Enhancing the thermal boundary conductance of Cu/Diamond interface via diamond surface amorphization by molecular dynamics simulation

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Abstract. Based on the non-equilibrium molecular dynamics simulation, a Cu/amorphous diamond/crystalline diamond sandwich model was established to investigate the effects of the amorphous degree diamond surface and the thickness of the amorphous layer on the thermal boundary conductance of Cu/crystalline diamond. The simulation results show that the thermal boundary conductance can be enhanced by diamond surface amorphization, and increases with the increase of the amorphous degree. For the fully amorphous layer, the thermal boundary conductance increases gradually with the increase of the thickness of the amorphous layer and can be enhanced up to 4 times. The analysis of the vibrational density of states, overlap energy and phonon participation ratio shows that the diamond surface amorphization promotes the vibrational coupling between diamond and Cu atoms at low frequencies, as well as the occurrence of phonon inelastic scattering, and thus improves the thermal transport capacity of interface.

Keywords: Cu/diamond composite; thermal boundary conductance; surface amorphization amorphous; molecular dynamicsfo

1. Introduction

Nowadays, the rapid development of 5G, flexible equipment, artificial intelligence, and other industries make chips, micro-nano electronics, and other equipment compact and integration higher and higher. In actual operation, the heat accumulated by these devices severely attenuates their performance, which leads to the increasing demand for efficient thermal management materials [1], and puts forward higher requirements for the stability and service life of heat dissipation equipment. In order to obtain greater heat dissipation capacity, heat dissipation equipment began to develop towards composite materials with high thermal conductance, such as Cu/Diamond composite materials. Cu (K = 398 W/m \cdot K) and diamond (K = 900 - 2000 W/m \cdot K) have excellent thermal conductance respectively. It is expected that a new generation of high thermal conductance composites can be obtained by combining the two materials (The high thermal conductivity of diamond will become an ideal reinforcing phase of high thermal conductivity composites). However, the large number of interfaces makes the heat transfer capacity of the composites extremely sensitive to the individual thermal boundary conductance (TBC) between Cu and diamond. Firstly, from the chemical perspective, Cu and diamond do not react with each other, the wettability is poor, and good interface bonding cannot be formed [2]. Secondly, from the physical point of view, Cu and diamond are different in thermal carriers. Cu mainly relies on electron heat conduction, while diamond depends on phonon heat conduction. In order to realize heat transfer at the interface of Cu and diamond, phonon coupling needs to occur at the interface, but poor phonon coupling between Cu and diamond interface leads to large interfacial thermal resistance [3].

For phonon-mediated interfaces, vibration coupling and bonding strength on the interface are the two most critical factors controlling the TBC [4-6]. Interface modification to enhance phonon coupling [7,8] or improve interface bonding strength [9-11] can significantly improve TBC. At present, the most utilized method to regulate the TBC of Cu/diamond is alloying of metal matrix or metallization of diamond surface [12], introducing carbide-forming elements into the Cu/diamond interface to form carbides in the middle layer, to make the physical properties of the middle layer

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between Cu and diamond. For example, transition group IV metals Ti [5,13], Zr [14], transition group VI metals Cr [15], Mo [16,17], W [18] and some semiconductor elements such as B [9] are used. In the process of the actual preparation of composite materials, using the sputtering and evaporation deposition technology lead to the axial thin film deposition, which will be formed in the interface layer between two solid disorderly films [20] near the interface changes, the crystallinity of materials, near the interface of the change of crystallinity damage will affect the vibration characteristics of materials, thus influence the interface thermal conductance. In some experiments, such as amorphous SiC:H/SiOC:H [21], amorphous SiO2/A12O3 [22], and amorphous SiO2/Si [23], the TBC is much higher than the typical value of the interface between crystalline solids. This may seem counterintuitive since the thermal conductance of amorphous materials is usually less than that of their crystalline counterparts. Due to the limited experimental ability and theoretical model to analyze the mechanism of heat transfer, the TBC over disordered interfaces has not received sufficient attention. In addition, the thermal conductance of the amorphous layer is low, and it is difficult to quantify the impact of amorphous materials on the TBC. As a result, the temperature drop at the interface is usually ignored, and it is difficult to calculate with low uncertainty in experiments and theory [24]. Therefore, amorphous diamonds of different states were constructed in this paper, the Cu/amorphous diamond/crystal diamond (Cu/A-diamond/C-diamond) sandwich model was established, and the TBC was calculated by non-equilibrium molecular dynamics simulation. The effects of different heat treatment temperatures and thicknesses of amorphous layers on the thermal conductance of the Cu/C-diamond interface were investigated by analyzing the vibrational density of states, overlap energy, and phonon participation ratio.

