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Communication

Strain effect on the heat transport properties of bismuth telluride nanofilms with a hole

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ABSTRACT

We investigated the mechanical behavior of bismuth telluride nanofilms with holes by using an equilibrium molecular dynamics (MD) approach. The holes had diameters of 20, 30, 40, and 50 Å. The thermal conductivity values of the nanofilms were calculated under different strains at different temperatures using a nonequilibrium MD simulation. The simulation revealed that the thermal conductivity of a bismuth telluride nanofilm with a hole decreases with an increase in hole diameter at different strains. For a film with a perfect structure at 300 K, a 48% reduction (from 0.33 to 0.17 W/m K) in the thermal conductivity was observed at a 7% tensile strain. In addition, the thermal conductivity increased by approximately 39% (from 0.33 to 0.46 W/m K) at a 7% compressive strain. A very low value (0.11 W/m K) of thermal conductivity is obtained for the nanofilm with a hole diameter of 50 Å at a 7% tensile strain at 300 K.

1. Introduction

Demand for clean energy is increasing; thermoelectric energy conversion is an alternative energy option. Furthermore, numerous people want reduced carbon emissions, and thermoelectric energy conversion can achieve this goal. In addition, thermoelectric energy conversion is an essential requirement for the next generation of photonic, electronic, and optoelectronic nanodevices. Therefore, thermoelectric materials have attracted considerable interest in the scientific and industrial communities during the past decade [1–5] because thermoelectric materials can directly convert thermal energy into electrical energy.

The energy conversion efficiency of thermoelectric devices is determined by the materials' dimensionless figure-of-merit (ZT), defined as $ZT = S^2\sigma T/k$, where S, σ, T, and k are the Seebeck coefficient, electrical conductivity, absolute temperature, and thermal conductivity, respectively [6]. To achieve a high ZT value, the material should exhibit a low k and high values of S and σ. Further research is required to improve the ZT value. Some low-dimensional thermoelectric materials exhibit higher thermoelectric performance levels than bulk materials do [7]. This is due to increased phonon boundary scattering and modified phonon dispersion in these low-dimensional materials [8].

To obtain a high ZT value, several researchers have recently developed experimental techniques and theoretical methods to study the thermal conductivity of nanostructures, especially bismuth telluride (Bi_2Te_3) and its alloys [9–14]. For example, Yu et al. [10] studied the strain effects on the thermal conductivity and local heat flux distribution in thermoelectric nanofilm using molecular dynamics (MD) calculations and found that the thermal conductivity of Bi_2Te_3 nanofilm can be effectively tuned by strain. Huang et al. [11] used the MD method to investigate the effect of Van der Waals bonding on the compressive mechanical behavior of Bi_2Te_3. Shao and Bao [13] performed MD simulations and normal mode analysis to study the thermal transport in quintuple layers of Bi_2Te_3 and found that the phonons in Bi_2Te_3 are strongly scattered by interfacial potential and the transport process is less strongly affected by the dynamics of the substrate.

Porous thermoelectric materials exhibit low thermal conductivity because of phonon scattering by pores; pores are useful for thermoelectric applications [15]. However, few studies have investigated the effects of pores on thermal conductivity [16]. In this paper, the thermal conductivity levels of Bi_2Te_3 nanofilms with nanoholes are studied using MD simulations. The effects of strain, temperature, and hole diameter on the thermal conductivity are investigated.

2. Simulation method

The atomic configuration of a nanofilm comprising bismuth and

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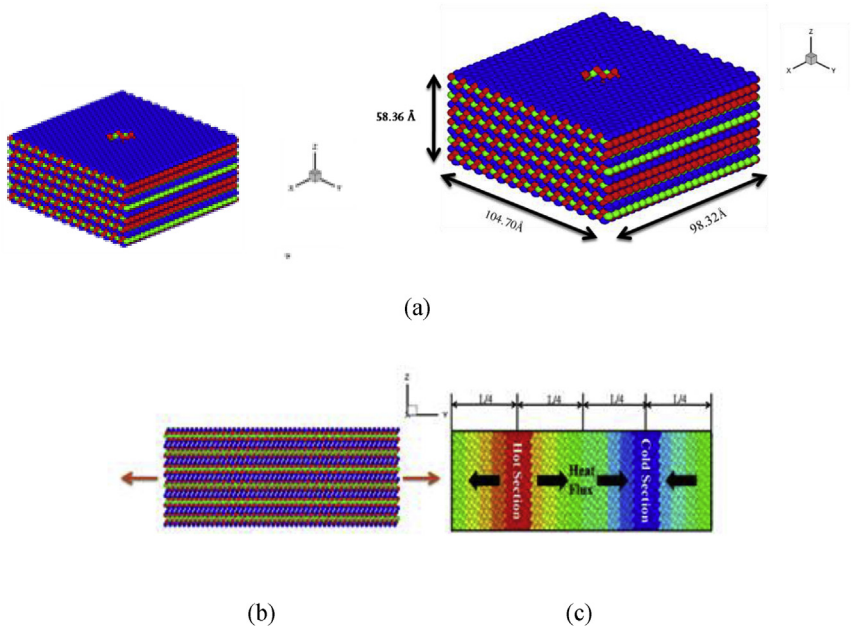

