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Influence of surface roughness on thermal properties of single crystalline Ge thin films

Zhang Xingli [a,*], Wu Xiande [b]

[a] College of Mechanical and Electrical Engineering, Northeast Forestry University, Harbin 150040, China
[b] College of Aerospace and Civil Engineering, Harbin Engineering University, Harbin 150001 China

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ABSTRACT

We use non-equilibrium molecular dynamics (NEMD) simulations to compute thermal conductivity of Ge thin films with rough surface. The analysis shows that the shape, height, and length of the surface roughness have an appreciable influence on the in-plane and cross-plane thermal conductivity of Ge thin films. The thermal conductivity significantly decreases with increasing the period height of roughness or with decreasing the period length of roughness. Phonon-boundary scattering mechanism could be used to explain our results.

1. Introduction

Single crystalline Ge thin films attract a great interest in the scientific community due to their potential applications in thin-film transistors, highly efficient solar cells, and three-dimensional on-chip optical interconnects [1–3]. In order to improve the performance and reliability of the devices manufactured by single crystalline Ge thin films, it is essentially important to understand and predict the thermal transport of them at nanoscale level. Since the characterization size is reduced to nanoscale, the heat transfer of single crystalline Ge thin films become unusual compared to bulk materials. Boltzmann transport equation (BTE) based methods and molecular dynamics (MD) simulations were used to measure the cross-plane or in-plane thermal conductivity of single crystalline Ge thin films [4,5]. It was found that thermal conductivity of nanofilms displays strong anisotropy and cross-plane thermal conductivity is lower than the in-plane thermal conductivity.

Single crystalline Ge thin films usually contain amorphous phase or oxides on their surface after being synthesized by CVD or PVD. The variation of surface roughness may considerably affect the thermal transport properties of the material. Many researchers simulated the effect of surface roughness on the thermal properties of nanoscale material using different methods. Liu and Chen demonstrated that the thermal conductivity of Si nanowires could be significantly decreased by introducing surface roughness using molecular dynamics simulations [6]. Aksamija and Knezevic calculated the thermal conductivity of graphene nanoribbons using the Boltzmann transport equation, and found that the physical width of the roughness along the line edges could be used to tailor the thermal conductivity value [7]. Wang et al. presented a phonon localization theory to explain the phonon scattering at the edges of graphene nanoribbon, and indicated that this theory could also affect phonon transport in the rough thin films [8,9]. Park et al. synthesized VLS-grown rough Si nanowires with various surface roughness and measured thermal conductivities. It was also found that the thermal conductivity of Si nanowires with rough surface was significantly lower than that of nanowires with smooth surface and decreased with increasing surface roughness [10]. Although the aforementioned studies have shown the influence of surface roughness on the nanoscale thermal transport, there is no comprehensive work on the study of the surface roughness effects on the single crystalline Ge thin films. Using non-equilibrium molecular dynamics (NEMD) simulations, the influence of surface roughness on cross-plane thermal conductivity and in-plane thermal conductivity of single crystalline Ge thin films is investigated in this study.

2. Methodology of NEMD simulation

The NEMD simulations of the Ge thin films are performed using LAMMPS code. Fig. 1 shows the simulation model used in the present study. The positions of each atom occupy in an FCC crystal. Periodic boundary conditions are used in Y and Z directions. The

* Corresponding author.
E-mail address: cindy07b@126.com (X. Zhang).

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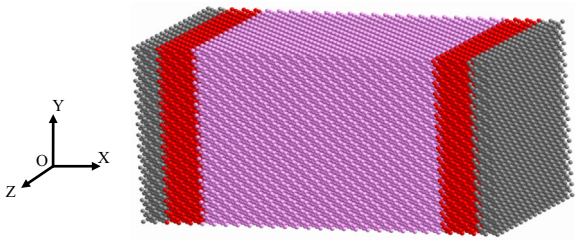

Fig. 1. NEMD simulation model of single crystalline Ge thin film.

cross-section area of *YOZ* is set to be 16 × 16UC (UC, unit cells). The heat transfer in the system occurs in *X* direction, and a hot and cold source with the thickness of 3UC is built to create a temperature gradient in the system by controlling the energy given or taken from these regions. Adiabatic walls with the thickness of 2UC are constructed to prevent the atoms escaping from the system, and the velocities of each atom in this region are 0.

The aim of our simulations is to calculate the thermal conductivity of single crystalline Ge thin films with different thicknesses and roughness. Several thin films with different thicknesses (10, 20, 30, and 40UC) and several roughness patterns are chosen in our simulation. Fig. 2(a) shows a 2D model of periodic isosceles triangle shaped interface in the *Z* and *X* axial directions with height H_1 and length L_1.In this case, the period length is dependent on the height ($L_1 = 2H_1$). Fig. 2(b) shows a 2D model of periodic square shaped interface in the (*Z*, *X*) planes with height H_2 and periodic length L_2. The lengths of convex and concave surfaces have same values in a single periodic length. As the main purpose of the present study is to show the effect of surface roughness on the thermal conductivity, thus the effects of the surface reconstructions will not be taken into account in this paper.

