New insights into thermal conductivity by non-equilibrium molecular dynamics\footnote{Supported by DOE grant No. DE-FG02-08ER46550} PHILIP ALLEN, Stony Brook University, YERONG LI, Nanjing University — Non-equilibrium molecular dynamics (NEMD) is often used to simulate thermal conductivity ($\kappa$). A steady state heat current and corresponding temperature gradient are created computationally over a simulation cell of thousands of atoms. We advocate a variation that gives directly $\kappa(q)$, the Fourier transform of the non-local $\kappa(x - x')$ that relates $J(x)$ to $\nabla T(x')$. The algorithm is tested on the Lennard-Jones liquid and crystal, and is efficient for extraction of the macroscopic $\kappa = \lim_{q \to 0} \kappa(q)$. Peierls-Boltzmann theory gives (in relaxation-time approximation) a closed-form expression for $\kappa(q)$ that can be used to study the $q$-dependence in the small $q$ limit, and how it depends on simulation cell dimensions in NEMD. The frequency-dependent relaxation rate $1/\tau_Q \propto \omega_Q^2$ was chosen for detailed comparison with simulation. For an isotropic cell ($N_x = N_y = N_z$), the behavior is $\kappa(q) = \kappa - A * q^{1/2}$. For the more typical anisotropic cell with one length ($N_z$) large compared to the others, there is an additional term $\propto q^{-1/2}/N_x N_y$. This divergent contribution disappears in the bulk limit. Strategies for extrapolation of simulations are suggested.

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