2. Simulation methods

2.1 Model building

In the process of model construction, an amorphous diamond is located in the middle of the Cu/C-diamond, and the model structure is a sandwich structure. In this paper, the effects of different sizes and states of amorphous diamond on the TBC of Cu/C-diamond are studied. To obtain diamond thin layers of different amorphous degrees, the diamonds were relaxed at high temperatures at 8000 K, 9000 K, 10000 K, and 11000 K for 0.25 ns. Then the temperature was lowered to 300 K, and finally, the diamond with a different amorphous degree was obtained by relaxation of 0.25 ns at a constant temperature of 300 K. All the conditions were consistent in the construction of amorphous diamonds with different thicknesses (1.5, 3, 4.5 nm). Using the vibration density of states (VDOS), overlap energy, and phonon participation ratio (PPR) explained and analyzed the changes of thermal conductance at the interface. The Cu/A-diamond/C-diamond interface model constructed in this paper at 10000 K heat treatment temperature and 1.5 nm amorphous layer thickness is shown in Fig. 1. Cu and diamond are $25.6 \times 25.6 \times 61.7$ Å, respectively.



Figure 1. Cu/A-diamond/C-diamond interface model with a thickness of 1.5 nm and heat treatment temperature of 10000 K for the amorphous layer.

2.2 Simulation process

The simulation work in this paper is completed on the open source LAMMPS (Large-scale parallel Atom/Molecule Simulator) [25]. In this paper, the EAM [26] potential function was used to describe Cu atoms, Tersoff [27] potential function was used to describe amorphous and crystalline diamonds, and L-J potential function was used to describe atoms on both sides of the interface [28]. Periodic boundary conditions are used in three directions. To achieve good energy conservation, we set 0.5 fs as the time step during the whole simulation. The Velocity Verlet integral method and conjugate gradient method were used to integrate the motion equation, and the simulation structure was optimized. First, an NVT ensemble was used to balance 1 ns at 300 K with a time step of 0.5 fs. After the equilibrium structure is reached, two 0.5 nm thick layers are fixed at both ends of z-direction to stabilize the system. The NVE ensemble was then used to continue balancing 1 ns. In the subsequent NEMD process, atoms within 0.5 nm near the fixed layer were selected as the heat source and heat sink. Langevin thermostat was used to set the temperature of the heat source and heat sink at 380 K and 220 K, respectively, to establish the temperature gradient. The NEMD process runs for 5 ns, the first 3 ns are used to make the system reach a steady state, and the last 2 ns data are used to obtain temperature distribution and heat flow for TBC calculation. The temperature distribution of the system, energy released by the heat source, and energy accumulated by the heat sink is shown in Fig. 2. The heat flux q was calculated by fitting the two curves, and then the interface thermal conductance was calculated according to Fourier's law:

$$TBC = \frac{q}{A\Delta T} \tag{1}$$

Where A is the interface area and ΔT is the interfacial temperature difference. Regardless of the presence of an amorphous layer, the total value of the interfacial temperature difference comes from the last point of the Cu temperature distribution and the first point of the crystalline diamond temperature distribution.



