Condensed Matter

The staff consists of 20 professionals and 2 technicians, plus a variable number of research students (at present: 5)

Projects on the move, all of them on solid state physics or condensed matter in general, include a variety of topics and techniques, with an important thematic inbreeding linking them. A brief description of the intervening Groups and Laboratories follows.

Laboratory Of Chemical Synthesis And Characterization:

A variety of perovskitic materials are obtained and characterized, in particular substituted manganese oxides. Among other materials of interst we find copper and alkaline earth metals. anhydrous formates, mixed copper and transition metals hydrated formates, and other related compounds of biological or technological interest. In this area some hydroxyapatites as well as their cationic and anionic substitution derivatives are also studied.

X-Ray Diffraction:

Areas of interest are: molecular structures of new coordination compounds with transition metals and polymorphs with a pharmacological interest, structural phase transitions and the study of compounds with modulated structures. The Laboratory runs a facility for the identification of third party crystalline samples by x-ray powder diffractometry.

Raman Spectroscopy:

Systematic studies are performed on thin films of amorphous carbon (diamond like) over different substrates, in order to fully chracterize them.

Mössbauer Spectroscopy:

The technique is applied to iron alloys and ferrites, minerals and soils, nanoparticles, etc.

Electrical Properties:

Measurements of dielectric constants, electrical conductivity and alternate magnetic susceptibility are performed on ceramics and single crystals, as a function of temperature (30-300 K), in the presence of a magnetic field of up to 1 Tesla. Presently, the interest is centered on the study of manganese oxydes with magnetoresistent properties.

Condensed Matter Theory:

The different lines include: electronic structure and magnetic properties calculations of different metallic systems of low dimensionality through ‘ab-initio’ methods (LMTO-FLAPW). Numeric simulation of transition metals. Calculation of transport properties tunnel effect on disordered systems and metallic superlattices. Dynamical properties of molecular crystals, using molecular dynamics. Static and dynamic properties of inconmensurate phases. Molecular dynamics as applied to C60-like molecules. Montecarlo calculations to obtain the phase diagram and dielectric constant of dipolar molecular liquids and antiferromagnetic systems with defects. Extended dynamical systems with self-criticallity. Study of the liquid-solid transition, from the point of view of a broken translation symmetry in a liquid. Order-disorder phase transitions in periodic systems with competing interactions which end up in a modulation of the disorder for intermediate temperatures. Structural and dynamical properties of C and Si compounds using semiempirical potentials

The polarizability and intermolecular potential of C_{60}

Z. Gamba

An intermolecular potential model of C60 that includes repulsive, dispersive and coulombic terms is proposed. The repulsive and dispersive terms are represented by one simple Lennard-Jones (LJ) interaction site that gives account of the almost spherical form of this molecule. The deviations of its spherical form are fully given by the coulombic interactions. A model of distributed polarizable dipoles that reproduce the ab initio electrostatic multipolar moment and polarizability of C60 molecule is proposed. The configurational energy, main molecular orientation and several barriers to reorientational motion of low temperature C60 crystals are well reproduced.

*Phys. Rev B **57** (1998) 1402.*

The ordered, orientationally disordered and glassy crystalline phases of P_4S_3

D.Bougeard [1] and Z. Gamba

The phase diagram of P4S3 crystals is studied by a series of constant pressure molecular dynamics simulations at several temperatures and zero pressure. The weak van der Waals intermolecular interaction forces are represented by a simple atom-atom semiempirical model. The calculations reproduce the experimental data on ordered α-P4S3 below 300 K, but also show the possible existence of a polymorph αP4S3. The structure and dynamical properties of orientationally disordered β-P4S3 are predicted. This work stresses the need of further experimental data in order to improve the potential model as well as clarify the issue of a possible new phase.

** Mol. Phys. **94** (1998) 815.*

[1] LASIR, Université de Sciences et Technologies de Lille, Bat. C5, 59655, Villeneuve D'Asq, France.

