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Investigation of wave interference effect in Si/Ge superlattices with interfering Monte Carlo method

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ABSTRACT

The recently proposed Interference Monte Carlo (IMC) method is a mesoscale particle simulation method that is capable of modeling wave interference effect in addition to phonons' particle behavior. Using the IMC, wave interference effect, which leads to a linear increase in thermal conductivity as the number of periods of superlattices increases, has been confirmed in Si/Heavy Si superlattices. Such a trend was also experimentally observed in AlAs/GaAs superlattices and has been regarded as the evidence of the coherent phonon heat conduction. In this work, wave interference effect in 1D Si/Ge superlattices at 300 K is investigated using the IMC method. First, the IMC method is further improved and validated with Molecular Dynamics simulations. It is then used to compute thermal conductivities of both periodic and aperiodic Si/Ge superlattices with fixed period length but varied number of periods. It is found that the nearly linearly increasing trend is present in both cases. However, this increasing trend is not caused by the wave interference, but is rather caused by the ballistic transport of low-frequency phonons due to their high transmission rates. Hence for Si/Ge superlattices with an average period length of 20 nm, the wave interference effect plays an insignificant role even when the interfacial scatterings are perfectly specular.

1. Introduction

Thermoelectric (TE) materials are an important class of materials that have various applications such as in thermal management and energy conversion. But the relatively low conversion efficiency of the many TE materials significantly limits their application scopes and degrades their commercial values. Searching for high-performance TE materials has been an active research area in the past a few decades. The efficiency of TE conversion is measured by the dimensionless figure of merit $ZT = \frac{S^2\sigma}{\kappa}T$, where S is the Seebeck coefficient, σ is the electrical conductivity, κ is the thermal conductivity, and T is temperature. Based on the figure of merit, an obvious strategy for improving the efficiency is to reduce the thermal conductivity while keeping the Seebeck coefficient and the electrical conductivity unimpaired. Superlattices (SLs), with their significantly reduced thermal conductivity and nearly unaltered electrical conductivity, are promising TE materials that may achieve high efficiency [1]. Understanding phonon transport in SLs is clearly important in the design of these materials. For large-scale systems, phonon transport is dominated by its particle nature. As the system size reduces to sub-microns, wave effects may become important. In an experimental study of AlAs/GaAs SLs [2], evidences of coherent heat conduction have been demonstrated, indicating the importance of considering wave effects in the modeling of SLs.

Molecular Dynamics (MD) is a popular tool to study phonon transport inside SLs, and many studies have been conducted on various systems using MD simulations [3–6]. A major advantage of MD simulation lies in that it naturally includes both effects and hence can provide a complete picture of phonon transport. However, since MD tracks the trajectory of every atom in the system, the computational cost is extremely high, greatly limiting the system size that can be simulated. In addition, it is difficult to obtain phonon transport mechanisms from MD simulation since it deals directly with atoms instead of phonons. In contrast, Monte Carlo (MC) method simulates phonons directly and thus it is much easier to extract phonon transport information. It is also much faster than MD due to its statistical nature. However, the conventional MC method is purely particle-based, which does not include any wave effect and is thus only valid for large systems in which the wave effect is insignificant. Several models have been proposed to include both wave and particle effects in the simulation of SLs, including modified Lattice Dynamics (LD) models [7,8], and a

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hybrid thermal conductivity model [9]. In the latter approach, wave and particle effects are modeled by separating phonons into two non-interacting groups: wave and particle groups. A holistic treatment of wave-particle duality of phonons was proposed recently [10]. This method, entitled as the Interfering Monte Carlo (IMC) method, incorporates phonon wave information into the conventional MC framework, and thus allows the modeling of both effects in a systematic and natural way. In the diffusion limit, the method recovers the conventional MC results, whereas in the coherent regime, it is able to capture the wave interference phenomena where the conventional MC fails. The SLs studied in Ref. [10] are composed of Si/heavy-Si with an artificial constant transmission rate of 0.6. These SLs have exhibited strong wave interference effects, and it has been shown that a thermal conductivity that is lower than the particle limit can be achieved by utilizing destructive interference occurred in aperiodic lattices. It would be interesting to examine if such a mechanism is applicable to more realistic and commonly studied SLs such as Si/Ge SL.

In the present study, the IMC method is further improved by feeding a more realistic transmission model. And quantitative validation of the IMC/MC methods using MD simulations is conducted for the first time. The IMC method is then applied to study phonon transport inside Si/Ge SLs. The particular focus is on the wave interference effect in both periodic and aperiodic SLs. We find that due to the high transmission rate and long relaxation time of low-frequency phonons, the wave interference effect plays a minor role in the phonon transport inside Si/Ge SLs with an average layer thickness of 20 nm.

