CMR is observed at temperatures below Tp1.
- (ii) Low-temperature low-field MR is highly sensitive for La0.63Y0.07Cao.30MnO3 films compared to La0.67Ca0.33MnO3 films on alumina substrate prepared under same condition.

Several repeat films were made and the reproducibility of the results obtained in the first batch were confirmed.

## Synthesis and Optical Properties of Polar acenes

Fred Wudl UCLA Department of Chemistry and Biochemistry 607 Charles E. Young Drive East Los Angeles, CA 90095-1569

## Abstract

We will describe blue azaanthracenes which have a smaller  $E_{gap}$  than pentacene. The azaanthracene exhibits very unusual photophysics with two luminescent bands; one in the blue and one in the red region of the visible spectrum



Theoretical calculations at the B3LYP with a 6-31G<sup>\*</sup> basis set were used throughout to predict the electronic properties of these and other molecules to be described in the talk. The benzoquinolone ( $l_{max}$  588) exhibits unusual photophysics, showing two emissions; one in blue and one red.

## The Electrochemistry of some organic compounds of biological importance at conducting polymer modified gold electrodes: Analytical performances study. Part II: Project of water pollutants detection"

Khalid Riffi Temsamani University Abdelmalek Essaâdi Faculty of Sciences of Tétouan Chemistry Department BP 2121, M'Hannech II. 93000 Tétouan-Morocco

#### **Abstract:**

With respect to dynamic electroanalytical techniques the concept of the modified electrodes is certainly one of the exciting developments in the end of the last century. The underlying motivation for electrode surface modification stem from the desire for improved electrocatalysis and freedom from surface fouling effects. Alternatively, electrode surfaces can be modified to prevent undesirable reaction from competing kinetically with the desired electrode process [1-3]. There is a multitude of polymeric coating for a wide variety of electrode applications in electrochemistry. Electrically conducting polymers, which constitute one group of a larger family of polymers (redox polymers, ion exchange polymers..), appear to have a distinct advantage over redox mediators for catalysis. This advantage is inherent in the fact that conduction, and therefor interfacial electron transfer, can take place over a broad potential window [4]. Our research group is working on a water quality control project based on the development of new electrochemical sensors. We realize the modification of a gold electrode with <u>poly(3-methylthiophene</u>) (P3MT), which is an electronically conducting polymer that is easily deposited onto the gold by electrooxidation of its monomer at + 1.6 volts. In this project we follow the electrochemical behavior of compounds of either biological or environmental importance at the Au/P3MT electrodes. Electrocatalytic effects under these conditions together with selective voltammetric determinations are giving interesting preliminary results. Also, non-reversible voltammograms obtained at bare gold for some neurotransmitters show perfect reversibility at conducting polymer-modified electrodes. In the near future, we plan to use the P3MT, as a matrix in which we will immobilize specific enzymes such as urease or polyphenoloxydase (PPO) at the electrode surface. By preparing these systems under the right substrate conditions( successively urea and catechol), we hope to be able to detect, indirectly, low water concentrations of well-known enzyme inhibitors such as heavy metals for urease or atrazine for PPO (by measuring pH, anodic or cathodic currents). The main electrochemical techniques we use are cyclic voltammetry, differential pulse voltammetry or potentionmetry. We believe that conducting polymers will open new horizons for surface electrochemists.

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**C7** 



## Strategies for Tailoring Chromophore-Chromophore Interactions in the Solid State

## Guillermo C. Bazan Department of Chemistry and Department of Materials Science UCSB

#### Abstract

The design of organic materials for optoelectronic applications requires control over the properties of individual molecules and the bulk morphology. To achieve the latter requirement, it is important to understand how interchromophore contacts affect the optical properties of the ensemble and how molecular shape relates to the arrangement of molecules in the solid state.



The paracyclophane family of compounds provides excellent study candidates for determining how bringing two chromophores into close proximity affect the photophysics of the pair. The paracyclophane compounds are well defined and their structures mimic a contact between two chromophores. It is possible to probe how the conjugation length, the orientation of the two chromophores and the location of contact affect the excitation energy and efficiency of

emission. The combination of synthesis, spectroscopic studies and calculational efforts (done in collaboration with Prof. Shaul Mukamel) provides important guidelines for maximizing, or minimizing, through space delocalization between chromophores in the solid state.



We have also found that molecules which incorporate optically active fragments within a tetrahedral environment have amorphous, glassy properties. It is possible therefore to solution cast films that have little tendency for crystallization. This type of materials combines the beneficial properties of small molecules (i.e. purity and precise structure) with the amorphous nature of polymers. The seminar will also discuss applications of organic glasses in the fabrication CMe<sub>3</sub> of optoelectronic devices.

#### PHOTO-VOLTAIC PROPERTIES OF A SINGLE LAYER POLY[3-(4-OCTYLPHENYL)-2,2'-BITHIOPHENE] (PTOPT)

#### ABAY GADISA AND BANTIKASSEGN WORKALEMAHU

DEPARTMENT OF PHYSICS, FACULTY OF SCIENCE, ADDIS ABABA UNIVERSITY P. O. BOX 32762, ADDIS ABABA, ETHIOPIA.

#### ABSTRACT

A Schottky contact is made from a single layer polymer PTOPT in its neutral state and a low work function metal (Al). The electrical and optical properties have been investigated by means of current-voltage measurements in the dark and under illumination. Various parameters were determined from the I-V curves in the dark of Al/PTOPT/ITO sandwich structure using thermionic emission theory. The reverse saturation current density  $J_q=4\times10^{-14}$  Acm<sup>-2</sup>, barrier height of 1.22 eV and diode ideality factor n=2.2 have been obtained.

Spectral response of the device was measured at various wavelengths giving a peak at 500 nm. The IPCE% at the peak value is 2.8% for illumination from the Al side and 4.7% for illumination through the ITO side.