The ordered and orientationally disordered crystalline phases of the flexible C_4F_8 molecule

Z. Gamba and B. M. Powell [1]

There is ample experimental evidence for the existence of several crystalline phases of C4F8, although they still have been not clearly identified. In this paper we report a series of molecular dynamics (MD) simulations using a partially flexible molecular model, which takes into account the mixing of the low frequency intramolecular modes and lattice modes. The calculations are carried out at constant pressure and constant temperature and the algorithm employed allows for volume and symmetry changes of the MD sample as a function of thermodynamic variables. Although several stable crystalline phases are found, their number is still less than determined by experiments.

** J. Chem. Phys, in press (1999).*

[1] B. M. Powell, National Research Council of Canada, Steacie Institute for Molecular Sciences, Neutron Program for Materials Research, Chalk River Labs. Canada

Test of a simple and flexible molecule model for α, β and γ-S_8 crystals

C. Pastorino and Z. Gamba

S_8 is the most stable compound of elemental sulfur in solid and liquid phases, at ambient pressure and below 400K. Three crystalline phases of S_8 have been clearly identified in this range of thermodynamic parameters, although no calculation of its phase diagram has been performed yet. α- and γ-S_8 are orientationally ordered crystals while β-S_8 is measured as orientationally disordered. In this paper we analyze the phase diagram of S_8 crystals, as given by a simple and flexible molecule model, via a series of molecular dynamics (MD) simulations. The calculations are performed in the constant pressure-constant temperature ensemble, using an algorithm that is able to reproduce structural phase transitions.

** J. Phys. Chem, in press (1999)*

Test of a simple and flexible S_8 model molecule in α-S_8 crystals

C. Pastorino and Z. Gamba

α-S_8 is the most stable crystalline form, at ambient pressure and temperature (STP), of elemental sulfur. In this paper we analyze the zero pressure low temperature part of the phase diagram of this crystal, in order to test a simple and flexible model molecule. The calculations consist in a series of molecular dynamics (MD) simulations, performed in the constant pressure-constant temperature ensemble. Our calculations show that this model, that gives good results for three crystalline phases at STP and Tsim>300K, fails at low temperatures, predicting a structural phase transition at 200K where there sould be none.

** Submitted to Chem. Phys. Lett. (1999)*

Cobalt impurities on noble metal surfaces

Mariana Weissmann, Andrés Saúl[1], Ana María Llois, and Javier Guevara

First principles calculations, based on the local spin density approximation, are performed for cobalt atoms deposited on noble metal surfaces. The local density of states at the cobalt site shows a narrow peak at the Fermi energy, which is of minority spin and *d* character. The *d* orbital of m = 0 symmetry, which must be mostly responsible for tunneling conductance from this surface site, makes a substantial contribution at E_f. Due to hybridization the same peak also appears, but reduced, at neighbor atoms. This result can be used for the interpretation of recent cryogenic scanning tunneling microscopy experiments.

[1] Centre de Recherche sur les Méchanismes de la Croissance Cristalline, CNRS, France

Model Hamiltonian for the conductivity oscillations of magnetic multilayers

Miguel Kiwi[1], Ana María Llois, Ricardo Ramírez[1], and Mariana Weissmann

The behavior of the electrical conductivity as a function of layer thickness of the superlattice systems Ni/Co, Ni/Cu and Pd/Ag is studied. Experimentally an oscillatory dependence was found for the first two, while the latter exhibited a monotonous behavior. In our calculations we find that, in these superlattices, the current is carried by the *sp*--character electrons, which are quite insensitive to the interfaces. To interpret the experimentally observed resistivity oscillations we suggest a scattering mechanism of these carriers against *d*--character quantum well states that are present in only one of the superlattice materials, when the well state energy is close to E_F.

