Soft Condensed Matter

6 - 1 – Thermally stimulated conductivity (TSC) IN Cu_3BiS_3 thin films deposited by co-evaporation: determination of trap parameters related with defects in the gap

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Thin films of Cu_3BiS_3 were produced by evaporating of precursor species of Cu and Bi in atmosphere of sulfur through a process that includes two stages. Thermally stimulated current (TSC) measurements are carried out on as-grown Cu_3BiS_3 crystals in the temperature range of 150-300 K. The measurements were performed while increasing the temperature at a rate of 5 K-min. Analysis of X-ray diffraction and thermal power measures to room temperature enabled the phase and the type of conductivity of the material respectively. The spectra obtained from the TSC showed the presence of trapping centers associated with the peaks in the currents curves as a function of temperature. Transport mechanisms as hopping and thermally active carriers were identified for low and high temperature regions, respectively. Three trapping levels around 1.04 eV were detected from the TSC spectra. These levels in Cu_3BiS_3 crystals may be associated with the presence of structural defects and-or unintentional impurities during preparation process. The trap parameters were determined by various methods of analysis, and they agree well with each other. A correlation between electrical properties and defects in the material were also studied.

6 - 2 – Percolation in insulating-conducting composites: modeling the conductance-strain dependence.

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One of the most interesting issues in theoretical and experimental studies of disordered insulator-conductor composites is the effect on the transport properties of external perturbations, like electric and magnetic fields, mechanical stress or molecular adsorption (1,2). We focus in the present work on composites of conducting particles embedded in an insulating elastomer matrix. The matrix is compressed by the action of an externally applied uni-axial pressure keeping constant the amount of conducting particles, a process that increases the electrical conductance of the composite, which can be used for obtaining a pressure sensor. These systems are usually considered as isotropic percolating networks where the dependence of transport properties, like the dc-electrical conductance, G, is expressed as function of the percolation probability between neighboring particles

Here a model for the dependence of the electrical conductance, G, with the strain induced by external mechanical stress in conducting particles-polymer composites is presented. The model assumes that the percolation probability between neighboring particles must depart from a scale-invariant behavior but saturate at moderated-high strains, reaching percolation path´s saturation, with sigmoid dependence. This dependence is obtained by proposing a dynamic picture where contacts or bonds between neighboring particles are created but also destructed when a stress is applied and relatively moderated or high strains are produced in the composite. The electrical conductance of prepared graphite-poly-dimethylsiloxane composites were measured as function of the applied pressure and fitted by the presented model. The elastic response to the uni-axial compression was studied using a texture analyzer. The possibility of non-universal effects in the conduction critical exponent, t, was taken into account. It is concluded that the saturation of the response in the G vs. strain plots can not be assigned to non-universal behavior of the exponent t, or to saturation of the elastic response. On the other hand the presented model accounts for all the main experimental features observed in these systems and for previously reported data of elastomer composites. The simulated behavior of the piezoresistivity coefficient is also in qualitative agreement with previous reports.

(1) N. Johner, C.Grimaldi, T. Maeder, and Peter Ryser, Phys. Rev. E, 79, 20104 (2009). (2) I. Balberg, J. Phys. D: Appl. Phys. 42, 64003 (2009).

6 - 3 – Ab initio study of Cd in bulk and at the (001) surface of metallic Indium: structural, electronic and hyperfine properties

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Nuclear techniques, such as Perturbed-Angular-Correlation spectroscopy (PAC), have proven to be versatile tools for the study of a broad set of phenomena in condensed matter physics and in many other fields. Through the detection of electric-field gradients (EFG), e.g., it is possible to obtain a fingerprint of the electronic structure near and at the site of a given probe-nucleus. In the last decade, ab-initio calculations have assumed an important role in supporting, improving or confuting the interpretation of experimental data. Especially for such very sensitive properties such as the EFG, the availability of these accurate and external-parameter-free calculations has opened new possibilities. For instance, by a combination of experiments and calculations, the systematic of the EFG at different impurities sites in oxides could be understood [1]. The structural and electronic properties of layers at and near surfaces are important to understand the interaction of atoms under these special boundary conditions. The reconstructions and surface states and changes of the electronic properties between different atomic layers (or even between atoms in the same layer) are of fundamental interest for both basic and technological reasons. Using PAC, monolayer-resolved studies are possible [2] and the measured EFG could give structural and electronic information of the system that cannot be obtained by other methods, but their interpretation is not straightforward. In the present work we present a study of the EFG at isolated Cd impurities in bulk and at the (001) surface of metallic In. Our study shows that the combination PAC - ab initio calculations gives a complete description of the surface reconstruction and the changes induced by the presence of the Cd probe with respect to the bulk undoped structure.

