



**International Workshop on
Magnetic Materials & Nanomaterials
MMN'2012**



BOOK OF ABSTRACTS

**BOUMERDES-ALGERIA
04-06 SEPTEMBER 2012**



**First International Workshop on
Magnetic Materials and
Nanomaterials
MMN'2012**

**Boumerdes, Algeria
04-06 September, 2012**

**Workshop Organizer:
Faculty of Sciences, M'Hamed Bougara University
of Boumerdes, UMBB**

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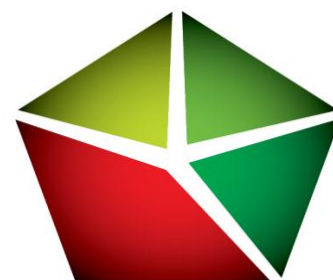
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Preface

The first international workshop on Magnetism and Magnetic Nanomaterials, MMN'2012, will be held from 04 to 06 September 2012 at M'hamed Bouguerra University of Boumerdes (UMBB). It will be an interdisciplinary forum for exchange of knowledge on the latest experimental results and theoretical advances in the fields of magnetism and magnetic nanomaterials. The main objective of the workshop is to bring together world recognized experts whose diverse expertise should stimulate discussions and push cutting edge research and collaborations in the field of magnetism in Algeria...

Over 100 participants, researchers, scientists and students made this conference a show case for the current state of the art of different field. The arrangement of time presentation of 30 minutes for the invited speakers and 20 minutes oral presentation allows the lectures to present their works, so that the experiences and the knowledge can be strongly exchanged and discussed.

In this proceeding, we have collected the extended abstracts with their references. The extensive scientific program and the support needed for some participants could not be covered by the registration fees alone. Contributions from sponsors, listed separately, were absolutely essential for the successful of MMN'2012 Workshop. To these sponsors the organisers, in the name of all participants, wishes to express their deep thanks.

Our particular thanks are addressed to: Dr. Ali Laggoun, President of the local organizing committee, Pr. O. Cherifi (Rectrice of UMBB University, honorary president of MMN'2012), Dr. Kamel Badari (Dean of Faculty of Sciences), Pr. A. Tairi (Vice-Recteur Relex) and Mohamed Hedibel (member of the organizing committee).

Finally, we would like to thank all speakers, contributors, session chairs and paper referees for their effort in making the MMN'2012 workshop a hugely successful. We hope all the participants will enjoy their stay in Algeria, profit from the discussion on magnetism and magnetic materials and of course do not forget to visit Boumerdes.

Welcome in Algeria, September 2012

Dr. A. Guittoum
Chairman (Algeria)

TOPICS

Topic 01: Elaboration of magnetic thin films and nanomaterials

Topic 02: Mössbauer spectroscopy in magnetic materials

Topic 03: Properties of magnetic thin films and nanomaterials

Topic 04: Theory and modeling in magnetism

Topic 05: Magnetism for engineering and environment

SCIENTIFIC PROGRAM

First International Workshop on Magnetic Materials and Nanomaterials

September 03, 2012 (afternoon)			
14h-19h	Registration, Reception, Opening ceremony		
September 04, 2012			
9h- 11h00	Topic 01: Elaboration of magnetic thin films and nanomaterials Chairman: R. Schäfer		
9h00- 9h30	PL01-T01	W. Kleemann	SUPERMAGNETIC STATES OF NANOPARTICLES
9h30- 10h00	PL02-T01	J. J. Suñol	MAGNETIC MATERIALS DEVELOPED BY RAPID SOLIDIFICATION
10h00-10h20	O01-T01	S. Boudinar	Mn-Bi THIN FILMS PREPARED BY ELECTROCHEMICAL METHODS
10h20-10h40	O02-T01	A.Younes	MAGNETIC PROPERTIES OF NANOCRYSTALLINE Fe ₆₁ Co ₂₁ Nb ₃ B ₁₅ ALLOYS POWDERS
10h40-11h00	O03-T01	M. Mebarki	STRUCTURAL AND MAGNETIC PROPERTIES OF ELECTRODEPOSITED Fe FILMS ON Al SUBSTRATE
11h00 -11h15	Coffee Break		
11h15- 12h55	Topic 03: Properties of magnetic thin films and nanomaterials Chairman: E. Hristoforou		
11h15- 11h45	PL03-T03	R. Schäfer	THE MAGNETIC MICROSTRUCTURE OF NANOSTRUCTURED MATERIALS
11h45- 12h15	PL04-T03	P. Gorria	STRUCTURAL TRANSFORMATIONS AND MAGNETO-VOLUME ANOMALIES IN NANOSTRUCTURED Fe ALLOYS STUDIED BY NEUTRON THERMO-DIFFRACTION
12h15-12h35	O04-T03	M. Belmeguenai	MAGNETIZATION DYNAMICS IN Co ₂ MnGe/Al ₂ O ₃ /Co TUNNEL JUNCTIONS GROWN ON DIFFERENT SUBSTRATES
12h35-12h55	O05-T03	A. Bourzami	STUDY OF STRUCTURAL, ELECTRICAL, MAGNETIC AND MAGNETO-OPTIC PROPERTIES OF COEVAPORATED Fe _x Co _{1-x} THIN FILMS
12h55-13h55	Lunch		
14h-16h00	Topic 03: Properties of magnetic thin films and nanomaterials Chairman: W. Kleemann		
14h-14h30	PL05-T03	W. Weber	ELECTRON-SPIN MOTION: A NEW TOOL TO STUDY FERROMAGNETIC FILMS
14h30-15h00	PL06-T03	S. M. Chérif	STATIC AND DYNAMIC MAGNETIC PROPERTIES OF FERROMAGNETIC NANOCYLINDERS
15h00-15h20	O06-T03	W. Bouzamouche	SYNTHESIS OF HYBRID CARBON NANOTUBES COBALT MATERIALS AND THEIR MAGNETIC PROPERTIES
15h20- 15h40	O07-T03	Z. Hamlati	PHASE TRANSFORMATION, STRUCTURAL EVOLUTION AND MICROSTRUCTURAL PROPERTY OF NANOSTRUCTURED FeAl AS A RESULT OF MECHANICAL ALLOYING

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15h40-16h00	O08-T03	N. Redjdal	STRUCTURAL AND MAGNETIC PROPERTIES OF THERMALLY EVAPORATED Fe ₃₅ Co ₆₅ THIN FILMS OBTAINED FROM MECHANICAL ALLOYING POWDER
16h00-16h15	Coffee break		
16h15-17h55	Topic 02 : Mössbauer spectroscopy in magnetic materials Chairman: A. Layadi		
16h15-16h45	PL07-T02	J. M. Greneche	MAGNETIC COMPLEX NANOARCHITECTURES
16h45-17h15	PL08-T02	M. Seredyuk	MÖSSBAUER SPECTROSCOPY AND ITS APPLICATION TO COORDINATION CHEMISTRY OF IRON(II)
17h15-17h35	O09-T02	O. Ould Fella	MAGNETIC AND STRUCTURAL PROPERTIES OF NANOSTRUCTURED ZINC FERRITES (ZnFe ₂ O ₄) Milled AT LOW ENERGY
17h35-17h55	O10-T02	M. Hemmous	STRUCTURE AND MÖSSBAUER SPECTROSCOPY OF (Fe ₆₀ Al ₄₀) _{100-x} Si _x NANOMATERIALS
17h55-18h10	Coffee break		
18h10-19h15	Topic 04: Theory and modeling in magnetism Chairman: K. Bouziane		
18h10-18h35	PL09-T04	N. Badji	ELECTRONIC TRANSPORT THROUGH A SPIN CROSSOVER MOLECULES
18h35-18h-55	O11-T04	A. Houari	SEMICONDUCTING (HALF-METALLIC) FERROMAGNETISM IN Mn(Fe) SUBSTITUTED Pt AND Pd NITRIDES
18h55-19h-15	O12-T04	Y. Bourourou	SPIN POLARIZATION EFFECTS ON THE STRUCTURAL AND ELECTRONIC PROPERTIES OF MONO BORIDES XB (X= Fe, Co, Mn)
September 05, 2012			
9h- 10h40	Topic 04: Theory and modeling in magnetism Chairmen: S. M. Chérif, W. Weber		
9h- 9h30	PL10-T04	Volker Sluka	SPIN-TRANSFER SWITCHING AND BACK-HOPPING IN MAGNETIC TUNNEL
9h30-10h	PL11-T04	D. Ledue	EXCHANGE BIASED BILAYERS: NUMERICAL INVESTIGATION OF THE TEMPERATURE AND MICROSTRUCTURE EFFECTS
10h00-10h20	O13-T04	M. Kharoubi	STRUCTURAL, MAGNETIC AND MAGNETO-OPTICAL PROPERTIES OF Fe/Pt[001] THIN FILM
10h20-10h40	O14-T04	M. Djermouni	ON THE ROLE OF EXCHANGE INTERACTION IN MAGNETIC ORDERING OF RARE-EARTH MONOCHALCOGENIDES
10h40- 11h	Coffee break		
11h00-11h30	PL12-T04	A. Layadi	STUDY OF SPIN VALVE SYSTEMS

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11h30-12h00	PL13-T04	K. Boukheddaden	ON THE SPATIO-TEMPORAL INVESTIGATION OF THE INTERFACE PROPAGATION IN A SPIN-CROSSOVER TRANSFORMATION INSIDE THE THERMAL HYSTERESIS LOOP: EXPERIMENT AND THEORY
12h00-12h20	O15-T04	B. Ouari	DYNAMIC MAGNETIC HYSTERESIS LOOPS AND NONLINEAR SUSCEPTIBILITY OF MAGNETIC NANOPARTICLES HAVING BIAXIAL ANISOTROPY
12h20-12h40	O16-T04	R. Tigrine	MAGNETIC SPIN WAVES SCATTERING INSIDE THE INHOMOGENEOUS 2D-HEXAGONAL MESOSCOPIC SYTEM
12h40-13h	O17-T04	M. Boukhelkoul	KERR EFFECT IN ULTRATHIN FILMS Fe _n /X(001) (X=Ag, Au)
13h00-13h55	Lunch		
14h00-16h10	Topic 01: Elaboration of magnetic thin films and nanomaterials Chairman: K. Boukheddaden		
14h-14h30	PL14-T01	A. Anane	ALL ELECTRICAL INJECTION AND DETECTION OF SPIN POLARIZED CURRENT IN GRAPHENE WITH OVER 100 μ m SPIN DIFFUSION LENGTH
14h30-15h	PL15-T01	A. Fnidiki	FINE SCALE MICROSTRUCTURE OF MAGNETORESISTIVE ALLOYS: RELATION WITH THE MAGNETIC PROPERTIES, EXAMPLE OF Cu ₈₀ Fe _x Ni _{20-x} (x=5, 10, 15 at %) RIBBONS
15h-15h30	PL16-T01	R. Hamzaoui	MECHANICAL ALLOYING AND MAGNETIC PROPERTIES OF Fe-Ni ALLOYS
15h30-15h50	O18-T01	M. Bouloudenine	POLYCRYSTALLINE Zn _{1-x} Co _x O DILUTED MAGNETIC SEMICONDUCTOR SYNTHESIZED BY CHEMICAL ROUTES
15h50-16h10	O19-T01	B. Benfedda-Mellil	EFFECT OF THE TARTARIC ACID ON THE MORPHOLOGICAL AND STRUCTURAL PROPERTIES OF THE Bi ELECTRODEPOSITED NANOWIRES
16h10-16h25	Coffee break		
16h25-18h05	Topic 03: Properties of magnetic thin films and nanomaterials Chairman: J. J. Sunol		
16h25-16h55	PL17-T03	F. Terki	MAGNETIC ANISOTROPY IN DILUTED MAGNETIC SEMICONDUCTORS AND PROMISING MAGNETOMETRY DEVICES
16h55-17h25	PL18-T03	K. Bouziane	ELECTRONIC AND MAGNETIC PROPERTIES OF MN-DOPED 6H-SiC: EXPERIMENT AND FIRST PRINCIPAL CALCULATION
17h25-17h45	O20-T03	F. Zighem	MAGNETIZATION REVERSAL OF FERROMAGNETIC NANOWIRES: A MAGNETIC FORCE MICROSCOPY AND MICROMAGNETIC SIMULATIONS STUDY
17h45-18h05	O21-T03	F. Otmane	MAGNETIC AND MICROWAVE PROPERTIES OF MECHANICALLY ALLOYED FeCo POWDERS
18h05-20h00	Poster session		

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September 06, 2012			
9h00- 12h00	Topic 05: Magnetism for engineering and environment		
Chairmen: P. Gorria, F. Terki			
9h-9h30	PL19-T05	E. Hristoforou	SPACE DETERMINATION OF SUPER-PARAMAGNETIC NANOPARTICLES IN HUMAN BODIES FOR TUMOR TREATMENT
9h30-10h	PL20-T05	N. Fenineche	SOFT MAGNETIC COATINGS FOR SENSORS AND MAGNETIC SHIELDING
10h-10h20	O22-T05	M. Aissaoui	ANALYSIS OF TOTAL LOSSES IN A EMBEDDED TRANSFORMER SUPPLIED WITH AN INVERTER AT NO-LOAD
10h20-10h-40	O23-T05	Z. Tigrine	CONTROL OF THE MAGNETIC FIELD EFFECT ON THE EUTECTIC ALLOY Pb-17Li FLOW
10h40 – 10h55	coffee break		
10h55-11h25	PL21-T05	E. Hristoforou	STEEL HEALTH MONITORING USING MAGNETIC TECHNIQUES
11h25-11h40	O24-T05	A. CheikhRouhou	MAGNETOCALORIC EFFECTS IN MANGANITES WITH PEROVSKITE STRUCTURE
11h40-12h00	O25-T05	F. Mokhtari	MAGNETIC FIELD EFFECT ON SPHERICAL CZ CRYSTAL GROWTH
12h00 – 12h45	Closing session		
12h45 – 14h00	Lunch		
14h to 19h30	Excursion around Algeria capital		

***PLENARY LECTURES
INVITED SPEAKERS***

PL01-T01
SUPERMAGNETIC STATES OF NANOPARTICLES

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ABSTRACT

Ensembles of single domained ferromagnetic (FM) nanoparticles, in which magnetic interparticle interactions are sufficiently weak, show superparamagnetic (SPM) behavior. However, at increased interactions the system eventually shows collective behavior, which overcomes the individual anisotropy properties of the particles. Different collective states of magnetism were first recognized [1] on so-called discontinuous magnetic metal-insulator multilayers (DMIMs) consisting of focused ion-beam grown $\text{Co}_{80}\text{Fe}_{20}$ nanoparticles on glassy Al_2O_3 . At sufficiently small interparticle distances as controlled by the nominal $\text{Co}_{80}\text{Fe}_{20}$ film thickness, $0.5 \text{ nm} < t_n < 1.1 \text{ nm}$, dipolar interaction enables superspin glass (SSG) properties. Similar to atomic spin glasses they reveal chaotic SSG ground states as corroborated by aging properties such as memory and rejuvenation. At increased concentration, but still below physical percolation, $1.1 \text{ nm} < t_n < 1.4 \text{ nm}$, stronger interactions give rise to superferromagnetic (SFM) states with domain formation similar to that in conventional FM films [2]. At $t_n > 1.4 \text{ nm}$ the metal-insulator multilayers (MIMs) become continuous owing to physical interparticle percolation. Owing to inherent layer roughness competing ANNNI-type dipolar interactions give rise to modulated magnetization profiles as evidenced by polarized neutron reflectivity and magneto-optical Kerr effect microscopy [3].

The talk will highlight the most important developments in the field of 'supermagnetism' [4] comprising superparamagnetism, superspin glass, super- and percolated ferromagnetism.

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PL02-T01
MAGNETIC MATERIALS DEVELOPED BY RAPID SOLIDIFICATION

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ABSTRACT

Magnetic shape memory alloys (MSMAs) have generated a continuously growing interest since their discovery [1]. Compared with the conventional actuator and shape memory alloys, MSMA offer the possibility of both large actuation strain (6-10%) and high response frequency [2]. Among the alloys that exhibit magnetic shape memory effect, the most extensively studied are those of the Ni-Mn-Ga system. Nevertheless, to overcome some of the problems related with practical applications (such as the high cost of Gallium and the usually low martensitic transformation temperature) the search for Ga-free alloys has been recently attempted, in particular, by introducing In or Sn [3-4]. In this work we present results of Ni-Mn-(In-Sn) alloys developed by rapid solidification. The control of the valence electron by atom e/a parameter determines the transformation temperatures range. Furthermore, texture is favoured by the ribbon shape. We also demonstrate that the martensitic transformation is highly sensitive to the applied magnetic field and to the annealing treatment, which means that the magnetocaloric effect can be tuned showing different behavior for each sample.

Acknowledgements

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PL03-T03

THE MAGNETIC MICROSTRUCTURE OF NANOSTRUCTURED MATERIALS

Rudolf Schäfer

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ABSTRACT

The magnetic microstructure and magnetization processes of nanostructured materials are reviewed in a phenomenological way, mainly based on domain observation by magneto-optical Kerr microscopy. This covers nanocrystalline soft magnetic ribbons and films as well as nanostructured hard magnetic materials. For comparison also the domain structure in coarse-grained material and amorphous ribbons are briefly touched to provide the frame for the nanostructured materials.

In nanocrystalline ribbons or films, the random magnetocrystalline anisotropy of the ultrafine grain structure is largely averaged out by exchange coupling. The soft magnetic properties are rather controlled by uniaxial, induced anisotropies that are uniform on a scale much larger than the exchange length. The interplay between these uniform and the random anisotropy results in a different degree of microscopic magnetization disorder which is reflected in the magnetization processes.

In high-anisotropy materials with exchange-coupled grains in the 10 nm regime (exchange-enhanced nanocrystalline permanent magnets), a highly irregular domain structure is found, consisting of immobile and high-coercive patch domains. If exchange coupling between the grains is interrupted, so-called interaction domains are observed due to the predominance of magnetostatic interactions between the (single domain) grains.