By illuminating the diode with a monochromatic light of wavelength 500 nm, the open-circuit voltage of 630 mV, short-circuit current density of 0.11 micro-ampere/cm<sup>2</sup>, power conversion efficiency of 0.7% and FF = 0.25 were obtained. The dependence of photo-current on light intensity was also recorded and analyzed.



## Pushing the limits of electronic structure theory; Can we design new spintronic materials?

## <u>Nicola Hill</u> Gerhard Theurich and Stefano Sanvito Materials Department University of California Santa Barbara CA 93106

## Abstract

Spin-polarized electronics is a rapidly expanding research area, both because of the fascinating fundamental physics observed in new spintronic materials, and because of their potentially far-reaching technological applications. There are two difficulties associated with the computational study of

spintronic materials. First most materials of interest are complex doped systems with many defects that can only be modeled using large unit cell sizes. Second, since we are specifically interested in spin properties, the usual scalar-relativistic approximation for spin-orbit coupling is not obviously justified.

In this talk we describe two recent advances in electronic structure theory which facilitate the study of spintronic materials; the clever use of localized atomic basis functions to incorporate realistic defects and doping levels, and the explicit inclusion of spin-orbit coupling and generalized non-collinear magnetism in pseudopotential density functional theory. These new computational tools allow us both to understand

the novel phenomena observed in spintronic materials, and design improved materials for specific technological applications.

## The Electrical and Optical Properties for Structural-Disordered Solids

Z.Q.Ma

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#### Abstract

Most of thin films in solid state manufactured by CVD (Chemical Vapor Deposition) or PVD (Physical Vapor Deposition) techniques are the atomic structural disordered in long distance, such as amorphous, nanometer, and micrometer materials. Their device application for electrical conduction and optical absorption / luminescence becomes more significant in recent years. The hopping conduction of carrier in amorphous semiconductor and Tauc plotting of disordered solids are always assigned to be the electrical conduction mechanism and the determination of optical band gap, respectively. However, the fluctuation of atomic potential and the spatial non-uniformity of optical density in those materials with lattice disorder in short distance are scarcely discussed in the past.

In our recent investigation, the "local features" of optical density of those impurity contained and / or irradiation damaged solids were experimentally resolved with a special optical topographical transformation and a surface scanning method applied to tetrahedral covalent bond of carbon. The difference of relative optical gap over all of bulk is associated with "local structure" of atomic bonding, which causes optical transition between localized states, and some "color centers" are formed in dispersed sites. The photoluminescence and cathodeluminescence emitted from modified "nano-volume" of insulator (SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, ZrO, etc.) is ascribed to localized band gap. The conductivity of amorphous structure being larger than its host in crystal is taken as the decrease of tunneling potential height, resulting in the increase of efficient carrier transport and the narrow of forbidden bands.

The impurity and defect in solids can induce a spatial distribution of electronic states as well as band gap (as figure), so as to lead to the variation of optical and electrical properties.

## Multiscale Structure and Function from Competing Short- and Long-Range Forces

## Alan Bishop Theoretical Division Los Alamos National Laboratory Los Alamos NM

#### Abstract

A significant change of philosophy from traditional solid state and manybody approaches appears necessary to describe many classes of complex electronic and structural materials, both inorganic and organic. This is evident from more than a decade of improving experimental data resolution, and increasing failures of traditional interpretative frameworks. We conclude that <u>multiscale complexity</u> is fundamental to the science of synthesis-structureproperty relationships in many "complex" materials. A large class of such multiscale complexity appears to be driven by competitions of short- and longrange forces, resulting in "landscapes" of spatio-temporal patterns and metastable states, and associated glassy, hysteretic dynamics. We briefly summarize various materials and condensed matter systems exhibiting these competitions, including examples from: Josephson junction arrays and flux flow; surface morphology and evolution; organic self-assembly; polyelectrolytes and biomolecules; and complex inorganic electronic materials.

In the last context, we emphasize an evolving view that transition metal oxides--including high-temperature superconductors, colossal magnetoresistance manganites, and ferroelectrics. Measuring, modeling and using this complexity will be the basis for a new generation of technology. Intrinsic, nanoscale patterning of spin, charge and lattice (and orbital) degrees-of-freedom (including filamentary "stripe" patterns) are key indicators of the complexity and the functionalities it carries. We describe: (1) several mechanisms responsible for this nanoscale patterning; (2) experimental signatures of these fibrillar "skeleton" patterns; and (3) possible macroscopic consequences, including inhomogeneous superconductivity and coexisting magnetism. We emphasize the collusion of spin, charge and lattice fluctuations in this scenario, and the inescapable considerations of nonlinear, nonadiabatic and nonequilibrium properties.

Finally, we describe mesoscopic structural patterns intrinsic to the elastic nature of these materials (twinning, tweed, etc.). We suggest that these scales and the above "stripe" scales are intimately coupled through the same competitions of anisotropic short- and long-range interactions, arising from the directional bonding and polarizability at unit cell scales. This coupling of scales controls both the electronic polarizability and elasticity, and defines novel classes of "electroelastic" materials with essential relationships between multiscale complexity and function.

## Incorporating polycrystalline plasticity in a finite element code for modeling polycrystals with complex microstructure

J.W. Signorelli

## Instituto de Física Rosario - Fac. de Ciencias Exactas Ingeniería y Agrimensura. Conicet-unr, bv. 27 de febrero 210 bis, 2000, Rosario, Argentina