Figure 2. (a) Temperature distribution of Cu/C-diamond at neutral layer; (b) The temperature distribution of the calculation model in the presence of amorphous layer, when the interface

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temperature difference ΔT values from Cu low-temperature side and diamond crystal high-temperature side; (c) The energy accumulated by the heat source and heat sink under Langevin method, and the slope is used to judge whether the energy is conserved. This heat flow corresponds to case (b) when the amorphous layer is added.

The TBC of Cu and diamond is controlled by lattice vibration. The relation between the TBC and diamond amorphization is discussed by calculating the vibrational dynamic density. Its expression is as follows [29]:

$$VDOS(\omega) = \int_{-\infty}^{+\infty} e^{i\omega t} VACF(t) dt$$
 (2)

Where, VACF is the velocity self-correlation function, which is defined as:

$$VACF(t) = \frac{1}{N} \sum_{i=1}^{N} \langle v_i(0) v_i(t) \rangle$$
(3)

N represents the total number of atoms in the computational domain, $v_i(0)$ is the initial velocity of the atom, $v_i(t)$ is the velocity vector of an atom i at time t, and () represents the average lineage.

Overlap energy can further quantitatively describe the matching degree of atomic vibration based on VDOS [30]. The larger the overlap energy is, the more harmonious the phonon vibration between them is, and the better the heat transfer is.

$$E_{\text{overlap}} = \int g_o(w) \frac{hw}{e^{\frac{hw}{k_B T}} - 1} dw$$
(4)

Where $g_o(w)$ represents the overlap region of VDOS image, h is Planck constant, w is frequency, T is absolute temperature, and $e^{\frac{nw}{k_BT}} - 1$ is Boltzmann distribution.

We also calculate the phonon participation ratio of diamonds in different amorphization states. Atomic defects, interface, surface, and structural changes all lead to phonon localization. It can be used as a criterion to study the degree of phonon localization and its influence on TBC [31]. Its calculation formula is as follows:

$$PPR(\omega) = \frac{1}{N} \frac{(\sum_{i} VDOS_{i}(\omega))^{2}}{\sum_{i} VDOS_{i}(\omega)^{4}}$$
(5)

Where N represents the total number of atoms and $VDOS_i(\omega)$ is the VDOS of a single atom calculated. When fewer atoms participate in heat transfer, the value of PPR is small. For example, when only one atom vibrates in local mode, the PPR is 1/N. When all atoms participate in the vibration, the PPR is calculated to be 1. The smaller the PPR value is, the more serious the localization of phonon mode is, and the more unfavorable the heat transfer is [32].

3. Results and Discussions

3.1 Effects of heat treatment temperature of amorphous layer on TBC of Cu/C-diamond

The disorder degree of atoms in the amorphous layer varies greatly with different heat treatment temperatures. For this reason, diamond films with a thickness of 1.5 nm were heat-treated at 8000 K, 9000 K, 10000 K, and 11000 K respectively, and then inserted into Cu/C-diamond as an intermediate layer to calculate the TBC. With the increase in heat treatment temperature, the disorder degree of atoms in the amorphous layer gradually increased. The calculation results of interface thermal conductance are shown in Fig. 3. When the heat treatment temperature is 8000-9000 K, the amorphous diamond body still maintains the ordered state, but disordered atoms appear at the boundary, and the TBC increases to a small extent. When the heat treatment temperature rises to 10000-11000 K, the atoms in the amorphous layer begin to show complete disorder. It is noteworthy that the TBC at this time reaches 80 MW/m2 • K, which is about 4 times that without the amorphous layer.

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Figure 3. The TBC and overlap energy of Cu/C-diamond at 1.5 nm were studied at different heat treatment temperatures.

