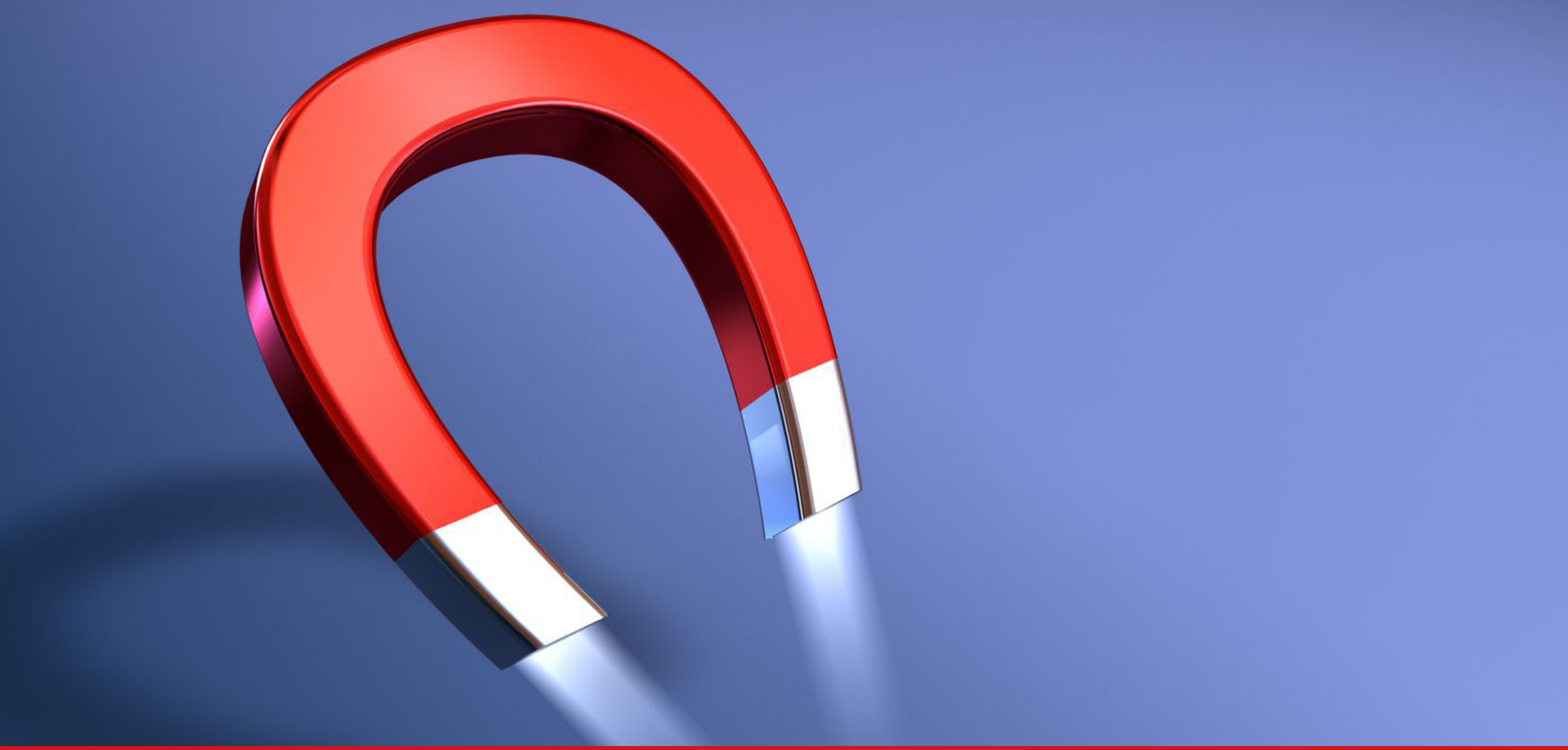

GCMMM2023

ABSTRACT BOOK

Global Congress on Magnetism and Magnetic Materials

August 10-12, 2023 | London, UK

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About Conference

Dear Colleagues,

On behalf of the Conference Organizing Committee and Avouch Conferences, it is our pleasure to invite all the world famous/leading scientists, outstanding researchers, academic people and industrialists from all over the world to attend the Global Congress on Magnetism and Magnetic Materials (GCMMM2023) which is to be held in August 10-12, 2023 in London, UK.