## **ABSTRACT**:

A Finite Element Method (FEM) code, coupled with a constitutive response given by a polycrystalline ViscoPlastic Self-Consistent (VPSC) model, is used to simulate forming processes. The resulting VPSC polycrystalline constitutive equation is used at each integration point of the FEM code. The mechanical properties at this level can be evaluated through appropriately averaging the individual grain responses. Finite element solver provides the velocity field compatible with the boundary conditions imposed at the workpiece level. Crystallographic texture and details of the microstructure are updated according to the spatial variation of velocity gradients, the anisotropic response and deformation-stress heterogeneity can be simulated. In the current work the introduction of the polycrystalline plasticity is achieved by replacing in the FEM code the strain rate, usually obtained through phenomenological constitutive equations, by the corresponding mesoscopic magnitudes calculated by the VPSC model. Two applications of this methodology are presented: texture evolution in cold wire drawing of a two-phase 25%Cu-75%Fe composite and compression of a high textured Zircalov-4 sheet. The first case assess/es the capability of the model to simulate a steady-state process using an Eulerian FEM approach and a 2-site VPSC model at the microscopic scale to consider phase interaction in the composite material. Particularly, in this case the mesh is structured from bidimensional sections with the same number of nodes to match the internal node coordinates with the material streamlines. The second application illustrates the implementation of a time-integration procedure to simulate the evolution of crystallographic textures in a non-steady compression test. In both cases, the simulations are performed starting from morphologic and crystallographic welldefined states. The resulting textures are in good qualitative agreement with the experimental ones and can be explained in terms of the initial texture, single crystal anisotropy and macroscopic heterogeneity.

## **Electronic Exotica in Strongly Correlated Materials**

## Matthew P.A. Fisher Institute for Theoretical Physics, University of California Santa Barbara, CA 93106

#### Abstract

The quantum theory of solids is primarily constructed in terms of weakly interacting electron and hole excitations. This framework works wonderfully in describing simple insulators, semiconductors and metals. But it is becoming increasingly clear that large classes of new materials - ranging from transition metal oxides such as the cuprate superconductors to novel one-dimensional conductors such as carbon nanotubes - are "misfits" which don't conform to the standard paradigm. A satisfactory understanding of these complex materials will surely require an incorporation of strong Coulomb interactions.

On the theoretical front, strongly interacting many-electron systems in one dimension are known to exhibit exotic properties, most notably the presence of excitations with fractional quantum numbers. In these instances the electron is ``fractionalized" - effectively splintered into consituents which behave as free particles. In this talk I will focus on the electronic properties of carbon nanotubes one dimensional molecular nanowires. I will describe some of the predicted signatures of fractionalization in nanotubes, and discuss several recent experiments which provide strong supporting evidence.

## JAMMING, DEFORMATION, AND FRACTURE IN AMORPHOUS MATERIALS

## J.S. Langer Department of Physics University of California, Santa Barbara

## Abstract

I shall summarize recent work by Falk, Lobkovsky and myself in an ongoing attempt to reformulate the theory of plastic deformation in amorphous materials. Our goal has been to produce a theory that is based on atomic-scale deformation mechanisms and, at the same time, provides a unified description of the wide range of phenomena that occur in deformable materials. We have been especially interested in the transition between viscoelastic and viscoplastic behaviors, the dynamics of plastic deformation near advancing crack tips, strain softening, and the possible formation of microstructural patterns of shear localization.

# THEORETICAL ANALYSIS OF THE COMPOSITION OF PLATES ISOTHERMALLY FORMED IN NON-FERROUS BINARY ALLOYS

# S.A. Mujahid Radiation Physics Division, PINSTECH P. O. Nilore, Islamabad, Pakistan

## ABSTRACT

The solute distribution near the plates that grow isothermally from solid solution in non-ferrous binary alloys has been investigated theoretically with a view to clarifying whether the plates grow without diffusion or whether the partitioning of solute occurs after transformation. To check whether the latter mechanism is plausible, calculations have been conducted of the diffusion profile of solute and of the time required for the plate to achieve its equilibrium composition. The calculations use a mathematical model based on a finite difference technique. The results have been compared with published experimental data.

## Semiflexible Equilibrium Polymers: A Self-Assembling Molecular Model

Rahul Pandit Centre for Condensed Matter Theory Department of Physics Indian Institute of Science Bangalore - 560 012 India

## ABSTRACT

In this talk I give an introduction to important issues in the statistical mechanics of semiflexible equilibrium polymers. I then discuss a continuum molecular model for self-assembling, semiflexible polymers that Apratim Chatterji and I have developed recently. I report on our detailed Monte Carlo studies of the equilibrium and nonequilibrium statistical properties of this model. We show that our model exhibits a first-order transition from a high-temperature disordered phase, in which the mean polymer length is small, to a low-temperature nematic phase, in which the polymer chains are longer and semiflexible. We show that, unless the system is cooled very slowly, disordered, glassy states can obtain at low temperatures; we study these by a Monte Carlo analogue of scanning calorimetry. We also use a dynamic Monte Carlo method to study shear alignment of polymers in our model.

## Deformation Studies in Rubber-Modified Polyester Resin Systems

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## ABSTRACT

The deformation mechanisms of rubber-modified polyester resins have been investigated using Real-Time Small Angle X-ray Scattering (RTSAXS) and Scanning Electron Microscopy (SEM). Results show craze-like deformation and debonding as occuring in the modified materials. Application of a mathematical model, to quantify the relative contributions of the different toughening mechanisms to the overall fracture energy increase, suggests that void formation is not the main energy dissipating mechanism in these materials.



## Synthesis and Self-assembly of BLock Copolypeptide Materials

## Tim Deming Materials and Chemistry Departments UCSB

## Abstract

The use of low-valent metal complexes for the polymerization of alpha-amino acid-N-carboxyanhydrides (NCAs) will be presented. Details of these polymerizations will be discussed in addition to studies on the initial reactions of NCA monomers with the various metals. These reactions will be analyzed to correlate how the chemistry of different metals, and different modes of monomer additions, affect the control of polypeptide formation. Using these initiators, we have prepared block copolypeptides containing a variety of both hydrophilic and hydrophobic domains. The hydrophilic chains are composed of either cationic, anionic, or custom non-ionic residues and the hydrophobic chains are composed of natural non-polar amino acid residues such as leucine, valine and phenylalanine. We have studied the self-assembly of these polymers in aqueous solution using a variety of techniques and will discuss the self-assembled structures that result as well as possible biomedical applications of these assemblies. **C13** 

