Towards a Deep Microscopic Understanding of Ferroelectric Alloys

Laurent Bellaiche, University of Arkansas, DMR-9983678

- We started a collaboration with two European experimental groups (in France and in the Netherlands) to investigate the high-pressure behavior of the technologically-important $Pb(Zr_{0.52}Ti_{0.48})O_3$ ferroelectric alloy.
- Two novel room-temperature phase transitions were observed, via synchrotron x-ray diffraction and Raman spectroscopy, under hydrostatic pressures up to 16 GPa. A monoclinic (M)-to-rhombohedral (R1) phase transition takes place around 2-3 GPa, while this R1 phase transforms into another rhombohedral phase, R2, at 6-7 GPa.
- Our first-principles calculations assign the R3m and R3c symmetry to R1 and R2, respectively, and reveal that R2 acts as a pressure-induced structural bridge between the polar R3m and a predicted antiferrodistortive R-3c phase.

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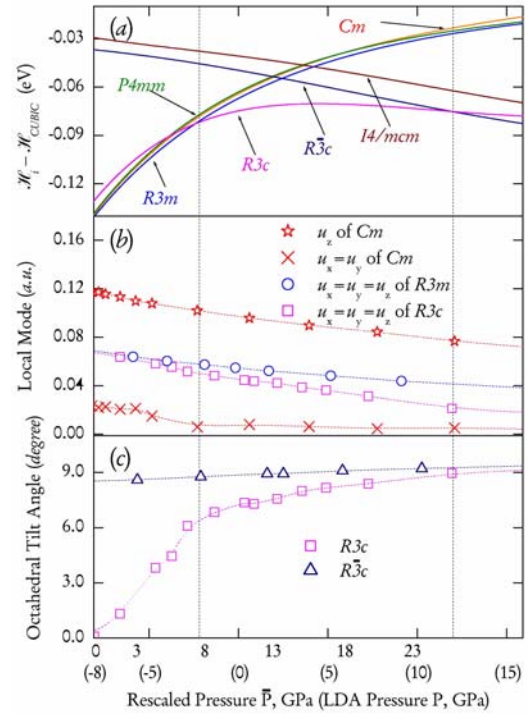

First-principles prediction of the pressure behavior of (a) ΔH for all the considered phases (the phase corresponding to a minimal ΔH at a given P is the most stable one for this pressure), (b) the Cartesian components of the polarization for the Cm, R3m and R3c phases, and (c) the rotation angle of the oxygen octahedra with respect to the pseudo-cubic [111] direction for the R3c and R-3c phases.

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Education:

- 7 graduate students (including two female students) and 2 research associates contributed to this work.
- Saad Bin-Omran received his Master of Physics in Fall 2004
- Alireza Akbarzadeh (Graduate student) was awarded a IBM-Zerner Fellowship, in Fall 2003, for his research on ferroelectrics.

Outreach:

The P.I.'s group participated in an outreach activity in Fayetteville high schools in the Fall 2003. More precisely, we were judging the BEST robotics competition. It was a competition between regional (Arkansas and surrounding states) high school and middle school students to promote science and engineering among local youth. Among the points on which the students were judged on were use of science and engineering process in robot construction and design, teamwork, presentation and sportsmanship.