References

R. Schäfer: "The Magnetic Microstructure of Nanostructured Magnetic Materials", in "Nanoscale Magnetic Materials and Applications", edited by J. Ping Liu, E. Fulerton, O. Gutfleisch, D. Sellmyer, Springer (2009)

STRUCTURAL TRANSFORMATIONS AND MAGNETO-VOLUME ANOMALIES IN NANOSTRUCTURED Fe ALLOYS STUDIED BY NEUTRON THERMO-DIFFRACTION

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ABSTRACT

Diverse metastable Fe-based alloys far from thermodynamical equilibrium, in either amorphous or nanostructured states, can be obtained by using the ball milling (BM) technique [1]. Moreover, BM allows the synthesis of alloys which are not miscible by other fabrication routes, such as nanostructured Fe–Cu solid solutions [2] or amorphous Fe–Zr metallic glasses [3], offering the possibility of studying new metastable compounds with interesting physical–chemical properties. Moreover, materials processing under severe mechanical stress (BM) can largely alter their microstructure (decreasing the mean crystalline size down to a few nanometers, and/or introducing a high degree of internal microstrain through the generation of a large number of defects), which provokes changes in the atomic environments, and therefore the physical properties can be significantly modified. However, most of these materials fabricated or processed by means of BM exhibit drastic structural changes on heating. Using *in situ* neutron powder thermo-diffraction, NPTD, these structural transformations can be easily observed in detail. In this talk we will discuss the power of NPTD technique when the understanding of the magnetic changes occurring during such structural transformations in Fe metastable alloys is pursued. Some examples of *in situ* NPTD experiments will be shown: (i) thermally-induced microstructural relaxation in nanostructured Fe [4]; (ii) segregation process in Fe-Cu [5]; (iii) crystallization and polymorphic transformations in FeZr metallic glasses [3]; (iv) enhanced Curie temperature in Fe-Ni compounds [6] or (v) magneto-volume anomalies in nanostructured Fe-Pr compounds [7].

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PL05-T03

ELECTRON-SPIN MOTION: A NEW TOOL TO STUDY FERROMAGNETIC FILMS

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ABSTRACT

When electrons are interacting with a ferromagnetic material, their spin polarization vector is expected to move. This spin motion, comprising an azimuthal precession and a polar rotation about the magnetization direction of the ferromagnet, has been studied in spin-polarized electron scattering experiments both in transmission and reflection geometry. We show that electron-spin motion can be considered as a new tool to study ferromagnetic films and we discuss its application to a number of different problems: a) the transmission of spin-polarized electrons across ferromagnetic films [1-3], b) the influence of spin-dependent gaps in the electronic band structure on the spin motion in reflection geometry [4], c) interference experiments with spin-polarized electrons [5,6], and d) the influence of lattice relaxations in ferromagnetic films on the spin motion [7-9].

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PL06-T03
STATIC AND DYNAMIC MAGNETIC PROPERTIES OF FERROMAGNETIC
NANOCYLINDERS

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ABSTRACT

Electrodeposited arrays of ferromagnetic nanocylinders (NCs) have been the object of intensive experimental and theoretical investigations [1-3]. Interesting magnetic properties have been observed such as giant magnetoresistance or spin transfer phenomena. Potential applications in data storage devices have also stimulated interest in magnetization reversal in individual cylinders. Such magnetic artificial materials are important class of active metamaterials needed for prospective data storage and signal processing applications. We present static and dynamic magnetic properties of two-dimensional arrays of ferromagnetic NCs, embedded into ordered nanoporous aluminum oxide (Al_2O_3) templates (figure 1), investigated by means of vibrating sample magnetometry (VSM) and Brillouin light scattering (BLS) techniques, respectively. The BLS spectroscopy gives access to spin waves modes with non-zero wave vector values in the 3-300 GHz spectral frequency range. The inelastic scattering by magnetic modes allows a detailed study of the dynamics of magnetization in NCs. The experimental results are explained within the frame of analytical model based on a mean-field approach including the dipolar coupling between the NCs in the array. Respective role of the direction of the applied field, of the magneto-crystalline and the shape anisotropies as well as the effect of the aspect ratio are pointed out and discussed.

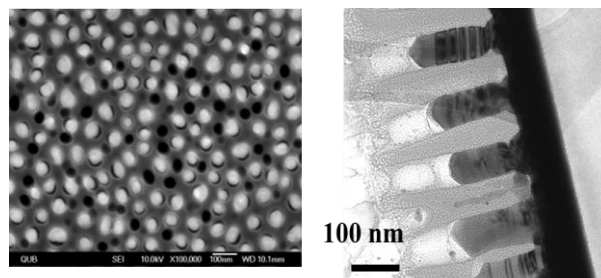


Figure 1: SEM (left) and TEM cross-section (right) images of Ni nanocylinders (NCs) grown in 70 nm pores. The aluminum oxide has been briefly etched to expose the NCs [4].

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PL07-T02

MAGNETIC COMPLEX NANOARCHITECTURES

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ABSTRACT

The increasing emergence of nanotechnology which refers to the design of functional nanomaterials from manipulation and self-assembly of atoms, molecules or clusters, originates new challenges. Because these nanomaterials exhibit unusual physical properties, the preliminary step consists in studying carefully their morphology and their chemical nature, controlling the temperature and time stability and then knowing how such parameters influence their physical and particularly magnetic properties which have to be tuned. One does first use complementary techniques to well characterize their whole structural and magnetic properties but local probe techniques have to be also considered to distinguish surface and bulk effects. ^{57}Fe Mössbauer spectrometry appears as an excellent tool to study Fe containing magnetic nanostructures. Indeed, it remains relevant to determine on the one hand the role of the surface or of the grain boundaries in the case of nanoparticles and nanostructured powders, respectively and on the other hand the hyperfine magnetic properties and their dynamics in correlation with superparamagnetic relaxation phenomena in the case of magnetic nanostructures. So we established the main features characteristics of the different types of nanostructures allowing thus to discriminate the relevant parameters which influence the physical properties and their changes compared to bulk microstructures. We illustrate then from selected examples how both the selectivity and the local probe character of ^{57}Fe Mössbauer spectrometry contribute to investigate in situ local atomic order and magnetic properties in different nanostructures. Particular attention will be developed in the case of nanostructured powders, nanoparticles and assemblies of nanoparticles, functionalized nanostructures and mesoporous hybrides (Metal Organic Frameworks, MOFs). In addition, some numeric modelling results are reported.

PL08-T02
MÖSSBAUER SPECTROSCOPY AND ITS APPLICATION TO COORDINATION
CHEMISTRY OF IRON(II)

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ABSTRACT

The recoilless emission and absorption of γ -ray photons was discovered by Rudolph Mössbauer in 1957. This led to the development of a new technique now known as Mössbauer spectroscopy which has an important influence in many branches of natural sciences. Its important characteristic is the production of monochromatic radiation with the narrow spectral line width and high sharpness of tuning which can be used to resolve minute energy differences. The application of the Mössbauer spectroscopy to chemistry arises from its ability to probe the tiny variations in the energy of interaction between the nucleus and its electron shell and provide precise information about the chemical, structural, and magnetic properties of a material [1].

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ABSTRACT

In conventional organic spin-valves, two magnetic electrodes sandwich an organic material, where the organic spacer serves as a spin and/or orbital filter while the electrodes are sources of spin polarized electrons. A new trend is to use non-magnetic leads sandwiching a magnetic molecule or magnetic molecular junction, where instead of the demanding control of the magnetization of lead, an easy control of the molecular states is affordable. The single-molecule junctions aim to harness the molecular bi-stability, i.e. molecule's ability to undergo a transition between a stable ground state to a long living meta-stable state by an external stimulus. If this change is accompanied by a detectable response then the junction can be used in the information processing and storage. Probably the most spectacular of the molecular bi-stability is the spin crossover phenomenon [1]. Some of the first-row transition metal ions in octahedral surroundings may display a spin transition from low spin state (LS), usually the ground state, to high spin state (HS), usually a meta-stable state. This LS-HS transition can be triggered by temperature, pressure or light irradiation. In this work we use NWCHEM [2] to characterise the LS-HS transition of a single molecule and the SMEAGOL code [3] for electronic transport calculations. We further investigate how the LS-HS transition can be detected by electric means. Our molecular junction consists of a single spin crossover molecule anchored by thiol groups to gold leads (Fig. 1). We show that the calculated current for the HS state is much larger than that of LS state (Fig. 2). We also demonstrate that by gating the molecule a significant increase of the current can be achieved [4].

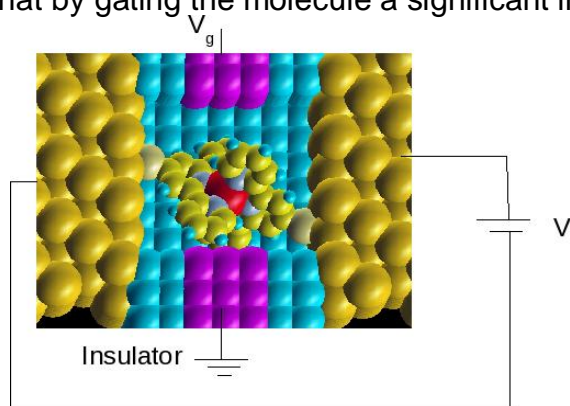


Fig. 1. Molecular junction: A typical spin crossover molecule sandwiched between two gold leads.

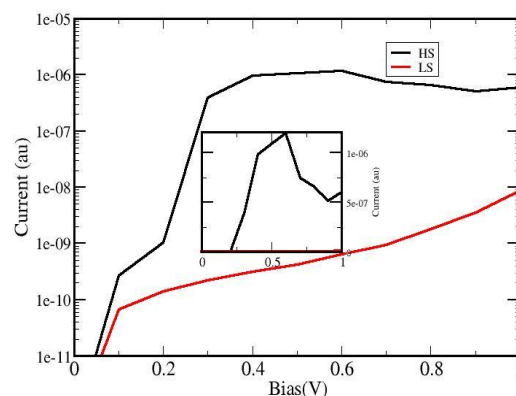


Fig. 2. Calculated current for LS (red) and HS (black) states on logarithmic scale (linear scale shown in the inset).

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PL10-T04
SPIN-TRANSFER SWITCHING AND BACK-HOPPING IN MAGNETIC TUNNEL
JUNCTIONS

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ABSTRACT

A spin-polarized current flowing through a ferromagnet can exert a torque on the local magnetization [1, 2]. This phenomenon is currently intensively investigated due to its potential application in magnetic random access memory (MRAM) or in telecommunication devices. Presently, the structure of choice for spin-torque devices includes a magnetic tunnel junction (MTJ) with an MgO barrier, due to their large magnetoresistance signals. However, a key step towards the practical implementation as MRAM elements is the reduction of the critical voltages, in order to keep the size of the selection transistor down and compete with existing technologies [3]. In addition, magnetic tunnel junctions also exhibit a somewhat obscure behaviour referred to as ‘back-hopping’, whereby reliable switching to the desired state is achieved for applied voltages of the order of the critical voltage, but a larger applied bias induces telegraph-noise behaviour. Back-hopping is characteristic for MTJs, as it has not been observed in metallic multilayers, and poses concerns for designing industrially-competitive MRAM devices. We evaluate the switching voltages and their temperature dependence by analytically and numerically solving the modified Landau-Lifshitz-Gilbert equation which includes both Slonczewski-like (in-plane) and field-like (out-of-plane) spin-torque terms. We demonstrate that the quadratic dependence of the field-like torque on the applied voltage translates into a more complex correlation between the critical bias and the external field, altering the shape of the phase diagram. It also explains back-hopping at a large bias for specific geometries, in agreement with experimental results.

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PL11-T04

EXCHANGE BIASED BILAYERS: NUMERICAL INVESTIGATION OF THE TEMPERATURE AND MICROSTRUCTURE EFFECTS

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ABSTRACT

Coupled F/AF bilayers exhibit exchange bias (EB). Exchange anisotropy which was discovered in 1956 by Meiklejohn and Bean [1], is unidirectional, and is evidenced by a shift in magnetic field (H_E) of the hysteresis loop. In such bilayers, the polycrystalline structure has an important influence on EB properties because the blocking temperatures of the grains strongly depend on their volume distribution. Recently, a study has evidenced a bimodal distribution of blocking temperature [2]. The low- T peak, which does not depend on the layer thickness, is attributed to a spin-glass like region at the F/AF interface with a freezing temperature of the order of 4-70 K. The high- T peak, which shifts towards higher temperature as the AF layer thickness increases, would correspond to the blocking of the AF grains.

In this study, we investigate the temperature effect on EB properties in polycrystalline bilayers by means of Monte Carlo (MC) simulations and compare our results to experimental data. It has to be noted that the MC technique allows taking into account thermal effects and is therefore well suitable in our investigation as far as the precession can be neglected. In our model, each F (AF) grain is modelled by one (two) macrospin(s). The F grains are ferromagnetically coupled to each other and to the AF grains at the interface. A temperature dependence of the F and AF anisotropy constants has been considered. Our results on monodisperse grain size distribution are in good qualitative agreement with experimental results on NiFe/NiMn [3]. The coercive field H_C is minimum at the blocking temperature of the F grains. At the blocking temperature of the AF grains, the exchange field H_E vanishes and H_C increases.

We have also determined the blocking temperature of the AF grains using the same procedure in our MC simulation than in the experiments [4] to achieve a better understanding on the bimodal distribution of blocking temperature [2]. We confirm using various volume distributions that the distribution of blocking temperature of the AF grains exhibits no low- T peak when only superparamagnetic relaxation of the grains is taken into account. As a second step, we have introduced, at the F/AF interface, regions which lose their magnetization above few 10 K because of roughness and frustration. Then, a bimodal distribution has been obtained as previously observed in the experiments.

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PL12-T04
STUDY OF SPIN VALVE SYSTEMS

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ABSTRACT

A spin valve or magnetic tunnel junction may consist of a stacking of an antiferromagnetic (AF) thin film and two ferromagnetic thin films [F(A) et F(B)] separated by a nonmagnetic interlayer. Such a system has been lately the subject of a lot of experimental and theoretical studies because, among other reasons, of its use as giant magnetoresistive (GMR) head in magnetic recording. Two magnetic phenomena arise in this system. First, the interaction at the interface of layer (A) with (AF) leads to a unidirectional anisotropy called exchange anisotropy; this anisotropy can be modeled as a magnetic field H_E , the exchange anisotropy field. Second, the magnetic coupling between two ferromagnetic layers separated by a nonmagnetic interlayer. This interaction will be described by the bilinear J_1 and biquadratic J_2 coupling parameters. The former may favor a parallel alignment (ferromagnetic coupling) or an antiparallel alignment (antiferromagnetic coupling) of the magnetizations M_A and M_B while the latter one may lead to a perpendicular configuration of M_A and M_B . Such a system has been investigated by a particular experimental technique, the Ferromagnetic Resonance (FMR). Analytical expressions have been worked out for the resonance modes [1] and for the magnetization curve [2]. It will be shown how J_1 , J_2 , H_E and other magnetic parameters affect the FMR spectra and how they can be derived. Experimental work has been done in this system; a good agreement is seen between the experimental results and the theoretical model [3].

Keywords: Ferromagnetic multilayers, exchange anisotropy, magnetic coupling, ferromagnetic resonance.

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PL13-T04

ON THE SPATIO-TEMPORAL INVESTIGATION OF THE INTERFACE PROPAGATION IN A SPIN-CROSSOVER TRANSFORMATION INSIDE THE THERMAL HYSTERESIS LOOP: EXPERIMENT AND THEORY

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ABSTRACT

We investigated single crystals of the dinuclear iron(II) compound $[\text{Fe}(\text{NCSe})(\text{py})_2]_2(\text{m-bpypz})$, which exhibits an incomplete thermal spin transition with hysteresis near 100 K. The robust character of the crystals made possible the investigation of both on-cooling and on-heating processes. We observed well-defined transformation fronts between macroscopic high spin (HS) and low-spin (LS) phases. The fronts are almost linear in shape, and propagate through the entire crystals, even in isothermal conditions (Fig.1). The interface orientation was \sim constant and its propagation velocity typically was \sim 1 and 10 $\mu\text{m/s}$ for the on-cooling and on-heating processes, respectively. The videos of the spin transition processes are very spectacular and will be shown in real (or accelerated) time.



Figure 1 : $[\text{Fe}(\text{NCSe})(\text{py})_2]_2(\text{m-bpypz})$ single crystal during HS \rightarrow LS transition at 107K,

We also investigated the evolution of the biphasic state inside the thermal hysteresis loop, by performing rapid temperature reversals which allowed to slow down the propagation of the interface. We measured the propagation velocity at several temperatures close to the equilibrium temperature (T_{eq}) and found that the motion occurred in opposite ways on the different sides of T_{eq} . The temperature dependence of the propagation velocity was determined all over the thermal hysteresis interval.

Using a microscopic elastic model [1] we simulated (Fig.2) the experimental data. The model is based on Monte-Carlo simulations of a Hamiltonian involving spin and lattice degrees of freedom in which each site can be in HS or LS state with an inter-site equilibrium distance depending on the spin states of the considered pair. The calculations were performed on a rectangular lattice. The results of the simulations will be discussed in relation with the experimental data and the multi-scale character of this transformation.



Figure 2: Simulated HS/LS interface

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PL14-T01

ALL ELECTRICAL INJECTION AND DETECTION OF SPIN POLARIZED CURRENT IN GRAPHENE WITH OVER 100 μ m SPIN DIFFUSION LENGTH

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ABSTRACT

Electronic devices based on spin transport are expected to play a major role in future Information and Communication Technologies (ICT). Those spintronics devices will use the spin degree of freedom to transport and process information. If one excludes magnetic read heads that have been the cornerstone of magnetic hard drives since 1996, all other concepts of spintronics devices have remained elusive. Datta and Das spin-transistor [1] for example is a very simple device based on spin injection and detection using ferromagnetic electrodes in direct contact with a semiconductor and on the manipulation of the spin information through the spin-orbit coupling (Rashba effect). It was, however, soon understood that fundamental constraints on the physics governing spin transport will make this concept very difficult to achieve with conventional semiconductors (GaAs or Si) [2][3]. Indeed it is only recently that the first step, namely the injection of spin polarized current directly in the conduction band of the semiconductor, has been demonstrated [4].

Here we will present a set of results on an alternative route where the channel is no longer a conventional semiconductor but graphene. Graphene is expected to be a good candidate for spin information transport as its mobility at room temperature outperforms that of any other material and its spin orbit coupling as well as the hyperfine interaction of ^{12}C are expected to be very small. Using Multilayer graphene grown on SiC wafers we experimentally demonstrate using spin transport experiments in the lateral spin-valve geometry that the spin diffusion length is at least of the order of 100 μm [5].