## Investigation of Vibrational Properties of Amino Acid Crystals Paulo de Tarso C. Freire Universidade Federal do Ceará

#### Abstract

Because some biological materials can be exploited in non-linear devices such as electro-optic phase modulators to generate frequency side bands in mode-locking of lasers [1], to avoid optical pumping in laser cooling techniques and to achieve correlated jitters in ultra-high resolution spectroscopy, there is a growing interest in their study. We are particularly interested in amino acid and aminosulfonic crystals because of their relatively simple structure. Our goal is to obtain a large amount of information related with optical and structural properties and from those try to tailor new materials with non-optical applications [2]. We have investigated Lalanine, L-threonine, monohydrated L-asparagine, L-serine and taurine (an aminosulfonic crystal) under several external conditions, such as temperature and hydrostatic pressure variations. From Raman spectroscopy analysis using a diamond-anvil cell we observed that up to 4.3 GPa the crystal of L-alanine undergoes a phase transition between 2.2 and 2.3 GPa [3]. Related with L-threonine we did an analysis of the normal mode vibrations [4] and identified that the orthorhombic original phase is stable up to about 2.0 GPa [5]. Also, our studies points to the possibility of a vibracional localization of energy for modes of low energy in Lthreonine crystal. By Raman scattering studies on monohydrated L-asparagine a complete assignment of the modes was performed at room temperature [6], while an investigation of the material under pressure showed that the crystal undergoes three different phase transitions, at 0.1 GPa, between 0.3 and 0.6 GPa and a third between 0.9 and 1.3 GPa [7]. Similarly, the taurine crystal was subject to investigation by light scattering both at room temperature and atmospheric pressure [8] and under high hydrostatic pressure conditions [9]. Under pressure conditions in a diamond-anvil cell we observed that taurine crystal undergoes a phase transition at about 0.7 GPa and possibly undergoes a second phase transition at about 5.2 GPa. For most of the amino acid crystal the molecules are tied together by hydrogen bonds from amino group to carboxyl oxygen atoms and, additionally, by ionic linkages. In some cases, it is also observed the occurrence of hydrogen bonds from hydroxyl groups to carboxyl oxygen atoms. A second goal of our studies is to understand the role played by hydrogen bonds in the stability of these simple biological crystals.

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## Silicon Biotechnology: New Routes for Structure-Directing Catalysis of Polysiloxane Synthesis

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Biological systems synthesize a diversity of silica structures with a precision of nanoarchitectural control that frequently exceeds the present capabilities of human engineering. In contrast to the conditions of industrial manufacture, these biological syntheses occur under mild physiological conditions of low temperatures and pressures and near-neutral pH. The biomolecular mechanisms controlling synthesis of these materials thus may offer insights for the development of new, environmentally benign routes for synthesis of nanostructurally controlled silicas and high-performance polysiloxane composites. Recent progress in elucidating and harnessing the molecular mechanisms underlying biosilicification now brings this goal within reach.

We found that the silica spicules made by a marine sponge each contain an occluded axial filament of protein composed of repeating assemblies of three similar subunits we named "silicateins." Analysis of the purified protein subunits and the cloned silicatein DNAs reveals that the silicateins are highly homologous to a family of hydrolytic enzymes. As predicted by this finding, we discovered that the silicatein filaments catalyze and spatially direct polycondensation to form silica, phenyl- and methyl-silsesquioxane from the corresponding silicon alkoxides at neutral pH and low temperature. Catalytic activity also is exhibited by the silicatein subunits obtained by disaggregation of the protein filaments, and those produced from recombinant DNA templates cloned in bacteria. Genetic engineering, used to produce variants of the silicatein molecule with substitutions of specific amino acid sidechains, in conjunction with computer-assisted molecular modeling, allowed us to probe the determinants of catalytic activity and confirm the identification of the amino acid sidechains required for hydrolysis of the silicon alkoxides. Based on these findings, we then predictively synthesized biomimetic diblock copolypeptides incorporating the essential features found to be required for catalysis. As predicted, these self-assembling synthetics mimic the activities of the native silicateins, catalyzing the polymerization of silica at neutral pH, while simultaneously directing the 3-dimensional structure of the resulting silicon-based-polymer composite. We now are using these structure-directing catalysts to write nanostructural features of silica on silicon chips for optoelectronic applications and biosensors.

These observations demonstrate that: (a) biological systems have evolved unique mechanisms capable of accelerating and spatially controlling siloxane polycondensation; (b) these systems can be resolved using the tools of biotechnology; and (c) harnessing these systems can prove useful in the design of synthetic catalysts for new routes to the synthesis and structural control of silica and organically substituted polysilsesquioxanes at low temperature and neutral pH.

## **Phase Behavior and Miscibility of Polymer Blends**

## <u>Karl F. Freed</u> Jacek Dudowicz James Franck Institute and Department of Chemistry, University of Chicago

#### ABSTRACT

While Flory-Huggins (FH) theory is widely used to describe the thermodynamic properties of polymer blends, the theory suffers from severe deficiencies. In particular, FH theory fails to explain the presence of an (often large) entropic contribution to the effective Flory interaction parameter, as well as the composition, pressure, and sometimes molecular weight dependence of the interaction parameter. Moreover, FH theory does not distinguish between linear, star, graft, or comb, polymers. Rectifying these deficiencies clearly requires a more sophisticated molecular formulation. The lattice cluster theory (LCT) accomplishes this task by virtue of two significant advances beyond FH theory. The first advance involves generating a more accurate, systematic solution for the lattice model of polymer systems, as is demonstrated in recent comparisons of Monte Carlo simulations with the LCT using no adjustable parameters. While many applications of the theory, such as a description of the pressure dependence phase diagrams and other thermodynamic properties, require incorporating compressibility into the theory, we discuss a simplifying (incompressible, high molecular weight) limit of the theory that is readily usable by experimentallists. The simplified LCT explains several examples of "anomalous mixing" in polyolefin blends, a new mechanism for lower critical solution temperature (LCST) behavior in polymer blends, unusual miscibility trends of random copolymer systems, including those containing cycloolefins, the transition from UCST to LCST behavior in isotopic polybutadiene blends as the degree of branching is varied, and the unusual ordering behavior exhibited by the homologous series of polystvrene-bpoly(n-alkyl methacrylate) as a function of n (i.e., lower and upper ordering transitions for different n).