We welcome you to join us and be a part of knowledge and views in respect to the theme "To Discuss the Latest Trends and Advancements in Magnetism". GCMMM2023 will provide a wonderful opportunity for academicians, researchers, scientists, engineers and pioneering students working in the fields of Magnetism and Magnetic Materials to exchange, share and discuss their unique ideas, new knowledge and cutting-edge science, unveiling recent trends and advancement for accelerating scientific discoveries in the area, offering the opportunity to all delegates for networking, also globalizing the research by installing a dialogue between industries and academics for launching new technologies and applications.

The conference will provide the ideal forum to stimulate ideas and establish collaborations as well as to initiate intense discussions to secure projects of the newest generations and to feature a highly interactive, stimulating and multidisciplinary program including workshops, plenary, Keynote, invited sessions and panel discussions.

We are sure that you will find the conference enlightening and inspiring. Come to share stimulating perspectives about the new frontiers in Magnetism and Magnetic Materials. We hope that, despite the intense scientific program, you will be able to get some glimpses of wonderful London, one of the fascinating cities in the world.

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Conference Chair
Prof. Arcady Zhukov
University of Basque Country and Ikerbasque, Spain
GCMMM2023 | London, UK
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Advanced Functional Magnetic Microwires with Amorphous and Nanocrystalline Structure for Technological Applications

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Abstract
Amorphous magnetic wires have attracted great attention owing to their superior soft magnetic, mechanical and corrosion properties. Excellent magnetic properties such as fast magnetization switching related to magnetic bistability or Giant Magnetoimpedance (GMI) effect are suitable for magnetic sensors applications [1]. Recent tendency in devices miniaturization stimulated development of thin (few μm diameters) microwires [1,2]. Better magnetic softness and higher GMI effect have been reported in Co-rich amorphous microwires, while Fe-rich amorphous microwires exhibit spontaneous magnetic bistability related to remagnetization process through fast domain wall propagation [1,3]. Less expensive Fe-rich microwires are preferable for the applications. However, amorphous Fe-rich materials exhibit rather high magnetostriction coefficient and consequently present quite low GMI effect.

Accordingly, we designed the post- processing allowing further optimization of magnetic properties of Fe- and Fe-Co based glass-coated microwires [1]. Conventional annealing allows considerable improvement of domain wall dynamics in Fe-rich microwires and slight decrease of coercivity, however remarkable magnetic hardening is observed after conventional furnace annealing of Co-rich microwires. Stress annealing of Fe-rich microwires allows considerable magnetic softening and GMI effect enhancement and even more remarkable improvement of domain wall dynamics. In Co-rich microwires stress-annealing allows improvement of GMI effect and even induction of transverse magnetic anisotropy at high enough annealing temperature, however the highest GMI effect is observed for stress-annealed Co-rich microwires which present rectangular hysteresis loops. Consequently, annealed Co-rich microwires can present both fast domain wall propagation and GMI effect.

For interpretation of observed changes of hysteresis loops after stress annealing we considered internal stresses relaxation and different mechanisms of stress-induced anisotropy. Observed versatile properties of properly processed glass-coated amorphous microwires with enhanced and tuneable soft magnetic properties make them suitable for various applications.

Keywords
Soft Magnetic Materials; Amorphous Microwires; GMI Effect; Domain Walls.

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[2]Y. Honkura and S. Honkura, “The Development of ASIC Type GSR Sensor Driven by GHz Pulse Current”, Sensors, 20 (2020) 1023.

Biography
Arcady P. Zhukov graduated in 1980 from the Physics-Chemistry Department of the Moscow Steel and Alloys Institute (presently National University of Science and Technology). In 1988 he received Ph.D. degree from the Institute of Solid State Physics (Chernogolovka) of the Russian Academy of Science, in 2010- Doctor of Science (habilitation) in Moscow State “Lomonosov” University. Present employment: Ikerbasque Research professor at the Department of Polymers y Advanced Materials of the University of Basque Country, Spain. Current fields of interest: amorphous and nanocrystalline ferromagnetic materials, magnetic micro-wires, giant magneto-impedance, giant magnetoresistance, magnetoelastic sensors. He has published more than 550 referred papers in the international journals (total number of citations of A. Zhukov’s papers, updated January 12, 2023: 10858(WOS), Citation H-index = 58(WOS)/66(Google)). A. Zhukov is an associate Editor of IEEE Magnetic

letters and International Journal on Smart Sensing and Intelligent Systems, member of several editorial boards and various committees of International Conferences, guest Editor of J. Alloys Compound., J. Magn. Magn. Mater., ... A. Zhukov wrote four books: (Springer, Nova Sci. Publ-, IFSA Publ.) few book chapters (the last one for the Handbook of Magnetic Materials ed. by Prof. K. Buschow).

