

**FA2-MS04-O1**

**Ab initio Simulations of Lattice Stability: An Effect of External Conditions.** Igor Abrikosov. *Department of Physics, Chemistry and Biology, Linköping University, Sweden.*  
E-mail: [igor.abrikosov@ifm.liu.se](mailto:igor.abrikosov@ifm.liu.se)

Ab initio electronic structure theory is known as a useful tool for prediction of materials properties and for their understanding. However, majority of simulations still deal with calculations of total energies at zero temperature. In this talk we show that for large number of problems it is necessary to take proper experimental conditions into account to obtain reliable theoretical results. In particular, we show that the problem of lattice stability, the energy difference between different crystal structures of a material, can be consistently described by theory and experiment if the former is done at elevated rather than at zero temperature [1]. A decisive role of lattice vibrations will be illustrated by theoretical search for metastable fcc-related Si-N phases [2], which are the tissue phases of (Ti-Si)N thin film nanocomposites, as well as in first-principles study of stability of newly synthesized ternary perovskite  $\text{Sc}_3\text{AlN}$  and a family of its isoelectronic compounds  $\text{Sc}_3\text{EN}$  (E=B, Ga, In) [3].

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**Keywords:** ab-initio calculations; crystal structures; lattice dynamics

**FA2-MS04-O2**

**Resonant X-ray Diffraction Distinguishes Inequivalent Iron Atoms in  $\text{Fe}_3\text{BO}_6$ .** V. E. Dmitrienko<sup>a</sup>, G. Beutier<sup>b</sup>, E. N. Ovchinnikova<sup>c</sup>, S. P. Collins<sup>b</sup>, J. E. Lorenzo<sup>d</sup>, J.-L. Hodeau<sup>d</sup>, A. Kirfel<sup>e</sup>, Y. Joly<sup>d</sup>, A. A. Antonenko<sup>c</sup>, V. A. Sarkisyan<sup>a,f</sup>, A. Bombardi<sup>b</sup>. <sup>a</sup>*Institute of Crystallography, 119333, Moscow, Russia.* <sup>b</sup>*Diamond Light Source, Harwell Science & Innovation Campus, OX11 0DE, United Kingdom.* <sup>c</sup>*Physical Department of Moscow State University, 119899 Moscow, Russia.* <sup>d</sup>*Institut Louis Néel, CNRS, F-38042 Grenoble, France.* <sup>e</sup>*Steinmann Institute, University of Bonn, Poppelsdorfer Schloss, D-53115 Bonn, Germany.* <sup>f</sup>*Beam Engineering for Advanced Measurements Co., 809 South Orlando Ave., Suite I, Winter Park, FL 32789, USA.*  
E-mail: [dmitrien@crys.ras.ru](mailto:dmitrien@crys.ras.ru)

It is demonstrated that, contrary to XANES and EXAFS, resonant X-ray diffraction can successfully distinguish atoms of the same element occupying inequivalent sites in the crystal structure. Forbidden Bragg reflections of

iron orthoborate  $\text{Fe}_3\text{BO}_6$  were studied theoretically and experimentally in the vicinity the iron *K*-edge. Their energy spectra are explained as resulting from the interference of X-rays scattered at two non-equivalent crystallographic sites occupied by the iron atoms. This particular structure property gives rise to complex energy and azimuthal dependences of the reflection intensities in the pre-edge region as they result from the interplay of site specific dipole-quadrupole and quadrupole-quadrupole resonant scattering. The interference is mainly constructive for the 300, 500 and 710 reflections, whereas the opposite holds for the 700 reflection. Best fitting of the main features of the intensity profiles was achieved by using different parameters for the excited states of the inequivalent iron atoms in the FDMNES code. Also evidenced is an anisotropic character of the absorption spectrum. Possible contributions of thermal vibrations and magnetic order are discussed. Particular care is given to extracting clean spectra from the data, and it is demonstrated that excellent results can be obtained even from measurements that appear corrupted by several effects such as poor crystal quality and multiple scattering. This work was supported by the grant RFBR 07-02-00324 and by Presidium of Russian Academy of Sciences.

