HB-2A

Neutron Powder Diffraction of Piezoelectric Ceramics at Hb2a

Piezoelectrics are a huge industry and their uses will expand if solutions can be found for a few limiting issues. Jennifer Forrester, a researcher at the University of Florida, and Krishna Nittala, a Ph.D. candidate at the university, used the Neutron Powder Diffractometer (NPD, at HB-2A) at HFIR to explore the structure and characteristics of piezoelectric ceramics that might lead to improved applications. Forrester used the NPD to examine crystal structures of lead-free piezoelectric ceramics with the aim of creating materials that can take more deformation and demonstrate improved properties. A limitation of currently used piezoelectrics is that at high temperatures they shift to a cubic structure, losing their piezoelectric properties. Nittala examined samples of piezoelectric materials at gradually increasing temperatures as part of an effort to develop materials with higher transition temperatures. The current temperature limit for piezoelectrics is around 400°C. He examined samples at temperatures ranging from room temperature to 600°C using the ILL vacuum furnace on HB2a. Their results have been published in APL and JACS.

J.Forrester (left) and K. Nittala (Right) at HB2a HFIR

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The Role of Spontaneous Polarization in the Negative Thermal Expansion of Tetragonal $PbTiO_3$-Based Compounds

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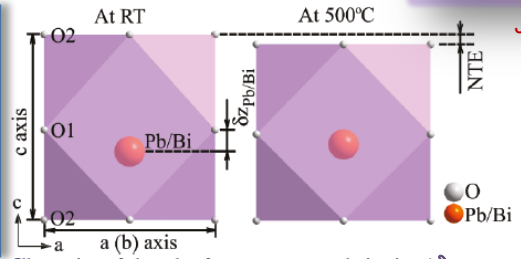

Illustration of the role of spontaneous polarization ($\delta z_{Pb/Bi}$) in NTE. The PbO_{12} polyhedron is projected along the b-axis

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Structural evidence for the nonmonotonic trend of T_C in tetragonal $PbTiO_3$—$BiScO_3$ solid solutions

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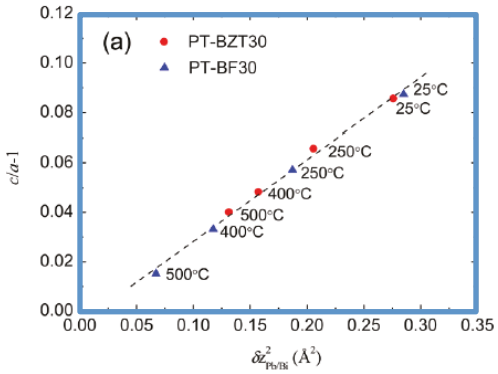

Linear correlation between (c/a - 1) and $\delta z_{Pb/Bi}^2$ for PTBZT30 and PTBF30 over the temperature range from RT to 500°C.

The mechanism of negative thermal expansion has been studied by high-temperature neutron powder diffraction performed on two representative compounds, $0.7PbTiO_3$-$0.3BiFeO_3$ and $0.7PbTiO_3$-$0.3Bi(Zn_{1/2}Ti_{1/2})O_3$, whose negative thermal expansion is contrarily enhanced and weakened, respectively. With increasing temperature up to the Curie temperature, the spontaneous polarization displacement of Pb/Bi ($\delta z_{Pb/Bi}$) is weakened in $0.7PbTiO_3$-$0.3BiFeO_3$ but well-maintained in $0.7PbTiO_3$-$0.3Bi(Zn_{1/2}Ti_{1/2})O_3$. There is an apparent correlation between tetragonality (c/a) and spontaneous polarization. Direct experimental evidence indicates that the spontaneous polarization originating from Pb/Bi-O hybridization is strongly associated with the negative thermal expansion. This mechanism can be used as a guide for the future design of negative thermal

The structure of (1-x)$PbTiO_3$-x$BiScO_3$ solid solutions was studied at HB2a. The cation displacements of Pb/Bi and Ti/Sc exhibit a coupling property and a different impact by the substitution content of $BiScO_3$. Its nonmonotonic trend of T_C is quantitatively related to the calculated spontaneous polarization in the whole tetragonal range. The unique role of Bi-substitution not only contributes to enhance the component of polarization of Pb/Bi but also to increase the T_C.