[1] Facultad de Física, Pontifícia Universidad Católica de Chile

On the magnetic contribution to the segregation energies in magnetic-nonmagnetic systems

Andrés Saúl[1] and Mariana Weissmann

The segregation energy of magnetic materials (Fe, Co, Ni) embedded in some nonmagnetic hosts (Pd, Ag, Cu) is calculated using an approximate procedure based on ab-initio calculations of three dimensional periodic systems, performed in the spin polarized and paramagnetic states. Slabs with full layers of magnetic impurities or with ordered alloy layers are considered, separated by sufficient empty space so as to simulate free surfaces. We find that the considered magnetic atoms always prefer to lie embedded in the host metal and not to be located at the surfaces (positive segregation energy). The ferromagnetic state has a systematically lower segregation energy than the paramagnetic state, but never so much as to change its sign. The resulting energies are compared to a simple Ising Model, whose parameters are the surface energies of the pure constituents and the effective pair interaction, that give the tendency of the alloy to phase separate. We found that a better agreement with the ab-initio segregation energies is found if we assume an enhancement of the effective pair interaction at the surface.

[1] Centre de Recherche sur les Mécanismes de la Croissance Cristalline, CNRS, France

Tight-binding molecular dynamics study of amorphous carbon deposits over silicon surfaces

Chu-Chun Fu and Mariana Weissmann

We report in this paper a procedure to simulate the deposit of carbon diamond-like films over the Si(001) surface. We use the method of tight-binding molecular dynamics and well know transferable C-C and Si-Si interactions. We propose for the Si-C interaction a weighted average of them and test it by studying crystalline SiC, the molecule SiC, some small mixed clusters and the surfaces of β SiC(001).

The first results of the deposition simulation are presented, showing the characteristics of the thin mixed interface layer, with a low carbon concentration.

Structural evolution of free Co cluster magnetism

J. Guevara and Ana Maria Llois, F. Aguilera-Granja[1] and J.M. Montejano-Carrizales[1]

We present a systematic study of the average magnetic moments of free Co_N clusters having different geometry: hexahedral, decahedral and octahedral. The spin polarized electronic structure is calculated with a parameterized Hubbard Hamiltonian with *spd* electrons within the unrestricted Hartree-Fock approximation, and spillover effects are considered.

We compare with our calculations with other theoretical calculations in the literature, we also comment the experimental results.

[1] Instituto de Física, *"Manuel Sandoval Vallarta"*, Universidad Autónoma de San Luis Potosí, México.

Large variations in the magnetization of Co clusters induced by noble metal coating

Javier Guevara, Ana Maria Llois and Mariana Weissmann

We report calculations of the electronic and magnetic properties of small Co clusters, coated with Ag or Cu, performed with a parametrized tight-binding method. For a given number of Co atoms in a cluster we obtain a large range of magnetization values, depending on the size and shape of the coating. The noble metal develops a net polarization that changes appreciably the total magnetic moment of the cluster. This result is reinforced by ab-initio calculations for Co slabs, where the corrugation of a non magnetic covering also produces important variations in the total magnetic moment.

Magnetic structure of small Fe-Ni clusters: calculations in the Ni rich region

Javier Guevara, and Ana María Llois

Small clusters present many novel properties absent in bulk materials. One of the most relevant features of small transition metal systems is their magnetic behavior. Monoatomic clusters show a magnetic moment per atom larger than the in the bulk. However, Fe-Ni clusters have experimentally a lower magnetization than the corresponding bulk alloy values. In this contribution we calculate electronic and magnetic structure of $Fe_{1-x}Ni_x$ clusters, for x > .5 We find ferro- and antiferromagnetic self-consistent solutions, in the antiferro solutions the Fe atoms are antiferromagnetically aligned among themselves, while the Ni atoms have a lower local magnetization than in the bulk.

