

s11.m33.o2 Pressure - Temperature Neutron diffraction studies of $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$ (PZT) system: polarisation rotation mechanism involving low symmetry phases.

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Due to their exceptional piezoelectric performances, compounds based on lead zirconate titanate perovskite solid solution $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ (PZT) (with x close to 0.48) represent one of the most important class of piezoelectric materials, which are used as piezoceramics (piezoelectric transducers and actuators), and thin films (MEMS system or high-frequency components). These particular compositions lie on what is termed the morphotropic phase boundary (MPB) between the ferroelectric rhombohedral ($R3m$) and tetragonal phases ($P4mm$). Up to now, the high piezoelectric coupling constants in these materials were attributed to the simultaneous presence of trigonal and tetragonal domains near the MPB. The recent discovery of a monoclinic phase (Cm) at this region of the phase diagram provides a new explanation of the high electromechanical response, based on a polarisation rotation mechanism in which the polar axis is oriented between the directions corresponding to the tetragonal and rhombohedral forms. Additionally, a second monoclinic phase (Cc) with a double unit cell has been observed at low temperature for $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$.

The morphotropic composition of lead zirconate titanate, $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$, was studied as a function of temperature (50-310K) and pressure (0.1 MPa-7.5 GPa) by neutron powder diffraction. A series of low symmetry phases, monoclinic (space groups Cm and Cc) and triclinic forms (space groups $F1$ and F) were observed at various points in the P - T phase diagram of $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$. The high-pressure behavior is characterized by two mechanisms, a rotation and reduction of the spontaneous polarization and the onset of octahedral tilting leading to unit cell doubling. The results show that pressure can, as in the case of temperature and external electric fields, induce polarization rotation.

s11.m33.o3 High pressure X-ray absorption spectroscopy: state of the art and future developments.

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Recently (December 2003) the D11 dispersive EXAFS beamline of LURE has been definitively closed. In the last three years a lot of modifications had been done in order to improve the acquisition of data under high pressure: (i) a new detector one order of magnitude more sensitive and with a larger energy range accessible, (ii) a new way for data collection which has strongly reduced the deformation of the spectra and the number of extra glitches on the spectra and (iii) the use of perforated diamonds to reduce the absorption of the diamonds and therefore give access to lower energy edges. Using the perforated diamonds, XAFS experiment can be performed at the LIII, LII rare earth edges and combined with XMCD, these experiments allow to study the effect of pressure on the material structure, on the electronic configuration and on the magnetic properties for ferromagnetic materials. The extension of the energy range available improves the accuracy of the determination of the bond length and of the disorder parameters. These points will be presented and illustrated by different examples: the γ - α transition of Ce, the zinc blend to rocksalt transition for nanocrystalline ZnSe, the coordination change in FePO_4 and the phase transitions in YbAl_2 , everything being induced by the application of pressure. This beamline will be transferred to the new French synchrotron (SOLEIL) and will be available for experiments in 2006.