In Section 2, an overview of the methodologies used in the study is presented. It is followed by the description of methods to obtain the key input parameters/properties required in the IMC simulations. Calculated thermal conductivities of various periodic and aperiodic SLs from MD, MC and IMC are showed and discussed in Section 4. In the last section, a summary is provided.

2. Methodology

2.1. Non-equilibrium molecular dynamic simulation

To validate the IMC/MC method, non-equilibrium Molecular Dynamic (NEMD) simulations are conducted to calculate the cross-plane thermal conductivities of several Si/Ge SLs with different total thicknesses but a fixed period length of 20 nm. In the MD simulations, the Stillinger-Weber (SW) potential [11,12] is adopted to model the interatomic interaction. Although more accurate potentials such as those obtained directly from First-principles calculations could be used, for simplicity, the empirical SW potential is used since the purpose of the MD simulations is to validate the IMC/MC method.

The SL is initialized by using the averaged lattice constant for both Si and Ge, and then relaxed to be free of internal pressure. The final lattice constant obtained is 5.5041 Å. Periodic boundary conditions are applied in the in-plane directions of SLs, and the size of cross section is set to be 4×4 unit cells to obtain the converged thermal conductivity. The MD system is relaxed in NPT ensemble at 300 K for 500 ps with periodic conditions applied in the cross-plane direction before the system is switched into NVE ensemble. Then, a layer of atoms is fixed at both ends of the structure to eliminate rigid-body motions. Meanwhile, thermal baths with 3 unit cells at two ends of the system are used to create a constant heat flux by adding and subtracting energy currents. After the system reaches steady state, the time-averaged temperature profile in the middle region is obtained and the effective thermal conductivity is calculated according to Fourier's law.

2.2. Overview of the interfering Monte Carlo method

Phonon MC is a stochastic solver for the phonon Boltzmann transport equation, which is:

$$\frac{\partial f}{\partial t} + \boldsymbol{v}_g \cdot \nabla f = \left[\frac{\partial f}{\partial t}\right]_{scat} \tag{1}$$

With the relaxation time approximation, this equation becomes

$$\frac{\partial f}{\partial t} + \boldsymbol{v}_g \cdot \nabla f = -\frac{f - f^0}{\tau} \tag{2}$$

where f is the distribution of phonons, f^0 is the equilibrium distribution of phonons, v_g is the group velocity and τ is the relaxation time.

In the conventional MC method, phonons are treated as particles. Only the momentum and the energy of each particle are monitored and updated when phonons undergo various scatterings. Hence, the conventional MC method doesn't include any wave effect.

However, when the period length of SLs reduces to submicrons, wave interference may occur as the wave packets split at interfaces when they travel along the SL. The IMC method is designed to include the wave interference within the conventional MC framework. We consider the cases when the spatial length of wave packets, that is, the coherence length, is smaller than the period length. In such cases, self-interference does not occur and wave packets can still be treated as point-wise particles as that in the conventional MC. A key feature in the IMC method is that both the amplitude and the phase information of packets that are essential for modeling waves are added into the particle model. These wave features are tracked and updated during the transport process based on their physical nature. Specifically, intrinsic phonon scatterings tend to randomize the phases and thus the phases of the scattered phonons are randomly set. At the interface, the reflection and the transmission of phonon wave packets can be partially coherent depending on the specularity. The coherent part of the transmitted or reflected phonon wave packet retains its phase, whereas the incoherent part has its phase been randomly set. After the interfacial scattering, two wave packets coming from different sides of the interface and having the same mode and wave vector may overlap and interference occurs. This process is handled by merging the two particles into one via wave superposition. In such a way, the wave interference and anharmonic scatterings are modeled naturally in the IMC method. A detailed description is provided in the following section.

2.3. Phonon-interface model

The phonon-interface model is critical in the modeling of phonon transport inside a composite material. For structures like SLs, interfaces between dissimilar materials play a key role in the reduction of thermal conductivity. Several interfacial models have been proposed [13–17]. Among them, the acoustic mismatch model (AMM) [13] and the diffuse mismatch model (DMM) [14] are the two most widely adopted models largely due to their simplicity. Both models assume purely elastic scatterings at the interface and thus the frequencies of the transmitted and reflected phonons remain unchanged. AMM assumes a perfect interface and the material is close to continua [18]. Thus, it is a good approximation for long-wavelength phonons but is not appropriate for high-frequency phonons. The transmission predicted by the AMM is:

$$t(\omega_i, \theta_i) = \frac{4Z_1 Z_2 \cos\theta_1 \cos\theta_2}{(Z_1 \cos\theta_2 + Z_2 \cos\theta_1)^2} \tag{3}$$