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PL15-T01

FINE SCALE MICROSTRUCTURE OF MAGNETORESISTIVE ALLOYS: RELATION WITH THE MAGNETIC PROPERTIES, EXAMPLE OF $\text{Cu}_{80}\text{Fe}_x\text{Ni}_{20-x}$ ($x=5, 10, 15$ at %) RIBBONS

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ABSTRACT

Granular magnetic systems consist of small magnetic precipitates embedded in a non magnetic (metallic or insulated) matrix. The sizes of the precipitates are usually in the range of a few nanometers. Those systems can be obtained by melt spinning, vapor deposition, mechanical alloying or electrodeposition [1, 2]. Their microstructure can be modified by performing specific heat treatments [3]. Such systems are of great interest for many physical properties, such as superparamagnetism, kinetics and phase transformation, or spin glass behavior. In the last decades, the discovery of giant magnetoresistance (GMR) in metallic granular systems such as CuFeNi, CuCo, CuCoNi, AuFe, or CoAg has increased their potential of interest. However, due to the complexity of their microstructure, the relation between the magnetic and transport properties and the microstructure is not fully understood yet. The aim of this study is to link the different structural parameters with magnetic and giant magnetoresistance properties of granular $\text{Cu}_{80}\text{Fe}_x\text{Ni}_{20-x}$ (at %) ribbons obtained by melt spinning. The microstructure of these ribbons was modified by annealing at 350°C, 400°C and 600°C. Firstly, the effect of the composition is presented. Then, the microstructure of a $\text{Cu}_{80}\text{Fe}_{10}\text{Ni}_{10}$ (at %) ribbon, presenting the highest magnetoresistance, was characterized precisely from a microscopic scale by means of X-Ray Diffraction (XRD), Transmission Electron Microscopy (TEM), to an atomic scale by means of Field Ion Microscopy (3DFIM), Atom Probe Tomography (APT) and Small Angle Neutron Scattering (SANS). The sample consists of fcc (Fe,Ni)-rich precipitates coherent with the matrix rich in copper. The magnetic behaviour was investigated through magnetic measurements, such as magnetization curves, Zero Field Cooled/Field Cooled (ZFC / FC) curves and GMR. In addition, Mössbauer spectroscopy has made possible a link between structural and magnetic observations. The study of the magnetic properties of this ribbon has shown that magnetic interactions are present which reduces GMR. Structural data (size and composition distributions, precipitate volume fractions and density, interface width...) were correlated with magnetic properties.

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PL16-T01

MECHANICAL ALLOYING AND MAGNETIC PROPERTIES OF Fe-Ni ALLOYS

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ABSTRACT

Influence of the milling time on the structure and the magnetic properties of the alloys Fe-10%Ni and Fe-20%Ni is carried out using a planetary high-energy ball mill (Retsch PM 400). For both alloys studied, a disordered body centred cubic solid solution forms after 24 h milling time. The steady-state grain size is: 10 nm. The reduction of the grain size increases the saturation magnetization (227 and 219 Am²/kg) and decreases the coercivity (200 A/m and 110 A/m) for Fe-10%Ni and Fe-20%Ni respectively [1]. Milling conditions effect (variation of the ratio Ω/ω , Ω speed rotation of the disc, ω speed rotation of the vials) on the magnetic properties of these same alloys for 36 h of milling is carried out using a planetary high-energy ball mill P4 vario ball mill from Fritch. The higher the shock power, the larger the bcc lattice parameter and the lower the grain size. In the friction mode, the lower the crystallite size, the lower the lattice strain conditions. In the shock mode, the lower the crystallite size, the higher the lattice strain. The highest values of the coercivity have been found in the shock mode [2]. In order to have local information on the magnetic behaviour of the studied alloys Fe-Ni, we have used the Mössbauer spectroscopy technique. The characterization is carried out at two temperatures from 77 K and 300 K [3]. Lastly an artificial neural network (ANN) methodology is applied to relate the power-milling process parameters to the magnetic properties of Fe-10%Ni and Fe-20%Ni alloys for 36 h of milling. An optimization procedure based on ANN training and testing steps has been developed to predict magnetic properties over a large range of process parameters [4].

Keywords: Fe-Ni nanocrystalline, mechanical alloying, magnetic properties, ball milling

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PL17-T03

MAGNETIC ANISOTROPY IN DILUTED MAGNETIC SEMICONDUCTORS AND PROMISING MAGNETOMETRY DEVICES

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ABSTRACT

During the last decade, considerable experimental and theoretical efforts have been devoted to the study of GaMnAs semiconductors due to their high ferromagnetic transition; "Curie temperature (T_c)" and their interesting magnetic properties. The potential implementation of structures based on GaMnAs diluted magnetic semiconductors as spintronic devices needs solid understanding of magnetic anisotropy and magnetization reversal processes. Nowadays, it is well established that the ferromagnetic interaction between magnetic ions is mediated by charge carriers, holes in this case. However, defects such as As antisites and Mn interstitials play a crucial role in determining the magnetic properties of GaMnAs. The objective of this study is to investigate the magnetic properties and anisotropy using magnetotransport measurements as well as the dynamics domain wall by high resolution magneto-optical imaging. Predicted theoretical models and developed ones by our team are in good agreement with experimental data. Finally, in this work, we emphasize the first evidence by transport measurements of two in-plane uniaxial axis reorientations. Another part of the talk will focus on new potential applications using magnetic multilayers structures to detect very small field, down to nanotesla, to investigate magnetic properties of spin-crossover materials.

PL18-T03

ELECTRONIC AND MAGNETIC PROPERTIES OF MN-DOPED 6H-SiC: EXPERIMENT AND FIRST PRINCIPAL CALCULATION

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ABSTRACT

The concept of diluted magnetic semiconductors candidates for efficient spin injection will be first introduced. Emphasis will be placed on recent results obtained for electronic and magnetic properties of 6H-SiC with Mn impurities using GGA and LDA+U formalism. The calculation addresses various configurations of Mn substitutional sites and Si and C vacancies. The magnetic coupling between two Mn atoms at substitutional and interstitial sites with and without vacancies is investigated as a function of Mn atoms interatomic distance using the calculated DOS. The band coupling model based on the *p-d* and *d-d* level repulsions between Mn (*d* band) and SiC (*p* band) has been used to describe the magnetism observed in each configuration.

Experimental results of Mn-implanted 6H-SiC for different Mn concentrations will also be addressed. Annealing effect is also explored. The experimental magnetic properties are analyzed on the light of the theoretical results.

PL19-T05
SPACE DETERMINATION OF SUPER-PARAMAGNETIC NANOPARTICLES IN
HUMAN BODIES FOR TUMOR TREATMENT

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ABSTRACT

The aim of this paper is the development of a reliable diagnosis tool for the space determination of super-paramagnetic nanoparticles using magnetic techniques. The method is needed for determining the position of super-paramagnetic nanoparticles (SPAN) onto the cancer cell surface and volume through the binding of specific protein molecules (with over expressed receptors on the cancer cell membrane and volume). Given that a breast or prostate cancer cell disposes two orders of magnitude more receptors than a healthy cell (1:100 ratio), the blood circulation and the nano-dimensions of the complex allow initially their extravasation through the existing pores of the incompletely developed blood vessels which feed cancer tumors and their attachment to the cancer cells by binding of the attached on their surface ligands (protein molecules) to the overexpressed protein receptors on cancer cell surface, , in a time interval of clearly less than an hour. An innovative magnetic method, subject of PCT pending patent, promises the measurement of the spatial distribution of super-paramagnetic nanoparticles. The sensitivity of the method could possibly touch the limits of monocytic measurement under given conditions (sensitive magnetometers), which is very important for micro-metastases diagnosis. Possible cancer cells found on breast epithelium or prostate can be killed applying increased inductive heating. The increase of temperature to healthy cells is minimum ($\Delta T < 2^{\circ}\text{C}$) due to the small amount of the mounted nanoparticles to them. On the contrary, the cancer cells are killed due to the huge increase of temperature to them ($\Delta T > 90^{\circ}\text{C}$). The released nanoparticles are eliminated from the body following the same process as the attached on their surface protein-ligand.

PL20-T05

SOFT MAGNETIC COATINGS FOR SENSORS AND MAGNETIC SHIELDING

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ABSTRACT

Soft magnetic materials are subject of great current interest because of their promising technological applications. Magnetic coatings have been applied to many applications, such as magnetic shielding, magnetic recording heads and media for hard disks [1,2], magnetic MEMS [3] and other magnetic devices. Materials used for manufacturing magnetic films sensors or inductors, magnetic shielding, need to present specific characteristics including high saturation magnetisation ($4\pi M_s$), low coercivity (H_c), high effective permeability, low magnetostriction, tuneable anisotropy, good thermal and temporal stability of magnetic properties, high corrosion resistance and adhesion to their substrate [4,5].

For example, magnetic sensors based on the Giant Magneto-impedance (GMI) are used in the non destructive testing where sensitivity to the weak field and high-resolution is required (Cerebral or muscular magnetic field measurements for example) [6]. These applications require a good control process for low dimension sensors. Accordingly, several ways are possible, in particular the development of thin films by magnetron sputtering. However, materials for magnetic shielding with higher thicknesses can be obtained by thermal spraying.

In this work we aim to optimize composition and to correlate the magnetic properties in the coating with process parameters both in PVD or thermal spraying processes. Also, we have to explore the reasons of the self magnetic domain orientation and the effect of the thickness on the properties of the coating.

Finally, we optimize the dimension of the sensors and test sensor performances for higher frequencies.

Keywords: thermal spraying, magnetron sputtering, magnetic shielding, coercivity, GMI sensors, magnetic properties, electrical resistivity.

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PL21-T05

STEEL HEALTH MONITORING USING MAGNETIC TECHNIQUES

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ABSTRACT

The current paper refers to the development of a non destructive technique able to predict the initiation of cracks and defects in pipelines and generally in critical magnetic steel structures, therefore aiming at the Steel Health Monitoring (SteHeMon). The proposed method is based on the correlation of magnetic properties with structure-microstructure of steels and may also be used for the detection of welding non-uniformities, impurities etc. Plastic deformation and residual stresses are due to the generation and propagation of dislocations in grains as well as to the presence of nano-precipitations in grains. Both of them generate stress fields which are responsible for the generation of cracks in the material: particularly, their gradient, i.e. their inhomogeneity in space is mainly responsible for the crack generation. Dislocations and nano-precipitations are also pinning centers for the mobility of the propagating magnetic domain walls, as well as the rotation of magnetic domains, wherever applicable. These pinning centers are observable in macroscopic (averaging) magnetic properties, when the size of accumulated dislocations (dislocation forests, subgrain etc) or precipitations in the grain are in the order or larger than the magnetic domain wall thickness, since they remarkably affect the magnetization process of the steel. In all ferrous steels (soft magnetic materials), the thickness of the magnetic domain wall is in the order of 20-30 nm. Despite the fact that, thermal history in some cases may counteract on the results of mechanical history and vice versa, in terms of stress field accumulation or release, the sum of the stress field due to both mechanical and thermal history, responsible for the possible generation of cracks, ought to be reflected on the bulk and surface magnetic properties. The same may apply even for different types of mechanical treatment, like plastic deformation or high-low cycle fatigue process. Therefore, dislocation and nano-precipitation defects of size comparable or larger than 20-30 nm, affect the bulk and surface magnetic properties of steels. The main bulk magnetic properties are the static or quasi-static magnetization hysteresis loop, particularly the minor hysteresis loops, as well as the magneto-acoustic emission (magnetostriction effect). The main surface magnetic properties are the Barkhausen noise and the surface permeability distribution. Different magnetic steels give different response on their magnetic properties under the same mechanical and thermal history. This is due to the different structure and microstructure of the material and suggests that a generalized method for determination of stress field gradient in an unknown ferrous material is practically impossible. Therefore a kind of "calibration" of the under test steel is required in order to obtain the correlation of magnetic properties with stress field gradient. After having correlated the magnetic properties with structure and microstructure, particularly with the stress field distribution in the material, the steel health monitoring of the particular steel under test, may become straightforward. For this reason, a magnetic model able to correlate the magnetic properties with the size distribution of stress field (pinning centers) in the under test steel is required. Such a model shall be based on the Preisach hysteresis modeling, accordingly aided by micromagnetic theory, physical meanings and critical coefficients. Having realized the model – algorithm of correlating the magnetic properties with the plastic deformation and stress field distribution, the instrument for field measurement and the necessary standardization procedure can furthermore be realized.

*ORAL
PRESENTATIONS*

O01-T01

Mn-Bi THIN FILMS PREPARED BY ELECTROCHEMICAL METHODS

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ABSTRACT

Recently, the electrochemical method has attracted much attention for the preparation of thin magnetic films and magnetic nonmaterials CoPt, FePt [1], FeNi, FeCo [2, 3] and recently Mn-Bi [4]. Indeed the equiatomic MnBi alloy in his hexagonal phase has attracted a lot of scientists for its very interesting magnetic properties, in particular its high uniaxial magnetic anisotropy [5] and its magneto-optical proprieties [6] which makes this material a potential candidate the magnetic recording field.

In this work the electrodeposition of Mn-Bi system from a mixed sulfate-nitrate bath was investigated by electrochemical method, under direct and pulse potentiostatic electrodeposition. Cyclic voltammetry (CV) and chronoamperometry (CA) were investigated. The morphology, composition and crystallographic structure of the electrodeposited Mn-Bi system were studied using scanning electron microscopy (SEM) with SE and BSE mode, energy dispersion spectroscopy (EDS) and X-ray diffraction (XRD).

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O02-T01

MAGNETIC PROPERTIES OF NANOCRYSTALLINE Fe₆₁Co₂₁Nb₃B₁₅ ALLOYS POWDERS

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ABSTRACT

The alloys compound Fe₆₁Co₂₁Nb₃B₁₅ (wt. %) powder mixture were prepared by mechanical alloying process in a high energy planetary ball mill P7. Morphological, structural and microstructural variations were followed by scanning electron microscopy and X-ray diffraction. Changes in the magnetic behavior as a function of milling time has been studied by vibration sample magnetometer (VSM) at room temperature and Mössbauer spectrometry. Morphological observations have shown the existence of a broad distribution of size and shape of the powder particles. Structural analysis shows a significant reduction of the crystallite size to the nanoscale and an increase of the internal strain level. Both XRD and Mössbauer spectrometry results reveal the formation, after 48 h of milling, a highly disordered like amorphous structure where nanometer-sized iron borides were embedded; like Fe₃B, Fe₂B and FeB phases. After 96 h, a mechanical recrystallisation process is also evidenced by the emergence of a sharp sextet gives rise to the formation of α -Fe and α -FeCo nanograins. The saturation magnetisation decreases rapidly during the first 6 h of milling to about 115 emu/g. After 96 h of milling, the coercivity, H_c, value of about 71.6 Oe and saturation magnetisation about 130 emu/g. The occurrence of disordering in the milled powders may be confirmed by broad exothermic reaction in the DSC scans which consists of several overlapping exothermic peaks and spreads over the temperature range 100-600 °C. Such behavior originates from recovery, strain relaxation, grain growth and recrystallisation.

Keywords: Nanomaterials; Mechanical alloying; Fe-Co-Nb-B alloys; Magnetic properties; Coercivity, H_c, saturation magnetization; Mössbauer spectrometry.

O03-T01

STRUCTURAL AND MAGNETIC PROPERTIES OF ELECTRODEPOSITED Fe FILMS
ON Al SUBSTRATE

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ABSTRACT

Series of Fe films have been prepared by electro-deposition onto porous and non porous Al substrate. Different solutions were used in the elaboration process. The Fe films are quite thick, in the micrometer range. The texture, the strain and the grain size values were derived from X-ray Diffraction (XRD) experiments. Two preferred directions ($\langle 200 \rangle$ and $\langle 110 \rangle$) were observed depending on the thickness, the solution and the type of substrate. For most samples, the strain values ϵ are positive (films subjected to a tensile stress) and ranging from 0.13 to 0.83 %. The grain size values D are found to be between 37 and 128 nm. Vibrating Sample magnetometer (VSM) has been used to obtain the hysteresis curves; the external magnetic field was applied in different directions in the film plane, and also perpendicular to the film. All samples show an in-plane magnetic anisotropy, however no preferred orientation within the film plane was detected. The in-plane coercive field H_C ranges from 38 to 78 Oe while the perpendicular H_C values are between 46 to 122 Oe. The squareness S values are very low (not exceeding 0.06) for the situation where H is applied perpendicular to the film, for the in-plane applied field, S is found to be between 0.03 and 0.12. For some of the samples, the magnetization curves were obtained for different temperatures (from 120°K to 350°K), we observe an increase in H_C and in S with decreasing temperature. All these results will be discussed and correlated; the contribution of different parameters such as the type of substrate (porous and non porous Al), the solution and the thickness to the structural and magnetic properties will be highlighted.

Keywords: Fe films, electro-deposition, XRD, Hysteresis curves.

O04-T03

MAGNETIZATION DYNAMICS IN Co₂MnGe/Al₂O₃/Co TUNNEL JUNCTIONS GROWN ON DIFFERENT SUBSTRATES

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ABSTRACT

Static and dynamic magnetic properties of Co₂MnGe (13 nm) / Al₂O₃ (3nm) / Co (13 nm) tunnel magnetic junctions (TMJ), deposited on various single crystalline substrates (a-plane sapphire, MgO(100), Si(111)), are presented. These TMJs are of great interest, due to their use in magnetic memories (MRAM) [1], in low field magnetic sensors [2] and in microwave components for spintronics [3]. The results are compared to the magnetic properties of Co and of Co₂MnGe single films lying on sapphire substrates. X-rays diffraction always shows a (110) orientation of the Co₂MnGe films. Our vibrating sample magnetometry (VSM) measurements reveal in-plane anisotropy only in samples grown on a sapphire substrate. Depending on the substrate, the ferromagnetic resonance spectra of the TMJs, studied by the microstrip technique (MS-FMR) show one or two pseudo-uniform modes. In the case of MgO and of Si substrates only one mode is observed: it is described by magnetic parameters (g-factor, effective magnetization, in-plane magnetic anisotropy) derived in the frame of a simple expression of the magnetic energy density [4]; these parameters are practically identical to those obtained for the Co single film. With a sapphire substrate two modes are present: one of them does not appreciably differ from the observed mode in the Co single film while the other one is similar to the mode appearing in the Co₂MnGe single film: their magnetic parameters can thus be determined independently, using a classical model for the energy density in the absence of interlayer exchange coupling. These results will be discussed using the structural observations obtained by High Resolution Transmission Electron Microscopy (HRTEM).

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O05-T03

**STUDY OF STRUCTURAL, ELECTRICAL, MAGNETIC AND MAGNETOOPTIC
PROPERTIES OF COEVAPORATED Fe_xCo_{1-x} THIN FILMS**

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ABSTRACT

Fe_xCo_{1-x} alloys have been deposited by coevaporation onto oxidized Si(100) and float glass substrates. The atomic composition has been evaluated from EDX and RBS analysis. From X-ray diffraction spectra, we show the coexistence of bcc and fcc phases for some compositions. All the films present (110) and (211) textures with a grain size varying with the composition. The lattice constant increases rapidly with x from the cobalt lattice constant to stabilize around the iron one. The electrical resistivity deduced from the resistance-four point probe, shows an oscillating behavior with composition. Magneto-optical and magnetic properties have been studied by recording the hysteresis loops of the longitudinal Kerr rotation and the magnetization. All the samples have in-plane anisotropy with no preferential direction. The in-plane coercivity and the saturation magnetization were studied as a function of composition.