Tersoff three-body potential model is employed to describe the interaction among different Ge atoms in the simulation film which is reliable to describe the semiconductor atoms potential properties [11]. For those atoms, Newton's classical equations of motion are solved using the Velocity-Verlet integration algorithm. The time step for the simulation is set as 1 fs. The simulations consist of two stages: the first stage is the constant-temperature simulation, in which the temperature is maintained at constant value with a coupling time of 2×10^6 MD steps; the second stage is the constant-energy one with a coupling time of 8×10^6 MD steps to ensure the whole system to reach an equilibrium state. The method proposed by Jund [12] is used to apply a specified heat flux by scaling the velocities of the atoms in the hot and cold source of the simulations. A specified amount of energy ΔE (set to 1% of K_BT) is added to hot source and subtracted the same amount from the cold source at each time step.

The velocities of all the atoms in the hot and cold sources are scaled according to the following equation:

$$v_{i,new} = v_G + \alpha(v_{i,old} - v_G) \tag{1}$$

where v_G is the velocity of the center of mass, which is set to be zero at the beginning of our simulations. A scaling factor α is calculated from the following equation:

$$\alpha = \sqrt{1 \pm \frac{\Delta E}{E_k}} \tag{2}$$

where $E_k = \sum_{i=1}^{N} \frac{1}{2} m_i v_i^2$ is the kinetic energy of atoms in the hot and cold source.

Based on the Fourier law of conduction, the thermal conductivity is given as:

$$\lambda = \frac{\Delta E}{2A\tau \cdot (\partial T/\partial x)} \tag{3}$$

where τ is the simulation step time; *A* is the cross-sectional area. To obtain the temperature distribution, the system is divided into numerous planes along the longitudinal direction, and the instantaneous temperature of each plane is calculated using the following equation:

$$T = \frac{1}{3K_B N} \left\langle \sum_{i=1}^{N} \left(\frac{1}{2} m_i v_i^2 \right) \right\rangle \tag{4}$$

where m_i is the mass of atoms; v_i is the velocity of atoms; *N* is the number of atoms in each plane; K_B is Boltzmann constant.

3. Results and discussion

The temperature level chosen for this study is 500 K. Single crystalline Ge thin films with periodic isosceles triangle shaped interfaces were first considered. Fig. 3 presents the variation in

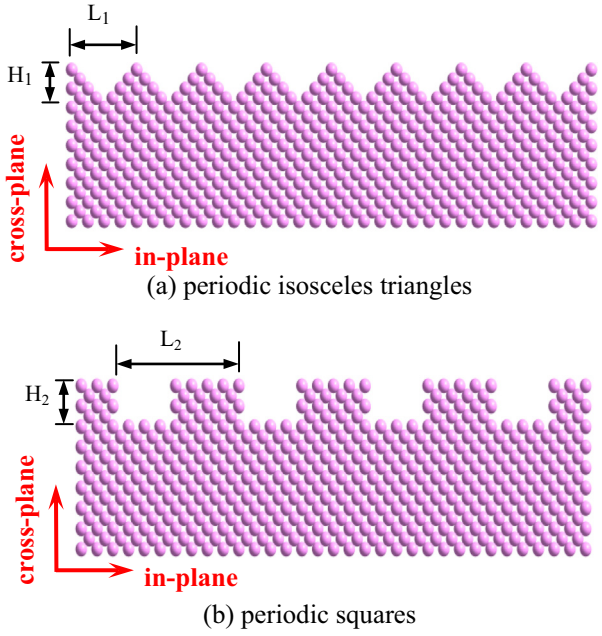

Fig. 2. The 2D simulation models of Ge thin films interfaces with roughness.

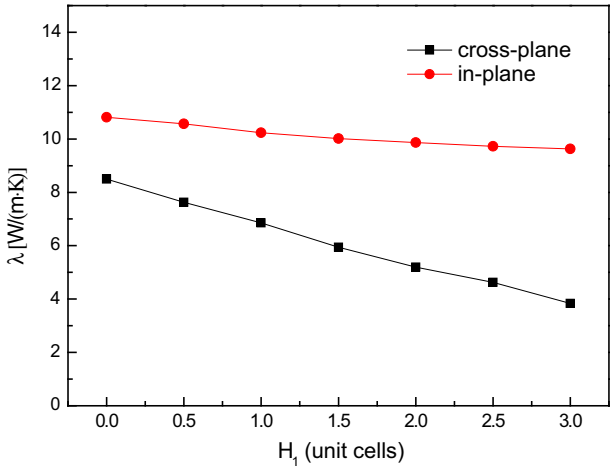

Fig. 3. Thermal conductivity as a function of the height of the roughness of the interface for periodic triangle shaped interfaces.