On the metallic behavior of Co clusters

F. Aguilera-Granja[1] and J.M. Montejano-Carrizales[1] J. Guevara and Ana Maria Llois

The nonmetal-metal transition in free Co_N clusters is studied by using a parameterized Hubbard Hamiltonian with *s*, *p* and *d* electrons within the unrestricted Hartree-Fock approximation considering spillover effects. The non-mental-metal transition occurs when the density of states at the Fermi level exceeds $1/k_BT$ and the discrete energy levels begin to form a quasi-continuous band. The role of the cluster structure in the nonmetal-metal is investigated by performing calculations for different geometries: hexahedral, octahedral and decahedral. We found that the metallic behavior in small clusters (N≤40) is strongly related with the geometrical structure of the cluster. We compare our calculations with Friedel's model and comment on the experimental results base on the Ionization Potential measurements.

[1] Instituto de Física, "Manuel Sandoval Vallarta" Universidad Autónoma de San Luis Potosí, México

Spin-flip contribution to the conductivity of magnetic multilayers

Ricardo Gomez Abal, Ana María Llois, and Mariana Weissmann

The conductivity of magnetic multilayers is calculated within the semiclassical approximation. The band structure is obtained with a tight-binding Hubbard Hamiltonian solved in the Hartree-Fock approximation. Once self-consistency is reached, the spin-orbit coupling term is added and a further diagonalization is performed. As it is well known, quantum well states appear in the band structure of superlattices. By calculating the conductivity as a function of the Fermi energy we find that there is a considerable influence of these quantum well states if their energy is close to the Fermi level when the spin- orbit coupling is taken into account.

Self-organization, resources and strategies in a minority game

Horacio Ceva

We find that the existence of self-organization of the members of a recently proposed minority game depends on the type of update rules used. The resulting resource distribution is studied in some detail, and a related strategy scheme is considered, as a tool to improve the understanding of the model.

** To be published in Physica A*

On the asymptotic behavior of an earthquake model

Horacio Ceva

We present evidence showing that there are important differences in the relaxation times associated with different aspects of the model of Olami, Feder and Christensen. The asymptotic behavior is characterized by a critical exponent that is independent of α, the degree of conservation of the model. The analysis of temporal series of avalanches gives helpful information to study the approach to self-organized criticality, and to put in evidence any quasi-periodic evolution.

** Physics Letters A **245** (1998) 413*

Hybrid quantum and classical mechanical Monte Carlo simulations of the interaction of Hydrogen Chloride with solid water clusters

Dario A. Estrin[1], Jorge Kohanoff[2], Daniel H. Laria[1,3], Ruben O. Weht.

Monte Carlo simulations using a hybrid quantum and classical mechanical potential were performed for crystal and amorphous-like HCl–water(n) clusters. The subsystem composed by HCl and one water molecule was treated within Density Functional Theory, and a classical force field was used for the rest of the system. Simulations performed at 200 K suggest that the energetic feasibility of HCl dissociation strongly depends on its initial placement within the cluster. An important degree of ionization occurs only if HCl is incorporated into the surface. We observe that local melting does not play a crucial role in the ionization process.

* *Chemical Physics Letters* ***280*** *(1997) 280.*

[1] Department of Chemistry, UBA

[2] ICTP, Trieste, Italy.

[3] Department of Chemistry, CNEA.

Correlations in the sand pile model: from the log-normal distribution to self-organized criticality.

Horacio Ceva and Javier Luzuriaga

We have studied the approach of the abelian sand pile model towards the stationary, self-organized criticality state. The uncorrelated limit is shown both numerically and by a simple analysis to follow the log-Normal distribution. We introduce and evaluate several correlation functions to study the correlated region.