**Keywords:** resonant diffraction; forbidden reflections; iron orthoborate

**FA2-MS04-O3**

**Pressure-Induced Phase Separation in High  $T_c$  Superconductors.** Maria Calamiotou<sup>a</sup>, Anestis Gantis<sup>a</sup>, Dimitrios Lampakis<sup>b</sup>, Eirini Siranidi<sup>b</sup>, Kazimierz Conder<sup>c</sup>, Irene Margiolaki<sup>d</sup>, Efthymios Liarokapis<sup>b</sup>. <sup>a</sup>*Solid State Physics Dept., University of Athens, Greece.* <sup>b</sup>*Physics Dept., National Technical University, Athens, Greece.* <sup>c</sup>*Paul Scherrer Institute, Villigen, Switzerland.* <sup>d</sup>*ESRF, Grenoble, France.*  
E-mail: [mcalam@phys.uoa.gr](mailto:mcalam@phys.uoa.gr)

It is now well accepted that structural and electronic inhomogeneities constitute intrinsic properties of cuprate superconductors. To this context the study of pressure-induced phase separation effects can improve our understanding on the role of lattice effects in the high  $T_c$  superconductivity. We present here the results of high pressure (up to 13GPa) synchrotron angle-dispersive powder diffraction experiments in comparison with high pressure micro-Raman data on different high  $T_c$  superconductors. 2D high quality diffraction images have been collected under high pressure using a diamond anvil cell (DAC) and a MAR345 image plate at the SNBL-BM01A beamline at ESRF. The *c*-axis of the optimally doped  $\text{YBa}_2\text{Cu}_3\text{O}_y$  (Y123) cuprate exhibits in the pressure range 3.7GPa < *p* < 10GPa a clear deviation from the expected equation of state while upon pressure release the data follow the anticipated dependence showing a strong hysteresis. At the pressure of ~3.7GPa new peaks appear in the diffraction pattern, which has being attributed to another apparently coherent phase that exhibits disorder and texture effects. Interatomic distances in the unit cell of Y123, such as the Ba distance from the basal plane, the Cu2-O<sub>pl</sub> bond length and

the Cu<sub>2</sub>-Cu<sub>1</sub> distance along the c-axis, exhibit also a non linear evolution with applied pressure that correlate with modifications of the in-phase oxygen mode and the apex oxygen mode frequencies respectively in the high pressure Raman spectrum [1],[2]. The correlation of the structural characteristics with the Raman frequency modifications and corresponding changes of T<sub>c</sub> imply that the trigger of lattice instabilities lies among the CuO<sub>2</sub> and BaO planes. Pressure-induced structural and microstructural modifications in the non-superconducting Pr123 cuprate, in the La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> (x=0.0, 0.15) compounds and in the YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub> superconductor has been found to correlate also with corresponding modifications of the phonon frequencies and widths in the high pressure Raman spectrum supporting a model of lattice distortions and possible pressure-induced phase separation at the nanoscale.

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**Keywords:** high pressure X-ray diffraction; phase separation; high-T<sub>c</sub> superconductors

#### FA2-MS04-O4

**Twining and Pseudosymmetry in Ferroic Materials at High Pressures.** Karen Friese<sup>a</sup>, Andrzej Grzechnik<sup>a</sup>. <sup>a</sup>*Department of Condensed Matter Physics, University of the Basque Country, Bilbao, Spain.*

E-mail: [karen.friese@ehu.es](mailto:karen.friese@ehu.es)

Ferroic phase transitions are characterized by the reduction of crystal symmetry as the material changes from the higher symmetrical to the lower symmetrical phase. This loss of symmetry is generally reflected in the appearance of a twin domain structure. In addition, the low-symmetry phase shows usually a strong pseudosymmetry with respect to the higher symmetry phase. Twining and high pseudosymmetry can thus be understood as an indication of the existence of structural instabilities in the material under certain temperature and/or pressure conditions.

