Phonons in Thermoelectric Devices
or
Anderson Localization in Random Multilayer Thin Films: a Phonon Story

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Seebeck Effect

\[ ZT = \frac{S^2 \sigma T}{\kappa_{ph} + \kappa_{el}} \]
\[ U = \frac{k}{2} \sum_{i} \left( (u_{i-1} - u_i)^2 + (u_i - u_{i+1})^2 \right) \]

\[ = \frac{k}{2} \sum_{i} 2u_i^2 + u_{i+1}^2 + u_{i-1}^2 - 2u_i u_{i+1} - 2u_i u_{i-1} \]

\[ m_i \ddot{u}_i = -\frac{\partial U}{\partial u_i} \]

\[ = -\frac{k}{2} \left( 4u_i - 2(u_{i+1} + u_{i-1}) \right) \]

With the ansatz \[ u_i(t) = A_i e^{ikia - \omega t} \],

\[ -m_i \omega^2 u_i = k \left( 2u_i - u_{i+1} - u_{i-1} \right) \]
\[-m_i \omega^2 u_i = k (2u_i - u_{i+1} - u_{i-1})\]

if we set \(m_i = M \forall i\),

\[-M \omega^2 e^{i(kna - \omega t)} = -k \left( 2 - e^{-ika} - e^{ika} \right) e^{i(kna - \omega t)}
= -2k(1 - \cos ka) e^{i(kna - \omega t)}.
\]

This furnishes

\[\omega(k) = \sqrt{\frac{2k(1 - \cos ka)}{M}}\]

\[= 2\sqrt{\frac{k}{M}} \left| \sin \frac{1}{2}ka \right|\]
1D Solid

Uniform Masses

Periodic Superlattice
1D Solid with random disorder

- Displacement vs. n
- $\omega$ vs. $ka/\pi$
- Fraction of Modes Localized vs. Mass Ratio
Four types of solids were examined in this work (Figure 1). In each case, 20% of the atoms were mass-altered as determined by a Gaussian probability distribution function with a standard deviation of one lattice plane. In the case of the random multilayer, 80 atomic planes (corresponding to 20% of the atoms) were randomly selected using a pseudorandom number generator that produced a uniform probability distribution in the atomic plane being altered when the random number generator produced values less than 0.2. Following initial equilibration, a RNEMD technique was employed for determination of thermal conductivity. In all cases, to eliminate artificially reduced phonon mean free paths provided by the finite size of the simulation box, thermal conductivities less than 1 W/m-K were verified to be free of size effects by doubling the length and width of the simulation box. For materials simulated here, thermal conductivities less than 1 W/m-K compared with the experimental data and the EMD simulated data generated out to 5 ns. The derived values for silicon containing its natural isotopes, in good agreement with previous equilibrium molecular dynamics simulations of this material.

Random multilayer, (b) disordered random multilayer, (c) superlattice, and (d) random alloy. FIG. 1. A schematic of the four silicon-like solids explored in this work. (a) ideal random multilayer (blue), mass/silicon mass) is shown in Figure 2 along with the experimental data at 300 K (Ref. 12) and other EMD for silicon containing its natural isotopes, in good agreement with previous equilibrium molecular dynamics technique, the details of which can be found in Refs. 35–37.

To verify the appropriateness of the Stillinger-Weber potential in these simulations, the thermal conductivity of the solid was determined from the extracted energy flux of the solid was determined from the extracted energy flux result of this energy exchange. In the case of an isotopically pure 28Si solid, thermal conductivity using this approach was 160 W/m-K which can be found in Refs. 35–37. A 512 atom system

The simulated thermal conductivity at 300 K as a function of mass ratio for the random multilayer shows a substantial reduction in lattice thermal conductivity when compared with the experimental data and the EMD simulated data. In the case of the superlattice structure, the thermal conductivity decreases from a size effect limited value of 20 W/m-K to a value of approximately 0.5 W/m-K as the mass ratio was varied from 1 to 0.1 (noting that C produces a mass ratio of 2.6), Sn (mass ratio 4.2), and Pb (mass ratio 7.4). A decrease in the mass ratio from 1 to 0.1 (noting that C produces a mass ratio of 0.43 and H a mass ratio of 0.03) also produces a noticeable reduction in the lattice thermal conductivity for the superlattice structure. In the case of the random alloy, the lattice thermal conductivity shows a reverse equilibrium molecular dynamics technique shows a negligible reduction in the lattice thermal conductivity for the random alloy structure and the superlattice structure with the ratio of 0.43 and H a mass ratio of 0.03 also produces a noticeable reduction in the lattice thermal conductivity for the random alloy structure. The simulated thermal conductivity as a function of mass ratio for the random multilayer shows a substantial reduction in lattice thermal conductivity when compared with the experimental data and the EMD simulated data.