# POSTERS

P1	O.B.G. de ASSIS
P2	N.M. BUTT
P3	N.H. DAN
P4	V. DUTTA
P5	T. EBADZADEH
P6	G.A. FATTAH (Ali)
P7	S.K. HASANIEN
P8	O. ILORI
P9	P. MANDAL
P10	S. TIONG-PALISOC
P11	B. BOUHAFS
P12	P. GALENKO
P13	A.P. PATHAK
P14	A. BHATTACHERJEE
P15	G.R. MOUSSA
P16	S.H. PEZZIN
P17	P. PREDEEP
P18	T.Z. RIZVI

## Development of Porous Vitreous Materials for Biopolymers Immobilization

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#### <u>Abstract</u>

Waste glass is a very recyclable material, quite amenable to be transformed into useful products. Although research and development on this topic are currently very active, until recently recycled glass uses were limited to bottle and glass fibers products. With regard to glass as raw material it can be demonstrated that when submitted to the suitable chemical treatments it exhibits more favorable hydrophilic or hydrophobic characteristics than metals or ceramics. These properties can be increased or even changed by an additional generation of charges or superficial free radicals. This is important in the sense that a large number of enzymes and other biopolymers of interest for application in biosensor and water purifying systems, possess amphifilic properties, that is, spatial charge distribution defining positive or negative molecular portion, leading to a tendency to be immobilized on oppositely charged interfaces. Therefore, glass appears to be a suitable material to be used as supporters for organic adsorption and trapping, which very strategic in biotechnological fields.

We are development process of manufacturing porous glass pieces suitable for enzyme and biopolymers coupling applications. The fabrication process here adopted follows the "filler principle", in which a non-sinterizable, water-soluble phase is added to the glass powder. After the heating cycle such phase is washed out generating the pore structure. The internal pore structure is characterized by electronic microscopy and tests of immobilization of enzymes and polysaccharides such as chitosan and carboxymethylcellulose are presented and discussed.

# Micro-macro properties of cubic materials

Dr.N.M.Butt PINSTECH.P.O.Nilore., Islamabad.PAKISTAN

## **ABSTRACT**

The mean square amplitude of atomic vibrations  $\langle u^2 \rangle$  in crystalline materials is an important fundamental parameter as this micro property  $\langle u^2 \rangle$  influences a variety of bulk physical and structural properties of the materials.

In recent studies it has been found that the micro parameter  $\langle u^2 \rangle$  in elements and binary cubic materials has systematic correlations with several bulk properties such as Young's modulous, hardness, compressibility, elastic constants, tensile strength etc. concerning mechanical properties, and other properties like melting point, activation energies, heat of fusion, and cohesive energies etc. [Butt, N.M et.al J.Mat.Sci. **28**,1595-1606, 1993 and Butt, N.M et.al.,J.Mat.Sci.Lett.,**13**,1440-1442,1994].

The correlations between this micro parameter for 21 cubic elements and 50 cubic compounds for bulk properties mentioned above describe the experimental data for  $\langle u^2 \rangle$  based on powder x-ray and neutron diffraction measurements *and* the experimental data of the **bulk parameters** based on their respective measuring techniques for those parameters.

## **FUTURE SCOPE OF INVESTIGATIONS.**

**Analytical aspects**:1. The above mentioned correlations observed between  $\langle u^2 \rangle$  and the bulk properties are based on the measured data but no analytical relations. have been derived for those observed correlations. Thus the derivation of analytical expressions for  $\langle u^2 \rangle$  from first principles involving the bulk parameters is a challenging task for theoretical investigation.

2. Correlations of  $\langle u^2 \rangle$  with ionic and defect parameters of materials. Electronic properties like ionic mobility, valencies, ionization potentials and defect properties, etc. may present interesting new scope for further research.

3.<u>Nano-technology</u>: The influence of  $\langle u^2 \rangle$  in the nano-material properties may be interesting to investigate. The atomic friction, self assembly problems in the area of nano-technology could be new ideas to examine.

# Some remarks on microstructure and magnetic property of the hard magnetic amorphous alloy Nd<sub>60</sub>Fe<sub>30</sub>Al<sub>10</sub>

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## **Abstract**

In 1997, Inoue et al [1-3] reported that,  $Nd_{60}Fe_{30}Al_{10}$  alloy can be fabricated in bulk amorphous form with thickness reaching 12 mm and in the bulk amorphous state the alloy exhibits hard magnetic behavior with maximum energy product of about 2.5 MGOe. This alloy attracted attention as a new kind of hard magnetic materials.

In our study, the Nd<sub>60</sub>Fe<sub>30</sub>Al<sub>10</sub> samples were prepared in ribbon and rod forms by melt-spinning and suction-casting methods, respectively, and characterized by X-ray diffraction, magnetization, ac-susceptibility and electric resistance measurements. The results obtained showed that the microstructure and magnetic property vary with spatial position in a rod sample. The hard magnetic behavior of the alloy is trongly dependent on quenching rate and very sensitive to microstructure. All the samples exhibit multi-magnetic phase behavior consisting of both hard and soft phases and fraction of the magnetic phases depends on quenching rate. In combination with magnetization measurement, the ac-susceptibility and transport measurements indecated an existence of various magnetic coupling in the alloy.

[1] A. Inoue, T. Zhang and A. Takeuchi, IEEE Trans. Magn., 33 (1997) 3814.

## **Cadmium Telluride Thin Films for Photovoltaic Devices**

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#### <u>Abstract</u>

Cadmium Telluride is an important semiconductor material for a variety of opto-electronic devices. Because of its band gap of 1.45 eV and Direct Band Gap optical absorption, thin CdTe films have attracted special attention for Photovoltaic devices. Since the polycrystalline thin films of CdTe deposited by a variety of techniques are of p-type, heterojunction solar cells of p-CdTe and n-CdS have been fabricated with efficiency > 15% over a small area. The technology of large area modules have also been developed which have been found to be stable under field conditions.

