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Effect of strain on thermal conductivity of amorphous silicon dioxide thin films: A molecular dynamics study

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ABSTRACT

The effect of strain on thermal conductivity of amorphous SiO_2 thin films is simulated by using molecular dynamics simulation (MD). The calculated results indicate that the thermal conductivity decreases monotonically as the strain varies from compression to tension and the thermal conductivity changes with thicknesses and temperatures under applied strain. Phonon density of states of strained thin films is used to explain the phenomena. The results can be potentially used to design the MEMS devices, which work at the enhanced temperature and use the amorphous SiO_2 film and other similar thin films.

1. Introduction

With the rapid progress in nanotechnology, nanomaterials have been applied in Micro-Electro-Mechanical System (MEMS) extensively. For materials used in MEMS, the heat transfer behavior becomes unusual, so the heat transfer at micro/nano scales has attracted increasing research focus. So, understanding thermal transport at micro/nano scales is essential to promote development of nanotechnology [1,2].

Many factors such as size, temperature, surface, interface, defect and impurity [3–9] had a major influence on thermal conductivity in the low-dimensional or nanoscale materials [10]. In recent years, researchers found that strain is also an obvious factor that affects the heat conductive properties [11]. Yang et al. [12] investigated the strain effect on thermal conductivity of nanoscale aluminum films. The strain decreases the mean free path of conductive electrons and it will lead to a decline in thermal conductivity. Murphy et al. [13] investigated the effect of uniform tensile strain and point defects on thermal conductivity in Si nanowires. It turns out that point defects have a far larger effect on thermal conductivity than the surface roughness or uniaxial strain. Bhowmick et al. [14] found that the thermal conductivity of insulating solid decreases with the increase of strain from compressive strain to tensile strain monotonically. Li et al. [15] investigated the strain effects on thermal conductivity of carbon and silicon nanostructures by molecular dynamics (MD) simulation. The strong coupling of strain and thermal conductivity was found. Further researches indicated that the thermal conductivities of amorphous silicon thin films increase with tensile strain [16], and those of amorphous silicon nitride thin films decrease with the increase of tensile strain [17].

Silicon dioxide (SiO_2) is one of the most common insulation materials, which has been widely used in many applications. Huang [18] measured the thermal conductivity of SiO_2 thin films through simulation and experiment. The results showed that the thermal conductivity of the films prepared by thermal oxidation is relatively stable. MD simulations were carried out to get the thermal conductivity of the ultra-thin films. Larkin et al. [19] investigated how the propagating and non-propagating vibrational modes contribute to the thermal properties of amorphous SiO_2 and amorphous Si. Kuryliuk et al. [20] calculated thermal conductivities of a-SiO_2 and a-SiO_2-based nanocomposite by MD. The changes of thermal conductivity were caused by the enhanced scattering of thermal vibrations at nanocrystal boundaries.

As mentioned above, on most occasions the thermal conductivity will decreases when a tensile strain is applied on the crystal material. It can be considered as a rule for most crystal materials. However, the rule is not applicable to all materials [13,15]. For amorphous materials, the conclusion is inconsistent [16–17]. According to the literatures review, so far, we have not yet found out the work that only considering on the effect of strain on thermal conductivity for the amorphous SiO_2 thin films and it is not easy to predicate the effect of the strain on the thermal conductivity of an amorphous thin film.

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In this paper, we investigate the influence of strain on the thermal conductivity of amorphous SiO_2 thin films by using the non-equilibrium molecular dynamics. All MD simulations are performed by LAMMPS package [21]. The work may be useful for designing the micro components with the a-SiO_2 thin film, which works under the fields of both strain and temperature.

2. Simulation procedure

As illustrated in Fig. 1, an amorphous SiO_2 model is considered (visualized by using software VMD [22]). The yellow larger spheres represent silicon atoms, and the pink smaller spheres represent oxygen atoms. The model of amorphous SiO_2 is based on reference [23]. Along the Z direction, cells are placed one by one to build the structure, and along the X and Y directions there is only one cell. Then Z-axis, which represents the thickness direction of the film, can be controlled by adjusting the number of the cells. The details of the modeling are described in Supplementary materials (see Supplementary materials Section 1). The dimension of initial simulation cell is 21.4 Å × 21.4 Å × 85.8 Å (XYZ). At this time, the film thickness is 85.8 Å. The strain is applied by deforming the simulation box. Then, the thermal conductivity can be given after applying the strain.

The thermal conductivity has been proved one of the most difficult transport coefficients to calculate [24]. The MD method is generally employed in two different ways to evaluate thermal conductivity of a specific system: equilibrium molecular dynamics (EMD) method and non-equilibrium molecular dynamics (NEMD) method. In this paper, both reversed nonequilibrium molecular dynamics (RNEMD) [24] and EMD are used.

