Development of Experimental and Computational techniques

7 - 1 – Numerical ab-initio approach to study hydrogen diffusion in 9Cr steels

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Recently, Hurtado Noreña et al [1] have studied the hydrogen (H) diffusion effects on 9Cr steels, candidates to futures conventional thermal power plants. Based on the numerical resolution of Fick's equations in presence of trapping sites, and from the fit of electrochemical H detection curves, these authors provided quantitative information about the binding energy between H and trapping sites during diffusion process. In the present work, we calculate the equilibrium configurations and migration barriers of H for soft-martensitic steeels. We have used a new theoretical approach based on ab-initio technique, employing the Monomer method [2] adapted to the SIESTA code as in Refs.[3,4]. Martensitic steel of BCT structure, containing 9%Cr in weight, is a complex system to be simulated. Our main difficulty arise in modeling such a system. For this purpose, we have considered an incremental approach, namely: the effect of c/a is not as relevant as the effect of substitutional Cr [5], then i) we start our calculation with a BCC-Fe structure in presence of an adequate environment of Cr; finally, ii) we calculate the migration barriers of H through BCC-FeCr crystallite relevant to diffusion process.

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[3] Ramunni, V.P.; Pasianot, R.C.; Bruzzoni, P.; Phys. B 404, 18, 2880-2882 (2009).

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7 - 2 – Experimental and theoretical interface interaction analysis of TiN/TiC bilayers

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TiN/TiC bilayers were grown by using the cathode vacuum arc technique. In order to study the interface interaction, depth profiles were obtained by XPS (X-ray photoelectron spectroscopy). An inter diffusion between TiN and TiC at the interface showing the formation of Ti-C-N bonds. For understanding the physical process present in such an interface, simulations employed the Gaussian 98W software, observing the interface behavior, using quantum mechanics tools as first order perturbation theory. Simulations showed the formation of several bonds in the TiN-TiC interface because of the existence of internal stress as those observed in the diffraction patterns. The atomic density at the interface is high. It implies bonds formation and destruction in order to stabilizing the system. Moreover, atomic reaccommodation is appreciated as a way of releasing stress.

7 - 3 – Simulation of the magnetic field influence on the magnetocaloric properties in $La_{1-x}Ca_xMnO_3$ thin films

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In this work, the magnetocaloric effect of $La_{1-x}Ca_xMnO_3$ as thin films varying the stoichiometry was calculated. For this aim, classical Monte Carlo simulations used in order to consider the interaction between nearest neighbors were implemented. Ions with valence Mn^{3+} and Mn^{4+} interacting with La^{3+} and Ca^{2+} respectively were considered. Terms like Zeeman effect and magnetocristalline anisotropy were included in the Hamiltonian. Moreover, Heisenberg hamiltonian was employed for obtaining a more realistic model. Curves of specific heat and entropy, ΔS and ΔT were obtained varying the external magnetic applied field for different values of x. Results show the magnetic, lattice and electron contributions to the total specific heat and entropy.

7 - 4 – Modeling Voltage Rectification Effects on Mesoscopic Superconducting Devices

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The general and central idea that motivates this work is the recent technological progress allowing the observation of ratchet effects in very complex systems such as cold atoms, electrons in semiconductors, vortices in superconductors just to mention a few. But the main question on this field is that "is not simple" in each case to know feasibly which are the mechanisms underlying these many bodies complex effects in condensed matter. In particular, motivated for recent experiments reporting voltage rectification effects in mesoscopic superconducting triangles [Schildermans *et al*, PRB **76**, 224501, 2007] we simulated an improved model for such a system. We studied thermal fluctuations effects and capacitive effects on a Small Josephson Junction Closed Loop that mimics the rectification phenomena observed experimentally due to the superposition of a field induced persistent current with the bias current. At finite temperature we predicted that the amplitude of the rectified signal depends strongly on the current contacts configuration on the Josephson Junction Ring (weak link type junctions), in coincidence with the observations on the mesoscopic superconducting triangle sample. In addition we analize the range of parameters where a closed loop of capacitive junctions is an appropriate model to explain the experimental observation. In short, in this work we conclude that the closed loop of SNS Josephson Junctions is a good and robust enough model in a considerable range of thermal fluctuations to explain the observed voltage rectification effects on mesoscopic superconducting samples.