* *Physics Letters A* ***250*** *(1998) 275*

An ab initio path integral Monte Carlo simulation method for molecules and clusters: application to Li_4 and Li_5^+

Ruben O. Weht, Jorge Kohanoff[1], Dario A. Estrin[2], Charusita Chakravarty[1,3]

A novel method for simulating the statistical mechanics of molecular systems in which both nuclear and electronic degrees of freedom are treated quantum mechanically is presented. The scheme combines a path integral description of the nuclear variables with a first-principles adiabatic description of the electronic structure. The electronic problem is solved for the ground state within a density functional approach, with the electronic orbitals expanded in a localized (Gaussian) basis set. The discretized path integral is computed by a Metropolis Monte Carlo sampling technique on the normal modes of the isomorphic ring-polymer. An effective short-time action correct to order τ^4 is used. The validity and performance of the method are tested in two small Lithium clusters, namely Li_4 and Li_5^+. Structural and electronic properties computed within this fully quantum-mechanical scheme are presented and compared to those obtained within the classical nuclei approximation. Quantum delocalization effects are significant but tunneling turns out to be irrelevant at low temperatures.

* *Journal of Chemical Physics* ***108*** *(1998) 888.*

[1] ICTP, Trieste, Italy.

[2] Department of Chemistry, UBA.

[3] Department of Chemistry, Indian Institute of Technology.

Extended moment formation and second neighbor coupling in Li_2CuO_2

Ruben Weht, W.E.Pickett [1]

Comprised of ferromagnetic edge-sharing CuO_2 chains that order in antialigned fashion at T_N=9 K, Li_2CuO_2 is found from local spin density calculations to display several surprising characteristics: (1) the ordered moment/f.u. of 0.92 μ_B is the largest for any low dimensional cuprate system, in agreement with experiment, (2) 40% of this moment lies on the neighboring O ions, making it the largest oxygen moment yet reported, and (3) the second neighbors couplings are larger than nearest neighbors couplings. All of these phenomena arise naturally due to a well defined effective d_{yz} type orbital that includes very strong O pσ character. We interpret the large moment as surviving reduction by quantum fluctuations due to extension caused by the d-p hybridization.

* *Physical Review Letters* ***81*** *(1998) 2502.*

[1] Department of Physics, University of California, Davis, USA.

Excitonic correlations in the intermetallic Fe_2VAl

Ruben Weht and W.E. Pickett[1]

The intermetallic compound Fe_2VAl looks non-metallic in transport and strongly metallic in thermodynamic and photoemission data. It has in its band structure a highly differentiated set of valence and conduction bands leading to a semimetallic system with a very low density of

carriers. The pseudogap itself is due to interaction of Al states with the d orbitals of Fe and V, but the resulting carriers have little Al character. The effects of generalized gradient corrections to the local density band structure as well spin-orbit coupling are shown to be significant, reducing the carrier density by a factor of three. Doping of this nonmagnetic compound by 0.5 electrons per cell in a virtual crystal fashion results in a moment of 0.5 bohr magnetons and destroys the pseudogap. We assess the tendencies toward formation of an excitonic condensate and toward an excitonic Wigner crystal, and find both to be unlikely. We propose a model is which the observed properties result from excitonic correlations arising from two interpenetrating lattices of distinctive electrons (e_g on V) and holes (t_{2g} on Fe) of low density (one carrier of each sign per 350 formula units).

* *Physical Review B* ***58*** *(1998) 6855.*

[1] Department of Physics, University of California, Davis, USA.

Half-metallic ferrimagnetism in Mn_2VAl

Ruben Weht and Warren E. Pickett[1]

We show that Mn_2VAl a compound for which the generalized gradient approximation (GGA) to the exchange-correlation functional in density functional theory makes a qualitative change in predicted behavior compared to the usual local density approximation (LDA). Application of GGA leads to prediction of Mn_2VAl being a half-metallic ferrimagnet, with the minority channel being the conducting one. The electronic and magnetic structure is analyzed and contrasted with the isostructural enhanced semimetal Fe_2VAl.

* *Physical Review B* ***60*** *(1999) 13006.*

[1] Department of Physics, University of California, Davis, USA.

