

Direct molecular dynamics simulation of thermal conductivity in ferroelectrics

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From the point of view of fundamental physics, thermal conductivity in ferroelectric materials with phase transitions may be interesting to understand. Here, we present a method to calculate the thermal conductivity directly by molecular dynamics (MD) simulations.

The effective Hamiltonian, constructed from first-principles calculations, and used in the present MD simulations is essentially the same as that in Refs. [1, 2]

$$H^{\text{eff}} = \frac{M_{\text{dipole}}^*}{2} \sum_{\mathbf{R}, \alpha} \dot{u}_{\alpha}^2(\mathbf{R}) + \frac{M_{\text{acoustic}}^*}{2} \sum_{\mathbf{R}, \alpha} \dot{w}_{\alpha}^2(\mathbf{R}) + V^{\text{self}}(\{\mathbf{u}\}) + V^{\text{dpl}}(\{\mathbf{u}\}) + V^{\text{short}}(\{\mathbf{u}\}) \\ + V^{\text{elas, homo}}(\eta_1, \dots, \eta_6) + V^{\text{elas, inho}}(\{\mathbf{w}\}) + V^{\text{coup, homo}}(\{\mathbf{u}\}, \eta_1, \dots, \eta_6) + V^{\text{coup, inho}}(\{\mathbf{u}\}, \{\mathbf{w}\}). \quad (1)$$

The true atomic structure has properties determined by the complex chemical bonding between the atoms, but in the model system the complexity is reduced; the collective atomic motion is coarse-grained by local soft mode vectors, $\mathbf{u}(\mathbf{R})$, and local acoustic displacement vectors, $\mathbf{w}(\mathbf{R})$, of each unit cell located at \mathbf{R} in a simulation supercell. Each term in the Hamiltonian is described in Ref. [2].

In Fig. 1, the supercell used in MD simulations is schematically illustrated. The procedure to estimate thermal conductivity involves two steps: First, constant-temperature MD is performed in the canonical ensemble using the velocity-scaling thermostat. Next, constant-energy MD using the leapfrog method is performed with adding energy Δe at each MD step into a single layer at $z = \frac{1}{4}L_z$ and removing the same amount of energy at $z = \frac{3}{4}L_z$. Temperature gradient and consequently heat flows appear between the energy source and sink. Typical time-averaged layer-by-layer temperature profile used to compute the thermal conductivity is shown in Fig. 2. MD simulations are performed with our original **feram** software. **feram** is distributed freely under the GNU General Public License (GPL) and can be found at <http://loto.sourceforge.net/feram/>.

References

- [1] U. V. Waghmare and K. M. Rabe, Phys. Rev. B **55**, 6161 (1997).
- [2] T. Nishimatsu, U. V. Waghmare, Y. Kawazoe, and D. Vanderbilt, Phys. Rev. B **78**, 104104 (2008).

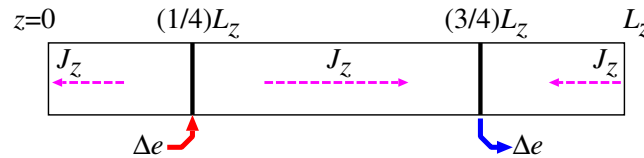


Figure 1: Schematic illustration of supercell used in MD simulations. The supercell of size of $L_x \times L_y \times L_z$ unit cells is placed in the periodic boundary condition. Energy Δe is pushed into the system through the $L_x \times L_y = 24 \times 24$ dipoles in a single layer at $z = \frac{1}{4}L_z$. Same amount of energy is pulled out from the system at $z = \frac{3}{4}L_z$. The heat flows J_z is indicated with dashed lines.

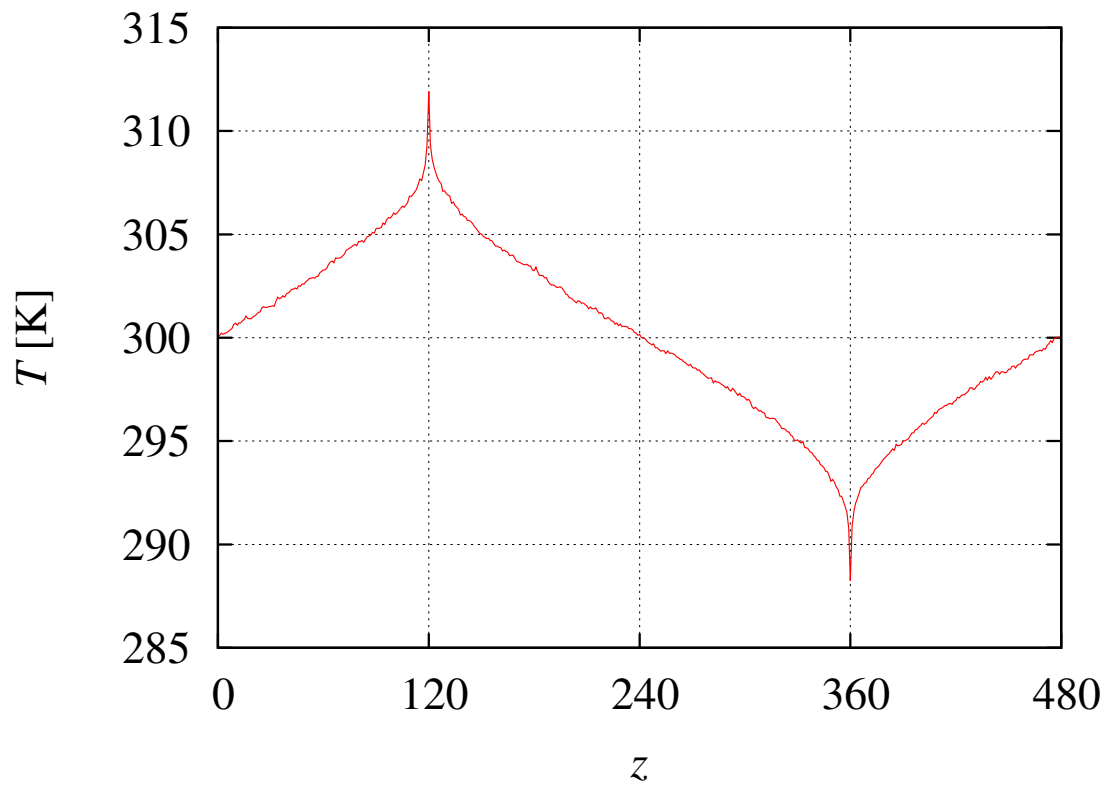


Figure 2: Typical temperature profile for a $48 \times 48 \times 480$ system at an average temperature of 300 K.