

catalysts without any sintering effects or changes in the size distribution. However, changes of the microstructure of the gold nanoparticles can be induced by chemical and thermal treatment. The effect of the microstructure properties of gold nanoparticles on the catalytic activity for CO oxidation has been investigated. Line profile analysis of powder diffraction data based on Whole Powder Pattern Modelling (WPPM) approach was used to determine both the domain size distribution and lattice defects present in this two phase system [2]. The different catalysts showed substantial variation in the activity towards CO oxidation depending on their microstructure. Lower dislocation densities and less stacking faults, but higher twin densities result in decreased catalytic activity.

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Keywords: microstructure, catalysts, nanocrystalline structure defects

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Lattice dynamics of multiferroic BiFeO₃. Elena Borissenko^a, Alexei Bosak^a, Pauline Rovillain^b, Maximilien Cazayous^b, Marco Goffinet^c, Philippe Ghosez^c, Dorothee Colson^d, Michael Krisch^a. ^a*European Synchrotron Radiation Facility, Grenoble, France.* ^b*Laboratoire Matériaux et Phénomènes Quantiques, Université Paris Diderot-Paris 7, France.* ^c*Département de Physique, Université de Liège, Belgium.* ^d*Service de Physique de l'Etat Condensé, CEA Saclay, France.*
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Materials with the coexistence of at least two ferroic orders (ferromagnetic, ferroelectric, ferroelastic) are known as multiferroics [1]. These materials represent a strong potential for devices based on the magnetic properties switch by an external electric field and vice versa. Among the multiferroics, Bismuth ferrite belongs to the *class* with the coexistence and coupling between magnetic order and electric polarization (ME: magneto-electric coupling).

This material is one of the most extensively studied multiferroic due to its unique property of ferroelectric and magnetic order at room temperature. Its dynamical properties have been studied by Raman [2, 3] and infrared spectroscopy [4], and have revealed some anomalies in the temperature dependence of the lowest optical phonon, which were interpreted as signature of magneto-electric coupling [2]. Here, we present an experimental study of the phonon dispersion in BiFeO₃ single crystals at ambient conditions by inelastic x-ray scattering. Phonon dispersions were recorded along several high-symmetry directions up to 35 meV. Our results compare favourably with *ab-initio* calculation performed using density functional theory (DFT) within the local-density approximation (LDA). We resolve a recent discrepancy concerning the symmetry of the lowest optical phonon branch observed by Raman spectroscopy [2, 3], determine the energy of the Raman- and infrared silent modes, and derive the elastic constants of BiFeO₃.

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Keywords: BiFeO₃, single crystal, lattice dynamics, Inelastic X-ray Scattering

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First Single-Crystal Neutron Diffraction Results on PZT Structure. A. M. Glazer^a, D. Phelan^b, X. Long^c, Y. Xie^c, Z. -G. Ye^c, H. Yokota^a, P.A. Thomas^d, P. M. Gehring^b. ^a*Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom.* ^b*NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA.* ^c*Department of Chemistry, Simon Fraser University, Burnaby, BC, V5A 1S6, Canada.* ^d*Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom.*
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The outstanding piezoelectric properties of PbZr_{1-x}Ti_xO₃ (PZT) perovskite ceramics have long been exploited in important device applications. The effort to understand the underlying piezoelectric mechanism has inspired a plethora of structural studies spanning decades. However, structure determination of PZT has always been problematic because single crystals have not been available, except for Zr and Ti-rich compositions near the end members PbZrO₃ and PbTiO₃, where the piezoelectricity is weakest. As a result, PZT has been the subject of literally thousands of powder and ceramic investigations. Despite these efforts, no consensus regarding the true PZT crystal structures has been achieved. Here we report the first neutron diffraction study of single-crystal PZT with $x = 0.325$ and 0.460 . Our measurements help to resolve a key debate on the structure of PZT by placing severe constraints on the magnitude of the structure factors of weak superlattice peaks and the splitting of fundamental Bragg peaks.

Keywords: perovskite structures, neutron diffraction, piezoelectrics

FA2-MS14-P33

Crystal structure of Li₂B₄O₇. Anatoliy Senyshyn^a, Björn Schwarz^b, Thomas Lorenz^c, Yaroslav Burak^d, Volodymyr Adamiv^d, Jūras Banys^e, Robertas Grigalaitis^e, Hartmut Fuess^a, ^a*Institute of Material Science, Darmstadt University of Technology, Darmstadt, Germany.* ^b*Leibniz-Institute IFW Dresden, Dresden, Germany.* ^c*II. Physikalisches Institut, Universität zu Köln, Köln, Germany.* ^d*Institute of Physical Optics, Lviv, Ukraine.* ^e*Physics Faculty, Vilnius University, Vilnius, Lithuania.*
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The crystal structure of lithium tetraborate Li₂B₄O₇ (mineral name diomignite) at room temperature is tetragonal with the space group *I4₁cd* (point group *4mm*) and with the polar axis along the crystallographic *c*-direction [1]. It is formed by a boron-oxygen network throughout the crystal with lithium atoms in the interstices; the anion B₄O₇²⁻ - the basic subunit of this net consists of four boron atoms, where two of them tetrahedrally and two other are triangularly linked to oxygens.