We have utilized four techniques to deposit CdTe thin films on CdS coated conducting glass. These are Electroplating, Closed Space Sublimation, Spray Pyrolysis and Pulsed Laser Deposition. In this presentation, the deposition techniques will be described to obtain photovoltaic quality CdTe thin films. The structural, optical and electrical properties of films deposited by these techniques will be presented with a particular emphasis on the cell characteristics. The effect of different post deposition treatments required for improved device performance will be discussed.

## Mullite-cordierite-zirconia composite materials from reaction sintering of multicomponent mixtures

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## <u>Abstract</u>

The effect of heat treatment on the phase evolution of the reaction sintering of zircon, clay, alumina and magnesium hydroxide mixed powders were investigated. The samples were fired with determined heat regime to 1450 °C (120 min). The fired samples were heat treated between 1200 ° and 1400 °C for 0.5, 1 and 2 h. Phase evolution results show that there are the boundary sintering conditions for cordierite phase development. The samples sintered at 1400 °C indicate the incomplete reaction behaviour. Increasing the sintering temperature to 1450 °C causes the dissociation of zircon associated with the removal of cordierite peaks. The sharp cordierite peaks were observed in the samples sintered at 1450 °C and heat treated after 2 h at 1300 °C, while at 1200 °C even after 2 h heat treatment the cordierite peaks were not observed. The flexural strength measurements show that the composite mixtures with expecting mullite and cordierite (50/50) and containing 20 wt % zirconia exhibit a positive effect on fracture strength at room temperature.

## Nanoparitcles Formed on Silicon Substrate by Direct Current Discharge

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## <u>Abstract</u>

Nanocrystalline silicon is produced on the surface of silicon substrate by direct current discharge at atmospheric pressure. The scanning electron microscope has been used to examine the formation of the dots on the silicon substrate. The formed structure show a wide photoluminescence (PL) spectrum with several feature in temperature range 20 - 300K, which found to be temperature independent. The estimated increase of the band gap energy of the formed dots is calculated (20 - 300K) following the effective mass approximation, consequently the average dot diameter can be calculated (4-7nm). The effect of the thermal expansion coefficient of silicon on the PL wavelength is studied. The distribution of the dot diameters is estimated from the integrated PL.

## Irreversible metal-insulator and magnetic transformations in charge ordering compositions

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## **Abstract**

The sensitivity of CMR compounds in the charge ordering regime to oxygen stochiometry is well established, with antiferromagnetism as well as ferromagnetic behaviour both being reported for the x=0.5 composition. We report the observation of *irreversible* transformation from metallic to insulating and ferromagnetic to antiferromagnetic behavior, as a function of time, in nominally charge ordered CMR compositions (La0.5Ca0.5MnO3 and La0.48Ca0.52MnO3). These are to be differentiated from the *reversible* transformations seen in the CMR compounds as a function of temperature and/or magnetic field. The transformation or relaxation is observed by us at temperatures in the charge ordering region and after few thermal cycles in this region or waiting for several hours at a fixed temperature,  $(T < T_{co})$  the insulating and canted spin state is stabilized. Once this latter state has been achieved, further heating and cooling above Tc or  $T_{co}$  produces no further changes. The initial metallic and ferromagnetic behavior is irreversibly erased. The behavior has been studied by dc resistivity and ac susceptibility measurements. X-Ray measurements show a single phase material with peaks indexed to a tetragonal perovskite structure and with lattice parameters consistent with the literature.

There is difference in detail between the 0.50 composition which is on the borderline for charge oredring and 0.52 which has the charge order more stabilized, even initially. The 0.52 composition goes from paramagnetic to antiferromagnetic at 200K and subsequently to antiferromagnetic alignment below 165K, in the fresh samples. The 0.52 samples show a weak maximum at 200 K followed by the ferromagnetic and metallic behavior, initially. The time dependence of the change in the susceptibility of the 0.52 composition is logarithmic over three decades of time and yields activation energy of about 110mev. The time variation for the 0.50 composition is more complex., suggestive of multiple barrier heights.

We interpret the behavior in terms of the instability of our samples prepared in air, with oxygen deficiency probably inhibiting the development of charge order even at low temperatures, initially. However when cooled down sufficiently (T<200K) the Jahn-Teller distortions at the microscopic level enable transfer of electrons between the Mn+3 ions and this diffusion of the carriers supports the stabilization of the highly resistive and antiferromagnetic state. This is the origin of the metastable behavior observed. Once the electron transfer and microstructural changes have taken place new energy barriers apparently develop which prevent the original metallic phase from being re-formed, even after heating to well above this region and cooling back to low temperature.

## SYNTHESIS, CHARACTERIZATION AND DEVICE APPLICATION OF MOCVD LIXMoYOz THIN FILM

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## **ABSTRACT**

The study involves the synthesis and characterization of thin films of LixMoyOz with emphasis on the magnetic, electrical and dielectric properties of the films, for possible application as a storage media. The LixMoyOz has been synthesized and deposited by a MOCVD technique. Characterization and modelling of the properties are in progress.