[1] See, for example, L.A. Errico, M. Rentería, and H.M. Petrilli, Phys. Rev. B 75, 155209, 2007. [2] W. Körner, W. Keppner, B. Lehndorff-Junges, and G. Schatz, Phys. Rev. Lett. 49, 1735, 1982.

6 - 4 – Electrical properties of AgGeSe films used in ion selective electrodes

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Chalcogenide glasses have been used as sensitive membranes in ion selective electrodes (ISEs) for more than three decades. Their chemical stability ensures high endurance even in aggressive acidic media and their remarkable glass forming ability enables the use of these materials, either as bulk or as thin films, in the development of sensitive membranes for micro-sensors or multi-sensor arrays. In order to understand the sensing properties of these materials it is necessary to know first its electrical properties.

The bulk chalcogenide glasses $Ag_x(Ge_{0.25}Se_{0.75})_{100-x}$ (0 at.% $\leq x \leq$ 25 at.%) have been studied as sensitive materials for ISEs. For $x \geq 8$ at.% the glasses exhibit sensibility to Ag^+ and Cu^{2+} ions in aqueous solutions. For $x < 8$ at.% the electrode's response was poor with almost no sensibility. On the other hand, this system behaves as ionic conductor (10^{-5} S/cm) for $x \geq 8$ at.% and as insulator ($< 10^{-13}$ S/cm) for $x < 8$ at.%.

Membranes with smaller resistance were prepared in order to study whether the sensibility of these materials is determined by the ionic conductivity exclusively or by the total electrical resistance of the membrane. Thin films of compositions $Ag_x(Ge_{0.25}Se_{0.75})_{100-x}$ (0 at.% $\leq x \leq$ 25 at.%) were deposited by PLD and the electrical transport of the films was analyzed by measuring the surface and bulk DC conductivity.

6 - 5 – Renormalized charge in spherical colloids with various boundary conditions

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The electrostatic force, long-range force is the principal responsible for phenomena in complex fluids. Complex fluids such as proteins and colloids in solutions presents a great variety of properties that make such an important and extensive field research at the industry in obtaining: aerosols, gels, foams, medicines and food, and the field of science in the description of colloids through the scattering of light, prediction of phases and structures.

The colloidal particles are of the order of micron size, sizes larger than atomic or molecular dimensions, in a solvent considered as a continuum, unstructured and characterized by a dielectric constant (ϵ). The charge of the colloids in an ionic solution (solvent)

is screened by the adherence of the micro-ions of opposite sign (screening cloud) from the solvent, thus changing the electrostatic interactions between colloids described by the nonlinear Poisson- Boltzmann equation (PB)

$$\Delta\Psi(r) = \kappa^2 Sinh[\Psi]$$

or linearization, approximation of Debye-Hückel (DH)

$$\Delta\Psi(r) = \kappa^2 \Psi$$

where $\Psi(r)$ is the potential, κ is the inverse screening length.

DH approximation approach becomes inadequate to describe highly charged colloids, but using the concept of charge renormalization (Z^*) this linear equation is valid at great distances from colloid (distances greater than the Debye length). This parameter that takes into account the colloidal charge (Z) as the screening due to the micro-ions (κ). We calculated renormalized charge of spherical colloids with different boundary conditions such as: colloids with constant density and colloid charge that allow the entry of ions inside, and we compare the potential obtained by the DH approach and PB equation.

6 - 6 – Thermal and magnetic behavior of Angustifolia Kunth bamboo fibers covered with Fe_3O_4 particles

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Several Angustifolia Kunth bamboo fibers, which have been previously treatment with an alkaline solution, were coated with magnetite particles. The coating of the fibers was achieved by an in-situ coprecipitation method with Fe^{2+} and Fe_{3+} in NaOH or NH_4OH. The fibers were evaluated by chemical analysis using atomic absorption (A.A.) technique, structural characterization by X-ray diffraction (XRD), morphology by scanning electron microscopy (SEM), thermal stability with thermo-gravimetric analysis (TGA) in nitrogen at temperature range between 23 °C to 800 °C, and magnetic behavior using vibrating sample magnetometry (VSM) applying a magnetic field between -27 KOe and 27 KOe at room temperature. We found that the thermal stability and magnetization depend of the synthesis method used to cover the Angustifolia Kunth bamboo fibers. In addition, it was observed an improved magnetic response when NaOH solution is used to generate the magnetite coating on the fiber surface.

6 - 7 – Thermomechanical behaviour of SBR reinforced with carbon nanotubes functionalized with polyvinylpyridine.