We are especially interested in the effect of pressure on ferroic materials. Due to the difficulties related to the in situ experiments at high pressures in diamond anvil cells, the characterization of pressure-induced ferroic phase transitions is not trivial [1,2]. We have analyzed the twinning and pseudosymmetry in a series of ferroic materials with a variety of crystal structures. The materials include mixed-valence vanadates with structures related to magnetoplumbite [1,2], disordered pyrochlore structures [3,4], scheelite related structures [5,6], ternary compounds in the system NaF-ThF<sub>4</sub> [7,8] and polar oxides with elements containing lone electron pairs [9].

We generally observe that, whether the pseudosymmetry is increased or decreased with increasing pressure depends –even within a family of isotypical compounds – entirely on the individual representative. The increase of pseudosymmetry might serve as an indication for the occurrence of a structural transition to a higher symmetrical phase at pressures not reached in the experiment.

Due to the limited information content of the high-pressure data it is not always possible to characterize the twinning in full detail. However, we were able to reliably refine twin

volume fractions as a function of pressure in a number of cases.

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**Keywords:** ferroics; twinning; high-pressure crystallography

#### FA2-MS04-O5

**Magneto-resistance and Magnetocaloric Properties**

of Ni<sub>50-x</sub>Cu<sub>x</sub>Mn<sub>36</sub>Sn<sub>14</sub>. Ilker Dincer<sup>a</sup>, Yalcin Elerman<sup>a</sup>.

<sup>a</sup>*Department of Engineering Physics, Ankara University, Ankara Turkey.*

E-mail: [idincer@eng.ankara.edu.tr](mailto:idincer@eng.ankara.edu.tr)

Compared with conventional refrigeration, magnetic refrigeration technology has many advantages, such as the absence of harmful gas, less noise, low cost and high efficiency. Magnetic refrigeration is based on the magnetocaloric effect (MCE) [1]. The giant MCE is observed when the transition is first order transition. The Heusler alloys Ni<sub>50</sub>Mn<sub>50-x</sub>Sn<sub>x</sub> show first order martensitic transition and giant MCE properties [2-3]. Since at the martensitic transition temperature, the resistance of these alloys shows a drastic change as a function of temperature and magnetic field, this type alloys show giant magnetoresistance effect (GMR). To improve magnetoresistance and magnetocaloric effect, we investigate the Ni<sub>50-x</sub>Cu<sub>x</sub>Mn<sub>36</sub>Sn<sub>14</sub> alloys (x=2, 4 and 6). The Ni<sub>50-x</sub>Cu<sub>x</sub>Mn<sub>36</sub>Sn<sub>14</sub> alloys are prepared by arc-melting under argon atmosphere. The compounds anneal at 950 °C for 2.5 days and then quench in ice water. The compositions of the compounds are found by EDS analysis. The Ni<sub>50-x</sub>Cu<sub>x</sub>Mn<sub>36</sub>Sn<sub>14</sub> alloys crystallize in the cubic L2<sub>1</sub> structure. The magnetic and resistivity measurements of compounds are performed by using PPMS between 5 and 350 K in ZFC, FC and FH modes. With increasing Cu content, the value of T<sub>Ms</sub> temperature decreases. The Ni<sub>50-x</sub>Cu<sub>x</sub>Mn<sub>36</sub>Sn<sub>14</sub> (x=2 and 4) alloys show ~45% and ~40% GMR effect at 7 T. These two alloys exhibit inverse giant MCE in continuous and noncontinuous modes. For the Ni<sub>48</sub>Cu<sub>2</sub>Mn<sub>36</sub>Sn<sub>14</sub> alloy, the magnetic entropy change is about 57 and 22 J/kg.K for continuous and noncontinuous modes, respectively.

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