Novel Tetragonal ($L1_0$) Magnets

Ian Baker*

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Abstract

Demand for high-performance permanent magnets for motors is increasing rapidly for applications such as wind turbine generators and motors in electric and hybrid cars. Sm-Co and Nd-Fe-B magnets are generally used for such challenging applications. While these rare earth (RE) magnets have the highest energy product (BH)max of any material, they are not without problems such as corrosion and brittle fracture. Other important issues are that over 95% of REs are produced in one country, and there has been substantial price volatility with RE elements. Finally, RE mining has been associated with severe environmental degradation. Here we discuss two tetragonalL10-structured materials that could replace RE magnets NiFe and MnAl. Both have long been identified as potentially-commercially useful, low-cost permanent magnets that could replace RE magnets, but there are problems associated with both. For NiFe, the issue is that the transformation from the high temperature f.c.c. phase to the L1o-structured phase occurs at around 600 K and, thus, is exceedingly slow. For tau MnAl, which is metastable, the issue is that researchers have shown, using different processing methods, high saturation magnetization or high coercivity but not both simultaneously. In this presentation, we will review previous efforts to produce these magnets and describe our efforts at alloying, based on ab initio calculations, and novel processing (equal channel angular extrusion, electropulse annealing) to produce the magnets. Funding was provided by the U.S. National Science Foundation, the Irving Institute for Energy and Society at Dartmouth.

Biography: Ian Baker obtained his BA and D. Phil in Metallurgy and Science of Materials from the University of Oxford. He is the Sherman Fairchild Professor of Engineering and Senior Associate Dean for Research and Graduate programs at the Thayer School of Engineering, Dartmouth College. He has published 400 papers and given over 300 presentations at universities, conferences and in industry, of which 180 were invited. He is a fellow of ASM, TMS, IOM3, MRS and AAAS. He was Editor-in-Chief of the journal Materials Characterization from 2008-2020. He is currently co-Editor in Chief of the journal High Entropy Alloys and Materials and Field Chief Editor for the Journal Frontiers in Metals and Alloys both of which were launched in 2022. He has published over 400 papers and one book entitled “Fifty Materials that Make the World”.

Progress of Spintronics with 2D Materials

Yongbing Xu*

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Abstract

The discovery of two-dimensional (2D) magnets opens the door for fundamental physics and next-generation spintronics. Here, we report our recent studies of the manipulation of the spin ordering in two prototype systems Fe3GeTe2 (FGT) and CrTe2, focusing on the enhancement of spin-ordering temperatures and new spin structures. We have found that the femtosecond pulsed laser can drive the emergence of ferromagnetism at room temperature in a few monolayers of FGT [1]. Both the saturation magnetization and the coercivity is strongly modulated by the excitation intensity of the femtosecond pulsed laser. The emerging room-temperature ferromagnetism is attributed to change of the carrier concentrations caused by the optical doping effect, which shifts the Fermi level to different density of states. In CrTe2, we have found that the bilayer graphene substrate can lead to room temperature intrinsic ferromagnetism with a Curie temperature (TC) above 300 K and perpendicular magnetic anisotropy (PMA) constant of 4.89×105 erg/cm3 at room temperature in these few-monolayer films grown by MBE [2]. The FM order is preserved with the film thickness down to a monolayer, benefiting from the strong PMA and weak interlayer coupling. With the strong spin-orbit coupling in Bi2Te3, we have obtained a giant THE signal of 1.39mWμcm in the van der Waals heterostructures of CrTe2/Bi2Te3, a prototype of two-dimensional (2D) ferromagnet (FM)/topological insulator (TI) [3]. Moreover, the engineering of the antiferromagnetic (AFM) interlayer exchange coupling between atomically thin FM CrTe2 layers in the 2D magnetic crystal, Cr5Te8 is realized [4]. By self-introducing interstitial Cr atoms in the vdW gaps, the emergent AFM ordering and the resultant giant magnetoresistance effect are induced. A large negative magnetoresistance with a plateau-like feature is revealed, which is consistent with the AFM interlayer coupling between the adjacent CrTe2 main layers in a temperature window of 30 K below the Néel temperature. We will also report our further studies of the dynamics process of the spin ordering in these 2D magnetic systems.