Fig. 1. (a) Atomic configurations of a bismuth telluride nanofilm with a nanohole at the center under (b) uniaxial tensile loading and (c) thermal loading.

telluride (Bi_2Te_3) atoms with a nanohole at the center is shown in Fig. 1(a). The atoms along the z-axis are in the sequence $Te_1 - Bi - Te_2 - Bi - Te_1$ [17] and the corresponding colors are blue, red, green, red, and blue, respectively. The subscripts 1 and 2 denote two types of differently bonded tellurium atoms. The atoms of the Te and Bi layers ($Te_1 - Bi$ and $Bi - Te_2$) are held together by strong ionic–covalent bonds. An extremely weak van der Waals interaction occurs between two adjacent Te_1 layers. The periodic boundary condition is set in the z-direction. The nanofilm has a length of 104.7054 Å, a width of 98.325 Å, and a thickness of 58.36 Å. Fig. 1(b) shows the nanofilm under uniaxial tensile loading along the y-direction. The atoms on each side of the nanofilm within 9.4 Å of the edges are assumed to be fixed whereas the other atoms are free. The fixed atoms have a positive displacement with a speed of 5 m/s in the y-direction when the force is applied to the atoms on the two edges. The uniaxial compressive loading is similar to tensile loading, but the displacement is negative; 150,000 time steps are required for the system to reach thermal equilibrium with a time step of 1 fs.

In addition, a nonequilibrium MD [18] simulation was adopted to calculate the thermal conductivity of a bismuth telluride nanofilm. A velocity-rescaling algorithm suggested by Jund and Jullien [19] was used to generate a constant heat flux in the nonequilibrium system, as shown in Fig. 1(c). The system was divided into slices along the y-direction, with each slice having a length of L/4. A local equilibrium was achieved at each slice when the system was stationary. An amount of heat $\Delta\varepsilon$ was added to the hot section centered at y = L/4, and the same amount of heat was removed from the cold section centered at y = 3 L/4 at every simulation time step. The heat flux in the nonequilibrium system can be expressed as

$$\dot{q} = \frac{\Delta\varepsilon}{2A\Delta t} \tag{1}$$

where A is the cross-sectional area of the nanofilm normal to the heat flux and Δt is the time step.

The thermal conductivity of the bismuth telluride nanofilm can be obtained from Fourier's law as

$$k = -\frac{\dot{q}}{dT/dy} \tag{2}$$

where dT/dy is the temperature gradient based on the temporal average

Table 1
The relevant parameters and their values used in the simulation.

Parameter	Value
Size (x, y, z) (Å)	98.32, 104.70, 58.36
Hole diameter, d (Å)	0, 20, 30, 40, 50
Atoms	19320, 18760, 18020, 17020, 15800
Time step, Δt (fs)	1
Cross-section area, A (Å^2)	5838
Temperature, T (K)	100, 200, 300, 400, 500
Strain, ε (%)	−7, −3, 0, 3, 7

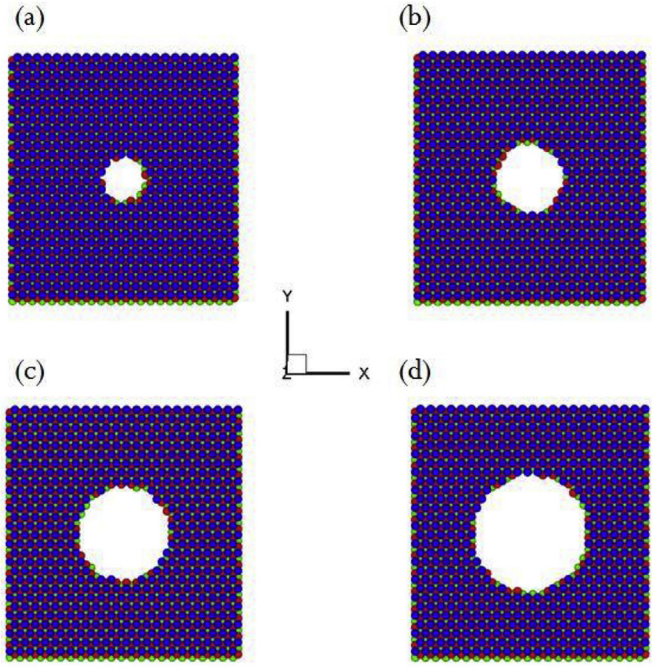

Fig. 2. Bismuth telluride nanofilms with nanoholes at the centers for different hole diameters of (a) 20 (b) 30 (c) 40, and (d) 50 Å.