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Ferroelectric and piezoelectric properties of $SrBi_2Ta_2O_9$

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Abstract – The phase transition sequence and the evolution of dielectric and piezoelectric properties of $SrBi_2Ta_2O_9$ are investigated using a shell model with parameters fitted to first-principles calculations. The simulated phase diagram shows the existence of an intermediate orthorhombic paraelectric phase between the high-symmetry tetragonal and the ferroelectric orthorhombic phase. We show that this intermediate phase can be also detected from the anisotropy of dielectric response of the material. Finally, piezoelectric properties along crystallographic directions are also investigated.

$SrBi_2Ta_2O_9$ (SBT) is very attractive material for FeRAM and piezoelectric device applications due to its low voltage operation, good reliability properties, and high T_C. It belongs to to the family of Aurivillius compounds, which are formed by bismute oxide Bi_2O_2 slabs separated by layers of perovskite-like blocks. The lack of crystal of sufficient quality makes theoretical studies highly desirable to determine single crystal properties.
We successfully develop a shell model potential for SBT with parameters fitted to first-principles calculations. The resulting model is able to reproduce correctly the T=0K structure of SBT, in good agreement with LDA but with values underestimated with respect to the experiments. The ground state is orthorhombic with lattice parameters *a*= 5.46Å, *b*=5.44 Å, *c*= 24.42Å while the experimental results are *a*=5.52Å, *b*=5.52 Å and *c*=25.02. In addition, the spontaneous polarization P = 8 μC/cm^2 of the model is considerable lower than the experimental one of 20 μC/cm^2 measured in single crystals.
The resulting lattice constants as a function of temperature obtained through molecular dynamics simulations are shown Figure 1. Discontinuities are clearly discernible in the plots of *a*, *b* and *c* parameters vs. T, suggesting the existence of two phase transitions, one at T_{c1} ~ 850K and another at T_{c2} ~1300 K. At low temperatures ($T < T_{c1}$) the structure is orthorhombic ($a \neq b \neq c$) and the polarization is different from zero, indicating the presence of the *A21am* ferroelectric phase. The lattice parameters show strong discontinuities at T_{c1}, despite the fact that the structure is still orthorhombic (*Amam* symmetry*)* up to T_{c2}. In this temperature range ($T_{c1} < T < T_{c2}$), the lattice parameter *a* is slightly different from *b* while the polarization is very close to zero. At T_{c2}, the lattice constant *c* shows a marked change of slope, and *a* and *b* have almost identical value. This is an indication for the transition to the tetragonal paraelectric *I4/mmm* phase.
We used the model to investigate the dielectric and piezoelectric properties of the SBT. Figure 2 shows the dielectric constants (ε_{11}, ε_{22}, and ε_{33}) determined by calculating the change in the polarization of the perfect crystal under an applied electric field. The *a*, *b* and *c* axes of the orthorhombic phase lie along the 1, 2 and 3 directions, respectively. The maximum of ε_{11} corresponding to the ferro-paraelectric phase transition is observed at T_{c1}, and no anomalies are observed in ε_{22} and ε_{33} at this temperature. In the intermediate phase ($T_{c1} < T < T_{c2}$) ε_{11} is considerable larger than ε_{22}.. Thus, the anisotropy of the dielectric constant provides an alternative way to identify intermediate phases. No dielectric anomalies are observed at T_{c2}, and $\varepsilon_{11} = \varepsilon_{22}$ in the tetragonal phase ($T>T_{c2}$).

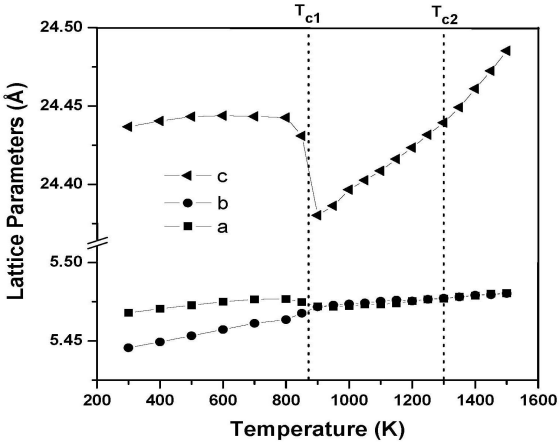

Figure 1: Thermal evolution of lattice parameters for SBT obtained by MD simulations. The vertical lines indicate the position of the structural phase transitions.

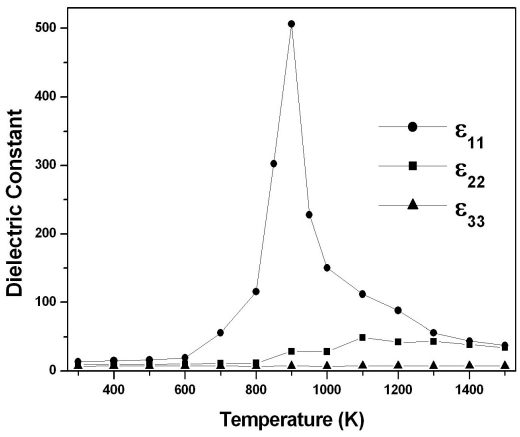

Figure 2: Temperature dependence of the dielectric permittivity along crystallographic directions for SBT obtained by MD simulations.