Electron doping in the honeycomb bilayer superconductors (Zr,Hf)NCl

Ruben Weht, Alessio Filippetti [1] *and Warren E. Pickett* [1]

Based on a virtual crystal treatment, we show that alkali doping introduces electron carriers into a single light mass (m* = 0.6), low density of states band in Li_xZrNCl and Na_xHfNCl (which have superconducting T_c up to 25 K) that is a symmetric interlayer combination of d_{xy}, d $d_{x^2-y^2}$ character. Doping leads to simple K-centered three-fold symmetrical cylindrical Fermi surfaces that concentrate low energy scattering into distinct regions of momentum. The lack of any observed magnetic tendencies, together with our calculation of small electron-phonon strength, suggests a pairing mechanism that is distinct from known superconductors.

* *Europhysics Letters* ***48*** *(1999) 320.*

[1] Department of Physics, University of California, Davis, USA.

Superconductivity in ferromagnetic $RuSr_2GdCu_2O_8$

W. E. Pickett[1]*, Ruben Weht and A. B. Shick*[1]

Relying on the inhomogeneous (layered) crystal, electronic, and magnetic structure, we show how superconductivity can coexist with the ferromagnetic phase of $RuSr_2GdCu_2O_8$ as observed by Tallon and coworkers. Since the Cu $d_{x^2-y^2}$ orbitals couple only to apical O p_x, p_y orbitals (and only weakly), which also couple only weakly to the magnetic Ru t_{2g} orbitals, there is sufficiently weak exchange splitting, especially of the symmetric CuO_2 bilayer Fermi surface, to allow singlet pairing. The exchange splitting is calculated to be large enough that the superconducting order parameter may be of the Fulde-Ferrell-Larkin-Ovchinnikov type. We also note that π-phase formation is preferred by the magnetic characteristics of $RuSr_2GdCu_2O_8$.

* *Physical Review Letters* ***83*** *(1999) 3713.*

[1] Department of Physics, University of California, Davis, USA.

Modulated phases in Ising lattices. Phase diagrams in the mean field approximation.

Vittorio Massida

Order-disorder transitions of Ising systems are studied in the mean-field approximation. Depending on the value of the interaction constants (J_i) between different sites, at intermediate temperatures these systems have a spatially modulated disorder. We applied the formalism to binary alloys and to magnetic systems with interactions up to third-nearest neighbours, investigating the dependence of the modulation wavelength on the temperature and on the J_i's.

Mössbauer spectra of intermolecular Fe in L-Alanine

D. Rodríguez Sierra, E. Winkler[1]*, C. Saragovi and C. Fainstein*[1]

Crystals of nominal 4%Fe:L-alanine have been grown from acqueous solution, introducing Fe as ferric nitrate. Mössbauer spectra of the powdered

crystals were obtained at 295K and 15K. The spectra were fitted with quadrupolar distributions, two at 295K, and three at 15K. For both temperatures, the found IS values indicate that Fe is in a state of charge 3+. Results of experimental EFG values are compared with calculations carried out for Fe at a possible site in the lattice. The spectra at both temperatures is discussed in terms of dynamic effects.

* *Hyperfine Interactions C* ***3*** *(1998) 65.*
1 CAB - CNEA and Instituto Balseiro, Argentina

Evaluation of pyrophosphate-extractable Fe from each horizon of an Argentinian soil profile

A. Mijovilovich, C. Saragovi, S.G. Acebal[1], E.H. Rueda[1] and M.E. Aguirre[2]

Sodium pyrophosphate (0.1M, pH10) is commonly used to extract iron and aluminium from soil organic complexes, but there is evidence that in some soils it also extracts non-organic forms. A Mössbauer study of the effect of Na-pyrophosphate treatment on the Fe extraction on a Mollisol (< 50μm fraction) from Bahía Blanca, Argentina is presented. Samples from different horizons, A_p, A_1, AC and C_k, were measured before and after treatment.. Spectra were fitted using two doublets and two sextets distributions. From the areas results, the variation of the Fe content with depth is discussed. Comparison with the obtained chemical data is made.

