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Interfacial thermal resistance between few-layer MoS_2 and silica substrates: A molecular dynamics study

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ABSTRACT

Interfacial thermal resistance (ITR) between molybdenum disulfide (MoS_2) and crystalline or amorphous silica as a substrate was studied using molecular dynamics (MD) simulation. To do so, pump–probe method, which is a MD technique inspired by an experimental method, was employed. The effects of substrate type, temperature, number of layers of MoS_2 and van der Waals (vdW) coupling strength on ITR between MoS_2 and its silica substrates were explored. It was observed that, obtained ITR values for crystalline or amorphous silica substrate were close to one another. Our findings showed that, by increasing the temperature from 200 K to 400 K, ITR between a single-layer MoS_2 and its crystalline or amorphous silica substrate decreases by about 20%, which might be due to better phonons couplings at the interface in higher temperatures. We also showed that, ITR between multilayer MoS_2 and crystalline or amorphous silica substrate does not differ by increasing the number of layers of MoS_2. It has been found that, by increasing Lennard-Jones coupling strength from 0.5 to 2, ITR between a single-layer MoS_2 and crystalline/amorphous silica substrate decreases by around 80%, showing better phonons couplings at the interface between the two structures.

1. Introduction

In recent years, two dimensional (2D) materials like graphene and transition metal dichalcogenides (TMDs) have attracted many attentions due to their thermal, mechanical, electrical and optical properties [1–6]. TMDs have 2D hexagonal MX_2 atomic structure in which M is a transition metal and X is a chalcogen like S, Se or Te. Because of their intrinsic 2D structure and their differences in atomic interactions along in-plane and out-of-plane directions, they show high anisotropy in physical properties. In-plane atoms have covalent bonds while interactions between planes are of weak vdW type. One of the most valid TMDs is MoS_2 which has suitable thermoelectric applications due to its high Seebeck coefficient and low thermal conductivity [7,8]. It has 1.8 eV energy band gap [9] and has found many applications including those in transistors [10], lithium batteries [11], photodetectors [12], photovoltaics [13] and memory devices [14]. Moreover, its interesting thermal and mechanical properties have attracted many attentions [15,16]. 2D structures like MoS_2 with a substrate (e.g. silica) are used in many instruments like photodetectors or field-effect transistors. In these applications, extra heat generated during the course of operating increases the temperature of the instrument, thereby decreasing its reliability and life-time. The rate of heat dissipation depends on the ITR between the 2D structure and its substrate [17] and the intrinsic thermal resistivity of the substrate itself. So, studying heat transfer phenomenon between the two structures can help improve their designs. Up to now, many researches have been conducted on the ITR between 2D structures and different substrates.

Zhang et al. [18] studied heat transfer between silicene and various crystalline and amorphous substrates using molecular dynamics simulations and pump–probe method [19–22]. Upon their results, the ITR between silicene and crystalline silica was equal to 1.888×10^{-8} m^2 K/W at 300 K. They further reported that the ITR between silicene and all substrates decreases by about 40% with increasing the temperature from 100 K to 400 K. In another study, the ITR of 3.52×10^{-8} m^2 K/W was reported between graphene and crystalline silicon at 300 K [23]. Chen et al. [24] studied the ITR between amorphous silica and crystalline silicon using non-equilibrium molecular dynamics (NEMD). They reported the value of 0.9×10^{-9} m^2 K/W for the ITR at room temperature with strong coupling strength. Ni et al. [25] measured the ITR between multi-layer boron nitride and silica about 2.2×10^{-8} m^2 K/W. Yuan et al. [26] calculated the ITR between multi-layer MoS_2 and crystalline silicon using Raman spectroscopy and molecular dynamics

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simulations. They measured the ITR values in the range 1.3–1.88 × 10^{-8} m^2 K/W. Taube et al. [27] investigated the dependence of thermal conductivity and interfacial thermal conductance (ITC) on temperature for a single-layer MoS_2 resting on SiO_2/Si substrate employing Raman spectroscopy. They observed that both thermal conductivity and ITC decreased by increasing temperature; from 62.2 W/m K and 1.94 MW/m^2 K at 300 K to 7.45 W/m K and 1.25 MW/m^2 K at 450 K, respectively. Besides experimental studies [27] and the theoretical research [17] on the ITR between MoS_2 and its silica substrate, there are some important factors affecting the ITR between these two structures which are yet to be studied.

In this paper, we begin with calculating thermal conductivity of a single-layer MoS_2 at different temperatures in the range 200–400 K using NEMD and employing Stillinger-Weber and ReaxFF potentials. In the following sections, the ITR between MoS_2 and crystalline or amorphous silica substrate is obtained utilizing pump–probe method. This quantity is further considered between a single-layer MoS_2 and its crystalline/amorphous silica substrate at different temperatures in the range 200–400 K. Then, the effect of number of MoS_2 layers on ITR is investigated. Finally, the effect of vdW coupling strength on ITR between single-layer MoS_2 and its crystalline or amorphous silica substrate is studied.