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SBR is a so called statistical polymer of styrene/butadiene (SBR) (75% butadiene in weight). SBR is superior to natural rubber regarding less ageing and greater resistance to heat and wear. The greatest limitation of SBR for industrial applications is in its high heat generation when subjected to cyclic loads. This is caused by its great plastic phase, which generates a high hysteresis. This disadvantage of SBR is critical when considering rubber products with great thickness subjected to repetitive stresses due to the poor thermal conductivity of rubber and its consequent inefficiency at heat dissipation, being this one of the most important points to be resolved with this material. One possible solution to this problem is the addition of carbon nanotubes (NT). In particular, if these NT are functionalized with a polymer akin to the styrene phase, they will position themselves in it, improving the response compared to the non functionalized NT. The purpose of this work was to study the mechanical and thermal response of SBR reinforced with different concentrations of NTs, functionalized and non functionalized. We used polyvinyl pyridine (PVP) because of its compatibility with the PS in SBR and having the extra benefit of being a conductor polymer. The influence of the addition of NT, functionalized or not, was studied at the temperature and energy associated to the cure of SBR by Differential Scanning Calorimetry (DSC). The composites, once cured at the temperature determined by DSC, were mechanical and thermally characterized.

6 - 8 – About the cure kinetics in Natural Rubber/Styrene Butadiene Rubber blends at 433 K

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Vulcanized blends of elastomers are employed in several goods mainly to improve physical properties and reduce costs. One of the most used blends of this kind are those composed by natural rubber (NR) and styrene butadiene rubber (SBR). The cure kinetic of these blends depends mainly on the compound formulation and the cure temperature and time. The preparation method of the blends can influence the mechanical properties of the vulcanized compounds. In this work the cure kinetic at 433 K of NR/SBR blends vulcanized with the system sulphur/TBBS is analyzed in sampled prepared by mechanical mixing and solution mixing. The two methods produce elastomer domains of NR and SBR which present different microstructure due to the cure level attained during vulcanization. The cure kinetics is studied by means of rheometer tests and the model proposed by Kamal and Sourour. The analysis of the cure rate is presented and is related to the structure obtained during the vulcanization process.

6 - 9 – Metastability of the vortex lattice in superconducting films containing competitive artificial and intrinsic pinning centers

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The vortex lattice (VL) in type II superconductors is known to model numerous other elastic systems in interaction with pinning landscapes. In most cases, pinning centers largely outnumber the vortex lines, and provide random weak potentials that give rise to complex dynamics, metastability and history effects. A new generation of patterned samples containing artificial arrays of strong pinning centers reveals new VL dynamics. The fingerprint of strong periodic pinning centers is an anomalous increase in critical current which generally occurs for applied "matching fields" producing a number of vortex lines equal to the number of artificial pinning sites. An open question is the effect of competing random defects on the matching anomaly. In this context we have studied the VL mobility in patterned Nb films containing periodic arrays of sub-50nm magnetic nanodots or holes, by means of ac susceptibility measurements. Nb films are chosen because compared to other unpatterned films, show quite strong random disorder and may lead to competing interactions. We observe matching effects in the patterned films within a wide temperature range, determined by the periodicity of the strong artificial pinning potential. In addition to these effects, we find a novel hysteretic behavior. Below a crossover temperature $t^* \simeq 0.75T_C$, the "matching field" not only depends on the geometry of the pinning array but depends on the sample thermo-magnetic history. This hysteretic response is examined in detail and we have consistently ascribed it to metastable VL configurations that arise from the competition between pinning by random intrinsic and periodic artificial arrays. By means of different measuring protocols, including small magnetic field loops, field cooling procedures or the application of a perturbation as an ac "shaking" field, we examine the response of the different VL configurations that are accessible with these pinning landscapes.

6 - 10 – Thermodynamic Behavior Above the Critical Temperature

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In this work, it was studied the thermodynamic properties above of the critical temperature of a magnetic bilayer (thim film), when submitted the actions of the interactions of exchange, the dipolar anisotropy (long range) and of a external magnetic field. The interaction of exchange between spins next neighbors is ferromagnetic. It was found numerically the magnetization in function of the temperature, and the relation of dispersion of the thim film. We use the Green's function theory dependents of two times and temperature, wich is a method very adysted for systems of many interagents bodies. The results showed that the system presents long-range order until a critical value of parameter of dipolar anisotropy. The behaviors of the magnetization and the relation of dispersion in the presence and the absence of a external magnetic field for diverse values of dipolar anisotropy have been showed.

6 - 11 – Transition from a dilute to a very dense liquid

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Adsorption on single planar walls and filling of slits with identical walls are investigated in the frame of a density functional theory. It was found that when for a given adsorbate-substrate combination the adsorption on a single wall exhibits a first-order wetting transition then asymmetric profiles always appear in the filling of an equivalent slit. Moreover, both these features terminate at the same temperature. The behavior is analyzed by varying the strength of the adsorbate-substrate attraction, the temperature T, and the coverage Γ_ℓ. It is shown that for a rather strongly attractive surfaces the adsorbed liquid becomes very dense and reaching densities characteristic of solids.