7 - 5 – Numerical simulation of Ge solar cells using D-AMPS-1D code

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A solar cell is a solid state device that converts the energy of sunlight directly into electricity by the photovoltaic effect. When light with photon energy greater than the band gap is absorbed by a semiconductor material, free electrons and free holes are generated by optical excitation in the material. The main characteristic of a photovoltaic device is the presence of internal electric field able to separate the free electrons and holes so they can pass out of the material to the external circuit before they recombine. Numerical simulation of photovoltaic devices plays a crucial role in their design, performance prediction, and comprehension of the fundamental phenomena ruling their operation. The electrical transport and the optical behaviour of the solar cells discussed in this work were studied with the simulation code D-AMPS-1D. This software is an updated version of the one-dimensional (1D) simulation program AMPS (Analysis of Microelectronic and Photonic Devices) that was developed at The Penn State University, USA, during the years 1988-1993. In AMPS the technique of finite differences and the Newton-Raphson iteration method are used to solve the Poisson and the continuity equations that are subjected to appropriate boundary conditions. The three unknowns were chosen as the quasi-Fermi levels and the electron potential. The letter D stands for new developments that were introduced in recent years. Structures such as homojunctions, heterojunctions, multijunctions, etc., resulting from stacking layers of different materials can be studied by appropriately selecting characteristic parameters such as the gap energy, carrier mobilities, absorption coefficients among others. The code evaluates the external device characteristic curves such as the current density-voltage (J-V) under dark and under illumination, the quantum efficiency (EQ), the reflectivity, and internal quantities such as the electric field, the free and trapped carrier concentrations, the recombination and generation rates, etc.. In this paper, examples of cells simulation made with D-AMPS-1D are shown. Particularly, results of InGaP and Ge photovoltaic devices are presented. It is important to mention that these structures can be use both in homojunction and multijunction devices. For the Ge cell, an example of the first scenario is the case of devices for thermophotovoltaics applications and an example of the second one is the triple junction InGaP-GaAs-Ge cells for space or terrestrial applications. In this work, numerical simulation of single junction n-p InGaP-Ge solar cells was performed. The optical reflectivity, the EQ and the role of the InGaP buffer on the device were studied. Moreover, a comparison of the simulated electrical parameters with experimental results was performed.

7 - 6 – Lattice Bhatnagar-Gross-Krook Model for Anomalous Subdiffusion

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A new lattice Boltzmann (LB) model is proposed for solving the anomalous subdifusion equation, mathematical development is shown from the BGK model that extends the simulation method for the normal diffusion equation, considering that the development of the Chapman-Enskog expansion of this model is based on some approximations and properties formulated from fractional calculus, this result is clearly discussed due to mean square displacement is not linearly dependent on time. The computational implementation shows that the method can be used to simulate the anomalous diffusion equation.

7 - 7 – Lattice Boltzmann Model for Fractional KdV Equation

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We propose a lattice Boltzmann model (LB) which simulates the fractional Korteweg-de Vries (FkdV) equation by using a method of higher moments of the lattice Boltzmann equation. For this model we developed the fractional Chapman-Enskog expansion, obtaining a series of lattice Boltzmann equations on different time scales, which recover exactly the macroscopic fractional KdV equation, taking into account the conservation law for t_0, we obtained the equilibrium distribution function. The numerical examples show that the method can be used to simulate the fractional KdV equation.

7 - 8 – Non equilibrium Thermodynamics and Entropy Production in Dielectric Breakdown process for polymer materials

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In the present paper we applied the non equilibrium thermodynamic theory in the analysis of the dielectric breakdown process. From the thermodynamic viewpoint all phenomena in nature have a tendency to reduce their energy, is the case of the propagation of electrical tree structure. As the tree channel front moves, the intense field near the front moves electrons and ions irreversibly in the region beyond the tree channel tips where electromechanical, thermal and chemical effects cause irreversible damage and from the non equilibrium thermodynamic viewpoint: entropy production. We choose the capacitive model (CDBM) to simulate the dielectric breakdown process. We select CDBM based on the special characteristics of the model: 1) Two different protocols are presented to select the capacitor that will be broken out of the set that meet breakdown conditions: 2) Protocol 1 is associated with the entropic contribution of the electrical tree growth process 3) Protocol 2 is identified with the corresponding internal energy contribution. 4) In the CDBM the dependence of the fractal dimension on the applied voltage has its thermodynamics origin in the interplay between energy injection and space charge formation process 5) The CDBM is also capable of qualitatively reproducing the temporal dependence of the breakdown process All of these combined give us an excellent framework for the entropy production evaluation in the tree growth process.