Keywords

Spintronics; 2D Magnet; AFM Ordering.

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Biography

Professor Yongbing Xu, Director of the Nanjing-York Joint Center in Spintronics and NanoEngineering, Nanjing University, China; Chair in Nanotechnology, also heads the Spintronics and Nanodevice Laboratory, The University of York. He was an EPSRC Advanced Research Fellow in Cavendish Laboratory, Cambridge University. His research interests are in the areas of nanomaterials, spintronics and nanofabrication. He has published more than 500 refereed papers in leading academic journals including Science Advances, Physical Review Letters, Prog. Mater. Sci., Nature Communications, Nano Letter, Advanced Materials, ACS Nano, Scientific Reports, Applied Physics Letters and IEEE journals and given many invited talks/seminars at major international conferences including MRS, WUNSPIN, EMN and Intermag. He was chair of five international conferences in spintronics. He was editor-in-Chief of "Handbook of Spintronics" by Springer, and edited the very first spintronics book "Spintronic Materials and Technology" by CRC Press. He had interviews with BBC News24 and New Scientists.

Rapid Quenched Soft Magnetic Ribbons for Power Electronics

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Abstract

Almost half century has passed since the amorphous ribbon fabricated by rapid quenching technique was developed. One of the most commercially successful applications would be an Fe-based amorphous alloy ribbon used in distribution transformers. The Fe-based amorphous alloy ribbon exhibits very suitable soft magnetic properties for this application such as low core loss with relatively high Bs of at around 1.6 T.1) There is demand of using this amorphous alloy ribbon in motor cores. However, there is big challenge to commercialize this application. The amorphous alloy ribbon exhibits high hardness as approximately 900 Hv.2) Moreover, the thickness of the ribbon is approximately 25-30 mm which makes difficult to make complicated core shape by punching process. However, if this process could be successfully accomplished, the motor with this core will exhibit unique characteristics. Especially, suppression of eddy current loss will enable rising the driving frequencies up to several kilohertz. This will help rising the rotation speed of the motor axis or also rising the torque of the axis. Namely, it will improve the power density of the motor. There is demand of improvement of power density of devises for inductors in power electronics as well. For this application, the Fe-based amorphous alloy will be one of candidates while Fe-based nanocrystalline alloy ribbons could be another candidate. Fe-based nanocrystalline alloy ribbons are fabricated by rapid quenching technique and amorphous phase is obtained at the as-quenched state. An annealing is applied for the nanocrystallization. There is also a composition that can reduce magnetostriction by half while increasing Bs compared to Fe-based amorphous alloys, and using this has the potential to improve the performance of inductors at medium frequencies.3) If magnetostriction can be lowered, megahertz switching will become possible and higher power densities will be achieved.

Keywords

Rapid Quenched Ribbon; Fe-Based Amorphous Ribbon; Fe-Based Nanocrystalline Ribbon; Motor.

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Biography

Motoki Ohta is a professor at Shimane University, Japan. He has completed his PhD from Tohoku University and Researcher at Hitachi Metals. Ltd.. He also has a cross-appointment Senior Researcher position at Company PROTERIAL. Hitachi Metals has changed its company name to PROTERIAL this year.