O06-T03

SYNTHESIS OF HYBRID CARBON NANOTUBES COBALT MATERIALS AND THEIR MAGNETIC PROPERTIES

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ABSTRACT

In this paper, we developed three strategies for filling carbon nanotubes with magnetic cobalt. In the first method, single and multiwalled carbon nanotubes were synthesised by direct arc discharge method [1], then nanotubes were opened by ball milling and heated in the presence of cobalt up to 1500 °C at controlled atmosphere. In the second technique, the conventional arc technique was modified to direct synthesis the hybrid structures. Different concentrations of cobalt acting both as catalyst and filling agent was incorporated to the anode. To improve filling process, catalytic quantity of sulfur was also added [2]. In the third technique, plasma enhanced chemical vapour deposition PECVD was used to grown nanotubes vertically from a thin cobalt layer. When heated, this continuous layer disaggregates and forms small cobalt nanoparticles where the growth of nanotubes occurs through the catalytic decomposition of methane. In order to determine the structural properties as well as to estimate the filling efficiency, the samples issued from each synthesis strategy were analysed by a combination of techniques including Atomic Force Microscopy AFM, Raman spectroscopy, X-Ray Diffraction XRD and Transmission Electron Microscopy TEM. Our results (Fig. 1) indicated that in ex-situ method, the cobalt is not encapsulated inside the internal channel of the nanotubes because of its high surface tension in the liquid state $\sim 1830 \text{ mN.m}^{-1}$. In the in-situ method, cobalt was encapsulated inside the nanotubes. The CNTs grown by PECVD have the cobalt nanoparticles at their top. Finally, the magnetic properties of the nanotubes Co samples were analyzed with a vibrating sample magnetometer (VSM). The Co@CNT showed ferromagnetic behaviour with a good normalized remanence ($M_r/M_s \approx 0.25$) and a coercive field H_c varying from $\sim 50 \text{ Oe}$ to $\sim 500 \text{ Oe}$ depending on the method used. The magnetic behaviour is analyzed within the frame of the coherent rotational model.



Fig. 1. Three different forms of cobalt: a) cobalt nanowires (*in-situ* filling), b) spherical particle cobalt (ex-situ filling), c) cobalt nanoparticles on the top of CNTs (PECVD).

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O07-T03

PHASE TRANSFORMATION, STRUCTURAL EVOLUTION AND MICROSTRUCTURAL
PROPERTY OF NANOSTRUCTURED FeAl AS A RESULT OF MECHANICAL
ALLOYING

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ABSTRACT

Objective of the work was to synthesize nanostructured FeAl alloy powder by mechanical alloying (MA). The work concentrated on synthesis, characterization, structural and microstructural properties of the alloy. Nanostructured FeAl intermetallics were prepared directly by MA in a high energy ball mill. To prevent oxidation phenomena, the mixed powder was sealed in a cylindrical vial under an argon atmosphere with stainless steel balls. Phase transformation, structural changes, morphology and particle size measurement during MA were investigated by X-ray diffraction (XRD), Mössbauer spectroscopy, Scanning electron microscopy (SEM) and Energy dispersive X-ray spectroscopy (EDX) respectively. XRD and SEM studies revealed the alloying of elemental powders as well as transition to nanostructured alloy. The complete formation of bcc-FeAl solid solution was observed after 4 h of milling. Crystallite size of 10 nm was obtained after 24 hours of milling. Longer milling duration introduces ordering in the alloyed powders.

Keywords: Mechanical Alloying; FeAl; Disorder; Order; Ball Milling; Nanostructured Powder.

O08-T03

STRUCTURAL AND MAGNETIC PROPERTIES OF THERMALLY EVAPORATED Fe₃₅Co₆₅ THIN FILMS OBTAINED FROM MECHANICAL ALLOYING POWDER

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ABSTRACT

The aim of this work is to investigate the microstructure and magnetic properties of Fe₃₅Co₆₅ thin films deposited by thermal evaporation using nanocrystalline mixture. The nanocrystalline mixture was a Fe₃₅Co₆₅ powder, prepared from Fe and Co powders by mechanical alloying process using high energy ball milling. The microstructural features of the obtained alloy were examined by X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM) techniques. The results showed homogeneous mixture with a mean crystallite size of 25 nm. Figure A shows an example of the obtained SEM photographs. The films were deposited on Si (100) substrate at different thicknesses. The characterization was carried out using Rutherford Backscattering Spectrometry (RBS), XRD and SEM coupled with Energy Dispersive Spectrometry (EDS). The analysis showed that the films were homogeneous and the stoichiometry of the powder was conserved. On another hand no contamination was found in the deposits. The film texture was [110]. Besides, atomic force microscopy (AFM) was used to probe the topography of the films. The static magnetic properties of the Fe₃₅Co₆₅ films were studied using Vibrating Sample Magnetometer (VSM) technique while the magnetic domains was imaged using Magnetic Force Microscopy (MFM). The obtained hysteresis loops showed a strong dependence of the coercivity on the film thickness. An example of the obtained hysteresis loops is shown in figure B.

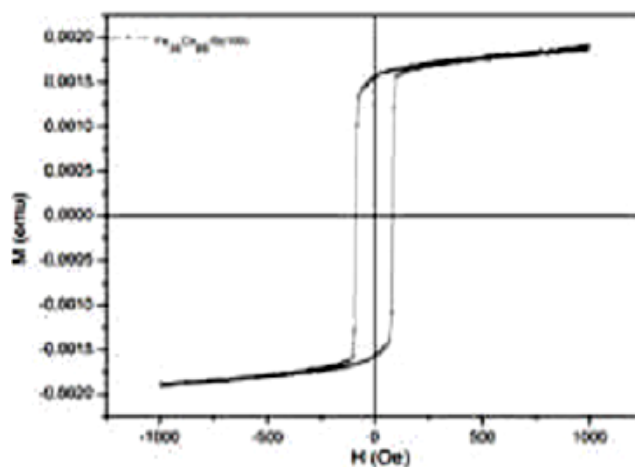
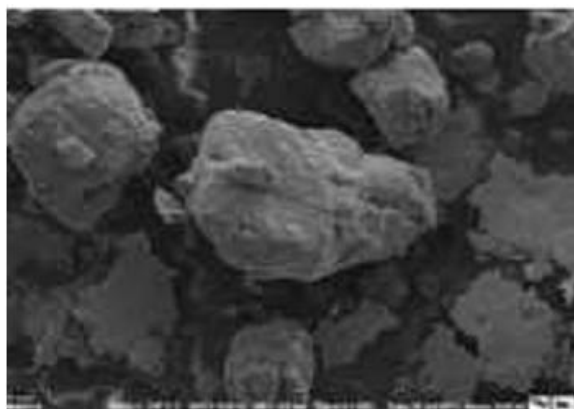


Figure A. SEM micrograph of nanocrystalline powder **Figure B.** Hysteresis loop for Fe₃₅Co₆₅ film

O09-T02

MAGNETIC AND STRUCTURAL PROPERTIES OF NANOSTRUCTURED ZINC FERRITES (ZnFe_2O_4) Milled AT LOW ENERGY

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ABSTRACT

Nanostructured ZnFe_2O_4 ferrites with different grains sizes were prepared using low energy ball milling for various milling times. The average grain size decreases with milling time. The inversion parameter is found to be 0.64 for 72 hours of milling. The lattice parameter increases with milling and decreases with further milling. ^{57}Fe Mössbauer spectra were recorded at 300K and 77K for all milled samples. For $T=77\text{K}$, Mössbauer spectra consist on a magnetically ordered component with a doublet characterising superparamagnetic behaviour of small crystalline particles. This doublet is reduced when the milling time increases. For $T=4.2\text{K}$ a magnetically blocked state is revealed and Mössbauer spectra under external magnetic field ($B=8\text{T}$) applied parallel to gamma rays direction and recorded for 12 and 48 hours milled samples depict ferrimagnetic ordering. Hyperfine field distribution correlated with angle distribution has been carried out in order to realise a qualitative adjustment for spectra. The results show that samples exhibit spin canting with large canting value, may be due to spin glass behaviour or the existence of grains boundaries. Schemes of magnetic moments distributions into grains and grains boundaries have been illustrated.

O10-T02
STRUCTURE AND MÖSSBAUER SPECTROSCOPY OF $(\text{Fe}_{60}\text{Al}_{40})_{100-x}\text{Si}_x$
NANOMATERIALS

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ABSTRACT

We report on a systematically study of the influence of Si addition on the hyperfine and structural properties of $(\text{Fe}_{60}\text{Al}_{40})_{100-x}\text{Si}_x$ ($x=0, 5, 10, 15$ and 20%) powders elaborated by high energy ball alloying for a milling time of 72 h. ^{57}Fe Mossbauer spectroscopy and X-ray diffraction (XRD) techniques were used for a better understanding of the competition between Si and Al. X-ray diffraction patterns show the formation of disordered bcc FeAlSi phase. The lattice parameter decreases monotonically with increasing Si content. When Si content increases, the mean grain sizes decreases slightly from 10 nm (for 0 % Si) to 6 nm (for 15% Si). The Mössbauer spectra clearly indicate that the ferromagnetism vanishes as Si (%) increases. Indeed, for $\text{Fe}_{60}\text{Al}_{40}$ (0% Si), the Mössbauer spectrum was adjusted by a sextet with a hyperfine magnetic field, $\langle H_{\text{hf}} \rangle$, equal to 22 T. This sextet was attributed to the ferromagnetic disordered $\text{Fe}_{60}\text{Al}_{40}$ phase. For Si content of (5, 10, 15 and 20%), the Mössbauer spectra show a dominance of the paramagnetic doublet that was attributed to B2 phase.

Keywords: Fe–Al–Si nanomaterials; Mössbauer spectroscopy; X-ray diffraction.

O11-T04
SEMICONDUCTING (HALF-METALLIC) FERROMAGNETISM IN Mn (Fe)
SUBSTITUTED Pt AND Pd NITRIDES

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ABSTRACT

Using first principles calculations as based on density functional theory, we propose a class of so far unexplored diluted ferromagnetic semiconductors and half-metals. These latter may be very interesting as a potential candidates for spintronic applications. Here, we study the electronic properties of recently synthesized 4d and 5d transition metal dinitrides. In particular, we address Mn- and Fe-substitution in PtN₂ and PdN₂. Structural relaxation shows that the resulting ordered compounds, Pt_{0.75}(Mn,Fe)_{0.25}N₂ and Pd_{0.75}(Mn,Fe)_{0.25}N₂, maintain the cubic crystal symmetry of the parent compounds. On substitution, all compounds exhibit long-range ferromagnetic order. While both Pt_{0.75}Mn_{0.25}N₂ and Pd_{0.75}Mn_{0.25}N₂ are semiconducting, Fe-substitution causes half-metallic behavior for both parent materials.

O12-T04

SPIN POLARIZATION EFFECTS ON THE STRUCTURAL AND ELECTRONIC PROPERTIES OF MONO BORIDES XB (X= Fe, Co, Mn)

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ABSTRACT

Metallic borides or Transition metal borides result from incorporation of boron into the surface of metal, This borides shows many interesting properties, such as high melting point, high melting hardness, wear resistance, corrosion resistance, catalytic properties, good electric and thermal conduction and magnetic properties [1,2]. These compounds can be used as reinforce phases in various materials to improve the mechanical strength, surface hardness and wear resistance of the metal matrix [3,4]. However, the bonding nature of these compounds is not very clear [5].

In this paper, spin polarization effects of Fe, Co and Mn elements on structural and electronic properties of mono-borides have been studied by using both the local spin density approximation (LSDA) and generalized gradient approximation (GGA) within the framework of density-functional theory (DFT).

Spin polarized and non-polarized calculations are performed to show the effect of magnetic moment on the structural and electronic properties. At equilibrium, non-magnetic and magnetic calculations of total energy versus volume show that the grounds states of the MnB, FeB are ferromagnetic. The calculated magnetic moments agree well with the experimental results. Finally we remarked that the spin polarization play crucially important role in determining the electronic and structural properties.

Keywords: Density functional theory; Spin Polarization; Transition Metals; LSDA

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O13-T04

STRUCTURAL, MAGNETIC AND MAGNETO-OPTICAL PROPERTIES OF
Fe/Pt[001] THIN FILMS

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ABSTRACT

By means of first principles calculation, we studied the structural and magnetic properties as well as the magneto-optical properties of Fe thin films deposited on Pt (001). We used the so-called FP-(L)APW+lo [1] method. In order to achieve the Kerr effect [2], we also included the spin-orbit interaction in the resolution of the electronic Kohn-Sham equations [3]. From the relativistic energy bands, we used the linear response Kubo-Greenwood formula [4] to calculate the complex Kerr angle as a function of the electromagnetic wave energy in the range [1-10] eV. We initially carried out the relaxation of the atomic planes in a self-consistent way, where we found that by increasing the number of Fe planes, the distances between planes tends to an average value between the bulk Fe-Fe and Pt-Pt distances. The obtained magnetic moments are in agreement with experiment. The magnetic moment of the central layer of Fe decreases to have a value closer to that of a bct-like bulk structure with the average lattice parameters between those of bulk Fe and Pt. The moment of the surface layer converges towards a value comparable with that of the free surface of Fe. At the interface Fe-Pt, The Fe moment is about $3 \mu_B$, and only the first interface plane of Pt polarizes with a magnetic moment of $\sim 0.3 \mu_B$. For all structures, we obtained a large Kerr rotation, whose behaviour of the signal according to the number of Fe planes was noted. At the end we showed the microscopic origin of the peaks of interest starting from the bands structure and the atomic densities of states in these films.

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O14-T04

ON THE ROLE OF EXCHANGE INTERACTION IN MAGNETIC ORDERING
OF RARE-EARTH MONOCHALCOGENIDES

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ABSTRACT

Rare-earths are chemically very similar due to an almost identical outer electron arrangement [1]. It remains, however, difficult to obtain impurity-free single crystals of the rare-earth elements or rare-earth compounds, and this may be responsible for some of the longstanding controversies concerning their physical properties. The electronic structures and magnetic properties of many rare-earth monochalcogenides REX (X= Te, Se, S, O) [2], which can be candidate materials for spintronics devices, are investigated in this work. We have attempted to provide a unified picture of the electronic properties of these strongly correlated systems. The relative merits of several ab initio theoretical methods useful in the study of the rare-earth monochalcogenides are discussed [3-5]. In addition, we have presented our current understanding of the possible half-metallicity, the semiconductor–metal transitions, and the magnetic orderings in the rare-earth monochalcogenides [6]. Finally, we have also applied a hydrostatic pressure to improve the magnetic and electronic properties of these candidate materials for spintronics devices, as well as, the enhancement of critical temperature T_c [7].

Keywords: Monochalcogenides, Magnetic ordering, Hydrostatic pressure, Critical temperature.

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O15-T04

DYNAMIC MAGNETIC HYSTERESIS LOOPS AND NONLINEAR SUSCEPTIBILITY OF MAGNETIC NANOPARTICLES HAVING BIAXIAL ANISOTROPY
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ABSTRACT

The nonlinear susceptibility $\chi_1^1(\omega)$ and dynamic magnetic hysteresis (DMH) of single domain ferromagnetic particles with biaxial anisotropy $\beta V = (\sigma + \Delta \cos^2 \varphi) \sin^2 \vartheta$ induced by an external ac field of arbitrary strength and orientation are treated via Brown's model of coherent rotation of the magnetization ($\sigma = \beta K$, K is the anisotropy constant, Δ is the biaxial parameter, $\beta = v / (kT)$, v is the volume of the particle, k is Boltzmann's constant, T is the absolute temperature, ϑ and φ are the polar and azimuthal angle, respectively). We demonstrated that the form of DMH loops and $\chi_1^1(\omega)$ strongly depends on the biaxial Δ , barrier σ , and damping α parameters at low, mid, and high frequencies.

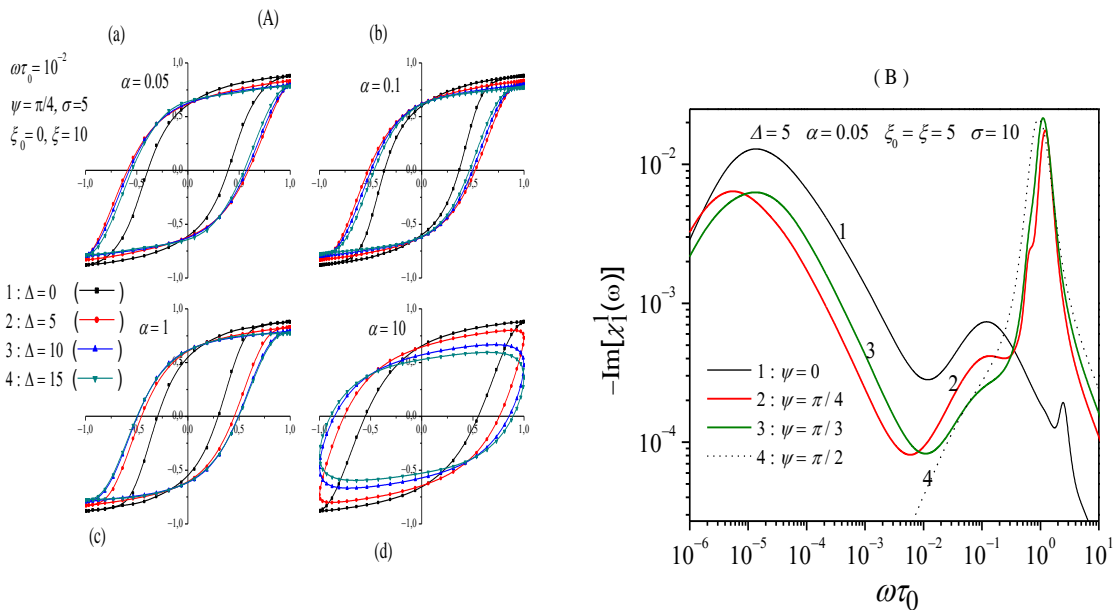


Figure. (A) : DMH loops [the magnetization $m(t)$ vs. the ac field $h(t)$] at the frequency $\omega\tau_0 = 0.01$ for various values of the biaxial Δ and damping α parameters [$\xi = \beta M_s H$ is the external field parameter; ψ is the angle between \mathbf{H}_0 and the Z axis, $\tau_0 = M_s / (2\gamma K)$ is a characteristic relaxation time with a typical estimation $\tau_0 \sim 10^{-10}$ s; M_s is the saturation magnetization, and γ is the gyromagnetic ratio]. (B) . Nonlinear dynamic susceptibility $-\text{Im}[\chi_1^1(\omega)]$ vs. $\omega\tau_0$ for various values of the angle ψ .

O16-T04

**MAGNETIC SPIN WAVES SCATTERING INSIDE THE INHOMOGENEOUS
2D-HEXAGONAL MESOSCOPIC SYTEM**

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ABSTRACT

We investigate the spin magnetic excitation at domain boundaries solitons that separate phase domains in hexagonal two dimensional lattices. The inhomogeneity breaks translation symmetry in the direction normal to the defect domain boundaries, which induces the localized magnons. The formalism of matching method [2-5], associated to Green functions, is used to calculate the curve of reflexion, transmission magnetic coefficients and associated magnonic conductance, for the spin components of the individual atomic sites that constitute a complete representation of the soliton domain boundaries. The variations of these spin precession as function of changes of exchange integral parameters at the soliton domain boundaries is determinate. It is shown that the calculated spin spectra are sensitive and explicit signatures for the softening, homogeneous and hardening effects. The coherent transmission coefficient is derived as elements of a Landauer- Buttiker type scattering matrix[6-7]. The numerical results show the interference effect between the incidents scattered magnons and the localized spin states at the perturbed domain, with are the characteristics of Fano_resonances. The numerical results are given according to the various parameters characterising the system. These spectra of the conductance of the system model may yield, from the theoretical and experimental points of view, useful information concerning the spins values and exchange integral parameters in the neighborhood of the perturbed region.

