

Magnetism from lodestone to plastics

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Abstract : Magnetism abounds in dichotomies. Humans have wondered about and used magnetism since the discovery of lodestone more than four thousand years ago. This invited talk aims to review the developments of the magnetic phenomena. Special importance is attached to recent advances in magnetic materials such as magnetic multilayers, half metallic magnets, coexistence of ferromagnetism and superconductivity, spintronics and, last but not the least, photo induced magnetism in plastic materials.

Keywords : History of magnetism, magnetic multilayers, half metallic magnets, spintronics and photo induced magnetism.

PACS Nos. : 75.20.-g, 75.70.Cn, 76.60.Cq, 78.20.Ls.

An electrical network model of plant intelligence

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Abstract : A simple electrical network model, having logical gate capacities, is proposed here for computations in plant cells. It is compared and contrasted with the animal brain network structure and functions.

Keywords : Artificial intelligence, neural networks, logic gates, membrane I-V characteristics, plant vacuolar membrane.

PACS NOs. : 84.35.+i, 87.10.+e, 87.18.Sh

Magnetic relaxation in nano-particles : a Mössbauer study

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Abstract : Ultra-fine superparamagnetic particles of iron compounds with size 50 to 125 Å probed through Mössbauer spectroscopy usually show magnetic relaxation effects at low temperatures. A magnetic sextet is observed for long relaxation times compared to nuclear lifetime whereas the magnetic interaction disappears for short relaxation times and this change usually occurs between 25 to 100 K. A theoretical model has been developed for the magnetic relaxation process considering that on microscopic level it involves an exchange of energy between magnon and phonon sub-systems *via* magnon-phonon scattering induced by dynamic exchange. It is seen that the relaxation rate increases with temperature in a complicated manner besides its dependence on the number of magnetic ions or particle-size. The calculated rates appear consistent with the observed Mössbauer results at low temperatures for some of the iron oxides.

Keywords : Nano-particles, superparamagnetic relaxation, magnon-phonon interaction, Mössbauer study.

PACS Nos. : 76.30.Fe, 76.80.+y

Critical behaviour of stiff polymer near the surface

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Abstract : We use the self-avoiding walk models to investigate the adsorption transition of semi-flexible homopolymer chain in two and three dimensions. The exact-enumeration method has been used to locate the transition points. The results obtained from this method have been compared with the exact results found for the directed walk model of semi-flexible polymer.

Keywords : Semi-flexible polymer, adsorption, stiffness.

PACS Nos. : 05.70.Fh, 64.60.Ak, 05.50.+q

Fano resonances in presence of dephasing and evanescent modes

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Abstract : In this work we analyze the effect of incoherent transport on Fano resonances. In close proximity to recent experimental results we find the transition from Fano to Lorentzian line-shapes with increasing incoherence. In the presence of evanescent wave propagation in the AB interferometer with a quantum well no Fano line shapes are observed. Only when one arm of the AB interferometer is made propagating do we recover Fano line-shapes.

Keywords : Dephasing, evanescent modes, Aharonov-Bohm rings, Fano resonances.

PACS Nos. : 72.10.-d, 73.23.-b, 05.60.Gg, 85.35.Ds

Mössbauer, EPR and IR studies of some (Pb,Fe)TiO₃ and (Sr,Fe)TiO₃ ceramic dielectrics

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Abstract : Perovskites of ABO₃ structure, like well known PbTiO₃ and BaTiO₃, have dielectric constants of a few hundred. Several ceramics synthesised partially with other divalent, tetravalent and pentavalent atoms show high dielectric constants and behave as relaxors, useful for electronic components, and hence their characterisation is important. Mössbauer, EPR and IR methods are effective for polycrystalline materials containing some iron, and therefore lead and strontium titanates with Fe were prepared for studies by these techniques. Strontium titanate, cubic at 295 K, was chosen as a reference lattice to see how iron doping changes its structural properties. Their IS, QS and g-values correspond to Fe(III) state. The strong IR bands at around 410 and 600 cm⁻¹ arise from the TiO₆ and FeO₆ polyhedra respectively.

Keywords : Dielectric materials, Mössbauer, EPR, IR spectra.