7 - 9 – Monte Carlo Studies of Critical and Dynamic Phenomena in Mixed Bond Ising Model

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The Hamiltonian of spin with mixed bond interactions [1] is used commonly to model several composed, such as $Co(S_pSe_{(1-p)})$ in the which atoms of Co interact amongst themselves through atoms either of S or Se [2], in that way, the interaction among the atoms of Co is modeled by two different exchange interaction. The mixed-bond Ising model also has been used to model composed that present modulated magnetic structures as the case of $Fe_pAu_{(1-p)}$, $Eu_pSr_{(1-p)}S$ and $Fe_pAl_{(1-p)}$[3]. In this work, we studied the thermodynamic properties and of our analysis we determined the critical exponents and we constructed the phase diagram for mixed-bond Ising model. The model was studied by means Monte Carlo simulation applied for cubic lattice by using Metropolis and Wolff algorithm with histogram technique and finite size scaling theory [4].

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[3] S. ABIKO; S. NIIDERA; F. MATSUBARA, Phys. Rev. Lett. 94 (2005) 227202.

[4] C. BERCHE, B.B. P CHATELAIN, W. JANKE, Eur. Phys. J. B 38 (2004) 463-474

7 - 10 – Modeling of high entropy alloys of refractory elements

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Reverting the traditional process of developing new alloys based on one or two single elements with minority additions, the study of high entropy alloys (HEA) (equimolar combinations of many elements) has become a relevant and interesting new field of research due to their tendency to form solid solutions with particular properties in the absence of intermetallic phases. To date, very few cases have been studied, but all show that the study of HEA is a promising and perhaps revolutionary area of growth in materials science. There are currently no theoretical or modeling studies of specific HEA which explain the formation, structure, and properties of these alloys, mostly due to the large number of constituents involved. In this work we focus on the HEA with refractory elements. While there is abundant experimental work concentrating on fcc-based HEA, there is only one experimental case that has been studied where all the constituents are refractory elements. To aid in the development of new compositions, as well as understanding the intricate details during the alloy formation process and the transition to what could be addressed as the high entropy regime, we show atomistic modeling results for W-Nb-Mo-Ta and W-Nb-Mo-Ta-V HEA for which experimental background exists. Such work indicates that these alloys exhibit unusual properties but the complexity of the system introduced unavoidable limitations in determining the role of each element, the transition to the high entropy regime characterized by the formation of extended solid solutions and, more importantly, limits the ability to identify the interactions and features responsible for such transition. We achieve this goal by means of atomistic modeling using the BFS method for alloys for the energetics. We show results for equimolar alloys of 4 and 5 elements (W, Nb, Ta, Mo, V), for which experimental results exist, and provide a straightforward algorithm for the determination of the features responsible for the characteristic HEA behavior.

7 - 11 – A potential for Th from inversion of cohesive energy: elastic constants

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An interatomic pair potential for fcc Th was derived by using the Chen-Mobius lattice inversion method. The cohesive energy vs lattice parameter relation required by this method was derived from first principles electronic structure calculations. Based on this potential the elastic constants of fcc Th were calculated by applying three differents types of strain to the starting crystal. In order to improve the accuracy of the validity of the potential a Salter-Kirkwood type non-additive three body correction was implemented. The computed elastic constants are found to be in a very good agreement with experiments.

7 - 12 – Magnetocaloric effect observed by differential thermal analysis

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The magnetocaloric effect (MCE) is the isothermal change of magnetic entropy and the adiabatic temperature change induced in a magnetic material when an external magnetic field is applied.

In this work, we study this effect using the differential thermal analysis technique (DTA), which consists in measuring simultaneously the temperatures of the sample of interest and a reference one while an external magnetic field ramp is applied. We calculate the temperature difference (ΔT) from these values.

By using this method, we study the MCE in $La_{0.305}Pr_{0.32}Ca_{0.375}MnO_3$, which presents phase separation effects at low temperatures (< 200 K).

We obtain ΔT vs H and ΔT vs t curves, and analyze how the MCE varies by changing the external pressure and the rate of the magnetic field ramp. Our results show that the effect is amplified by working at lower pressures ($< 10^{-4}$ Torr) and at high velocity. However, at high vacuum a temperature gradient appears and makes it difficult to set the temperature properly. Also, self-heating of the sensor becomes relevant at this condition. Therefore, we decide to work at pressures of the order of 1 Torr. We also measured MCE at different temperatures, finding an inverse MCE, characterized by a $\Delta T < 0$ on increasing magnetic field, in the region between 140 K and 180 K.