# Structural, transport and magnetic properties of $Ru(Sr_{1-x}La_x)_2GdCu_2O_8$ superconductor

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(March 23, 2001)

## Abstract

The structural, electrical and thermal transport and magnetic properties have been investigated systematically in the ferromagnetic superconductor  $\operatorname{Ru}(\operatorname{Sr}_{1-x}\operatorname{La}_x)_2\operatorname{GdCu}_2O_8$ , as a function of La doping, of temperature and of external magnetic field. Pure compound is characterized by superconductivity ( $T_c = 45$  K) in the CuO<sub>2</sub> planes coexisting with weak ferromagnetism in the  $RuO_2$  planes. Doping with La gives no significant structural changes but reduces the carrier density. With increasing x both the resistivity and thermopower (S) are found to increase whereas superconducting transition temperature  $T_c$  shows a considerable decrease and the system becomes more and more underdoped. Superconductivity is completely suppressed at x = 0.03 whereas magnetic transition temperature is observed to increase with x. The large value of S, the shape of S(T) curve and the appearance of the broad maximum at high temperatures are the signatures of underdoped cuprates where normal-state transport properties are strongly dominated by the presence of a pseudogap and the gap opening temperature increases with decreasing hole concentration. Based on our results, we conclude that similar to other high- $T_c$  materials, superconductivity appears in the vicinity of insulator to metal transition point at around 0.04 holes/Cu.

# **P10**

## FABRICATION AND CHARACTERIZATION OF MELT QUENCHED LEAD-DOPED BSCCO SUPERCONDUCTING CERAMICS

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## **ABSTRACT**

The melt quenched method was applied in the fabrication of  $Bi_{1.6}Pb_{0.4}Sr_2Ca_n$ .  $_1Cu_nO_y$  superconducting ceramics with n = 2.0,2.5,3.0 and 3.5. Each sample was prepared as determined by its stoichiometric composition by melting it at 1080°C. The melt was poured immediately onto a stainless steel plate and quenched to room temperature. Each sample was ground, pelletized and annealed at a constant temperature of 840°C for 24 hours. T<sub>c</sub> SEM and XRD measurements were made. XRD results showed the coexistence of the low T<sub>c</sub>, high T<sub>c</sub> and several non superconducting phases. An increase in Ca and Cu facilitated the growth of the high T<sub>c</sub> phase.

# Effects of d electrons on the electronic structure of GaAs, ZnS and CuCl compounds

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## <u>Abstract</u>

The cation d electrons play a fundamental role in the electronic structure of II-VI and I-VII semiconductors, since the d character modify in host the band structures. In order to investigate the effects of d-like bands in the electronic structure of the zinc-blende prototype compounds, especially, GaAs, ZnS and CuCl as III- V, II-VI and I-VII materials, we report a systematic study using a fullpotential linearized augmented plane waves method (FP-LAPW). In our calculation, the d-electrons are treated on the same footing as other valence electrons and therefore we can investigate quantitatively and qualitatively the importance of the hybridization between cation d- electrons and anion p-electrons. The effects of d character are demonstrated via the p-d repulsion. However, GaAs is characterized by a p-p repulsion and the cation d levels are negligeable. II-VI compounds such as the ZnS compound exhibit a cation d subbands inside the main valence band, but the p-p repulsion remain more important. In CuCl, the cation d electrons occupy the upper valence band and concequently, the p-d repulsion becomes more important than the p-p one.

# **P12**

## Modeling of Rapid Dendritic Growth using the Boundary Integral Method

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#### <u>Abstract</u>

Microsctucture of casted materials consists, as a rule, of dendritic pattern. These structures determine the properties of materials and quality of many man made objects. Particularly, the microstructure of casted materials influence the mechanical properties strongly. Thus, understanding how the dendrites form is theoretically and practically relevant.

In the present report, a process of rapid solidification from a supercooled liquid in a binary system is examined. In order to describe rapid solidification, the model for local nonequilibrium dendrite growth is used [1]. This model takes into account deviations from local equilibrium both at the solid-liquid interface and bulk phases.

Presently, the boundary integral method (BIM) is well-established model for prediction of the fractal and dendritic pattern formation and is related to the models of the sharp interface (see, e.g. [2]). In order to describe evolution of dendrite pattern in detail, the BIM is developed analytically and numerically for rapid dendritic solidification. A modeling of the detailed evolution of pattern of a free-growing dendrite is realized in the two dimensions.

A main attention in modeling is paid to the examination of the influence of anisotropy of the solid-liquid interface energy on the selection of the structure of a free-growing dendrite. As it follows from the results obtained in the modeling, with the decreasing of the anisotropy of surface energy the gradual transition from a smooth needle-like dendrite to a branching dendrite occurs . As the anisotropy of surface energy is decreasing lower than some critical value, the dendrite is growing with the oscillating tip velocity and tip radius. A comparative analysis of the predictions of the microscopic solvability theory (MSC) [3] with the results of the present modeling shows a clear desagreement for low anisotropy of surface energy. As soon as the anisotropy vanished, the tip of the dendrite tends to a splitting phenomenon. These results obtained in the modeling confirm qualitatively the outcomes of the interfacial wave theory [4] in accordance with which there is a critical number for anisotropy lower of which the oscillated dendrite is predicted instead of the steady-state smooth needle.

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- 2. Y. Saito, G. Goldbeck-Wood, H. Müller-Krumbhaar, Phys. Rev. A 38 (1988) 2148.
- 3. D.A. Kessler, J. Koplik, H. Levine, Advances in Physics 37 (1988) 255.
- 4. J.J. Xu, Interfacial Wave Theory of Pattern Formation (Springer, Berlin, 1998).

## Theoretical and Experimental Studies of Semiconductor Multilayers using Energetic Ion Beams

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#### **Abstract**

The semiconductor multilayers, superlattices(both strained layer as well as lattice matched) are broad new class of materials where the band gap engineering is possible by adding a controlled amount of impurity in a III-V compound.. like Indium in the alternate layers of GaAs. The strain thus generated in the successive layers can be accurately studied by using energetic charged particles.. Mostly alpha particles. For thicker layers, the strain relaxes and gives rise to misfit dislocations.

We have been working on various theoretical aspects of these studies using resonance channeling, catastrophic dechanneling to study the strain/defects in a comprihensive way. For last few years, with availability of accelerators and IOP Bhubaneswar and NSC New Delhi, we have also undertaken, exeperimental programm to measure the strain/defects on the samples which are grown at TIFR and SSPL. One student has already graduated under tghis experimental programme.