PACS Nos. : 76.30.Fe, 76.80.+y

Effect of static Jahn-Teller distortion on magnetism in the manganite system : $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$

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Abstract : The colossal magnetoresistance manganite system is described by a simple Hamiltonian containing the hopping term arising out of the itinerant e_g electrons of Mn atom in presence of a static band Jahn-Teller lattice distortion and the external magnetic field in the same e_g band. The ferromagnetism originates due to the more localized core t_{2g} electrons. The itinerant e_g electrons are hybridized with the on-site t_{2g} electrons with a strong hybridization. The magnetization (m) and lattice strain (ϵ) are considerably influenced by the model parameters of the system : *i.e.* the t_{2g} level (d), hybridization (v), magnetic coupling (g_1), J-T coupling (g), external magnetic field (b) and the impurity concentration (x). In same situations the ferromagnetic metallic state is pushed to higher temperatures. The results are discussed.

Keywords : Electron-electron interaction, magnetically ordered materials, exchange and super exchange.

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Superconducting gap excitations in Raman spectra of CDW systems: 2H-NbSe₂ revisited

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Abstract : The phonon spectral function for charge density wave (CDW) system in the superconducting (SC) phase is calculated for finite wave vectors (q). An exact expression for the q dependent phonon self-energy is obtained. The analysis is carried out with $q = 0$ limit. The spectral function shows a peak for frequency ω less than the SC energy gap ($2D$) for $q = 0$. The temperature dependence of the Raman peak is discussed with variation of the electron-phonon coupling (s), superconducting gap parameter (z), temperature (t), half-width of the peak (e) and the charge density wave frequency (p). The results are discussed in context with the Raman scattering observations of SC gap excitations in 2H-NbSe₂ (a layered compound exhibiting both CDW and SC transitions) by Sooryakumar and Klein.

Keywords : Charge density wave superconductor, Raman spectra, electron-phonon interaction.

PACS Nos. : 71.45.Lr, 78.30.-j, 71.38.-k

A model study of gap equation in the heavy fermion superconductors

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Abstract : The superconducting order parameter due to conduction electrons and the sub-lattice staggered field parameter due to the weakly delocalized f -electrons are calculated by Zubarev type Green function method for the heavy fermion magnetic superconductors. We solved the self-consistent mean field equations for the superconducting gap and the staggered field. The mutual influence on each other is studied by varying model parameters of the systems : the superconducting coupling (g_1), antiferromagnetic coupling (g_2), the hybridization (v) for various temperature ranges. The results show a strong correlation between them through the suppression and enhancement of the order parameters and transition temperatures as well as a few anomalous results. This model can explain the strong coupling between magnetism and superconductivity in the UM_2Al_3 and similar U-based systems.

Keywords : Heavy fermion superconductor, narrow band system, local moment in heavy fermions.

PACS Nos. : 74.70.Tx, 71.28.+d, 75.20.Hr

Normal state Raman spectra of high- T_c cuprates

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Abstract : We present a microscopic theory to explain Raman spectra of high- T_c cuprates $R_{2-x}M_xCuO_4$ in the normal state. We used electronic Hamiltonian prescribed by Fulde in presence of anti-ferromagnetism. Phonon interaction to the hybridization between the conduction electrons of the system and the f -electrons has been incorporated in the calculation. The phonon spectral density is calculated by the Green function technique of Zubarev at zero wave vector and finite (room) temperature limit. Parameter dependence of Raman active phonon frequencies are studied by varying model parameters of the system *i.e.* the position of f -level ($\hat{I}_f$), the effective electron-phonon coupling strength (g), the staggered magnetic field (h_1), and the hybridization parameter (v). The four Raman active peaks (P_1 to P_4) represent the electronic states of the atomic sub-systems of the cuprate systems. They show up as phonon excitations due to the coupling of the phonon to the electrons and the anti-ferromagnetic gap.

Keywords : Anti-ferromagnetic order, electron-phonon interaction, Raman scattering.