VDOS of amorphous diamond and Cu/C-diamond at different heat treatment temperatures were calculated according to Equation (2), as shown in Fig. 4. The results show that the VDOS of crystalline diamond and Cu are weakly coupled in the range of 0-10 THz, while the VDOS of amorphous layer change significantly in the temperature range of 9000-10000 K. When the heat treatment temperature is 8000 K and 9000 K, the VDOS of the amorphous layer are similar, and the vibration of the amorphous layer increases slightly at low frequency, which leads to a slight increase in the thermal conductance of the interface. When the heat treatment temperature is 10000 and 11000 K, the VDOS of the amorphous layer is completely different from that of the crystalline diamond. VODS is flatter in the whole frequency distribution and there is no obvious characteristic peak. The cutoff frequency of crystalline diamond increases to about 50 THz, while that of an amorphous diamond increases to about 60 THz. The larger cutoff frequency indicates that more phonon modes are involved in the vibration. In addition, compared with crystalline diamond and amorphous diamond heat treated at 8000-9000 K, its VDOS at low frequency is higher than that of crystalline diamond, which further improves the TBC of Cu/C-diamond. Moreover, in the VDOS the of amorphous layer at the calculated four heat treatment temperatures, a decrease at high frequency and an increase at low frequency appear, as shown by the black dotted line in Fig. 4. Interface amorphous can be considered as a kind of interface defects. It has also been found in relevant reports that with the increase of interface defects, the TBC of graphene/h-BN [33], Si/Ge [34], Si/Al [35] increases, and the defects lead to more phonon scattering, especially high-frequency phonons [36]. For Cu/C-diamond systems with high phonon vibration mismatch, the phonons responsible for the interface heat transfer are mainly low-frequency phonons less than ~ 8 THz, and the conversion of high-frequency phonons to low-frequency phonons increases the phonon coupling between the two in the low-frequency region. Therefore, it can be concluded that the presence of an amorphous interface promotes the inelastic scattering process at the interface (high-frequency phonon conversion to low-frequency) [37]. With the high-frequency phonon conversion to low frequency, the phonon coupling between Cu and diamond is enhanced and the TBC is increased. In addition, the TBC strongly depends on the overlap of VDOS in the interface region [38]. In order to further clarify the change of the TBC, we calculated the overlap energy under different thicknesses according to Equation (4), as shown in Fig. 3. The greater the overlap energy, the more harmonized the vibrations between the two atoms, the more conducive to energy transfer. Obviously, the vibration mismatch between Cu and diamond is larger without the addition of an amorphous diamond. However, the higher the heat treatment temperature of diamond amorphous is, the more intense the inelastic scattering occurs, and the greater the coupling degree between amorphous diamond and Cu at low frequency, which increases the overlap energy and ultimately increases theTBC of Cu/C-diamond.



Figure 4. VDOS variation of interface model at different heat treatment temperatures.

3.2 Effects of amorphous layer thickness on TBC of Cu/C-diamond

It can be observed from Fig. 4 that the TBC of amorphous layer has little difference at 8000-9000 K, but increases greatly at 10000 K, and then changes little at 11000 K. Therefore, we focused on the study of the influence of thickness changes on the TBC when the heat treatment temperatures of the amorphous layer were 9000 K and 10000 K. The calculation results are shown in Fig. 5. When the amorphous layer is treated at 9000 K, the TBC decreases gradually with the increase of its thickness, and the sensitivity of the TBC to the thickness of the amorphous layer is low, but it is still higher than that of the amorphous layer. On the contrary, when the heat treatment temperature is 9000 K, the TBC increases with the increase of the amorphous layer thickness when the heat treatment temperature is 10000 K. The TBC is much higher than that of the amorphous layer.



Figure 5. Effect of thickness variation of amorphous layer on TBC and overlap energy at different heat treatment temperatures.

In order to further study the influence of these two heat treatment temperatures on the TBC, VDOS at Cu/A-diamond/C-diamond interface are shown in Fig. 6. Vibration frequency and VDOS at the interface can further understand the enhancement mechanism of interface heat transfer. The VDOS of the amorphous layer show a great difference with different heat treatment temperature, and the main changes are described in the previous section. With the increase of heat treatment temperature, the matching degree of Cu and amorphous diamond is improved, and the interfacial heat transport efficiency is improved. The presence of amorphous layers at the two heat treatment temperatures still improves the vibration mismatch of Cu/C-diamond at low frequencies, and to some extent compensates for the vibration gap of Cu/C-diamond in the range of 10-20 THz, which is especially obvious at 10000 K.