* *Hyperfine Interactions C* ***3*** *(1998) 336.*
[1] Department of Chemistry and Chemical Engineering, Universidad Nacional del Sur - Bahía Blanca, Argentina.
[2] Department of Agronomy - Universidad Nacional del Sur- Bahía Blanca, Argentina.

Magnetic and Mössbauer experiments on disperse hematite nanoparticles

R. D. Zysler [a] , C. Arciprete [a] , M. Dimitrijewits [a] , C. Saragovi and J. M. Greneche [b]

Nanoparticles of hematite with sizes comprised in the range 4-5 nm were prepared and dispersed in a non-magnetic polymer matrix. Magnetic studies and Mössbauer measurements were performed on three samples with following concentrations: 10%, 1%, 0.1%wt, respectively, in order to follow the influence of the interparticle interactions. The magnetic studies show a maximum in the DC magnetization as a function of the temperature measured under zero-field cooling (ZFC) at Tm=16K. This maximum was associated to the blocking of the nanoparticles magnetic moment. First series of Mössbauer spectra were performed at 300K and 15K. The obtained results were presented and discussed.

* *Hyperfine Interactions C* ***3*** *(1998) 33.*
[a] CAB - CNEA and Instituto Balseiro.
[b] Laboratoire de Physique de l'Etat Condensé, Le Mans Cedex 9, France

Magnetic fraction of an ultisol from Misiones, Argentina

A. Mijovilovich, H. Morrás (1), C. Saragovi, G. Santana(2) and J.D. Fabris (2)

The magnetic fractions of the B1 horizon from three profiles of a subtropical soil derived from a basaltic rock from Misiones Argentina were studied. The samples were separated by particle size into their sand, silt and clay fractions. Magnetic concentrates of sand and silt were extracted with a hand magnet. Measurements by XRD and Mössbauer spectroscopy and of saturation magnetization were performed. The results indicate the presence of large amounts of hematite and magnetite, but maghemite is very likely also present. To contrast other results on soils of neighbouring areas, magnetite appears pedogenetically stable in this environment.

* *Hyperfine Interactions C* ***3*** *(1998) 332.*
(1) INTA-CIRN, Castelar, Argentina.(2) Dept of Chemistry, UFMG, Belo Horizonte, MG, Brazil

Magnetic interaction evidence in α-Fe_2O_3 nanoparticles by magnetization and Mössbauer measurements

M. Vasquez-Mansilla[1], R. D. Zysler[1] , C. Arciprete[1], M.I. Dimitrijewits[1], C. Saragovi and J. M. Greneche [2]

Magnetic properties of α-Fe2O3 antiferromagnetic particles of 5 nm mean diameter prepared by sol-gel method were investigated by means of static magnetic measurements and 57Fe Mössbauer spectrometry. The large magnetic moment as well as the anisotropy energy are attributed to the lack of compensation of the antiferromagnetic arrangement essentially located at the surfaces. Zero-field and in-field Mössbauer experiments reveal the existence of magnetic interaction among antiferromagnetic nanoparticles in the sample with higher particle concentration and established the presence of a 2 atomic thick surface magnetic layer estimated from a core-shell model.

* *J. Magnetism and Magnetic Materials* ***204*** *(1999) 29*
1 CAB - CNEA.
2 Laboratoire de Physique de l'Etat Condensé, Université du Maine, France

Mössbauer spectroscopy of the Zr-rich region in Zr-Nb-Fe Alloys with low Nb contents

C. Ramos[1], C. Saragovi, M. Granovsky[2] and D. Arias[2]

Intermetallic phases and solid solutions in the Zr-rich region of the Zr-Nb-Fe system with low Nb content are studied by Mössbauer Spectroscopy complemented with X-ray diffraction, optical and scanning electron microscopy and electron microprobe analysis.