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Annealing effect on the Giant magnetoimpedance of amorphous microwire

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Abstract : Giant magnetoimpedance (GMI) effect in positive magnetostrictive glass-coated amorphous $\text{Co}_{83.2}\text{Mn}_{7.6}\text{Si}_{5.8}\text{B}_{3.3}$ microwire has been studied as a function of a dc magnetic field $-140 < H_{dc} < 140$ Oe and frequency $0.1 < f < 12.85$ MHz. A maximum change of 43% in MI of the as-quenched sample has been observed around 5 MHz frequency. Heat treatment of the sample by passing a dc current of 50 mA through it enhances the MI value to a large extent (maximum change ~94%) by increasing the outer domain volume and inducing a transverse anisotropy. The magnetization of the as-quenched and heat-treated samples has also been studied to understand the domain structure and magnetoimpedance results.

Keywords : Giant magnetoimpedance, amorphous, microwire.

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Effect of alloying on the kinetics of CO + O₂ and CO + NO reactions on Pt-Rh nanocatalysts : a theoretical model

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Abstract : Surface Chemistry Reaction Model has been used to study the kinetics of CO + NO and CO + O₂ reactions on Pt-Rh nanocatalysts. For CO + O₂ reaction the alloy particles evince an intermediate behaviour; however, for the CO + NO reaction the alloy particles show no synergistic effect of alloying. The inherent rate of CO + O₂ reaction is much higher than that of CO + NO reaction on the Pt₅₀Rh₅₀ nanoparticles. The kinetics of the CO + NO + O₂ and CO + NO reaction on the alloy particles are almost the same. NO inhibits formation of CO₂ molecules. The simulated results are in qualitative agreement with the experimental findings.

Keywords : Surface Chemistry Reaction Model, nanocatalysts, Monte Carlo simulation.

PACS Nos. : 68.43.Mn, 82.20.pm, 82.65.+r, 82.45.Jn, 82.20.Wt

Ordering potential – the anomalous structure and properties of liquid LiNa alloy

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Abstract : Using pseudopotential theory the *ab initio* calculation for ordering potential of liquid LiNa alloy is presented. Taking into account the electronic charge transfer and also charge neutrality condition we find the effective valencies in the alloy. We then use the model to obtain the Bhatia-Thornton structure factors, particularly at null alloy concentration ($\text{Li} = 0.61$). The calculations of concentration fluctuation and other related thermodynamic properties show that this ordering potential approach works reasonably for this phase-separating (ps) liquid alloy system.

Keywords : Ordering potential, structure, liquid alloy.

PACS Nos. : 61.25.Mv, 61.20.Gy

Variation of the intermolecular distance with temperature of the mesogen CCH₅

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Abstract : The cyanocyclohexyl cyclohexane CCH₅ (C₁₈H₃₁N) shows the following phase transitions :

62°C 85°C
Solid $\rightarrow$ nematic $\rightarrow$ isotropic
Smectic 1 $\xrightarrow{39^\circ\text{C}}$ smectic 2 $\xrightarrow{50^\circ\text{C}}$ nematic

X-ray diffraction studies have been conducted on the mesogen in the solid and liquid phases. However, the temperature variation of its parameters namely apparent molecular length/layer thickness/and intermolecular spacing D in the liquid mesophase has not been determined to date. In the present work, X-ray photographs of the sample in the liquid phase has been taken at different temperatures and the variation of intermolecular separation with temperature determined. The results have been compared with X-ray data in the solid phase.

Keywords : Mesogen, thermotropic, X-ray, intermolecular distance.

PACS Nos. : 61.30.-v, 61.10.Nz.

Structural and dielectric properties of KLiMoO₄ ceramic

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Abstract : Potassium lithium molybdates (KLiMoO₄) ceramic has been prepared by solid state reaction technique. Preliminary structural study suggests the formation of single phase (monoclinic) compound at room temperature. The variation of dielectric constant and loss as a function of temperature (from room temperature to 250 °C) at 1 kHz and 10 kHz exhibits dielectric anomaly and sequential phase transitions at $T_{C1} = 134^\circ\text{C}$ and $T_{C2} = 48^\circ\text{C}$ respectively. A comparison of various properties of KLi(Mo_xW_{1-x})O₄; $x = 0$ [*J. Mater. Sci. Lett.*, **16** 1807 (1997)], 0.5 [*J. Mater. Sci. Lett.*, **18** 501 (1999)] and 1.0 ceramics have also been made. The ferro-paraelectric phase transition (T_{C1}) has been found to be first order Curie-Weiss type.

