

MO-POS-81

Effect of Chain Unsaturation on Bilayer Response to Pressure: A Deuterium NMR Study*, **Michael R. Morrow**, I.D. Skanes, J. Stewart and K.M.W. Keough, *Memorial University of Newfoundland* — The effect of chain unsaturation on bilayer response to pressure has been investigated via wide-line deuterium NMR observations of 16:0-18:1 PC- d_{31} (POPC- d_{31}) and 16:0-18:2 PC- d_{31} (PLPC- d_{31}). For bilayers of each lipid, saturated chain orientational order was measured as a function of pressure for selected temperatures and as a function of temperature for selected pressures up to 193 MPa. For POPC- d_{31} , the main transition temperature increased by ~ 0.18 K/MPa, a rate that is similar to that found for bilayers of disaturated PCs. For PLPC- d_{31} , the increase in transition temperature with pressure was slightly smaller at ~ 0.13 K/MPa. To investigate the isothermal response of chain orientational order parameters to pressure, spectra for each lipid were obtained for three pressures (ambient, 55 MPa, and 110 MPa) at 25°C and for three pressures (ambient, 110 MPa, and 193 MPa) at 40°C. Application of a given pressure was found to increase orientational order for each methylene group on the saturated chain of a particular lipid by roughly similar amounts. This corresponds to an approximately uniform shift of the saturated chain orientational order parameter profile with pressure. Within the liquid crystalline phase, the response to pressure decreased with increasing temperature. Comparison of the responses of POPC and PLPC to pressure at corresponding temperatures relative to their respective ambient pressure transition temperatures showed that PLPC saturated-chain orientational order was less sensitive to pressure than that of POPC.

These observations suggest that increasing levels of chain unsaturation may reduce the sensitivity of bilayer order to variations in pressure.

* Supported by NSERC (MRM) and CIHR (KMWK).

MO-POS-82

Characterization Of Anisotropy In Foams: An Ultrasonic Approach*, Hussein Elmehdi, J.H. Page AND M.G. Scanlon, *University of Maitoba* — We use low frequency ultrasonic waves (50 kHz) to investigate the mechanical properties of anisotropic freeze-dried bread foams that were prepared by applying uniaxial stress to fresh breadcrumb. Longitudinal ultrasonic velocity and amplitude measurements were taken in directions parallel and perpendicular to the compression direction. The velocity was found to decrease as the amount of compression is increased, with the decrease being greater in the parallel direction. The velocity data were interpreted using two theoretical models, one based on the static compression of a simplified strut model of foams and the other including the effects of tortuosity on wave propagation through anisotropic media. Both models allowed the velocity anisotropy to be directly related to the anisotropy of the foam structure, and give predictions in good overall agreement with the data. The results also allowed us to conclude that there must be a weakening of the cell walls caused by the uniaxial compression in addition to the effects resulting from the anisotropy alone.

* This work is being supported by NSERC.

MO-POS-83

Structure of a Homologue Series of Banana Mesogens Studied By C13 NMR Spectrum*, J. Xu and R.Y. Dong, *University of Manitoba* — C13 NMR spectroscopy was used to obtain the geometrical information in three members of a homologue series of banana molecules, 9CIPBBC, 8DCIPBBC and 9DCIPBBC. The orientational order parameter S, bending angles and tilt angles between the biphenyl rings were determined from the temperature dependent chemical shifts in the nematic phases. Although the temperature dependence of S was found to be different for these molecules, the S values at Tc were almost identical. It was also found that tilt angles depend linearly on temperature, and the bending angle in the mono-substituted molecule is about 14 degree smaller than the di-substituted molecular. A SUPER (Separation of Undistorted Chemical-Shift Anisotropy Powder Patterns) technique was used to determine the chemical shift tensors of carbons of model compounds (e.g. 4-Chlororesorcinol). These tensorial components are required for fitting the temperature dependent chemical shifts in aligned samples.