Magneto Optic Imaging Film (MOIF) Technique: Latest Advances and Applications

Lev Dorosinskiy*

National Metrology Institute, Turkey

Abstract

Magneto Optic Imaging Film (MOIF) technique was developed in the early 1990's to study the penetration and behaviour of magnetic flux in high temperature superconductors. In first studies, films with perpendicular magnetic anisotropy having a labyrinth domain structure were used. Later, films with in-plane anisotropy having no magnetic domains were developed. The magneto optical Faraday effect arises in such films due to the rotation of magnetization vector away from the film plane under the effect of external magnetic field. This Faraday rotation produces an optical image in crossed polarizers and, by measuring the light intensity using digital cameras of photomultiplier tubes, one can convert the local magnetic flux density into an electrical signal. Thus, not only qualitative observations can be done but numerical maps of the local magnetic flux density can be obtained. Due to the absence of domains and zero of coercivity for the magnetization rotation process, a high sensitivity of the order of 10 mT and a high spatial resolution near the optical resolution limit can be achieved in such measurements. However until recently, the exact calibration of the magneto optical signal with respect to the local magnetic field was not possible because such factors as the effect of the MOIFs non-zero thickness and the interplay between normal and in-plane field components could not be accounted for. Our recent metrological studies have solved these issues and have made it possible to perform traceable calibrated measurements of local magnetic fields using MOIF sensors. In our presentation we show the latest achievements in understanding the underlying physics of MOIF sensors and in establishing the metrology of magneto optical measurements. We further demonstrate applications of MOIFs for studies of the magnetic structure and behaviour of magnetic materials, such as transformer steels, and for the industrial applications, like calibration of magnetic scales.

Biography

Lev Dorosinskiy was born in Moscow in 1966. He graduated from the Moscow Institute of Steel and Alloys 1989 and began his research career in the Russian Academy of Sciences at the Institute of Solid State Physics. In 1994 he completed his PhD work, which was entitled "Investigation of the defect structure of YBa2Cu3O7-d single crystals and its effect on the superconducting properties". Since 1998 he has been working at the National Metrology Institute of Turkey, TÜBİTAK-UME. Lev has 56 publications in peer reviewed journals.

Magneto-Fluorescence Coupling in Coordination Complex

Zhao-Bo Hu[1,2], You Song[1,*]

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2Chaotic Matter Science Research Center, Faculty of Materials Metallurgy and Chemistry, Jiangxi University of Science and Technology, Ganzhou 341000, P. R. China

Abstract
Fluorescent materials are widely used in LED lighting, biomedicine and other fields. Under magnetic field, some of them can show magneto-optical properties, such as Zeeman effect, Faraday effect, magneto-optical Kerr effect, etc. However, the reported compounds with magneto-fluorescence are basically concentrated in pure inorganic materials. Molecular materials can also exhibit magneto-fluorescent properties, but related researches are very rare, mainly because spin often quenches fluorescent properties in coordination complexes. In one complex, magnetism and fluorescence always seem in conflict with each other. Even though there have been some molecular magneto-fluorescence materials, most of them are pure organic radicals, and few examples have been reported. Meanwhile, the materials mentioned above shows that magnetic field stimulation can only change their fluorescent intensity, while other interesting phenomena relative magnetism are rarely reported.

As is well known, the electronic structure of [MnIICl4]2− can be converted from (t2g)3(eg)2 to (t2g)4(eg)1 after being excited by light, thus showing fluorescence properties. MnII ions have single electrons before and after excitation. So, the fluorescence of complexes containing [MnIICl4]2− groups may be sensitive to changes of magnetic fields. Based on this strategy, we studied the magneto-fluorescence coupling under pulsed magnetic field for a series of the layered perovskite complexes, (NR4)2MnCl4. The experiment shows that not only the stimulation of the external magnetic field can change the fluorescent intensity of the material, but also the red shift of the luminescent spectrum can be observed obviously. Even, the magneto-florescent hysteresis can be generated even under very low field, which proves that these complexes are the candidate material for low energy consumption magneto-optical devices.

Keywords
Magneto-Optical; Fluorescence; Magnetic; Manganese.

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Biography
You Song obtained his Ph.D. degree from Nanjing University in 2000. From 2000 to 2002, he worked in Hashimoto Laboratory as a STA and JSPS fellow in Tokyo University and Kanagawa Academy of Science and Technology. He went back to Nanjing University in 2003 and became an Associate Professor in 2005. In 2005 and 2006, he visited Academic Sinica and National Taiwan University for twice as a short-time academic visitor of "Aim for Top University Project". In Dec. 2009, he was moved up to a full professor of Nanjing University. He works in the area of functional coordination chemistry. Much of his works focuses on the design, synthesis and properties of molecule-based magnets, in which the main topics are on spin-frustration and molecular qubit.

