A first-principles-based study of thermal conductivity in PbTiO₃

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PbTiO₃ is a well studied ferroelectric perovskite. This work is about its lattice thermal conductivity, $\kappa_L$. We can expect $\kappa_L$ 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 PbTiO₃ may additionally contribute to lowering $\kappa_L$. In this work I use a Boltzmann transport equation solver for phonons, ShengBTE[1], to estimate $\kappa_L$ 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 PbTiO₃ 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 $\kappa_L$ 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 $\kappa_L$ of PbTiO₃. Encouraged by the preliminary results indicating a low $\kappa_L$, I also look at the thermoelectric behavior of PbTiO₃. If it is possible to enhance the electrical conductivity of PbTiO₃ through doping, we could expect very good thermoelectric properties.