A first-principles-based study of thermal conductivity in $PbTiO_3$

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$PbTiO_3$ is a well studied ferroelectric perovskite. This work is about its lattice thermal conductivity, κ_L. We can expect κ_L to be low because of the presence of Pb, a heavy element. The structural instability associated with the transition from the paraelectric (PE) to the ferroelectric (FE) phase of $PbTiO_3$ may additionally contribute to lowering κ_L. In this work I use a Boltzmann transport equation solver for phonons, ShengBTE[1], to estimate κ_L of lead titanate. A key ingredient to this program is the force constant matrix of the material under study, obtained using harmonic approximation of the lattice vibrations. Density functional theory-based methods (at zero temperature) is used to calculate the above force constant. However, the cubic phase of $PbTiO_3$ shows a number of soft modes indicating its structural instability associated with the PE/FE phase transition. The presence of soft modes renders the above machinery unusable for the cubic phase. While we cannot calculate κ_L for the cubic phase, we can study the tetragonal phase. All the soft modes harden in the tetragonal phase, and harmonic approximation is generally valid again. More importantly, we can controllably soften the phonon branches in this structure by applying strain along the z direction. This exercise, albeit artificial, can tell us how the interaction among the acoustic and optic branches of phonons influences κ_L of $PbTiO_3$. Encouraged by the preliminary results indicating a low κ_L, I also look at the thermoelectric behavior of $PbTiO_3$. If it is possible to enhance the electrical conductivity of $PbTiO_3$ through doping, we could expect very good thermoelectric properties.

[1] Li W., Carrete J., Katcho N. A., Mingo N., Comp. Phys. Comm. **185**, 1747-1758 (2014).