* Research is supported by NSERC and Brandon University

MO-POS-84

On the Physical Mechanism of Vortex Stirring in MHD-Driven Two-Fluid Molten Metal Flows, David Munger and A. Vincent, *Université de Montréal* — Magnetohydrodynamic (MHD) instabilities such as those observed in aluminum reduction cells have been thoroughly studied, for instance by means of linear analysis by Sneyd (1992) and numerical simulation by Potocnik (1989) using industrial codes, as well as by Gerbeau (2001) using finite elements. Though its understanding is critical for efficient aluminium production, the physical mechanism is still unknown. We focus on the stability of vortex stirring that naturally occurs in MHD-driven systems of two fluids with a large electrical conductivity ratio, traversed by an intense vertical electric current and under a strong background magnetic field. We perform three-dimensional nonstationary numerical simulations of the conservative equations, using a levelset technique to track the position of the interface between the two fluids. Periodic transport of large eddies occurs, in which we observe an oscillation of vortex energy arising from a balance between the dissipation forces and the supply from the imposed electric current. The corresponding frequencies are orders of magnitude smaller than those observed in typical metal pad roll, so that long-lasting simulations are necessary to track slowly growing instabilities. We are able to find a stability threshold in terms of the electrical conductivity of the fluids, and we are currently trying to correlate it with the cell's dimensions. We conjecture that an increase of the latter will compensate a decrease of conductivity in the triggering of instabilities. Simulations are underway and results will be presented at the conference.

MO-POS-85

Spin Wave Dispersion of the 2D Hubbard Model at Intermediate Coupling*, Walter Stephan, *Bishop's University* — The spin wave dispersion relation for the 2D square lattice Hubbard model at half-filling is calculated using an "exact" linked cluster expansion method. The approach used is most reliable at strong coupling, but still converges reasonably well when the Coulomb repulsion is of the same order of magnitude as the band width. Results are compared to those of other approximate calculations as well as neutron scattering measurements of undoped cuprates.

* This work is being supported by NSERC.

MO-POS-86

The Giant Magnetocaloric Effect (GMCE) in Ni-Mn-Ga, Wei Li, Xuezhi Zhou, H P Kunkel and Gwyn Williams, *Univeristy of Manitoba* — Several previous investigations have demonstrated that a giant magnetocaloric effect (GMCE) – a large isothermal entropy / adiabatic temperature change associated with the application of an external magnetic field to a system – is most often linked to the substantial entropy change accompanying a first-order phase change. However, it appeared plausible that in systems exhibiting sequential magnetic transitions – specifically a continuous paramagnetic to ferromagnetic transition followed by a first-order / discontinuous (order-order) transition - this effect might be enhanced if these two transitions could be brought into close proximity, or better still, merged. The veracity of this suggestion has been demonstrated in the Ni-Mn-Ga system where such a coincidence can be achieved through careful compositional tuning, thus for Ni_{55.2}Mn_{18.6}Ga_{26.2} an entropy change of $\Delta S_M = -20.4 J kg^{-1} K^{-1}$ is observed at 317K in a field of 5T, one of the larger values measured at or above room temperature.

MO-POS-87

Comparison of Electron Mobility in Zincblende and wurtzite GaInN, A. Somaee², M. Sadeghi², H. Arabshahi¹, M. Ghazi², ¹Tarbiat Moallem University and ² *Shahrod University, Shahrod, Iran* — GaN has received much attention in recent years because of its potential for a wide range of applications in high power and optoelectronic devices. The demands of device designs have encouraged numerical studies of electron transport in the material. In this research a numerical iteration method has been developed and used to model electron transport in zincblende and wurtzite GaInN at low electric fields. Our results show that the electron drift mobility of wurtzite GaInN is lower than that for the zincblende structure at all temperatures. This is largely due to the higher G valley effective mass and a higher electron scattering rate in the wurtzite phase.

MO-POS-88

Low-Field Electron Transport Calculations in Bulk Wurtzite GaN Using Iterative Technique, Hadi Arabshahi, *Tarbiat Moallem University* — Temperature and electric field-dependent electron transport in bulk wurtzite GaN structure have been calculated using an iterative technique. The following scattering mechanisms, i.e. impurity, polar optical phonon, acoustic phonon, piezoelectric and electron plasmon are included in the calculation. Ionized impurity scattering has been treated beyond the Born approximation using the phase-shift analysis. The low electron drift mobility is calculated for temperatures in the range of 300-600K and for ionized impurity concentrations between 10¹⁶ and 10¹⁸ Cm⁻³. The low temperature value of electron mobility increases significantly with increasing doping concentration. The iterative results are in fair agreement with other recent calculations obtained using the relaxation-time approximation and experimental methods. Compensation effects on the mobility are also examined. Due to the freezout of deep donor levels the role of ionized impurity scattering in bulk wurtzite GaN is suppressed and the role of phonon scattering is enhanced, compared to zincblende structure. Electron transport properties have been modelled with an electric field applied both parallel and perpendicular to the (0001)c-axis. The extracted model parameters can be used for electron transport simulations in GaN-based transistors.