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O17-T04

KERR EFFECT IN ULTRATHIN FILMS $Fe_r/X(001)$ ($X=Ag, Au$)

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ABSTRACT

Structural, magnetic and magneto-optical properties of ultrathin films of iron grown by pseudomorphic epitaxy on semi-infinite noble metals $X(001)$ with ($X=Ag, Au$) are investigated. Calculations are performed within the framework of relativistic approach using the local spin density approximation (LSDA). To calculate the band structure, we have used the Spin-Polarized Relativistic (SPR) Linear Muffin-Tin Orbitals (LMTO) with the Atomic Sphere Approximation (ASA) method [1]. The Hamiltonian and the overlap matrices corresponding to Dirac equation are expressed in terms of the basis set of the so-called relativistic muffintin orbitals centered on the atomic sites. The crystalline structure was calculated by relaxation of the studied systems using an optimization process of the total energy with respect to inter-plane spacing. A body centered tetragonal (bct) pseudomorphic crystalline structure with a tetragonality ratio c/a larger than unity was found and the pseudomorphic growth is found to be larger than 3 monolayers. The magnetic behaviour is characterized by an enhanced magnetic moment with a ferromagnetic interlayer coupling. Using the Kubo-Greenwood linear response [2]; the dispersion of the optical conductivity tensor $\sigma_{\alpha\beta}(\omega)$ as a function of the frequency ω of the incoming electromagnetic radiation is calculated from the energy band structure and The polar magneto-optical Kerr effect [3] spectra are given over a photon energy range extended to 15eV and the microscopic origin of the most interesting features of Kerr rotations are interpreted by interband transitions.

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O18-T01

POLYCRYSTALLINE $Zn_{1-x}Co_xO$ DILUTED MAGNETIC SEMICONDUCTOR
SYNTHESIZED BY CHEMICAL ROUTES

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ABSTRACT

We have used chemical methods like hydrothermal and co-precipitation techniques to synthesize polycrystalline $Zn_{1-x}Co_xO$ diluted magnetic semiconductor [1, 2]. For both techniques, X-ray diffraction indicates that the maximum Co concentration that can be inserted in the würtzite structure without any significant change and without apparition of secondary phases is 10%. Optical absorption measurements show several absorption bands that are due to the transitions between the crystal-field-split 3d levels of tetrahedral Co^{2+} substituting Zn^{2+} ions, forming a solid solution with würtzite structure instead of Co precipitates. Room- and low-temperature magnetization measurements reveal a paramagnetic behavior for the Co-doped ZnO samples and not the expected ferromagnetic behavior. For all samples the paramagnetic Co amount was smaller than the nominal concentration. χT versus T curves evidenced that the remaining Co is anti-ferromagnetically coupled through oxygen. This is further supported by a simple model that shows that as the Co concentration increases the amount of nearest neighbors Co atoms increases thus giving anti-ferromagnetic coupling and reducing the paramagnetic contribution [3].

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O19-T01

EFFECT OF THE TARTARIC ACID ON THE MORPHOLOGICAL AND STRUCTURAL PROPERTIES OF THE Bi ELECTRODEPOSITED NANOWIRES

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ABSTRACT

Nanostructured materials such as nanoparticles, nanowires and nanoarrays have attracted much attention due to their new interesting physical properties. In this context, much attention has been paid recently to the preparation of Bi nanowires because of their extraordinary thermoelectric and magnetotransport properties which are strongly depended on their diameter and orientation [1, 2].

Generally, both physical and chemical methods are used to synthesize Bi nanowires. Electrodeposition is a low cost technique and a very interesting way specially when using anodic porous alumina membranes (AAM) as a substrate. Indeed AAM are known to exhibit controllable pore diameter, extremely narrow size distribution for pore diameters, and ideally cylindrical pore shape.

For this purpose, nanoporous alumina templates are prepared beforehand by anodic oxidation of pure aluminum foils in an oxalic acid. As the oxide layer of the AAM is non-conductive, a thin gold layer was sputtered onto one side of the AAM in order to make an electrical contact for the electrochemical deposition. Bi nanowire arrays were fabricated in a three electrode plating cell from a chlorid acid solution in the presence and absence of tartaric acid. The kinetic study of the deposit, according to the tartaric acid concentration in the bath, was performed by voltammetry measurements using a rotating disk electrode. Several deposits of bismuth nanowires have been elaborated at different concentrations of tartaric acid. The nanowires arrays were characterized by X-ray analysis (XRD) and scanning electron microscopy (FESEM). The results obtained revealed that the pores filling, the morphology and structural properties of the Bi nanowires are strongly dependent on the tartaric acid concentration in the electrolytic bath.

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O20-T03

MAGNETIZATION REVERSAL OF FERROMAGNETIC NANOWIRES: A MAGNETIC FORCE MICROSCOPY AND MICROMAGNETIC SIMULATIONS STUDY

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ABSTRACT

Arrays of magnetic nanostructures, such as of nanowires (NWs), are extensively investigated due to their potential applications in magnetic storage and microwave devices. Amongst the various issues at stake for a comprehensive understanding of these arrays is the influence of long range dipolar interactions because these interactions between NWs strongly influence the switching field distributions (SFD) which play a significant role for information storage. Two dimensional arrays of ferromagnetic nanowires of different diameter, ranging from 40 to 100 nm, embedded inside low porosity ($P < 1\%$) polycarbonate nanoporous membranes have been fabricated by using electrodeposition technique. The magnetization reversal of these arrays has been studied by in situ magnetic force microscopy and micromagnetic simulations. For such low packing factor of the arrays, the nanowires are sufficiently isolated from each other to neglect the dipolar interactions between them. This helps to avoid the difficult corrections which are necessary for dense nanowires arrays, thus leading to an easier analysis and interpretation of the MFM data. In these conditions, the micromagnetic simulations can be performed by considering only one isolated nanowire. The MFM data of the nanowires were analyzed for different magnetization states, successfully measured at the same spot through in situ measurements, to get the switching field distribution (SFD) by counting the number of nanowires having reversed their magnetization after each increment of applied magnetic field. The magnetization/magnetic field curves obtained from the in situ MFM images after calculating the number of wires in each magnetization direction is square-shaped as expected and the broadening of the curves could be ascribed to the intrinsic switching field distribution. We observed a nice agreement between the MFM results with the bulk magnetic hysteresis curves. The measured SFDs are significantly reduced compared to the previously studied strongly interacting magnetic nanowire arrays [1, 2]. The influence of wire diameter has also been investigated.

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O21-T03
MAGNETIC AND MICROWAVE PROPERTIES OF MECHANICALLY ALLOYED
FeCo POWDERS

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ABSTRACT

In this research an investigation of the formation, microwave and magnetic properties is conducted for a series of nanocrystalline FeCo powders with least grain size of 15 nm. nanocrystalline FeCo powders are obtained by Mechanical Alloying (MA) route in nominal compositions Fe_xCo_{100-x} ($x=85,75,65,55,50,35,15,5$) using planetary ball mill. Alloying formation is confirmed by X-Ray Diffraction (XRD) analysis. Powders morphology is examined by the mean of Scanning Electron Microscopy (SEM). Reflection losses for bulk samples obtained by cold compaction are measured in X-band metallic wave guide whereas magnetic experiments of Hysterisis loops are carried out using Barkhausen noise system measurement. Discussed XRD results according to milling time show that α solid solution of substitution with disordered bcc structure is formed after a least 2 hours of milling with related mixing factors confirming that structural properties are governed by internal strain accumulated during high energy mechanical alloying. Produced powders are larger agglomerations of refined particles with high surface area. Measured refection losses according to Co concentrations show that maximum reflection losses are observed between 55% and 75% Co concentrations. Obtained Hysterisis loops for 60% Co concentration are enhanced according to milling progression with decreased coercivity.

O22-T05

ANALYSIS OF TOTAL LOSSES IN A EMBEDDED TRANSFORMER SUPPLIED WITH AN INVERTER AT NO-LOAD

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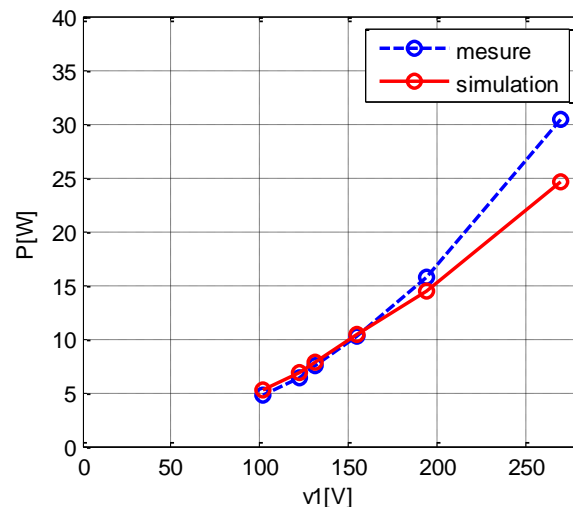
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ABSTRACT

The aim of the proposed paper is to present the model of an embedded electrical transformer supplied by voltage frequency inverter. The model is used to simulate an embedded transformer behavior at no-load. The eddy currents and hysteresis are considered on the magnetic core model [1], [2]. The theoretical losses are obtained by calculating the static hysteresis from the measured B (H) curve while the dynamic losses are obtained from the eddy-current formula together [1], [3]. The parameters of characteristic B (H) are identified by a genetic algorithm (GA).

The experiments are performed by feeding the transformer through an inverter, which was designed in the laboratory. The measured and calculated core losses are compared for 400 Hz (fig 1). The results obtained can be used when designing transformer to optimize these performances.

Index Terms—transformer, magnetic hysteresis, eddy currents, core losses.



Measured and simulated total losses in iron core as function of voltage at 400 Hz.

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O23-T05
CONTROL OF THE MAGNETIC FIELD EFFECT ON THE EUTECTIC
ALLOY Pb–17Li FLOW

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ABSTRACT

In fusion blankets, eutectic alloy lead–lithium Pb-17Li is used as breeder and coolant, it is an attractive option due to potentially higher thermal efficiency. Using a strong magnetic field to confine the plasma in the water-cooled blankets for fusion reactors, this liquid alloy has been proposed as breeder material. The Magnetohydrodynamics coupled with heat and mass transfer, have a great importance in the operation, safety and performance of the blanket. A better understanding and prediction of MHD effects during blanket operation could allow significant improvements of fusion blanket systems. The main goal of this work is to investigate numerically the laminar magnetohydrodynamic flow flowing in a parallelepiped duct filled with LiPb. Fluent computational fluid dynamics software based on the finite volume method is employed in simulations. The effect of different values of the magnetic field on the eutectic Pb–17Li alloy flow, heat and mass transfer is studied for small and moderate value of the magnetic field strength. The study was performed for various Hartmann number Ha in the range $0 \leq Ha \leq 104$ corresponding to a range of interaction parameter $N=Ha^2/Re$ of $0 \leq N \leq 9$.

Keywords: Magnetic field, Magnetohydrodynamics, Pb–17Li alloy, Liquid Metal, Instability, CFD, fluent software.

O24-T05

MAGNETOCALORIC EFFECTS IN MANGANITES WITH PEROVSKITE STRUCTURE

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ABSTRACT

Magnetic refrigeration is becoming a promising technology to replace the conventional expansion-compression technique since it presents higher energy efficiency with no harmful gases. This technology employs environmentally friendly and affordable non-toxic materials. Magnetic refrigeration is a method of refrigeration based on the magnetocaloric effect. This effect, discovered in 1881, is defined as the response of a solid to an applied magnetic field which is apparent as a change in its temperature. This effect is obeyed by all transition metals and lanthanide-series elements. When a magnetic field is applied, these metals, known as ferromagnets, tend to heat up, favoring the alignment of magnetic moments. On the contrary, when the field is removed, the ferromagnet cools down as the magnetic moments become randomly oriented. Gadolinium, a rare-earth metal, exhibits one of the largest known magnetocaloric effects and is considered as prototype material for magnetic refrigeration. It was consequently used as the refrigerant for many of the early magnetic refrigeration designs. However, pure gadolinium presents some disadvantages essentially related to his expensive cost.

More recently, considerable efforts were focused on the research of new materials presenting low cost, high chemical stability and operating near room temperature. Manganites are considered as potential candidates since they can present high magnetocaloric effect extended to a large temperature range near room temperature. In our work, we have studied different manganese oxide systems with perovskite structure synthesized using the solid-solid elaborating technique at high temperature or using the sol-gel method. We studied especially the effect of monovalent doping on the magnetocaloric effects in these manganites. In order to obtain large magnetocaloric effect on a wide temperature range around room temperature, we elaborated and studied the magnetocaloric effect in composite materials based on manganites. The elaborated materials are suitable enough for applications in the magnetic area.

O25-T05

MAGNETIC FIELD EFFECT ON SPHERICAL CZ CRYSTAL GROWTH

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ABSTRACT

The silicon crystals used in the technology of semiconductors are produced primarily by the Czochralski technique. During the Czochralski process three modes of heat transfer are present [1], namely, conduction in melt and crystal, natural convection due to the temperature gradient between the crucible wall and the melt/crystal interface, forced convection due to crystal and/or crucible rotation, thermocapillary convection known as Marangoni convection due to the surface tension gradients on the free surface of the melt, finally the heat transfer by radiation between various surfaces of the furnace. A direct current magnetic field is used to reduce undesired turbulent flows and fluctuations associated with melt convection during solidification to help eliminating solidification defects and striations [2]. Striations are growth-induced inhomogeneities that hamper the applications of crystals in numerous technologies. They are caused by the presence of convective instabilities which are damped with convection decreasing via magnetic field application. Inhomogeneities are thus reduced and the crystal quality is improved [3]. The silicon Czochralski crystal growth in spherical crucible is found to be of better advantages relatively to the cylindrical system when non magnetic field is applied and seems to be adapted for the growth of a good quality crystal [1,5-7]. This work aims to report the effect of transverse and axial magnetic fields of different intensities on silicon Czochralski crystal growth in hemispherical crucible with rotating crystal and thermocapillary convection in the bulk flow, the growth interface and the free surface.

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***POSTER
CONTRIBUTIONS***

P01

THEORETICAL PREDICTION OF STRUCTURAL, ELECTRONIC, MAGNETIC AND ELASTIC PROPERTIES OF Co₂-BASED FULL HEUSLER COMPOUND WITH THE 4D TRANSITION-METAL ELEMENT

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ABSTRACT

In this work, first principles calculation of structural, electronic magnetic and elastic properties of the half-metallic ferromagnetic Heusler compounds with 4d transition elements T , Co_2TZ ($T = \text{Y, Zr}$ and $Z = \text{Si, Ge}$), are presented. We have applied the full-potential linearized augmented plane waves plus local orbitals (FP-L/APW+lo) method based on the density functional theory (DFT). For the exchange and correlation potential generalized-gradient approximation (GGA) is used. The computed equilibrium lattice parameters agree well with the available theoretical data. The electronic band structures and density of states indicate half-metallic behavior with vanishing electronic density of states of minority spins at Fermi level.

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P02

STRUCTURE AND MÖSSBAUER STUDY OF NANOCRYSTALLINE Fe₉₀Ni₁₀
POWDERS

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ABSTRACT

Nanocrystalline Fe₉₀Ni₁₀ powders were prepared by the mechanical alloying process using the Vario-planetary high-energy ball mill P4 FRITICH. The alloys formation and the different physical properties were investigated as a function of the milling time, t, (in the 0 to 48 h range) by means of the X-ray Diffraction (XRD) technique, Mössbauer Spectroscopy. From X-ray diffraction we showed that centred-cubic (cc) nanocrystalline Fe₉₀Ni₁₀ alloy is completely formed after 18 h of milling. However the Mössbauer spectra show that complete formation of disordered Fe₉₀Ni₁₀ was achieved after 27 h of milling time. When milling time increases, the lattice parameter increases while the grain size decreases from 71nm for 0 h to 12 nm for 48 h. All these results will be correlated and discussed.

Keywords: Fe₉₀Ni₁₀ alloy, nanostructured powders, X-ray diffraction, microscopy Mössbauer effect.

P03

ELECTROMAGNETIC INTERFERENCE FROM SHIELDING EFFECTIVENESS OF A RECTANGULAR ENCLOSURE WITH APERTURES: FDTD AND FIT MODELING

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ABSTRACT

Apertures in a rectangular enclosure can be the coupling path of electromagnetic Interference (EMI) [1]. The development and investigation of approximate phenomenological models used to estimate the electromagnetic energy coupling through apertures into enclosures is presented in this paper. The FDTD method has been widely applied to solving different types of electromagnetic field penetration into a rectangular enclosure through apertures [1], [2], [3]. It is give good predictions of the shielding effectiveness of a rectangular enclosure with apertures. Both the magnetic and electric shielding may be calculated as a function of frequency, enclosure dimensions, apertures shapes, positions within the enclosure, plane wave incidence mode [4], and the "loaded aperture" approach was investigated.

The results of shielding effectiveness predictions obtained by the FDTD method are compared and validated with full-field simulations using the software CST/EMC . The software code is based on the finite integration technique (FIT)

Keywords: Electromagnetic compatibility, shielding effectiveness, enclosures, FDTD, FIT.

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P04

FIRST-PRINCIPLES INVESTIGATION OF LOCALIZED *D*-STATES IN MnVO₃
PEROVSKITE

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ABSTRACT

First-principles calculations have been performed for different magnetic orderings of orthorhombic manganite MnVO₃ perovskite [1] containing localized $3d^5$ Mn²⁺ and itinerant $3d^1$ V⁴⁺ states. This phase has a distorted *Pnma* crystal structure and is metallic. In this work, magnetic phase stabilities and chemical bonding of MnVO₃ have been investigated. In addition, LDA+*U* [2] band structure and densities of states are determined and discussed. We confirm the results of recently synthesized orthorhombic compound [3].

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P05

STRUCTURAL AND MAGNETIC PROPERTIES OF FE-PD THIN FILM

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ABSTRACT

We report on the structural, microstructural and hyperfine properties of Palladium rich Fe-Pd films. A serie of FePd films has been prepared by RF magnetron sputtering. The morphology and composition of the films were investigated by scanning electron microscopy (SEM). The structure of the FePd films was determined by the grazing incidence X-ray diffraction (GIXD). The hyperfine properties were investigated by Mossbauer spectroscopy in the CEMS mode.