We wish to continue this comprehensive programme and It will be good to interact with the experts in the field during the ICTP miniworkshop. I can also give some lectures on our recent work

# **P14**

## Mobile Charge Density Wave Model for Third Order Non-Linearity of $\pi$ - Conjugate Polymers

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## <u>Abstract</u>

A theoretical one dimensional model based on Huckel's molecular orbital theory applied to one electron delocalized  $\pi$  electron hamiltonian in a conjugate chain of regular polyene (ignoring electron-electron repulsion) is developed that demonstrates the dependence of third order nonlinearity on the (a) the chain length (b) linear correlation plot of v (c=c) vs.  $1/\lambda_{max}$  ( parameters measured from linear spectroscopic technique of Raman and absorption spectroscopy) (c) ratio of the electron velocity to the sound velocity in the chain. (d) deformation potential coupling of the phonons to the on-site electronic charge density.

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# Temperature Effect on Photonic Band Gap in Polymer Photonic Lattices

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#### **Abstract**

Using the transfer matrix method we have studied the effect of the temperature on all the appearance, the width, and the emplacement of the photonic band gap (PBG) for the air cylinders embedded in a slab of vinyl chloride polymer. For two different lattice parameters we have found that the behavior of the this polymer with respect to the temperature in the visible region is strongly different from that of the far-infrared region. Furthermore results of comparison in the farinfrared region with the PBG material which is constructed with methylpentene polymer are reported.

## Development of Multiphase Polymer Blends and Fiber-Reinforced Thermoplastics at the Santa Catarina State University - Brazil

#### <u>Sérgio Henrique Pezzin</u>

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#### **Abstract**

This work aims to describe the most recent developments in the production of new polymer materials, as multiphase blends and polymer composites, at the Santa Catarina State University (UDESC) in Brazil.

The development of multiphase polymer blends is of major economic importance in the polymer industry. The most widespread examples involve a modification of a thermoplastic by the microdispersion of a rubber into a brittle polymer matrix. In this sense, we are studying the physical-mechanical properties of NBR/SAN blends, and the product morphology, that is mainly determined by the processing method. Three types of morphologies have significant potential for industrial polymer blends: core-shell, multiple discrete particle, and dual semicontinuous. The core-shell structure can simultaneously increase the volume of the dispersed phase and the matrix-elastomer interface for a given amount of elastomer and is the most researched morphology. Multiphase blends can be made using a variety of methods; however, our research has focused on phase separation, melt compounding, and solid-state extrusion. Other modified SAN blends are being investigated, in order to obtain new materials that are resistant to HFC, the new hermetic compressor's refrigerant. The mechanical, morphological and chemical behaviors of polyvinyl chloride (PVC)/polyamide-6 (PA-6) blends were also studied. The samples were prepared by casting, phase separation and solid-state extrusion, showing a typical morphology of a binary blend containing one crystallizable polymer. When the PVC is the major constituent of the blend, a crystalline hedritic structure (PA-6) dispersed on a amorphous matrix (PVC) is observed. With a higher PA-6 content, SEM shows spherical PVC particles dispersed on a fibrous PA-6 matrix. Films obtained by phase separation show a better interaction between the polymers, with non distinguishable phases.

An alternative way to develop polymer materials with better mechanical properties is the production of reinforced polymer composites by the insertion of fibrous materials in a polymer matrix. We present an experimental study of the incorporation of fibers of recycled poly(ethylene terephtalate) – PET in polypropylene. Composites of PP/PET with 3, 5 and 7% of PET fibers (m/v) were prepared by monoscrew extrusion followed by injection moulding and the mechanical behavior was estimated by the measurement of the tensile strength, the Izod impact strength and the surface hardness (Shore D). The morphology was determined by scanning electron microscopy, showing good dispersion of the fibers but no interaction between the polymer phases. It was observed that the incorporation of recycled-PET fibers in PP is an efficient way to recycle PET, increasing significantly the mechanical properties of polypropylene.

## SPECIFIC HEAT, ENTHALPY AND ENTROPY OF LDPE/ NATURAL SISLAL FIBRE COMPOSITES

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#### **ABSTRACT**

Investigation of thermophysical properties of polymers and their composites in the cryogenic temperature region is of much importance in deciding the serviceability of the composites. The efficiency of the thermal design of a cryogenic system depends on the accurate estimation of such properties. Study of he variation of heat capacity thus helps to make an efficient and optimized design. Similarly the variation of entropy and enthalpy with temperature will be helpful to understand the intermolecular interactive phenomena, the different vibrational modes of the molecules and their arrangements in the different temperature regions and the calculation of various thermodynamic functions. In this study composites of Low Density Polyethlyene (LDPE) and Natural Sisal fibre are prepared and their specific heat are measured using Differential Scanning Calorimetry in the low temperature range of 120 to 300K. Specific heat is seen to increase monotonously from the vicinity of the glass transition of these composites. A simple polynomial equation is found to be capable of fitting the variation of specific heat with temperature. Variation of entropy and enthalpy of the composites with temperature are also evaluated and an attempt is made to explain the observed variation of these properties with respect to temperature.

**P18** 

# STRUCTURES AND TEXTURES IN THERMOTROPIC LIQUID CRYSTAL POLYMERS

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# <u>Abstract</u>

Although lyotropic liquid crystal polymers were recognized almost half a century ago, it was only in the mid eighties that polymers with thermotropic liquid crystalline properties were synthesized. The two major classes of themotropic liquid crystal polymers; the main chain liquid crystal polymers (MCLCPs) and side chain liquid crystal polymers (SCLCPs) have found vast applications in many high technology fields. MCLCPs have been used as structural elements in systems forming ultra high modulus fibres whereas SCLCPs due to their tailorable intriguing electro-optical and visco-elastic properties, have high potential to be employed in an immense range of new electrically switchable polymers for electronics and optical computing etc.

This paper gives a brief introduction to liquid crystal polymers with emphasis on structures of major classes of thermotropic liquid crystals and their recent hybrid variants with special reference to their typical characteristic textures under a polarizing microscope.