Dimerization and Magnetization Plateaus in $Ni_2V_2O_7$ Observed at 120 T

Z. W. Ouyang[1,*], Y. H. Matsuda

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Abstract
Quantum magnetism and its interplay with topological structure are of particular interesting. Representative examples are the spin Peierls effect and the formation of clusters in many antiferromagnetic spin systems such as one-dimensional chain NaTiSi2O6, triangular lattice LiVO2, kagome lattice LiZn2Mo3O8, and spinel lattice MgTi2O4 driven by particular orbital order. Reduction of dimensionality and clusterization-related physics renew interests in quantum magnets.

Ni2V2O7 is a skew chain compound in structure. Magnetically, Ni2V2O7 is a 3D antiferromagnet with long-range ordering at TN = 7 K and spin-flop-like transition at low fields. For such a classical antiferromagnet, one takes it for granted that above the spin-flop transition the magnetization will increase linearly until saturation. However, we recently observed a wide 1/2 magnetization plateau within 8-30 T, which is difficult to understand. Puzzled by the wide 1/2 plateau, we have measured the ultrahigh field magnetization of Ni2V2O7 up to 120 T. Intriguingly, in addition to the wide 1/2 plateau within 11.7–34.8 T, a new and wider 3/4-like plateau within 55.6–87.0 T is observed. With the density function theory, exact diagonalization and quantum Monte Carlo simulations, the magnetization process can be described satisfactorily, which yields main exchange interactions — the intrachain J1/kB = −1.0 K, J2/kB = 6.3 K, and the interchain J3/kB = −78.5 K. Thus the skew chain Ni2V2O7 can be described by a "dimer + monomer" model: the 1/2 plateau is due to weakly coupled Ni2 monomers, while 3/4-like plateau is the result of dimerization of Ni1 ions originating from large overlap of 3d-orbital along the Ni1-Ni1 bond.

Keywords
Dimerization; Magnetization Plateaus; Skew Chain; 120 T High Field.

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https://doi.org/10.1103/PhysRevB.106.184409

Biography
Zhongwen Ouyang obtained his Ph.D. degree from Institute of Physics, Chinese Academy of Sciences in 2004. From 2004 to 2006, he worked as a postdoc research associate in Ames Laboratory & Iowa State University, USA; from 2006 to 2008, he worked as a JSPS postdoctoral researcher at the Institute for Materials Research, Tohoku University, Japan. From Dec. 2008 to present, he worked as professor of physics in Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, China. His research interest includes low-dimensional quantum magnetism, frustrated magnets and nano-sized molecular magnets.

Structure and Magnetism of an Ideal One-dimensional Chain Antiferromagnet $[C_2NH_8]_3[Fe(SO_4)_3]$ with Large Spin of $S = 5/2$

Zhenxing Wang*, **Zhongwen Ouyang**
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Abstract
One-dimensional (1D) spin chains have been a lasting research topic due to the diverse magnetic properties. According to the Haldane's conjecture, spin energy gaps open in a Heisenberg antiferromagnetic (AFM) spin chain with integer spins, which were confirmed by earlier model materials with S = 1 such as CsNiCl3 and Ni(C2H8N2)2NO2(ClO4), and subsequent ANi2V2O8 (A = Pb, Sr) and Y2BaNiO5. For chain with half-integer spins, spin gap is absent. Large spin 1D chains are not extensively investigated because quantum magnetism in these systems decays with increasing S and even a very small interchain interaction can stabilize long-range AFM ordering.

We report an S = 5/2 linear chain antiferromagnet [C2NH8]3[Fe(SO4)3] with trigonal lattice (space group R3c) using the traditional solvothermal method. The magnetic susceptibility μ(T) curve exhibits a broad maximum at Tmax = 18 K with the Curie-Weiss temperature μCW = −25.5 K, showing dominant antiferromagnetic interaction. However, no long-range magnetic ordering is observed down to 2 K. High-field magnetization at 2 K increases nearly linearly until saturation at 30 T. Zero-field spin gap is absent in the high-field ESR spectra. Ratio of interchain to intrachain interactions is determined as Jμ/J < 2.5×10−3. Thus, [C2NH8]3[Fe(SO4)3] is an ideal 1D uniform linear-chain antiferromagnet.