P06

**STUDY OF THE ELECTRONIC STRUCTURE AND MAGNETIC BEHAVIOUR OF
CUBIC $\text{Al}_{1-x}\text{Yb}_x\text{N}$**

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ABSTRACT

First-principles calculations of the electronic structure and magnetic interaction of substitutional ytterbium rare-earth impurity in cubic AlN have been performed using density functional theory within LSDA+ U approach (local spin density approximation with Hubbard- U corrections). The electronic structure is characterized by occupied $4f$ -Tm states located in the valence band for majority and minority spins, and minority unoccupied states located in the conduction band. The magnetic interaction of the rare-earth ion with the host states at the valence and conduction band edges has been investigated and found to be weak in comparison with Mn impurities. Finally, the magnetic moment is analysed.

P07

STUDY OF A FERROMAGNETIC PROPERTIES IN THE $(\text{CrN})_1/(\text{GaN})_1$
SUPERLATTICES

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ABSTRACT

The ab initio full potential linearized augmented plane wave (FP-LAPW) method within density functional theory was applied to study the structural and electronic properties of a zinc-blende $(\text{CrN})_1/(\text{GaN})_1$ superlattices.

Structural, electronic and magnetic properties of a zinc-blende $(\text{CrN})_1/(\text{GaN})_1$ superlattices have been studied using ab initio method. Calculations have been made using full potential linearized augmented plane wave (FP-LAPW) [1] method within the framework of spin-polarized density functional theory (SP-DFT) [2]. For exchange-correlation energy and corresponding potential, generalized gradient approximation (GGA). These calculations as employed in WIEN2k code [3].

The results including equilibrium lattice parameter, band structures, total and partial densities of states for spin majority and spin minority, and the total magnetic moment of $(\text{CrN})_1/(\text{GaN})_1$ superlattices in ferromagnetic state.

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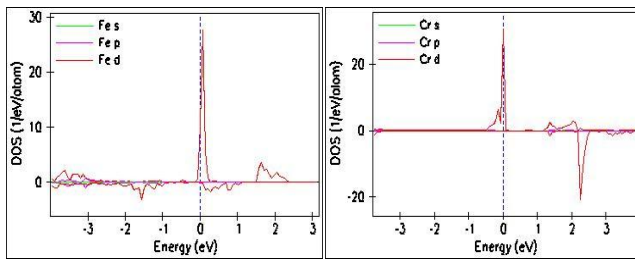
AB-INITIO CALCULATION OF MAGNETIC PROPERTIES OF $BaTi_{1-x}M_xO_{3-\delta}$; $M= (Fe, Co, Cr, Mn)$

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ABSTRACT

The magnetic properties of TM-doped $BaTiO_3$ with $TM= Fe,Co,Cr$ and Mn have been studied by means of a first-principles calculations based on density functional theory using the linear muffin-tin orbital method in the atomic sphere approximation with combined correction[1] LSDA for exchange –correlation potential. We studied spin polarization induced by replacement of titanium atoms by a transition metal (TM) ($TM= Fe$ or Cr or Mn or Co) in non magnetic tetragonal $BaTiO_3$ which gives the chemical formula of $BaTi_{0.9375}TM_{0.0625}O_3$. We give in that work a real approach of theoretical prediction to the experimental work of B,Xu et al [2] with different dopant and oxygen vacancies



Tetragonal Symmetry

Figure: Density of states of Fe and Cr in compound

$BaTi_{0.9375} Fe_{0.0625} O_3$ $BaTi_{0.9375} Cr_{0.0625} O_3$, with spin orbit

in For all samples we have found that the coupling spin-orbit enhances moderately the magnetic moment of Fe and Mn but enhances considerably the moments for Cr and Co. In the case of oxygen vacancies we noticed an overall increase of the total magnetic moment of the compound. We have compared our results to the experimental results.

Table: magnetic moment studied with

<i>Magnetic moment</i>	<i>TM(μ_B)/atom</i>	<i>Theo/exp</i>
$BaTi_{0.93} Fe_{0.06} O_3$	2.108	3.05/0.75
$BaTi_{0.93} Cr_{0.06} O_3$	2.528	-/-
	-0.017	-/-
	2.731	-/-
$BaTi_{0.93} Fe_{0.06} O_{2.5}$		
$BaTi_{0.93} Cr_{0.06} O_{2.5}$		

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P09

THE FIRST-PRINCIPLES OF THE ELECTRONIC PROPERTIES, MAGNETIC AND STRUCTURAL PROPERTIES OF COMPOUNDS OF THE TYPE IIA-V

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ABSTRACT

Ferromagnetic materials are of great interest to materials science, because their structure is relatively simple reflects various properties: electronic, and magnetic. The properties of these materials have made possible the development and manufacture of various technological devices. Studies of these new materials are of great importance to obtain information on their physical properties in order to improve their devices for their immediate applications. This work has the aims to study the first-principles of the electronic properties, magnetic and structural properties of compounds of the type IIA-V (CaN, SrN, BaN), This study has been done using a method of first-principles type ab-initio. The ab-initio methods, or the first principle has been used for over a decade, they form a powerful tool for the prediction and study of materials, and that under the effect of different conditions where experience becomes impossible or dangerous, destructive or polluting. Among the ab-initio methods, we find the method FP-LAPW (linearized Full Potential Augmented Plane Wave), based on the method LAPW (linearized Augmented Plan Wave) developed by Andersen, it is basically an improved method of augmented plane waves APW (Augmented Plan Wave), developed by Slater [1-2], it remains the most accurate method at present for calculating the electronic structure of solids within the framework of the theory of density functional theory (DFT), by Honenberg 1964 and Kohn [3], Kohn and Sham in 1965 [4] as amended LDA, local density approximation [5] as well as in its GGA generalized gradient approximation [6] the FP-LAPW method is Wien2K implemented the code [7] with which we perform our calculations. This code has successfully treated the systems high-temperature superconductors, minerals, the surfaces of transition metal oxides, non-ferromagnetic, and the molecules the electric field gradient.

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SYNTHESIS OF MAGNETIC MATERIALS

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ABSTRACT

The widespread contemporary interest in metal phosphonate materials [1–3] reflects their potential applications as ion exchangers [4] ionic conductors [5] nonlinear optical materials [6] and catalysts. The vanadyl organophosphonate system has proved particularly fruitful and is represented by molecular clusters of various nuclearities, and one-, two- and three-dimensional phases.^{7–9} In common with metal organophosphonates in general, The vanadyl organophosphonates possess structurally well defined internal void spaces and coordination sites which allow intercalation of substrate molecules. Modifications of organic substituents, introduction of templating reagents, and variations in metal–phosphonate compositions can be exploited to change substrate-specific recognition and to design novel phases. It is also apparent that variations in reaction conditions can result in significant structural reorganization.^{10–11} The novel material $(\text{H}_3\text{O})[(\text{V}_3\text{O}_4)(\text{H}_2\text{O})(\text{PhPO}_3)_3] \cdot x\text{H}_2\text{O}$ ($x = 2.5$) was determined by X-ray single-crystal analysis. The crystals belong to the trigonal system, space group P-3, with $a = 18.6845(4)$ Å, $c = 13.8330(4)$ Å, $V = 4182.25(2)$ Å³, and $Z = 6$. At low temperatures, magnetic interactions are observed between ions V^{4+} ($S = 1/2$) with antiferromagnetic coupling.

Keywords: Hydrothermal Synthesis ; VPO ; Exchange Interaction ; Magnetic Susceptibility; Antiferromagnetisme ; Metal transition.

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P11

FIRST PRINCIPLES INVESTIGATION OF Co AND Mn DOPED SnO₂

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ABSTRACT

Based on first-principle spin-polarized density functional theory calculations (DFT), the electronic and magnetic properties of Mn and Co-doped SnO₂ with rutile structures are investigated using the full-potential linearized augmented plane wave method (FP-LAPW) within the GGA approximation for treating the effects of exchange correlation. Our calculations predict that the spin-polarized state is more favorable in energy than the non-spin polarized state. The doped Mn and Co results in reduction of the band gap, which can be attributed to a series of impurity bands at the bottom of the conduction band caused by the strong hybridization between Mn 3d and O 2p. The results also show that the Mn-doped systems tend to convert into p-type semiconductor with direct band gaps.

Keywords: First principle, FP-LAPW, DFT, spin-polarized, semiconductor

P12

MAGNETIC SPIN WAVE SPECTRA OF SOLITON BOUNDARIES AT 2D HEXAGONAL STRUCTURE

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ABSTRACT

We investigate the spin wave spectra at domain boundaries called heavy and super heavy solitons that separate phase domains in hexagonal two dimensional lattices. The defect breaks translation symmetry in the direction normal to a soliton domain boundary, which induces the localized modes effects. The technical formalism of matching method and Green functions, are used to calculate the characteristic vibration, spectral densities and densities of states, of the spin precession components of the individual atomic sites that constitute a complete representation of the heavy and superheavy soliton domain boundaries. The variations of these spin vibration spectra due to changes of exchange integral parameters in the soliton domain boundary are determinate. It is shown that the calculated spin vibration spectra are sensitive and explicit signatures for the softening and hardening effects. Numerical results show characteristic interference effects between the incident spin-waves and the localized spin states of the soliton boundary.

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P13

EFFECT OF YTTRIUM DOPING ON PROPERTIES OF $\text{Bi}_2\text{Sr}_{1.9}\text{Ca}_{0.1-x}\text{Y}_x\text{Cu}_2\text{O}_{7+\delta}$
(Bi-2202) CUPRATE CERAMICS

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ABSTRACT

The properties of Bi-Sr-Ca-Cu-O (BSCCO) superconductors can be changed by substitutions of elements having different ionic radii and different bonding characters. Many research groups have investigated of the effect of Y^{3+} doping on the properties of the Bi-based superconductors [1-5]. In comparison with the 2201, 2212 and 2223 compounds that have been extensively studied, only one paper was published on the Bi-2202 phase [6].

In this work, we report on the effect of Y^{3+} doping on structural, mechanical and electrical properties of this phase. Samples $\text{Bi}_2\text{Sr}_{1.9}\text{Ca}_{0.1-x}\text{Y}_x\text{Cu}_2\text{O}_{7+\delta}$ with $x = 0, 0.025, 0.05, 0.075$ and 0.1 are then elaborated in air by conventional solid state reaction and characterized by X-ray diffraction (XRD), Scanning Electronic Microscopy (SEM) combined with EDS spectroscopy, density, Vickers microhardness and resistivity measurements.

The study shows that the samples are composed of only Bi-2201 and Bi-2202 phases, in accordance with previous results [6]. The cell parameters a and c are reduced by the doping while the b increases. A good correlation between the variations of the bulk density and the Vickers microhardness with x is obtained. The SEM photograph shows that the samples are composed of grains with a flat shape that characterizes the Bi-based compounds. Quantitative EDS analysis confirms the reduction of Ca content and the increase of Y^{3+} content when x is increased. The variation of resistivity with temperature shows that only samples $x=0.025, 0.05$ and 0.075 present an onset transition to the superconducting state. The higher onset critical transition temperature is obtained for $x = 0.025$ is about 96.11K.

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P14

**X-RAY DIFFRACTION AND MAGNETIZATION STUDIES OF NANOSTRUCTURED
(Fe₇₅Al₂₅)_{100-x}Si_x POWDERS**

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ABSTRACT

Nanocrystalline (Fe₇₅Al₂₅)_{100-x}Si_x powders with 0 ≤ x ≤ 20 at % were prepared by mechanical alloying process for a milling time of 72 h. The formation, structural and magnetic properties of FeAlSi alloys were investigated, as a function of Si content, by means of the X-ray diffraction (XRD) technique and vibrating sample magnetometer (VSM). From XRD spectra, the complete formation of bcc Fe(Al,Si) phase was evidenced after 72 h of milling. The mean grains size exhibit a weak decreasing as Si content increases. The lattice parameter decreases with increasing Si content. From hysteresis curves, we derived the saturation magnetization, Ms, and the coercive field, Hc. It is observed that Ms monotonously decreases with increasing of Si content. It is also noted that Hc decreases and reaches a minimum for x=10 at % then increases for x=15 and 20 %.

Keywords: (Fe₇₅Al₂₅)_{100-x}Si_x nanomaterials, mechanical alloying, XRD, magnetic measurement

P15

FIRST-PRINCIPLES STUDY OF ZnO:TM(TM:Co,Mn) ON THE ELECTRONIC AND MAGNETIC PROPERTIES

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ABSTRACT

The results of first-principles theoretical study of structural, electronic and optical properties of $Zn_{1-x}TM_xO$ $X=0.25$, have been performed using the full-potential linear augmented plane-wave method plus local orbitals (FP-APW). In this approach both the local density approximation (LDA) and the generalized gradient approximation (GGA) are used for the exchange-correlation (XC) potential. Results are given for structural and electronic and magnetic properties.

The lattice constants, the bulk modulus, elastic constants and their related parameters are in good agreement with the available results. The electronic structures show ZnO have direct bandgap insulator. Finally, the values of dipole magnetic moment per supercell of $Zn_{0.75}Co_{0.25}O$ compound was obtained about 3.01 and 3.02 μB

Keywords: ZnO, first-principles study, magnetic moment.

P16

THE SOMMERFELD CONSTANT AND THE INITIAL MAGNETIC SUSCEPTIBILITY
ARE LINKED TOGETHER

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ABSTRACT

Using the approach based on molecular field calculations for $S = \frac{1}{2}$ resonant level model; a close relationship between the two ratios $\frac{\gamma}{\chi(0)}$ and $\frac{|J_m|}{T_K}$ is obtained. Where γ represents the electronic contribution in the specific heat, $\chi(0)$ is the susceptibility at zero temperature, J_m is the molecular field parameter and T_K is the Kondo temperature.

P17

THE IDD EFFECT ON MAGNETIZATION SWITCHING OF FERROMAGNETIC
NANOCLUSTER ASSEMBLY

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ABSTRACT

We have studied by Monte-Carlo simulation (MC) the ac-susceptibility of monodisperse assembly of nanoclusters of Cobalt located at the vertices of 2 different shape lattices (oblate and prolate). Thanks to comparison of our results with theoretical ones [1], we have deduced the time δt_0 associated to one MC step. Then we have studied dipolar interactions effect (ID) on the dynamic magnetization (magnetization switching). We have found that the peak position of the out-of-phase component of ac-susceptibility shifts towards lower temperatures with increasing the strength of ID for oblate sample, which means magnetization dynamic is accelerated, and the opposite behavior have been shown for prolate one.

Keywords: ac-susceptibility, nanoclusters, dipolar interaction, magnetization dynamic, MC simulation.

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PREDICTION OF CUBIC L₆₀ STRUCTURE OF Ni₃N AND MAGNETIC PROFILE OF Ni₃N (001) SURFACES

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ABSTRACT

We present *ab initio* spin-density-functional calculations of the magnetic profile of the Ni₃N (001) surface. We use the Tight Binding Linear Muffin-Tin Orbital (LMTO) in the Atomic Sphere Approximation (ASA) [1] within the generalized gradient approximation (GGA) for the exchange and correlation functional [2]. From energetic and mechanical stability calculations, we show that Ni₃N nitride in the cubic L₆₀ structure (space group P4/mmm, $a = 3,63 \text{ \AA}$, $c/a = 0,84$) can also be stabilized as well as the hexagonal structure (P6₃22 space group) [3]. Then, we investigated the electronic and magnetic properties of Ni₃N thin layers with the L₆₀ structure for both Ni-N and Ni surface terminating, and by considering also the Ni-N mixing possibility at the top most layer. Our results show that the magnetic moment of the Ni atoms at the surface is very sensitive to the nature of the surface (Ni-N or Ni terminating) and to the number of the atomic layers considered. The Ni magnetic moment at the surface is reduced as compared to the bulk value when the outer layer is a pure Ni, and it decreases when going from the middle to the surface of the slab (Fig.1a, 1d).

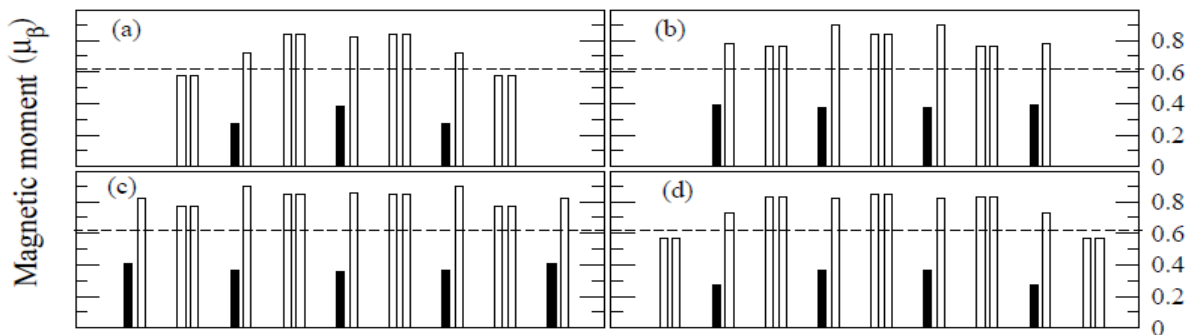


Figure 1. Magnetic profiles of Ni₃N (001) surfaces for: (a)-7 layers with a mixed central plane and with a pure Ni atoms plane at the surface, (b)- 7 layers with a pure Ni central plane and with a mixed Ni_{0.5}N_{0.5} plane at the surface (c)- 9 layers with a mixed Ni-N central plane and a pure Ni surface layer, (d)- 9 layers with a pure Ni central plane and a mixed Ni-N atoms plane at the surface. Open and dark bars atoms represent the Ni and N magnetic moments respectively whereas the horizontal dashed line indicates the Ni bulk moment.

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ELECTRODEPOSITION OF THIN MAGNETIC Ni₄₅Fe₅₅ LAYERS ONTO n-Si (111)

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ABSTRACT

Electrodeposition of NiFe film directly on n-Si (111) from acidic sulphate solutions was studied by electrochemical measurements at room temperature. Mott-Schottky measurements was used to determine the flat band potential (E_{Fb}) of the n-Si(111) in contact with the free metals-ions electroplating bath. The kinetic of deposition process was investigated by voltammetric study. The deposits were prepared under galvanostatic conditions and the effects of Fe^{2+} content on the deposit composition was studied. The morphology, structural and composition of the film were investigated by Scanning electron microscopy (SEM), Grazing X-ray diffraction and Energy dispersive spectroscopy (EDS). Magnetic characterization was investigated with a vibrating sample magnetometer (VSM), a coercivity less then (10Oe) is measured in a 350 nm Ni₄₅Fe₅₅ film thickness.

