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Molecular dynamics study on interfacial thermal conductance of unirradiated and irradiated SiC/C

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ABSTRACT

SiC_f/SiC composite materials have been considered as candidate structural materials for several types of advanced nuclear reactors. Both experimental and computer simulations studies have revealed the degradation of thermal conductivity for this material after irradiation. The objective of this study is to investigate the effect of SiC/graphite interface structure and irradiation on the interfacial thermal conductance by using molecular dynamics simulation. Five SiC/graphite composite models were created with different interface structures, and irradiation was introduced near the interfaces. Thermal conductance was calculated by means of reverse-NEMD method. Results show that there is a positive correlation between the interfacial energy and interfacial C–Si bond quantity, and irradiated models showed higher interfacial energy compared with their unirradiated counterparts. Except the model with graphite atom plane parallel to the interface, the interfacial thermal conductance of unirradiated and irradiated (1000 eV) models, increases as the increase of interfacial energy, respectively. For all irradiated models, lattice defects are of importance in impacting the interfacial thermal conductance depending on the interface structure. For the model with graphite layer parallel to the interface, the interfacial thermal conductance increased after irradiation, for the other models the interfacial thermal conductance decreased. The vibrational density of states of atoms in the interfacial region was calculated to analyze the phonon mismatch at the interface.

1. Introduction

Continuous silicon carbide (SiC) fiber-reinforced SiC-matrix (SiC_f/SiC) composites have been considered as one of the most important candidate structural materials for nuclear reactors, such as light water reactor (LWR) [1], high-temperature gas-cooled reactor (HTGR) [2] and future fusion reactor [3], for their low radioactivity, high-temperature strength and chemical inertness, high radiation stability, low induced-activation and low after-heat properties [4,5]. But there are still numerous challenges such as their thermal conductivity, radiation stability, hermetic behavior and joining technology [6,7]. Many efforts have been made in these decades including extensive worldwide cooperation.

As we all know, the fiber/matrix interfaces play an important role in accommodating fiber-matrix load transfer, debond, and sliding. For most ceramic materials, SiC in particular, due to a relatively low density of valence electrons [8], the thermal transport across conductor (Graphite)/semiconductor (SiC) interface is primarily by interphonon transport [9]. But the interface phonon scattering, arising from the poor mechanical or chemical adherence between fiber and matrix, is the main mechanisms to create thermal resistance, "Kapitza-type", for heat conduction [10–12]. More important, interface thermal resistance has the huge negative influences on the thermal conductivity of the composites [13]. Therefore, if the interface thermal resistance is too high, it will lower the thermal conductivity of the composite components and degrade the heat removal and thermal stress reduction in fusion reactors.

It is difficult to study detailed thermal energy transport across these small scale interfaces through physical experiments, but molecular dynamics (MD) simulations offer the possibility to understand the detailed mechanisms of the interfacial transport phenomena [14]. There are two main approaches to analyze thermal transport through MD [15]: (1) equilibrium molecular dynamics (EMD) based approach that uses fluctuation dissipation theorem or the Green-Kubo method and (2) non-equilibrium molecular dynamics (NEMD) based approach that imposes a

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temperature gradient and subsequently measuring thermal conductivity using the classical Fourier law of thermal conduction. However, compared to EMD, NEMD is more suitable to study an inhomogeneous system, such as the interface studied here, because the Kapitza conductance, which is a local property, cannot be correctly treated under the assumption that the system is homogeneous [16]. In this work, reverse NEMD (rNEMD) is used. In rNEMD, the heat flux is imposed on the system by the unphysical velocity exchange, after reaching steady state, the energy exchange and heat flux is balanced in the opposite direction, and then the resulting temperature gradient is measured to calculate the thermal conductivity. The advantages and disadvantages of rNEMD have been discussed in detail elsewhere [17], and not to be repeated here.

In this paper, all work has been done by classical MD modeling of interfacial heat transport between SiC-fibre and pyrolytic carbon interphase (SiC/C). Five composite models with different crystal orientations were systematically studied; besides, effect of irradiation on the interfacial thermal conductance was also discussed.

2. Methodologies

Five SiC/C composite models were established and studied in this work, each model includes three parts and two SiC/C interfaces. On each side is single crystal 3C-SiC with a lattice spacing of 4.359 Å (named a_0). The middle part is graphite, with carbon atoms arranged in a honeycomb lattice, 1.42 Å separated in each layer, and 3.35 Å between planes. In order to ensure SiC and graphite to meet the periodic boundary condition (PBC) in all directions at the same time, there are only several specific angles and cross-section sizes that can satisfy the requirement. As shown in the top panel of Fig. 1, α is the angle between the graphite plane and SiC, which is 56.705°, thus this model is denoted as M56. The other four angles are 90.000°, 77.315°, 28.560° and 0.000° (denoted as M90, M77, M28, M0), respectively. The M0, $8a_0 \times 82a_0 \times 10a_0$, involves 29744 graphite atoms and 26720 SiC. The M28, M56, M77, $8a_0 \times 82a_0 \times 7a_0$, involve 21728, 21000, 21252 graphite atoms, respectively, and 9352 SiC each. The last one, M90, $8a_0 \times 82a_0 \times 9a_0$, involves 26624 graphite atoms and 11880 SiC.

