

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.*
E-mail: elena.borissenko@esrf.fr

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.*
E-mail: glazer@physics.ox.ac.uk

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

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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.*
E-mail: anatoliy.senyshyn@gmail.com

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.