MO-POS-89

Design and Modelling of Inductively Heated Substrate Holders for Advanced Plasma Materials Processing Applications*, Ajay K. Singh and Michael P. Bradley, *University of Saskatchewan* — Plasma processing of materials will be one of the key enablers for advances in electronics and photonics technology in the 21st century. Effective plasma materials processing requires careful control of process parameters, including the temperature of the target material. For example, a minimum target temperature ~ 800 Celsius is required for plasma deposition of diamond films. Unfortunately, in high pressure (~ 10 Torr) microwave plasma systems (such as the diamond film growth system at the University of Saskatchewan) the ultimate target temperature may be limited to ~ 500 Celsius because ion-neutral collisions limit the amount of heat delivered to the target, and because of relatively high convective cooling rates. Thus it is necessary to directly heat the target to achieve the high temperatures required. Direct heating via heating wire may be difficult to implement because in most cases the substrate must be biased with respect to the grounded chamber walls to achieve good film growth. Inductive eddy current heating provides a solution. Heating energy is efficiently coupled into the substrate via induced eddy currents, providing rapid and potentially highly uniform heating. The purely inductive coupling means that the substrate can be biased to arbitrary voltages as required. This presentation will discuss our design efforts on heated substrate holders. We will present results of thermal modelling calculations (i.e. heating curves, mean temperature, temperature uniformity) and will discuss their implications for advanced target holder design.

* This work is being supported by NSERC.

MO-POS-90

Elastic Fields from Reconstructed Terraces of a Semi-Infinite Solid*, R. Arief Budiman, *University of Calgary* — Two-dimensional problem of a semi-infinite solid with surface reconstruction boundary condition is considered. Surface reconstruction produces sinusoidal displacement fields on a terrace and attractive interaction due to the reconstruction is

found. Stress fields and surface forces due to the surface reconstruction are presented. With the addition of the step-step interaction model by Marchenko and Parshin, the equilibrium surface configuration under the presence of step array and reconstructed terraces is presented.

* This work is being supported by NSERC.

MO-POS-91

High Resolution Oxide Single - Crystalline X-Ray Screens, **S. Nedilko**, *Kyiv National Taras Shevchenko University, Ukraine* — There are well known applications of scintillating materials in imaging devices: X-ray imaging, X-ray computed tomography (X-ray CT), single photon emission computed tomography (SPECT) and positron emission tomography (PET). Here we will talk only concerning X-ray imaging with micrometer resolution. Decreasing of exposure dose during diagnostics, medical, biological *in vivo* etc., when ionizing irradiation is used, can be achieved by increasing of spatial resolution of the screens used for visualization of X-rays image. At present X-rays screens are made, as a rule, on the polycrystalline powder luminophors base with the 5 – 200 μ grain dimensions which determine spatial resolution of the screens. Essential increasing of spatial resolution became possible by using of screens those are the single crystalline thin film (SCF) scintillator with a high coefficient of X-ray absorption applied on the surface of non-luminescent single crystalline substrate by means of liquid phase epitaxy method. At first, the X-ray image detector with resolution near 1.3 – 1.5 μ with the screen on the doped with Ce ions yttrium aluminum garnet SCF with thickness $h = 5 \mu$ was described by A. Koch *et al.* in 1998. The further increase of resolution can be achieved by thickness decreasing that requires higher SCF X-ray absorption (the last is proportional to effective atomic number of SCF) and by increasing of SCF light output. In this paper the results of investigation the set of doped oxide materials with the garnet and perovskite structure which allow significant improving of the X – ray screens parameters are presented and the perspectives of their using are discussed as well.

MO-POS-92

Thermostimulated Self-Assembled Formation of Semiconductors Micro – Inclusions in Matrices of Oxide Dielectric Sulphate Crystals, **V. Sheludko**¹ and **S. Nedilko**², ¹*Glukhiv Pedagogical University, Ukraine* and ²*Kyiv National Taras Shevchenko University, Ukraine* — Paper reports about formation of the CdS semiconductor micro-inclusions in the dielectric matrix of CdSO₄. The formation of the CdS is a result of the CdSO₄ annealing. Temperature diapasons and atmosphere effects on results of the thermal treatment were established. The excess of the sulfur is necessary condition of the CdS formation. Control of the micro-inclusions formation and determination of their spatial and energy parameters was carried out by observation of the optical (luminescent) properties of the samples. Spectral distribution and decay parameters reveal a recombination character of this emission - luminescence of the donor-acceptor pairs in semiconductors of the A(II)B(VI) group. Obtained results are analyzed from the point of view of formation of other compound micro-inclusions in a volume of the initial crystal matrix. A close similarity of observed characteristics to characteristics of the so called "green" edge emission of very well known material as the cadmium sulfide CdS don't allow any doubts concerning the fact that thermal treatment results the inclusions just of cadmium sulfide semiconductor phase into volume of the CdSO₄. The same luminescence properties had been observed for the K₂SO₄ and Rb₂SO₄ crystals. K₂S and Rb₂S are formed there after thermal treatment. Energy characteristics and the sizes of the clusters (25 - 50 nm) of the inclusions were estimated.