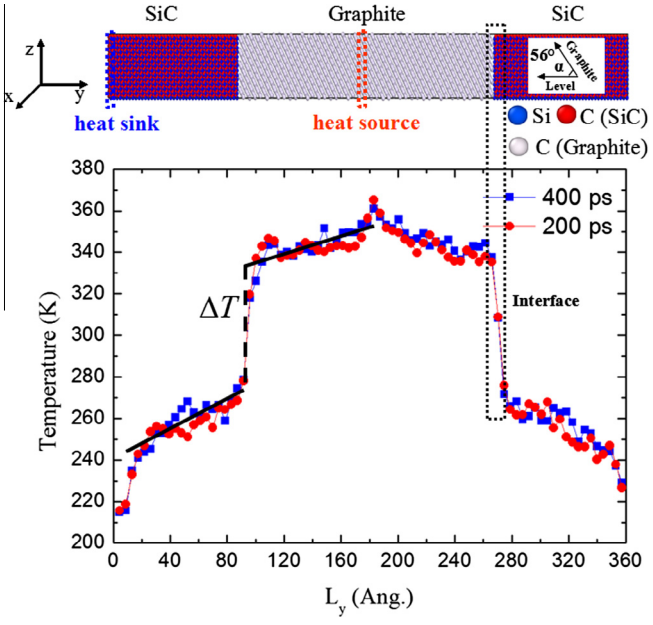

Fig. 1. (Top) Typical structure of SiC/C composite model. (Bottom) Temperature profile of SiC/C composite system. ΔT: temperature drop between SiC and graphite interface.

All MD simulations were performed using the LAMMPS package [18]. The SiC in each system was modeled using the modified analytical bond-order Tersoff-type potential (for thermal conductivity) [19] and hybrid Tersoff-ZBL potential (for irradiation) [20,21]. The graphite was modeled using the adaptive intermolecular reactive empirical bond order (AIREBO) potential [22]. The same potential was used for graphite-SiC interactions as in SiC. All initial molecular systems were equilibrated at a temperature of 300 K by NPH (constant number of particles, pressure, and enthalpy) ensemble and Langevin thermostat for 2 ns with a time step of 0.5 fs. After NPH relaxation, the systems were converted into NVE ensemble for calculating interface thermal conductance. In order to maintain the energy conserved, a value of 0.1 fs was chosen as the time step throughout the NVE simulations.

In order to impose a heat flux perpendicular to the interface, the system was divided into 82 slabs after the NPH relaxation, whose thickness was about 1 a_0, along the direction of heat flow. Slab 1 is defined as the "heat sink" and slab 42 as the "heat source". The constant heat flux (J_Q) was imposed through Müller-Plathe method [17]. As shown in the bottom panel of Fig. 1, the temperature profile does not change significantly from 200 to 400 ps, i.e., the systems had reached the steady-state. Also, the temperature drop near the interface (ΔT) was obtained from the temperature profile. The interfacial thermal conductance G can be obtained from the relationship [23]

$$G = J_Q/\Delta T \tag{1}$$

The interfacial energy E_{if} denotes the excess energy per unit interface area due to the existence of interface interaction as given by

$$E_{if} = \frac{1}{S_{interface}}(E - E_0) \tag{2}$$

where S is the total interface area, E and E_0 is the energy of the system with and without interface interaction, respectively.

The vibrational density of states (VDOS) denote the strength of phonons vibration mode in different frequency. It can be obtained from the fast Fourier transformation of the velocity autocorrelation function (VACF) [24].

$$\mathrm{VDOS}(\upsilon) = \int_{-\infty}^{\infty} \mathrm{VACF}(t) e^{-2\pi i \upsilon t} dt \tag{3}$$

where υ is the phonon frequency, t is the correlation time of VACF(t).

The systems equilibrated by NPH ensemble were used for the irradiation simulations. In order to ensure the system was sufficiently large to contain the cascades within the box and near the interface, the primary-knock-on atom (PKA), an energetic Si in the interface, was given a small kinetic energy of 250 or 500 eV projected through the interface between SiC and graphite. After irradiation, all the models were used for calculating the interfacial thermal conductance by the same method as above.

3. Results and discussion

3.1. Interfacial thermal conductance

The typical temperature profile of the SiC/C composite system with two interfaces is shown in the bottom panel of Fig. 1. As can be seen, there is no significant difference between 200 and 400 ps temperature profile, i.e., the whole system had reached the equilibrium state after 200 ps. By extrapolating to infinite length, an approach proposed by Schelling et al [15], the thermal