The periodic boundary condition (PBC) is performed along the three directions. The thermal conductivity of bulk material is calculated by using EMD method. The thermal conductivity of thin films is calculated by using NEMD method (the periodic boundary condition of heat transfer direction will be no longer working). After the minimum energy configuration is attained, the model is equilibrated in the NPT ensemble at interesting temperature. MD simulations then are used to deform the model [25] at strain range [26]in uniaxial tension at a constant strain rate of 1×10^{-3} ps^{-1}, which is applied in the Z- direction. Then, the MD should run in 0.5 ns NVT dynamics to equilibrate at temperature of interest. After the state reaches to equilibrium, the program performs about 5 ns run under NVE conditions to generate raw data for computing property of interest. The run duration depends on the specific method and the state of material. For NEMD, it requires sufficient time to achieve steady velocity or temperature profiles.

3. Results and discussions

3.1. The effect of interatomic potential

There are several choices of interatomic potential for our simulation. Although those potentials have been employed to obtain the thermal conductivity of amorphous SiO_2, the deviation of simulation predictions and experimental measurements are not understood yet [27]. BKS interatomic potential is the most commonly used one. The simulation using the BKS potential has reported about 2.1 W/mK of the thermal conductivity, but the experimental value is around 1.4 W/mK at 300 K. Tian et al. [26] used MD to obtain about 2 W/mK, 2.3 W/mK, and 1.3 W/mK for BKS, Teter, and ReaxFF, respectively. For a system containing element Si and O, there are also tersoff potential [28] and vashishta potential [29], which can be used for simulation. The calculation results used tersoff potential [30] are in good agreement with the results of other potentials used in the literatures [18–19,23,27].

The thermal conductivity of bulk amorphous SiO_2 is calculated by using BKS potential, in our work. For our model, the value is 2.15 ± 0.19 W/mK for the bulk material (see Supplementary materials Section 2), the value is in accordance with the results of the literature [19,27]. This means our model structure is reasonable at 300 K. However, BKS potential will not be our choice because its low accuracy (more than 50% overestimation for the experimental value) and long computing time. ReaxFF also takes a long time to calculate, even though it has good accuracy. Tersoff potential will be our optional and the tersoff potential (around 1.2 W/mK, 13% underestimation for experimental value [31]) is much more capable of reproducing bulk thermal properties than the BKS potential.

3.2. The effect of temperature and film thickness

In this part, we first use the MD method to calculate the thermal conductivity of amorphous SiO_2 thin films at different temperatures, and compare them with the results from other literatures.

RNEMD method requires a reasonable temperature distribution as shown in Fig. 2. A reasonable temperature distribution should be linear. At this time, the temperature gradient is acceptable. The transfer direction is divided into several slabs due to the size of model. Every slab should contain enough atoms to exchange energy. In this simulation, the number of slabs is 10 (at 85.8 Å thickness). There are about 261 atoms in every slab.

Thermal conductivities at different temperatures (100 K, 300 K, 500 K, and 700 K) are compared with the literatures [23,30] as

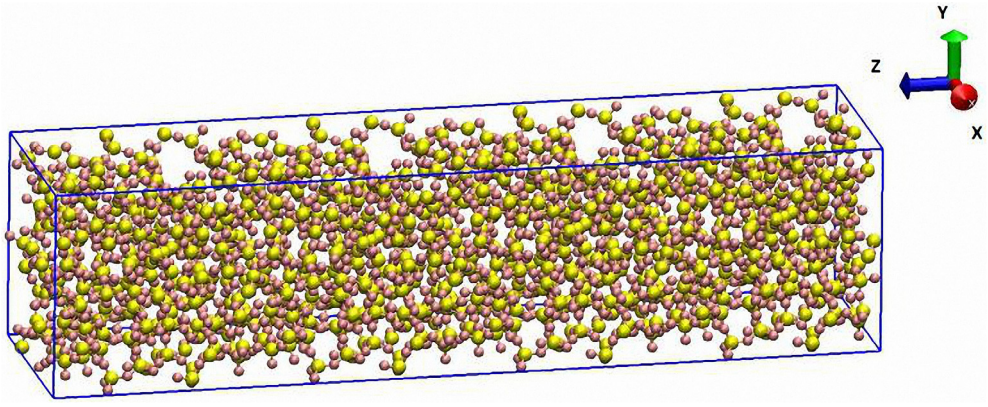

Fig. 1. Schematics of amorphous SiO_2 thin film. The yellow larger spheres represent silicon atoms, and the pink smaller spheres represent oxygen atoms. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)