Then, from DTA measurements of samples with different masses and a description of the thermal coupling of our system, we obtain the effective specific heat of the system. With this analysis, we are able to describe the influence of the environment and subtract it to calculate the adiabatic temperature change of the sample.

Finally, we propose a thermodynamic model which allows us to relate the DTA results with magnetization measurements.

7 - 13 – Microstructure and hard magnetic properties in bulk rods of $Nd_{60}Fe_{30}Al_{10}$ glass forming alloy

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The $Nd_{60}Fe_{30}Al_{10}$ alloy exhibits a large glass forming ability which allows to obtain relatively thick cast rods containing large volume fractions of amorphous phases. In this work the microstructure and the hard magnetic properties of as-cast rods are characterized. The alloy is processed by suction casting onto chilled copper mould to obtain cylinders 5 mm diameter and 50 mm length. This diameter is selected because it is an upper limit for this processing route, beyond which the hard properties largely deteriorate. A room temperature coercivity of 0,34 T is obtained. The sample microstructure is heterogeneous, with very different size scales near the surface and along the central zone. However, in both regions a large fraction of an amorphous ferromagnetic phase is observed; it is found that paramagnetic nanocrystalline phases - mainly Nd or Nd-rich particles, embedded in the amorphous matrix - are somewhat coarser in the central zone. These larger nanocrystals, less efficient to pin domain walls, are proposed to be responsible for the lower coercive fields observed, as compared with those found in cylinders 1-3 mm diameter where no inhomogeneities are found. This conclusion is supported by microstructure, calorimetric and magnetic domain observations.

7 - 14 – Simulation of magnetorheological fluids to a magnetic field

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A magnetorheological fluid (MR) is a liquid with a density greater than water, which passes an oily state to a quasi-solid to be exposed to a magnetic field. Currently, the use of MR fluids is extended to different industries, engineering, medicine, etc., Depending on the scope.

The mathematical program to use is a computer simulation technique that uses a numerical system called finite element method (FEM) or finite-difference numerical procedure to obtain approximate solutions for problems can be represented by a system of equations differentials, these programs lead to better products at lower costs, improve existing processes, to study the structural component failure or a computer, widely used in engineering and physics.

In this research, a mineral magnetite, which were determined by percentage of iron using two methods: physical test (magnetic separation) and chemical testing (chemical gear), the first we worked with two grain sizes (100 mesh and mesh 200), with a score of 78.26% and 86.63% respectively and magnetite in the second we worked with 200 mesh, resulting in an average of 94.1% magnetite, which were found very high content of magnetite. Then he prepared another part of the magnetite mesh sizes 400 and 500, which are derived magnetorheological fluid 8 which has a variation in the concentration (30:70 and 50:50), also working with two liquids different (SAE 20 and SAE 50) finding the best behaved fluid to the applied magnetic field in the final design team and determining the value of the variables that are at stake.

As a final result expected from a model and simulation of a magnetorheological fluid to a magnetic field.

7 - 15 – Point defect properties in the vicinity of an Al/U interface

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The static and dynamic properties of vacancies and interstitials have been studied in the neighborhood of an Al/α-U interface using classical atomistic techniques. A suitable interatomic EAM potential for uranium and aluminum have been used for this purpose. First, a bicrystalline Al(fcc)/α-U(A20) simulation block is built in such a way that the two compact planes and two directions are correspondingly parallel, i.e., (111)Al//(001)αU and [110]Al//[100]α-U. Vacancies and interstitials are generated in the proximity of this planar defect to study properties and interaction with the interface as a function of distance. To characterize their properties far from the interface, the same defects have also been studied in bulk Al and α-U. We observed that the vacancy is stable in the first (001)U interfacial layer and unstable up to the second layer on each phase. Regarding interstitials, the final configurations depend both on the initial unrelaxed position chosen and on atomic species. They can take the form of mixed crowdions or simple interstitials. Point defects generated beyond around the third plane of each phase recover their corresponding bulk value. Taking into account the previous formation studies, only point defect jumps in the first layers of the interface are studied. We have applied the monomer method, a recently developed static calculation technique, to find point defect migration energy barriers in the same Al/α-U interface structure. The advantage of this new calculation methodology over other more familiar techniques resides in which, given an initial equilibrium position of the jumping defect, no assumption is made upon the final equilibrium position. Results show that in both bulk and interface α-U the presence of an Al impurity decreases the vacancy jumping barrier. On the other hand, the interchange between a vacancy and a first neighbor U impurity in Al is not favorable with respect to other jumps. These results suggest a faster diffusion of Al in α-U than viceversa.