Keywords
Spin chain; Heisenberg Antiferromagnetic; Large Spin; High-Field ESR.

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M.-Y. Liu, Z.-W. Ouyang, X.-C. Liu, J.-J. Cao, T.-T. Xiao, Z.-C. Xia, Z. Wang, Inorg. Chem. 61, 38, 15045–15050 (2022). https://doi.org/10.1021/acs.inorgchem.2c02001

Biography
Zhenxing Wang obtained his Ph.D. degree from Florida State University in 2012. From 2012 to 2014, he conducted postdoctoral research at the University of California, Los Angeles. Since 2014, he has been an associate professor at the National High Magnetic Field Center, Huazhong University of Science and Technology. His research interests include: molecular-based magnetic materials, molecular-based quantum bits, and high-magnetic field ESR technology.

Novel Sensing Technique for Non-Destructive Composites Monitoring

V. Zhukova [1,2,3], P- Corte-Leon [1,2,3], A. Allue [4], K. Gondra [4], M. Ipatov [1,2], J. M. Blanco [2,3], J. Gonzalez[1,2,3] and A. Zhukov [1,2,3,5]

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5 IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Spain

Abstract

The real time non-destructive monitoring of stresses and temperature is one of the most demanded solutions in the field of sensor technologies. One of the most prospective technologies addressing this problem is a novel sensing technique for non-destructive monitoring utilizing ferromagnetic wire inclusions presenting the high frequency Magnetoimpedance, MI, effect quite sensitive to tensile stress and magnetic field [1]. One of the advantages of this technology is that proposed free space microwave spectroscopy allows remote monitoring of external stimuli, like stress, magnetic field or temperature.

The glass-coated microwires with typical diameters from 1 to 50 μm can provide new functionalities such as improved mechanical and corrosive properties, adherence with polymeric matrices and biocompatibility [2].

In the present paper a novel sensing technique for direct non-destructive and non-contact monitoring of the composite polymerization utilizing ferromagnetic glass-coated microwire inclusions with magnetic properties sensitive to tensile stress and temperature is described. We provide in-situ studies of the evolution of the hysteresis loop of arrays consisting of Co- rich (Fe3.8Co65.4Ni1B13.8Si13Mo1.35C1.65) microwires during the composites matrix polymerization. We observed remarkable change of the hysteresis loops upon matrix polymerization: remarkable coercivity change and transformation of linear hysteresis loop into rectangular in the arrays with Co-rich microwires placed inside the matrix. Using the free space microwave spectroscopy technique we observed considerable variation of the Transmission parameter of the microwires array in the range of 4-7 GHz upon the matrix polymerization. Observed dependencies are discussed considering heating during the matrix polymerization measured using the thermocouple and the matrix shrinkage and their influence on magnetic properties and MI effect of glass-coated microwires.

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Biography

Valentina Zhukova is a researcher of the Department of Polymers y Advanced Materials of the University of Basque Country, Spain. Graduated as an engineer in the Metallurgy in Moscow Steel and Alloys Institute in 1982 and received PhD degree in 2003 in the Basque Country University, Spain in the studies of transport and magnetic properties of glass-coating microwires. Her expertise is technology, magnetic properties and applications of glass coated magnetic microwires, being documented in more than 300 scientific publications (total number of citations of V. Zhukova`s papers, updated March 02, 2022: 6434, Citation H-index = 40(WOS)/47(Google)) in indexed international scientific journals. Current fields of interest: novel magnetic materials, amorphous and nanocrystalline ferromagnetic materials

Towards Room Temperature Magnets: The Exchange Properties of d7 Transition Metal Phthalocyanines