2. Simulation details

In the present study, molecular dynamics simulations were carried out utilizing LAMMPS package [28]. Molecular dynamics is a powerful technique that is widely used to investigate thermal [29,30] and mechanical [31,32] properties of nanostructures. In order to describe atomic interactions between molybdenum (Mo) and sulfur (S) atoms in MoS_2 structure, modified Stillinger-Weber potential developed by Jiang et al. [33] has been utilized. Also, in order to compute atomic interactions between silicon (Si) and oxygen (O) atoms in crystalline and amorphous silica structures, Tersoff potential with parameters reported by Munetoh et al. [34] has been employed. This potential and its parameters have been widely used for calculating atomic interactions between silicon and oxygen in many studies [24,35–40]. For vdW interactions between MoS_2 and Silica, 6–12 Leonard-Jones (LJ) potential, $U(r) = 4\chi\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6]$ was exploited, in which ε is energy parameter, σ is distance parameter, r is interatomic distance and χ represents vdW coupling strength between MoS_2 and Silica. The ε and σ parameters were calculated from the universal force field (UFF) [41] for different atomic interactions, as presented in Table 1. Cut-off radius (r_c) was assumed to be 2.5 σ. For initial atomic hybrid configuration, a single-layer MoS_2 with the dimensions of 20.22 × 5.23 × 0.6 nm and a crystalline or an amorphous silica with the respective dimensions of 20.19 × 5.17 × 5.5 nm and 20.29 × 5.28 × 5.55 nm were utilized. In order to create an amorphous structure of silica, BKS [42] potential was employed along with a 6–24 Leonard-Jones potential [43–46]. The coefficients of 6–24 Leonard-Jones and BKS potentials were extracted from references [43,47]. In this simulation, firstly, temperature of the crystalline silica was increased by Nosé-Hoover thermostat for 100 ps from 300 K to 5000 K (above melting point). After reaching the temperature of 5000 K, the silica was equilibrated for 50 ps. Then, in 1 ns, the structure was quenched at the rate of 4.7 × 10^{12} K/s from 5000 K to 300 K. Next, NPT ensemble was imposed for 50 ps at 300 K and zero stress to equilibrate the silica.

After preparing the substrates structure, MoS_2 was placed on the crystalline and amorphous silica substrates at 3 Å and 2.59 Å distance, respectively. In these simulations, periodic boundary conditions and free boundary condition were considered in in-plane and out-of-plane directions, respectively. In all simulation runs, time step was set to 0.5 fs.

Table 1
LJ parameters for different vdW interactions [41].

	ε (eV)	σ (Å)
Si-Mo	0.00562	3.27
Si-S	0.01242	3.71
O-Mo	0.004	2.93
O-S	0.00884	3.37

3. Results and discussion

3.1. Thermal conductivity of suspended single layer MoS_2

In order to validate the results of computations, thermal conductivity of the suspended single-layer MoS_2 was calculated using the modified SW [33] and the recently developed ReaxFF [48] potentials separately. In this case, a single-layer MoS_2 with the length of 20.22 nm was used and NEMD method was employed to calculate the thermal conductivity. After setting the initial conditions according to the temperature of 300 K, corresponding structure was relaxed with NPT ensemble for 50 ps at 300 K and zero stress in horizontal direction. Then, employing Nosé-Hoover thermostat (NVT ensemble), temperature of the first and the last regions of the structure with the width of 7.5 Å were set to 270

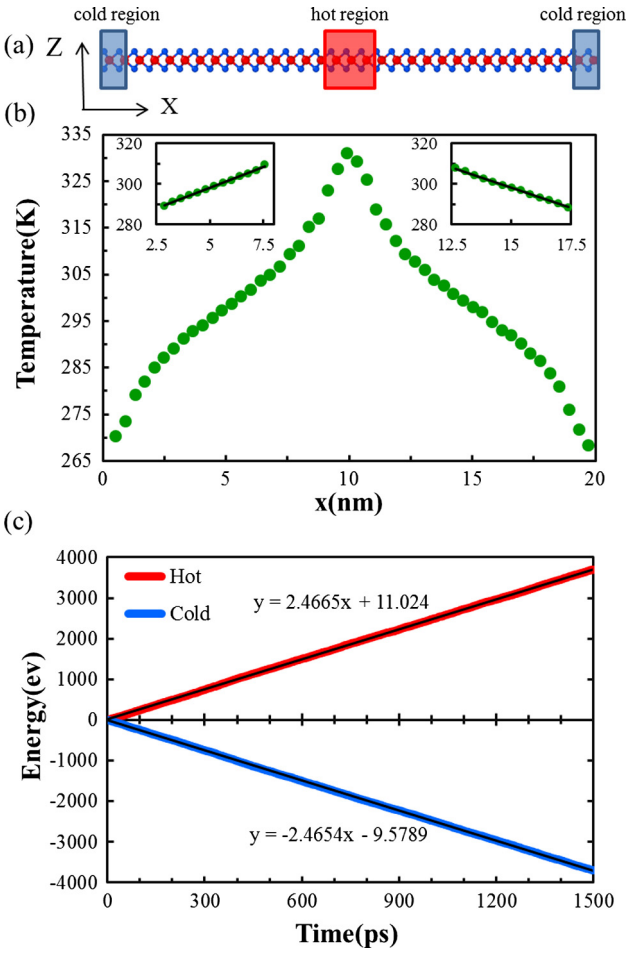

Fig. 1. (a) Front view of suspended MoS_2 and applied thermostatic regions. (b) Steady state temperature profile along the structure due to the imposed temperature difference using NEMD method with SW potential. (c) Energy added to the hot region and subtracted from the cold region during the NEMD simulation time and the equations of fitted lines for calculating the heat flux.