The phases found in each sample were those expected from the corresponding binary Zr-Fe system. Furthermore, one of the samples showed a ternary cubic Ti_2Ni type phase with a similar stoichiometry to the tetragonal Zr_2Fe compound. Mössbauer parameters were suggested to this phase [IS: -0.12 mm/s, QS: 0.30 mm/s], to the bcc Zr(β) phase [IS: (-0.11±0.01) mm/s, QS: (0.23±0.02) mm/s] and to the hcp Zr(β^T) phase [IS: (-0.24±0.02) mm/s, QS: (0.45±0.02) mm/s].

* *Hyperfine interactions* ***122*** *(1999) 201.*

[1] FCEyN, UBA

[2] Departmento de Materiales, CNEA

Mössbauer study of the Fe mineralogy in two different argentine soils

A. Mijovilovich, H. Morrás(1) , H. Causevic (2) and C. Saragovi.

Two Argentine featuring different characteristics and compositions (Mollisols and Ultisols) have been studied by Mössbauer Spectroscopy and X-ray diffraction. The first type has a weakly developed profile with a solum thickness of 40cm; the Fe oxyhydroxides are present in low concentrations in mixtures with other slightly weathered minerals (e.g. quartz, feldspars, 2:1 phyllosilicates, etc). The second one is a Typic Kandihumult, which is a highly weathered red coloured, deep soil. The Fe oxyhydroxides are abundant, mixtured mainly with kaolinite clay minerals. Analyses of iron mineralogy show hematite and goethite in both soils. Their ratio is low in the first case and high in the last case. Magnetite-maghemite are also present in both situations, but in the Mollisol their content is much lower than in the Ultisol. The mineralogy found is related to the different lithological characteristics and processes of pedological evolution on both soils.

* *Hyperfine Interactions* ***122*** *(1999) 83.*

(1) Instituto de Suelos, INTA-CIRN Argentina.

(2) FCEyN, UBA.

Iron oxide mineralogy of a mollisol from Argentina by selective dissolution techniques, X-ray diffraction and Mössbauer spectroscopy

Silvia G. Acebal (1), Ana Mijovilovich, Elsa. H. Rueda (1), María. E. Aguirre (2) and Celia Saragovi.

Selective dissolution techniques using ammonium oxalate (OX), DCB and D-EDTA together with X-Ray diffraction and Mössbauer spectroscopy are applied to identify and characterize iron oxides and oxyhydroxides in the <2 mm, <50 μm and <2 μm fractions of a Mollisol from Bahía Blanca, Argentina. Iron compounds are present at low concentrations in mixtures with other main minerals, such as quartz, illite-montmorillonite, *etc*. Total Fe and Al content increase as soil particle size decreases, from 4.3 and 13.3 wt. % in <2 mm fraction to 8.5 and 22.8 wt. % in clay fraction respectively. No more than 25% - 30% of the total Fe is associated with crystalline and amorphous Fe oxides. Hematite and goethite are identified in the different fractions, both small sized and/or of low crystallinity and Al subtituted. Crystalline magnetite-maghemite are scarce. These Fe compounds are probably coating coarser particles. In all fractions, the efficiency for Fe removal is highest for the D-EDTA treatment whereas for the OX is the least, regardless of particles size. The opposite is true for Al removal. OX-extracted amorphous oxides are only present in coarser fractions. DCB and D-EDTA-extracted amorphous and crystalline oxides are present in coarser fractions disappearing completely only in the clay fraction**.** In illite, DCB treatment dissolves Fe and Al hydroxy interlayers while D-EDTA does not.

* *Clays and Clay Minerals (1999).*

(1) Departmento de Química e Ingeniería Química. Universidad Nacional del Sur. - Bahía Blanca, Argentina.

(2) Departmento of Agronomía Universidad Nacional del Sur - Bahía Blanca, Argentina.