MO-POS-93

Modelling the Magnetic Response of Fe Nanoparticles in Alumina: A Preisach Approach, **Candice A.H. Viddal** and **R.M. Roshko**, *University of Manitoba* — Measurements of the field cooled moment, the zero field cooled moment, the isothermal remanent moment, the thermo remanent moment, and hysteresis isotherms, were performed on a thin film of nanodimensional Fe particles embedded in Al₂O₃ over a temperature range 10K ≤ T ≤ 300K and a field range |H_a| ≤ 2kOe. The data were analyzed within the framework of a Preisach model, which assumes that the free energy landscape can be decomposed into an ensemble of bistable Barkhausen elements, each with two moment configurations ±μ, a dissipation barrier W_d = μH_d, which measures energy dissipated as heat, and a level splitting W_s = 2μ H_s, which measures energy stored reversibly. Numerical simulations based on the Preisach model, assuming a lognormal distribution of dissipation fields H_d and a Lorentzian distribution of bias fields H_s, were able to replicate all of the principal structural features of the experimental data, and their systematic variation with field and temperature. In particular, fits to the experimental data yield the temperature dependence of the mean dissipation field H_d(T), and the dispersions of dissipation fields σ_d(T) and bias fields σ_s(T), and show that the magnetic response below T ≈ 150K is dominated by field activated transitions over free energy excitation barriers which collapse rapidly with increasing temperature, and which are most likely related to disordered spin configurations on the surfaces of the Fe nanoparticles. By contrast, at temperatures above 150K, the response is dominated by thermal relaxation of Barkhausen elements with an average moment μ ≈ 10⁻¹⁰ emu, which probably originates from the ferromagnetic cores of the Fe nanoparticles.

MO-POS-94

Thermally Activated Diffusion of Indium into 2H-TaSe₂, **Onkar Rajora**, *University College of the Cariboo* — We have studied the thermal diffusion of indium into the layered compound 2H-TaSe₂ single crystals parallel to the layers.¹ Measurements were done *in situ* in a scanning electron microscope equipped with an x-ray energy dispersive system. The distance of the diffusing indium front into the crystal was determined as a function of time from secondary electron image as well as from x-ray line scans for indium taken at different time intervals. The diffusion coefficients D were found by fitting the data to $\langle r^2 \rangle = 2D t$, where $\langle r^2 \rangle$ is the mean square displacement in time t. The diffusion coefficients thus obtained were 1.5 x 10⁻¹², 3.8 x 10⁻¹², 7.7 x 10⁻¹², and 17.5 x 10⁻¹² m²/s with an uncertainty of about 10 percent at 351, 375, 411, and 458 K respectively. The activation energy E₀ of indium diffusion into TaSe₂, using $D = D_0 e^{-E_0/k_B T}$, was calculated to be 0.32 ± 0.04 eV. The results show that diffusing indium atoms put severe stress on the layers as they intercalate between them. This stress is relieved by buckling of the layers and these buckling features are clearly visible in secondary electron images.

1. O. Singh and A.E. Curzon, *J. Appl. Phys.*, 17, 1415, 1984.

MO-POS-95

Magnetic Properties of ErFe₂/DyFe₂ Superlattices Studies by Neutron Diffraction*, **Z. Yamani**¹, **H. Fritzsche**¹, **W.J.L. Buyers**¹, **Z. Tun**¹, **R.A. Cowley**² and **R.C.C. Ward**², ¹*Neutron Program for Materials Research* and ²*Oxford Physics, Clarendon Laboratory, UK* — Magnetic structure of two superlattices of the form [60Å ErFe₂/60Å DyFe₂]₄₀ and [80Å ErFe₂/40Å DyFe₂]₄₀, prepared by molecular beam epitaxy on a sapphire (1120) substrate, is determined by neutron diffraction technique using the triple-axis spectrometer C5 at the NRU reactor in Chalk River. The experiments were performed at zero field, in a horizontal field of 2.63 T applied along [001] (the easy axis for bulk DyFe₂), along [111] (the easy axis of bulk ErFe₂), and along the surface normal [110]. The temperature dependence of several Bragg reflections both at zero field and non-zero field was determined in the range of 4 K to 250 K. The data analysis shows that the easy magnetization direction is determined by a competition between the Zeeman energy favoring the field direction, the crystalline anisotropy favoring either the [001] or [111] directions, the exchange interaction at the interface favoring a parallel orientation of the magnetizations of both layers, and finally the magnetoelastic energy.

* This work is being supported by NRC.