Keywords: Electrodeposition, NiFe, Silicon, Mott-Schottky, Voltammetry, magnetization

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EFFECT OF Y DOPING ON STRUCTURAL AND MAGNETO-ELECTRICAL
PROPERTIES OF $\text{La}_{0.55}\text{Bi}_{0.15}\text{Ca}_{0.3}\text{MnO}_3$ MANGANITES

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ABSTARCT

In the last years, many attentions have been given by the scientific community to the study of simple perovskite manganites that exhibit the colossal magnetoresistance (CMR) effect. These materials are very promising candidates for technological applications such as read heads for magnetic information storage, low and high magnetic field sensors and spintronics. It has been shown that the doping of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ phase by rare earth elements such as Y, Eu and Gd changes magneto-electrical properties and improves its magnetoresistance (MR) [1-3]. On the other hand, the doping by Bi raises MR to nearly 100% for an applied magnetic field of 5 Tesla [4]. In the aim to test the double effect of doping by Y and Bi in this phase, ceramic samples of nominal composition of $\text{La}_{0.55-x}\text{Y}_x\text{Bi}_{0.15}\text{Ca}_{0.3}\text{MnO}_3$ ($x= 0$ and 0.1) are prepared in air by solid state reaction and characterized. The analysis of X ray diffraction patterns shows that the samples are of high purity. The scanning electronic microscopy reveals that the doping by Y causes a significant change in the microstructure of the samples. The temperature of magneto-resistivity curves are registered from room temperature down to 50K under a magnetic field up to 5 Tesla. The doping causes a great increase of resistivity and lowers the temperature of the insulator-metal transition (T_p). In the insulating region ($T>T_p$), the resistivity curves are well fitted by the small polaron hopping mechanism while in the metallic region ($T<T_p$), the simple model of small hopping of spin-polarons is used. Some physical parameters are extracted and their evolution with doping and magnetic field are presented and discussed. The highest obtained MR values is about 91.81% and 81.73% at 5 Tesla for the undoped and the doped samples, respectively. For the undoped phase $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ and even for a higher magnetic field of 7 Tesla, the MR value does not exceed 44% [3].

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**OSCILLATIONS PERIODS OF EXCHANGE COUPLING IN ONE DIMENSIONAL
FREE STANDING CHAINS Fe_5Cr_n , $n=1-5$**

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ABSTRACT

Since the discovery of the giant magnetoresistance (GMR) in Fe/Cr trilayers [1,2], numerous investigations on Fe/Cr system, even at nanometer scale, have been performed. The interlayer exchange coupling between two successive ferromagnetic Fe layers in Fe/Cr trilayers oscillates between parallel (P) and antiparallel (AP) with a two-monolayer period of the spacer thickness of Cr layer. In this communication we performed *ab initio* calculations of the exchange coupling in one dimensional free standing linear chains Fe_5/Cr_n , $n=1-5$, in the collinear magnetic approximation while allowing inter-atomic relaxations. We find similar behavior than that obtained in Fe/Cr multilayers layers, i.e the magnetic coupling between two successive 5-Fe atoms through the Cr atoms, oscillates between AP and P with two Cr atom period (see figure). The origin of such oscillations is discussed and preliminary results with non-collinear magnetism will be reported.

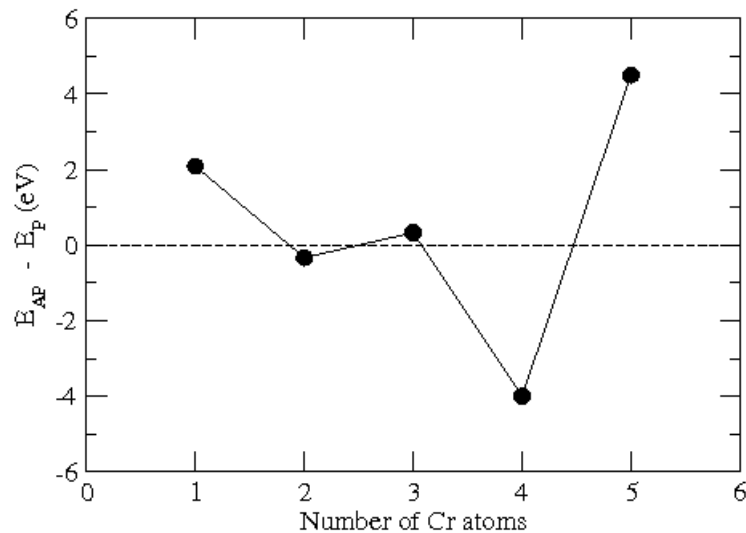


Figure: Exchange coupling in linear chains Fe_5Cr_n , $n=1-5$, as function of the number of Cr atoms

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THE RELATIONSHIP BETWEEN THE IMPURITY AND THE MAGNETIC TRANSITION
IN $\text{MnAs}_{1-x}\text{Sb}_x$ COMPOUNDS: DFT+ U CALCULATIONS

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ABSTRACT

In this work, we have performed a first-principles study to evaluate the electronic and magnetic properties of hexagonal $\text{MnAs}_{1-x}\text{Sb}_x$ up to $x = 0.125$. We have employed LDA+ U approximation within the framework of density functional theory. Calculations have been carried out in different configurations. Our results show that, with increasing the concentration of Sb, the ferromagnetic \rightarrow paramagnetic transition is localized which is in excellent agreement with the recent experimental data. The electronic properties of pure MnAs and $\text{MnAs}_{1-x}\text{Sb}_x$, such as projected densities of states, band structures and charge distribution in various $\text{MnAs}_{1-x}\text{Sb}_x$ compounds, are discussed. A model structure of 64-atoms supercell is used.

Keywords: APW+lo Method; Magnetic stability; Electronic properties; Compounds.

P23

SURFACE SPIN DYNAMICS OF SEMI-INFINITE ($S=1$) HEISENBERG FERROMAGNET UNDER THE INFLUENCE OF BIQUADRATIC EXCHANGE

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ABSTRACT

Calculations within the framework of both non-interacting spin-wave theory and random phase approximation have been carried out to investigate localized modes associated with surface spin dynamics. The context of semi-infinite ($S=1$) Heisenberg ferromagnet is considered. Emphasis has been laid upon the advantage of handling bulk and surface spin precessional fields, characterized by their symmetry in particular. The solutions are described considering the presence of both surface anisotropy and biquadratic exchange. The focus is on the existence, the nature as well as the form of bulk and surface magnetic waves. Also, the obtained solutions are discussed qualitatively by observing the response of the energy branches to the variation of both biquadratic exchange and surface anisotropy field as well as exchange parameters occurring on the surface. The theoretical formulation presented in this work provides an accurate and practical scheme for calculating surface spin dynamics and demonstrates that the occurring localized spin wave modes remains independent of the biquadratic coupling value and therefore only the surface exchange parameters play an important role in the existence of acoustic and optical surface modes. Results in some particular cases are discussed and reflect a qualitative agreement with those obtained in the literature when the Green functions approach is employed.

Keywords: Heisenberg ferromagnet. Biquadratic coupling. Magnetic surface. Elementary excitations.

EFFECT OF MAGNETIC FIELD ON CARBON NANOTUBES

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ABSTRACT

For 15 years, the fervor generated by the carbon nanotubes, at the boundary between the macro-molecule and solid, has continued to grow. The involvement of the scientific community was created after the discovery in 1991 by Sumio Iijima [1] of a new crystalline form of carbon. At that time, only three crystal forms were identified by the scientific community, and generally used in everyday life: the diamond formed by Sp^3 hybridized carbon, graphite formed by Sp^2 hybridized carbon, and fullerenes C_{60} discovered in 1985 [2], and very similar to the structure of the nanotubes.

Although derivatives of the same compound atomic, these different crystal structures have completely different properties. Carbon nanotubes are generally defined as graphene sheets rolled up, although having no reality in terms of synthesis, this view of the mind allows a simple approach of their main physical properties. In this work, we investigated the effect of applying a magnetic field on the nanotubes based on the tight-binding method combined with the Peierls substitution under a magnetic field, it is equivalent to using Bloch orbitals which satisfy the periodicity condition on the equivalent sites of the network as the basis of the system. Then we deduce electronic properties of nanotubes such as modulation of their electronic band structure. We observe in the case of a metal nanotube, opening a gap energy at the Fermi level and in the case of a nanotube semiconductor closing the gap, and the nanotube will undergo transitions metal-semiconductor. These will be made periodically with the field [3]. When the magnetic field applied is parallel to the axis of the nanotube, a metal-insulator transition Periodic in B is predicted, is the Aharonov-Bohm effect. By against, if the field is applied perpendicular to the axis of the nanotube, the rotational symmetry is broken and there is formation of Landau levels comparable to those of graphene [4].

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P25

**STUDY OF MICROSTRUCTURE AND MAGNETIC PROPERTIES OF
ELECTRODEPOSITED CoFeCu IN SELF-ASSEMBLED MESOPOROUS SILICON**

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ABSTRACT

The development of novel magnetic material has been subject of wide scientific research which has led to reduce physical dimensions. The fabricated arrays of high aspect ratio have a great interest for use as sensors and ultra high density information storage. Self assembled mesoporous silicon open new opportunities to prepare novel composite nanostructured materials exhibiting an ordering arrangement.

In this paper we report the preparation and the characterisation of CoFeCu nanostructured inside self assembled mesoporous silicon. CoFeCu thin films were electrodeposited from sulphate baths. Self-organized quazi-2D regular pore arrangements, with a diameter about 80 nm and a depth 3 μ m have been fabricated by electrochemical anodization process. The effect of current density on the morphology, microstructure and magnetic properties of CoFeCu were studied by SEM, EDS, DRX and VSM. The images SEM show the filling of CoFeCu into mesoporous layer. From hysteresis loops, the CoFeCu deposit exhibit soft magnetic properties.

P26

NUMERICAL SIMULATION STUDY FOR THE EFFECT OF APPLIED MAGNETIC FIELD ON FREE CONVECTION IN NON NEWTONIAN FERROFLUIDS

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ABSTRACT

Ferrofluids (known also as magnetic fluids) are a special category of smart nanomaterials, in particular magnetically controllable nanofluids. These types of nanofluids are colloids of magnetic nanoparticles, such as Fe₃O₄, γ -Fe₂O₃ or CoFe₂O₄, stably dispersed in a carrier liquid such as kerosene, heptane or water. Consequently, these nanomaterials manifest simultaneously fluid and magnetic properties. This fluid combines three main properties: (i) it is an efficient contrast agent for magnetic resonance imaging (MRI); (ii) its magnetic behaviour allows possible magnetic guiding towards biological site under magnetic field gradient; (iii) it can be used for treatment by hyperthermia by applying alternative magnetic field. The possibility of controlling the position and properties of a fluid using a magnetic field has opened up diverse fields of applications research. The preparation, characterization and application of MFs has attracted much attention (Vishista and Gnanam, 2004; Larachi and Desvigne, 2006; Deshpande et al., 2005; Jhon et al., 1996; Zhou et al., 2001; Meziani et al., 2006; Bossis et al., 2002b). Rheology of MFs is a major subject of investigating the flow and deformation of materials under external forces (R.Y. Hong et al., 2007; X. Yang and Aldrich, 2005; Machac et al., 1995; Dan and Mihaela, 2000). Most studies have been focused on measurement of shear stress versus shear rate (Vlaev et al., 2007; Hassanpour et al., 2007), yield stress threshold (Dang et al., 2000; Si et al., 2005; Harzallah and Dupuis, 2003; Alan et al., 2004; Byung and Winter, 2002; Vicente et al., 2004).

The present study concerns the numerical analysis of the effect of magnetic gradient field of hydrodynamic and thermal characteristics of the natural convection of an incompressible ferrofluid of constant physical and rheological properties. The MFs is confined in square cavity. The governing equations were solved using the finite volume technique developed by Patankar [1980]. The rheological model of Herschel-Bulkley are used to describe the MFs.

MAGNETIC AND STRUCTURAL PROPERTIES OF Zn DOPED Bi(Pb)₂₂₂₃ CERAMIC SUPERCONDUCTORS

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ABSTRACT

Doping with Zn change strongly the superconducting properties of high temperature superconductors reducing the critical temperature and the critical density of current. Explanations have been proposed based on very strong quasi-particle scattering rates and dramatic reduction in the order parameter near the Zn site. Scanning Tunneling Measurements in Zn doped Bi₂Sr₂CaCu₂O_{8+d} (Bi2212) crystal seems to confirm suppression of superconductivity at the Zn site[1]. Doping by Zn on Cu site of whiskers of Bi₂Sr₂Ca₂Cu₃O_{10+d} (Bi2223) phase has the same effect on the superconducting properties and particularly the transition temperature T_c which is reduced [2]. On the other hand, co doping by addition of ZnO in a lead doped Bi2223 phase (Bi_{2-x}Pb_xSr₂Ca₂Cu₃O_{10+d}) shows no influence on the T_c but a reduction of the critical current density J_c [3].

The samples of Bi_{1.6}Pb_{0.4}Sr₂Ca₂Cu_{3-y}Zn_yO_{10+d} where y varies from 0 to 0.05, have been prepared using the conventional solid-state reaction technique. Microstructure of the prepared samples was investigated by X ray diffraction (XRD) and scanning electronic microscopy (SEM). AC susceptibility measurements were made on a SQUID magnetometer. Indexation of the peaks and determination of cell parameters has been made by use of CELREF software. The results show an effect of the doping on the microstructure and the critical temperature T_c. Cell parameters c diminishes when the rate y of zinc increases. Zn doping has an effect on the critical temperature T_c and on the apparent superconducting volume fraction.

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P28

CARBON COMBUSTION SYNTHESIS OF SOME FERRITES: A SIMPLE METHOD TO GET NANOSIZED GRAINS BULK MATERIALS

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ABSTRACT

In this work we present a fast, novel, and economical process to produce nanostructured bulk materials of some spinel ferrites MFe_2O_4 ; this so called method: Carbon Combustion Synthesis of Oxides (CCSO) is a modified SHS process (Self propagating High temperature Synthesis). Several perovskite oxides have been successfully obtained by this easy synthesis method, introduced by Martirosyan and Luss [1-4], which uses carbon as a fuel instead of a pure metal such as in standard SHS. In CCSO of nanostructured materials, the exothermic oxidation of carbon nanoparticles generates a thermal reaction wave with temperature of up to 1200°C that propagates through the solid reactant mixture, converting it to the desired complex oxide product. The carbon is not incorporated in the solid product and is released in CO_2 gas from the sample. As it is well established nowadays, nano-materials had better performances, but the challenge is still to obtain a good product with better properties together with minimizing the cost of fabrication and with tailoring the physical properties of the material according to the desired application. In CCSO synthesis method, characteristics of the obtained materials, especially the particle size, depend on the concentration of carbon used, together with rate of oxygen flux necessary to propagation of combustion wave.

Keywords: Carbon combustion synthesis, spinnel ferrite, MFe_2O_4 , nanomaterials.

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EFFECT OF SUBSTRATE ON THE STRUCTURAL AND MAGNETIC PROPERTIES OF EVAPORATED Ni THIN FILMS

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ABSTRACT

Series of Ni thin films have been deposited by thermal evaporation onto glass, Si(100), Cu, mica and Al₂O₃ substrates. The Ni thicknesses, t , are in the 5.5 to 100 nm range. The effects of substrate and thickness on the structural and magnetic properties of Ni are investigated. The texture, the strain and the grain size values were derived from X-ray Diffraction (XRD) experiments. The Ni films grow with the $\langle 111 \rangle$ texture on all substrates. The Ni grain sizes D increase with increasing thickness for the glass, Si and Mica substrates and decrease for the Cu one. The strain ϵ is positive for low thickness, decreases in magnitude and becomes negative as t increases. Magnetic properties were inferred from the Vibrating Sample magnetometer (VSM) set-up. Hysteresis curves show an in-plane magnetic anisotropy for all samples. There is a monotonous increase of the coercive field H_C with increasing thickness regardless of the substrate. For the thinnest sample (5.5 nm), the smallest H_C value (about 4 Oe) seems to be independent of the substrate (glass, Si, Cu). As t increased, the Ni/Si(100) system shows the highest H_C value. The squareness S depends on substrate and t and seems to be relatively large in Ni/glass and small in Ni/Cu. All these results will be discussed and correlated.

Keywords: Ni thin films, Evaporation, XRD, Hysteresis curves.

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**MICROSTRUCTURE AND MÖSSBAUER SPECTROSCOPY OF NANOSTRUCTURED
Ni₃Fe INTERMETALLIC**

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ABSTRACT

Ni₃Fe samples were elaborated at different milling times (0-96 h) by using the vario-planetary ball mill system. The intermetallic Ni₃Fe formation and different physical properties were investigated as a function of milling time, t, by means on the Scanning Electron Microscopy (SEM), Energy Dispersive X-ray (EDX) and Mössbauer Spectroscopy. Particles morphology at different formation stages was observed by SEM. From SEM micrographs, we show that the particles becomes round in shape and finer in size when the milling time increases. Elemental mapping experiments (EDX) were performed on the samples. After 6 h of milling, it becomes difficult to distinguish between Ni and Fe particles; this indicated the beginning of Ni and Fe alloying process; however, elemental Ni and Fe are still observed. For milling time of 24 h, the elemental maps indicate that the Fe and Ni elemental distributions are closely correlated indicating that the two elements are completely alloyed and the Ni(Fe) solid solution is formed. The Mössbauer experiments were performed in order to follow the formation of Ni₃Fe compound as a function of milling time. From the adjustment of Mössbauer spectra, we extracted the hyperfine parameters (hyperfine magnetic field and isomeric shift). The evolution of hyperfine magnetic field shows that the magnetically disordered Ni₃Fe phase starts to form after 6 h of milling and grow in intensity with milling time. For the milling time greater than 24 h, only the Ni₃Fe disordered phase is present with a mean hyperfine magnetic field of about 29.5 T.

Keywords: Ni₃Fe intermetallic compound, nanostructured powders, SEM, microstructure, Mössbauer spectroscopy, hyperfine parameters.

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ELABORATION, MICROSTRUCTURE AND MAGNETIC PROPERTIES OF
(Fe₇₀Al₃₀)_{100-x}Si_x NANOMATERIALS

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ABSTRACT

Nanocrystalline (Fe₇₀Al₃₀)_{100-x}Si_x alloy (with x= 0, 5, 10, 15 and 20) were synthesized by mechanical alloying method (MA) for a milling time of 72 h. The milled samples were characterized by X-ray diffraction (XRD), Electron Scanning microscopy (SEM) and Vibrating sample magnetometer (VSM). From X-ray diffraction (XRD) spectra, we have shown that as Si content increases from 0 at.% to 20 at.%, the grain size decreases slightly from the 11 nm to 8 nm and the lattice parameter decreases monotonically from 0.2890 nm to 0.2842 nm. From SEM micrographs, we showed that the particle becomes more finer and rounded in shape with increasing Si at.%,. The saturation magnetization, Ms, and coercive field, Hc, values were extracted from hysteresis curves. The behaviors of Ms and Hc were discussed as a function of Si at.%.