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Abstract

Owing to their modular nature, thermal and chemical stability and relative ease of fabrication, metal phthalocyanines have been extensively studied within the context of spintronics. However, their application in possible devices is hindered by their low magnetic transition temperatures. Alpha phase cobalt (II) phthalocyanine has exhibited a much stronger exchange interaction (J / kB = 78 K [1]) than its 1st row transition metal counterparts. The underlying interaction is thought to arise from a direct hopping superexchange mechanism, whereby outof-plane dz 2 derived a1g molecular orbitals align antiparallel to one another. By capturing the interaction dynamics using Hubbard model parameters, directed modifications to the system may be made in order to raise the magnetic transition temperature. Presented here is a theoretical study in which hybrid-DFT has been used to evaluate the exchange energy of a set of d7 transition metal phthalocyanines. It has been shown that by replacing the Co2+ central ion with its 2 nd row analogue rhodium (Rh2+), the underlying exchange interaction within an alpha-phase geometry has been markedly strengthened. The underlying cause of this increase has been linked to the decrease in the on-site Coulomb repulsion (U) arising from the occupation of rhodium's more diffuse 4dz 2 derived singly occupied orbital. The smaller U facilitates a lower "energy penalty" from double occupation thereby increasing the strength of the superexchange interaction. The results of this theoretical study present a promising candidate for applications in spintronic semiconductor materials.

Keywords
Spintronics; Semiconductor; Phthalocyanine; Hubbard; High-temperature magnetism.

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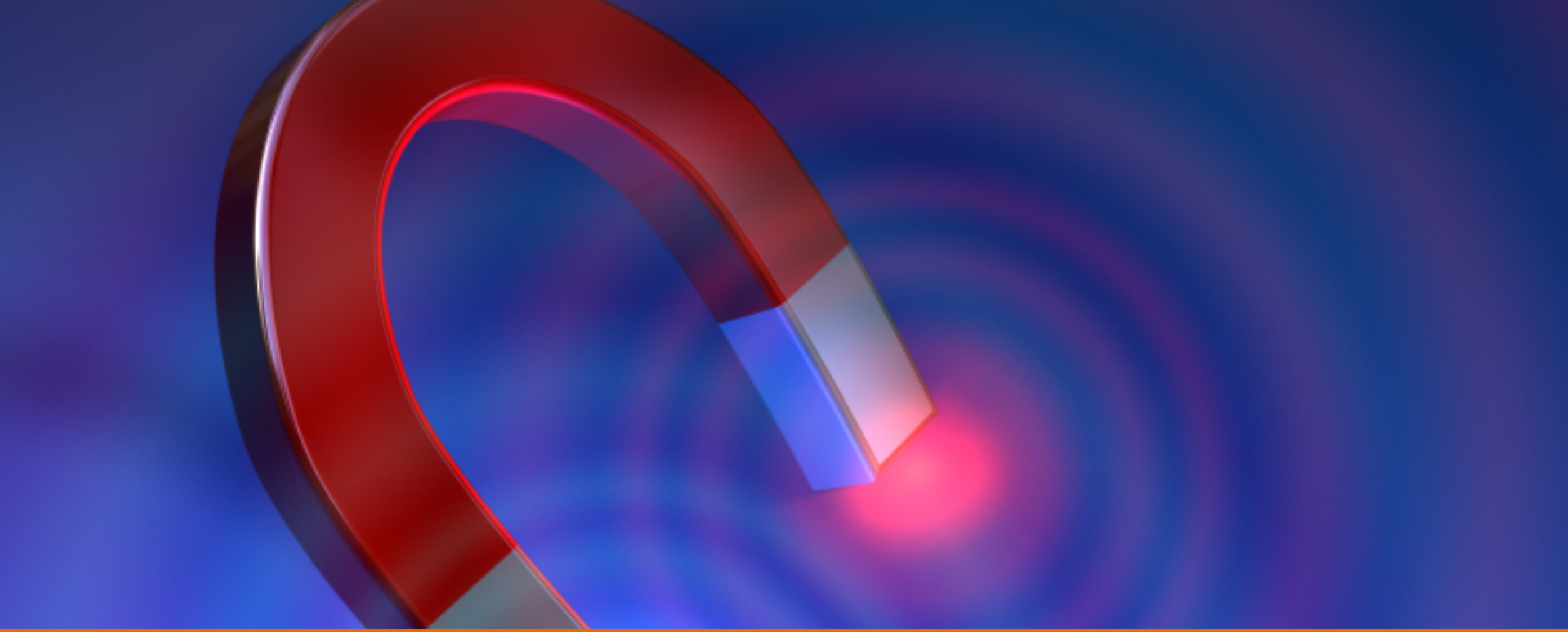
Biography: My name is James Broadhurst. I am currently studying for a PhD in the Department of Chemistry at Imperial College London. My fields of research include spintronics and organic/hybrid magnetic materials. I received my MSci in chemistry from the University of Bristol.



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