Keywords : Phase transition, dielectric constant, structure.

PACS Nos. : 77.22.Gm, 61.10.Nz, 77.80.Bh.

Phase transition in $\text{Pb}(\text{Mg}_{1/4}\text{Co}_{1/4}\text{W}_{1/2})\text{O}_3$ ceramics

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Abstract : Polycrystalline samples of $\text{Pb}(\text{Mg}_{1/4}\text{Co}_{1/4}\text{W}_{1/2})\text{O}_3$ ceramics were prepared by the high-temperature solid-state reaction technique. Preliminary crystal structure and microstructure of the compound at room temperature were studied using the X-ray diffraction (XRD) technique and scanning electron microscopy (SEM) respectively. Detailed dielectric studies suggest that the compound undergoes successive phase transitions at 87°C and at 105°C. Variation of dc conductivity as a function of temperature suggests the semiconductor characteristics of the material.

Keywords : Successive phase transitions, orthorhombic, dielectric, dc conductivity, XRD.

PACS Nos : 77.22.Gm, 61.10.Lx, 77.80.Bh

Studies of structural and electrical properties of some tungsten-bronze ferroelectric ceramics

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Abstract : Polycrystalline samples of $\text{Ba}_5\text{RTi}_2\text{ZrNb}_7\text{O}_{30}$ [R=Sm, Gd] of Tungsten Bronze (TB) structural family have been prepared by a high temperature solid-state reaction technique, X-ray diffraction (XRD) analysis as a function of temperature shows the orthorhombic structure of the compounds at room temperature. Dielectric studies at four different frequencies, 1, 10, 100 kHz and 1 MHz, show that the above compounds have ferroelectric phase transition of diffuse type, and also have relaxor properties.

Keywords : Ferroelectric, tungsten-bronze, diffuse phase transition, orthorhombic.

PACS Nos : 77.22.Gm, 61.10.Nz, 77.80.Bh

Sensitivity of piezoelectric transducers

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Abstract : A theoretical analysis based on an established transducer model has revealed a mathematical expression for sensitivity (*e.g.*, volts. per unit signal force) of piezoelectric plate transducer operating in its thickness mode and air as its surrounding medium. The sensitivity is found to be a strong function of frequency, with the principal peak being at the plate's fundamental thickness resonance. Other peaks of sensitivity are found to be at the odd multiples of this fundamental resonance frequency, whereas at even multiples of this frequency, the sensitivity is practically zero.

Keywords : Sensitivity, piezoelectric transducers, Laplace transform, thickness mode, resonance.

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Piezoelectricity and electron mobility in ZnO

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Abstract : Piezoelectric scattering mobility of electrons for the zinc blende structure is found to vary as $T^{-1/2}$ for all range of low temperatures. This signifies a very high conductivity of the sample and a very high velocity of electrons in it at suitably low temperatures. So substances like ZnO have enormous prospect in searching for room temperature super conductivity.

Keywords : Piezoelectricity, dynamical matrix, electron mobility, phonon.

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Energetic Harrison's first principle approach to the transport properties of metals : Mg and Ga

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Abstract : Harrison's First Principle (HFP) method owes its existence to the concept of orthogonalised plane wave (OPW). In this technique, the beauty lies in the factorization of the matrix element of the crystal potential into form factor $w(k,q)$ and the structure factor $a(q)$. The latter is available from experimental measurements either through X-ray or neutron diffraction but the former is to be calculated theoretically by suitable theoretical framework.

In Harrison's First Principle method, there is no arbitrary adjustable parametrization and no arbitrary model of potential is chosen, rather all the contributing potentials are derived from basic considerations. However, there is a controversy regarding the choice of eigenvalues of the core states. This is due to the fact that different self-consistent computations lead to eigenvalues which differ markedly, amongst themselves.

Thus in the present work, the impact of various eigenvalues have been studied both on the form factor $w(k,q)$ and electrical resistivity (R) derived from Ziman's formalism and also Knight shift (K) of Mg and Ga. The study reveals interesting features.

Keywords : Pseudo-potential, liquid metal, electrical resistivity, Knight shift.

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