Keywords: (Fe₇₀Al₃₀)_{100-x}Si_x alloy; mechanical alloying; XRD, SEM, hysteresis curves

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**MICROSTRUCTURE AND MOSSBAUER STUDY OF NANOCRYSTALLINE
Fe₈₀Ni₂₀ POWDERS PREPARED BY MECHANICAL ALLOYING**

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ABSTRACT

Nanostructured Fe₈₀Ni₂₀ powders were prepared by mechanical alloying of elemental powders in a vario-planetary high energy ball mill under argon atmosphere. The formation of alloy, morphology changes and hyperfine properties were investigated as a function of milling time (in the 0-25 h range) by scanning electron microscopy (SEM), energy dispersive X-ray analysis and ⁵⁷Fe Mössbauer spectroscopy. The powder particle morphology and the maps of Ni and Fe distribution were observed by SEM at different milling times. From the adjustment of Mossbauer spectra, we have shown that the Fe₈₀Ni₂₀ phase starts to form after 3 h of milling and grow in intensity with milling time. The complete formation of Fe₈₀Ni₂₀ compound was observed after 10 h milling. We have also show that the Mossbauer spectroscopy is able to detect the grain boundaries.

Keywords: FeNi alloys; nanostructured powders; microscopy; Mössbauer effect.

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MAGNETISM IN ULTRA-THIN FILMS OF FeGe(111)

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ABSTRACT

We investigated the magnetic structure of Fe ultrathin films on Ge(111) in diamond structure, using *ab initio* density functional theory within SIESTA code. From total energy calculations, it is showed that the magnetic ground state is determined by chemical composition of the atomic surface. Contrary to tetragonal Fe₂Ge₄ (100) films [1, 2] which present a magnetic transition from ferromagnetism to antiferromagnetism when the thickness of the film is increased, the FeGe(111) films are ferromagnetic when Fe atoms are on the surface. Concerning Ge terminated films, the ground state is antiferromagnetic. A strong increase of the magnetic moments, up to 3 μ_B on Fe atoms present at the surface is observed.

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**MAGNETO-ELECTRICAL PROPERTIES OF THE DOUBLE LAYERED MANGANITES
La_{1.2}Re_{0.2}Ca_{1.6}Mn₂O₇ (Re=La, Pr, Y)**

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ABSTRACT

The magneto-electrical properties of the double layered manganites La_{1.2}Re_{0.2}Ca_{1.6}Mn₂O₇ (Re=La, Pr, Y) showing the colossal magnetoresistance effect have been investigated from room temperature down to 4K. The metal to insulator transition temperature (T_{MI}) increases with increasing magnetic field H. A combination of residual resistivity, weak localization, electron-electron and electron phonon interactions models [1] is found to be the best way to fit the resistivity versus temperature curves in low temperature range ($T < 50K$), while the 3D variable range hopping is the best model fits well resistivity curves in the high temperature range ($T_{MI} < T < 300K$). Mott's activation energy decreases with increasing H, while the density of states near the Fermi level $N(E_F)$ increases, which explain the difference in the resistivity curves for the samples at high temperatures. These results are consistent with earlier report [2]. The ferromagnetic fraction phase $f(T,H)$, which is estimated from the fit of resistivity curves in the entire temperature range by use of the percolation model [3], increases with increasing magnetic field in accordance with the observed increase of T_{MI} .

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ELECTRONIC AND MAGNETIC PROPERTIES OF IRON ATOMS IN SILICON CAGE CLUSTERS

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ABSTRACT

In this his work we present a theoretical investigation of electronic and magnetic properties of different $Si_{n-m}Fe_m$ clusters with different sizes ($19 \leq n \leq 24$), ($1 \leq m \leq 3$) using a molecular dynamics (MD) simulation based on density functional theory with generalized gradient approximation (GGA) implemented in SIESTA packages [1-2]. We find that the encapsulation of Fe atoms within silicon clusters leads to stable silicon cage clusters when compared to the clusters with the same size of pure silicon [3-4]. This suggests that the impurity Fe atom increases the stability of some doped silicon clusters. This is due to the improvement of some bond strength, particularly in the case of one and two Fe atoms. It is also seen that the Fe doped silicon clusters have large HOMO-LUMO gap for spin up electrons while those with spin down electrons have a very small HOMO-LUMO gap. This trend will have an interesting repercussion on electronic conductance through these clusters which could be considered as interesting properties in spin electronics applications for example as spin filter. The silicon clusters which are not magnetic in their pure state become magnetic after the substitution of Fe atoms in the structures and the magnetic moment increases with increasing the number of Fe atoms in the cluster. The magnetic character observed in our clusters is due to the charge transfer between d atomic orbitals of Fe atoms and the s atomic orbitals of Si atoms which implies that Fe atoms act as electron donors [5].

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ELECTRONIC AND MAGNETIC STRUCTURE OF ABO_3 PEROVSKITES

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ABSTRACT

The electronic and magnetic structures of orthorhombic perovskites ABO_3 ($A = \text{Er, Gd, Tb}$ and $B = \text{Mn, Fe, Co}$) are studied using *ab initio* density functional theory in the local density approximation (LDA) with the on-site Hubbard U_{eff} parameter (LDA+ U). To show A and B -cation effect, we have analyzed the structural parameters, spin and charge density and total and partial density of states. We also show how the results can be made relatively insensitive to the choice of cation and to ion size. The effect of the Hubbard correction is investigated and is found to be a necessary requirement for the accurate description of both the unit cell structure and the magnetic moment. Valence electronic structures obtained from subsequent LDA+ U calculations are compared and discussed.

Keywords: DFT+ U ; APW+lo; Magnetic structure; Strongly correlated systems; Perovskites.

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HYDROMAGNETIC STABILITY IN CONICAL TAYLOR-COUPETTE FLOW SYSTEM

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ABSTRACT

Taylor vortices have been studied experimentally and theoretically by G.I Taylor [1]. There have many experiment, theoretical, and numerical investigations of the formation of Taylor vortices in axisymmetric cells other than that formed by coaxial concentric circular cylinders. Among these geometries cones [2-7], M.A. Sprague et al. [7] investigated the stability of circular Couette flow in discontinuous asymmetric geometries using numerical simulation and physical experiment.

We present a set of three dimensional numerical simulations of the Taylor Couette flow between concentric cylinders with different apex angles, so we go from classical cylinder T-C to conical T-C system, We seek the onset of the first instability and we compare the obtained results for different velocity rates, we calculate the critical Taylor number corresponding to each geometry then we apply an axial magnetic field of different intensities in order to show his effect on flow patterns and pressure field.

The flow is subjected to the influence of the magnetic field; we note radical change in the flow structure. It would be interesting to extend the prediction for a fixed taper angle α versus a magnetic induction variable and vice versa.

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**THEORETICAL STUDY OF ELECTRONIC AND MAGNETIC PROPERTIES
OF THE HALF-HEUSLER ALLOYS PdCoX (X= Ga and Sn)**

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ABSTRACT

The electronic structure and magnetic properties of the half-Heusler alloys PdCoX (X= Ga and Sn) were calculated by using the self-consistent full potential linearized augmented plane wave method within the generalized gradient approximation (GGA) for the electronic exchange and correlation. The total energy minimization of the two phases non-magnetic and ferromagnetic indicates that the latter is the most stable one. Densities of valence state, magnetic moment and band structure are analyzed and discussed.

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MONTE CARLO STUDY FOR MAGNETIC THIN FILMS

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ABSTRACT

Today, the theoretical study and modeling of physical phenomena of major interest in technology is the basis of scientific research. Using mathematical models and by numerical simulations to treat different systems: spin systems, particle systems, magnetic materials, polymers, membranes, etc...

We have done during our work a theoretical study on Monte Carlo methods based on their applications in statistical physics. These methods are consisted to simulate a stochastic phenomenon on computer, it allows us to generate a large number of spins configurations in a magnetic material, according to a probability proportional to the Boltzmann law, and make statistical averages of the macroscopic characteristics quantities of the system: magnetization, mean energy, specific heat, etc [1].

To indicate the confidence intervals that can be obtained for numeric values and the precision that the Monte Carlo method provide; studying the magnetic properties of trilayer Fe/Ag/Fe by this code was our implementation, we determined their spin configurations and plotting the corresponding hysteresis curves.

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ELECTROCHEMICAL PRODUCTION OF Co-Mo FILMS: EFFECT OF THE DEPOSITION POTENTIALS ON THE DEPOSITS PROPERTIES

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ABSTRACT

In the nanometer scale, magnetic materials show new physical and chemical properties that are different from those obtained in the bulk state. Generally, these materials are elaborated by physical vapor deposition techniques such as sputtering or molecular beam epitaxy (MBE). Recently, the electrodeposition has been employed as an alternative technique in the production of nanostructures with very interesting magnetic properties [1, 2]. Various works on the electrodeposition of Co-Mo thin films on metallic surfaces have been carried out [3, 4]. The film growth was controlled by deposition parameters such as electrolyte bath composition, pH, deposition potential or current density, temperature, agitation or electrodeposition dynamics. In the present study, a Co-Mo thin films with metallic appearance were obtained on Ru substrates from aqueous sulphate solution without additives at pH=4. The reaction of electrodeposition of Co-Mo alloy is controlled by the diffusion of the electrochemical species. Thus, the process of nucleation is in good agreement with the instantaneous nucleation and three-dimensional (3D) diffusion-limited growth. The morphology and the degree of cristallinity depended on the applied potential: when the potential was more negative the deposit was will crystallized. The Co-Mo coatings showed lower values of coercivity which are suitable for magnetic applications. Its well established that the electrodeposition parameters such as the applied potential have a great influence on the structure, morphology and magnetic properties.

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SPIN WAVES TRANSMISSION BY AN INTERFACE IN FCC ULTRA THIN FILMS

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ABSTRACT

Spin wave excitations through the (001) interface between two Fcc thin films ferromagnetic, is investigated in the context of the Heisenberg model. The model system A/B/A consists of two thin films FCC (001) ferromagnetically ordered crystal A joined by an interface B. It is applied to the system Ni / Fe /Ni .

The thin film dynamics and the spin waves diffusion, which are the magnetic excitations being propagated collectively on the atomic sites of the plans constituting the ferromagnetic film, by the magnetic interface are the subject of our study. The spin dynamics, localized spin states, magnon transmission and the localized density of spin states (LDOS), are calculated and analyzed for the ultra thin film.

The theoretical calculations are carried out using the matching method. The spectrum of these bound states was calculated for a number of different sets of parameters. The spin waves associated to the interface zone interact with each other, leading to interesting magnetic behaviors. For the system, we analyze the magnon conductance under three different possibilities as regards the inter-atomic magnetic exchange on the interface domain in comparison with that for the bulks of the Fe and Ni systems. We found that the spin waves are localized in the neighborhood of the interface, and this system can be used as a filter to the spin waves.

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THERMAL HYSTERESIS IN SPIN CROSSOVER NANOPARTICLES USING A DEFORMABLE LATTICE MODEL: A MONTE CARLO STUDY

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ABSTRACT

We analyzed the size effect of spin-crossover nanoparticles in a two-dimensional core-shell model, where the edge atoms are constrained to the HS state. By Monte Carlo(MC) simulations, the obtained step transition is analyzed in term of LS-LS, LS-HS and HS-HS populations. We have also investigated the size dependence of the transition temperature, and found that the later decreases drastically for small sizes, also we have shown in this work, the thermal behavior of the HS fraction, calculated for various particle sizes. The experimental behaviors [1,2] are reproduced: upon decreasing particle size the transition temperature is downward shifted.

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EFFECT OF LI DOPING ON ELECTRONIC AND MAGNETIC PROPERTIES OF SMALL Pt CLUSTERS

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ABSTRACT

Density functional theory is used to study electronic, geometric, and magnetic properties of pure Pt_n ($n=1-4$) and Pt_mLi ($m=1-3$) clusters in their ground state and those of their closest states. Optimised equilibrium bond lengths, adsorption and binding energies, and total magnetic moment are determined. The chemical properties of the clusters are tested via adsorption of atomic hydrogen, where a systematic study of the preferred adsorbate adsorption site is performed. The adsorption energy of hydrogen atom is found to be higher for the Li doped clusters. The small size of hydrogen may favor top or bridge sites depending on the cluster morphology. Our calculations are in good agreement with results reported by other authors [1-7]. An analysis of the charge transfer and the distribution of the electronic population show that the clusters become more polarised after H adsorption.

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SPIN WAVE DYNAMIC AT THE ATOMIC STEP

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ABSTRACT

We investigate the spin wave spectra at domain boundaries of the isolated atomic step. The defect breaks translation symmetry in the direction normal to the defect domain boundary, which induces the localized modes effects. The theoretical model of matching method and Green functions, are used to determinate the characteristic spin wave deviation, spectral densities and densities of states, of the spin precession components of the individual atomic sites that constitute a complete representation of the inhomogeneity domain boundaries. The variations of these spin precessional deviation spectra due to various values of exchange integral parameters in the soliton domain boundary are determinate. It is shown that the calculated spin wave spectra are sensitive and explicit signatures for the softening and hardening effects. Numerical results show characteristic interference effects between the incident spin-waves and the localized magnons at the step boundary.

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STUDY OF THE THERMO-MAGNETIC FLUCTUATIONS IN CARBON NANO-TUBES
ADDED BI-2223 SUPERCONDUCTORS

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ABSTRACT

We have investigated the effect of addition of carbon nano-tubes (*CNT*) on the properties of $\text{Bi}_{1.6}\text{Pb}_{0.4}\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_y$ superconductors. The samples are prepared from commercial powders with addition of zero and 0.1 wt% of *CNT*. They are characterized by XRD, SEM and magneto-resistivity in the transition region. As it was reported for *CNT* added Y-123 compounds [1], the refined cell parameters are practically independent of this kind of addition. Under applied magnetic field, a large broadening of resistive transition is observed. This is a direct evidence for the thermal fluctuations in the vortex system. The modified vortex-glass to liquid transition theory is used to calculate the values of the glass-transition temperature T_g and the temperature and magnetic field dependent activation energy $U_0(B, T)$ [2]. These parameters are seen to decrease with *CNT* addition and applied magnetic field. Also, we have found that the undoped sample proves a better transition width, residual resistivity (ρ_0) and a higher onset critical transition temperature of about 119.1 K. Also, the appearance of a double resistive transition for both samples is a confirmation of the existence of a secondary phase which plays the role of the weak links at the grain boundaries [3].

Keywords: Bi-2223 phase, addition, flux pinning.

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MAGNETIC PROPERTIES OF Fe-S FREE STANDING CLUSTERS

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ABSTRACT

Iron-sulfur clusters are best known for their properties in the electron transfer process [1]. They have even been postulated to have played a key role in the evolution of life [2, 3]. Today we know that they are also involved in many other functions such as substrate binding, catalysis, regulation, and sensing [4]. This work reports density functional calculations of geometric, electronic and magnetic order in free standing iron-sulfur clusters with stable composition $Fe_nS_m^{-/+}$, $n=m$, $m\pm 1$, ($n=1-4$) observed experimentally in gas phase. We investigate neutral, anionic and cationic clusters using a method that employs linear combination of atomic orbitals as basis sets, non-local norm-conserving pseudopotentials and a generalized gradient approximation to exchange and correlation. The results are discussed in connection with available experimental data. In all cases, anti-ferromagnetic (-ferrimagnetic) order between Fe atoms is always preferred to ferromagnetic and paramagnetic ones. For Fe_2S_2 , Fe_3S_4 and Fe_4S_4 clusters which are the most frequently contained ones in proteins, the geometric distortions induced by magnetism decrease with cluster size and the maximum deviation between Fe-Fe distances is 11% in Fe_2S_2 , but only ~3% in Fe_4S_4 . Similar tendencies are obtained for other Fe:S compositions.

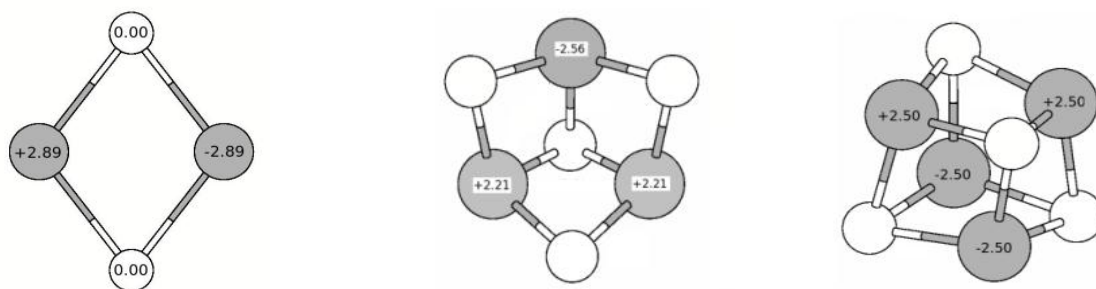


Figure: Optimized geometries of neutral Fe_2S_2 , Fe_3S_4 , and Fe_4S_4 clusters in their anti-ferromagnetic (-ferrimagnetic) spin arrangement with their corresponding moments. The grey and white spheres represent the Fe and S atoms respectively.

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NON-COLLINEAR MAGNETISM IN MnS FREE STANDING CLUSTERS

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ABSTRACT

Transition-metal sulfur clusters are appealing in many fields ranging from catalysis to biology and material science. Their potential relationships with biology and nanotechnology, in particular, are exemplified by the iron-sulfur clusters which are involved in the electron transfer process as well as in many other functions such as substrate binding, catalysis, regulation, and sensing [1-4]. Manganese sulfur clusters have shown to form similar gas phase species [5,6], and thus are also expected to have important technological applications. In the present communication, we report density functional calculations, within the local spin density approximation for the exchange and correlation, of the equilibrium geometries and non-collinear spin-polarized electronic structure of Mn_xS_2 clusters ($x=1-4$). We investigate clusters with stable compositions observed in gas phase and we show that, as in the pure Mn clusters, non-collinear magnetism is also present, a fact that was not reported before.

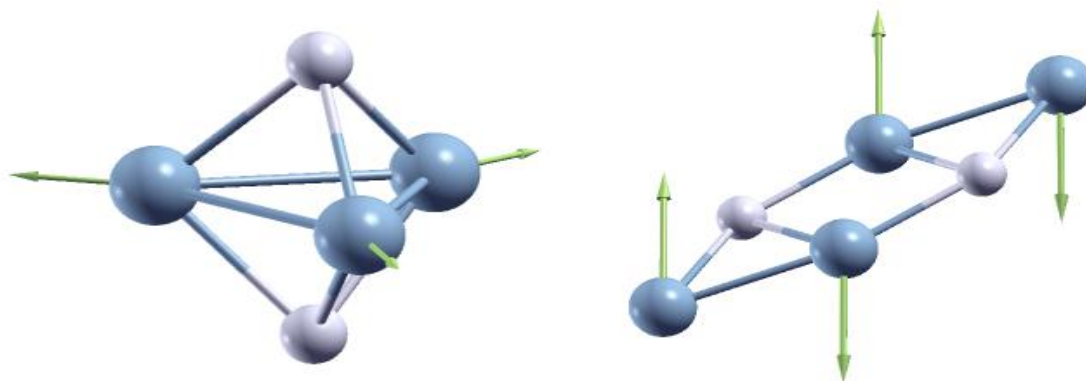


Figure: Lowest-energy isomers of Mn_3S_2 and Mn_4S_2 with the direction and magnitude of the magnetic moments on the Mn atoms. The S atoms remain unpolarized

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