Lithium tetraborate attracts considerable interest in nonlinear optics as an element of surface acoustic wave devices, a frequency-conversion material for 2nd-5th harmonic generation from a high-power Nd:YAG laser, as a high power ultraviolet light source based on SHG and SFH of the visible laser radiation *etc.* Possible applications for Li₂B₄O₇ require deeper understanding of its properties, especially at non-ambient conditions.

Thus in the literature there is plenty of controversial data on Li₂B₄O₇ reporting anomalous behaviour in the different temperature ranges, e.g. thermal scintillations have been observed in Li₂B₄O₇ when not excited by hard quanta [2], incommensurate structure modulation [3], anomalies in thermal expansion and thermal evolution of bond lengths [4, 5], numerous phase transitions [6, 7], anomalies in sound velocities and Raman spectra [8], strong anisotropy of ionic conductivity [9] *etc.* The existing discrepancies between the experimental results of different authors lead us to perform systematic studies of lithium tetraborate.

Structural studies were performed using coherent elastic neutron scattering on ¹¹B enriched Li₂B₄O₇ (99.6% ¹¹B). Powder diffraction examinations unambiguously indicated isostructurality of Li₂B₄O₇ structure type in the temperature range from 3 K to its melting point at ca. 1170 K. Despite this fact, an evidence for anomalies in thermal dependencies of lattice parameters, bond lengths and displacement parameters has been deduced.

In the current contribution we report on complex studies of lithium tetraborate doped with ¹¹B in the broad temperature range 3-1200 K using neutron powder/single crystal diffraction, dilatometry, specific heat, calorimetry and impedance spectroscopy together with an attempt to present our view on the nature and origin of anomalies in Li₂B₄O₇.

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Keywords: neutron diffraction, noncentrosymmetric oxides, boron compounds

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Structural, magnetic, electrical and magnetocaloric properties in Pr_{0.6}Sr_{0.4}MnO₃/BaTiO₃ composites. M. Triki^a, E. Dhahri^a, M.P.F. Graça^b, M.A. Valente^b. ^a

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Composites with varying composition of ferromagnetic Pr_{0.6}Sr_{0.4}MnO₃ and ferroelectric BaTiO₃ have been prepared using a solid-state ceramic method (1-x)(Pr_{0.6}Sr_{0.4}MnO₃)/x(BaTiO₃), with x is the molar ratio and x = 0.0, 0.03, 0.05, 0.10 and 0.30 using conventional ceramic double sintering process. We report the structural, magnetic electrical and magnetocaloric properties of all samples. The presence of the two phases of Pr_{0.6}Sr_{0.4}MnO₃ (PSMO) and BaTiO₃ (BTO)

was confirmed by X-ray diffraction (XRD) technique and the structural analysis. Magnetic measurements of magnetization versus temperature and applied field were performed. The temperature dependence of magnetization reveals that the composite samples show paramagnetic to ferromagnetic transition when the temperature decreases at the same Curie temperature as the parent PSMO compound (T_c ≈ 273K). The magnetic entropy change $|\Delta S_M|$ has been deduced from the M(H) data by the Maxwell relation. Close to T_c, large change in magnetic entropy has been observed in all samples. The maximum value of the magnetic entropy is $|\Delta S_M^{\max}|$ decreases from 2.88 J.kg⁻¹.K⁻¹ for x = 0 to 1.86 J.kg⁻¹.K⁻¹ for x = 0.3 for an applied magnetic field of 2T. At this value of magnetic field the relative cooling power (RCP) decreases also from 63 J.kg⁻¹ for the parent sample to 38.3 J.kg⁻¹ for x = 0.3. The temperature dependence of the Landau coefficients have been deduced using the Landau expansion of the magnetic free energy, indicating the second order nature of the magnetic transition.

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FA2-MS14-P35

Twin structure and conductivity in LSGM. T. Tataryn^a, D. Savvitskii^a, E. Schmidbauer^b, C. Paulmann^c, U. Bismayer^d. ^a

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The aim of our investigations was to study the arrangement and distribution of twin boundaries during mechanical and thermal treatment in order to examine reversibility phenomena in larger ferroelastic crystal plates (5x6x0.87 mm³) as well as the influence of the domain structure on ionic conductivity. In a selected La_{0.95}Sr_{0.05}Ga_{0.9}Mg_{0.1}O_{3-x} (LSGM) - crystal plate the submicron twin structure was studied using white synchrotron radiation at the Kappa-diffractometer F1 equipped with a MAR CCD-detector (HASYLAB, DESY). Scanning of the sample under the beam (0.05x0.05mm²) and collecting diffraction data at each step with 45 micron spatial resolution was used to map the domain pattern in the LSGM-plate after mechanical and thermal treatment. Conductivity measurements were done between ~ 70 °C and 710 °C in air. Impedance spectroscopy was applied using a HP4284 LCR-meter in the range 20 Hz – 1 MHz. Data were recorded applying AC amplitudes of 80 mV and 1V to the electrode. It was shown that before mechanical treatment mainly twin walls normal to the largest surface of the plate occurred. The observed domain structure was partially switched to another twin configuration with domain walls parallel to the surface or to certain domain states during polishing. After annealing the domain configuration with prevalent domain walls normal to the largest plate surface was fully restored.

Impedance plots show two semicircular arcs. The first high frequency arc corresponds to the bulk conductivity while the second low frequency one corresponds to the conductivity on domain boundaries.

Our results show that strain can relax completely by forming