Figure 6. VDOS of Cu, C-diamond and A-diamond at different heat treatment temperatures and thicknesses.

In addition, we calculate the overlap energy at different thicknesses, as shown in Fig. 5. The overlap energy results show that, firstly, the matching degree between amorphous layer and Cu increases with the increase of heat treatment temperature, which is mainly due to the increase of VDOS at low frequency due to the amorphous diamond. However, with the increase in the thickness of amorphous layer, the overlap energy at different heat treatment temperatures shows an opposite trend. When the heat treatment temperature is 9000 K, the overlap energy decreases with the increase of the thickness. When the heat treatment temperature is 10000 K, the overlap energy increases gradually with the increase of thickness, thus improving the interface heat transfer efficiency. This is also the internal reason why the TBC increases with the increase of the thickness of the amorphous layer. Finally, no matter what the heat treatment temperature or thickness of the amorphous layer is, it improves the weakest link in the heat transfer process, thus improving the vibration matching of the weakest part of the heat transfer, and thus enhancing the TBC.

When the amorphous layer is inserted, the temperature difference of the TBC is taken from both sides of the amorphous layer. In this calculation method, the thermal transport characteristics of the amorphous layer will further affect the TBC, so we calculate according to Equation (5) under different heat treatment temperatures and different thicknesses of amorphous diamond PPR, in the amorphous layer on its heat transfer characteristics of TBC should be, as shown in Fig. 7. If PPR = 0.4, the boundary is the delocalized mode, and if PPR is greater than 0.4, it is local mode [39]. The delocalized mode plays a positive role in heat transfer. Firstly, no matter what the heat treatment temperature is, the PPR of the amorphous layer is closer to the local mode than that of the crystalline diamond. For example, at 9000 K, the PPR of the amorphous layer in the range of 0-15 THz is much smaller than that of the crystalline diamond. For example, at the heat treatment temperature of 10000 K, in the range of 20-50 THz, although most phonons are in the delocalized mode, the PPR of the amorphous layer is close to the localized mode. All these indicate that the existence of the amorphous layer weakens the heat transfer to a certain extent. Although the thermal transfer characteristic of the amorphous layer is not as good as that of crystalline diamond, the use of the amorphous layer as an intermediate layer to regulate Cu/C-diamond can indeed improve its TBC. According to VDOS and overlap energy calculation, it can be concluded that: The improvement of the thermal conductance of the interface is due to the improvement of the vibration coupling between the amorphous layer and Cu in the low-frequency range and the filling of the vibration mismatch, and the competition between the improvement of the vibration coupling and the decrease of the thermal transmission performance of the amorphous layer is dominant. When the heat treatment temperature of the amorphous layer is 9000 K, with the increase of the thickness of the amorphous layer, the PPR in the range of 20-30 THz gradually increases and is in a delocalized mode, which promotes the heat transfer. Therefore, the increase of its own thermal transport

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performance partially offsets the decrease of TBC caused by the decrease of overlap energy, and finally makes the TBC less sensitive to thickness. When the heat treatment temperature of the amorphous layer is 10000 K, PPR changes little with the increase of thickness. At this time, the improvement of vibration coupling plays a major role in the TBC, the increase of overlap energy leads to the increase of the TBC. More amorphous layer under different heat treatment temperatures on the influence of TBC results can be seen that defects in amorphous layer (atomic arrangement from order to disorder), the defect will greatly change the VDOS amorphous layer of the whole frequency, defects in amorphous layer (layer amorphous atomic disorder) on the Cu/C-diamond, the effects of the TBC is greater.



Figure 7. PPR with different thickness at 9000 K and 10000 K.

4. Conclusion

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The heat transport across individual interface inside the composites of composites are very important for the application of micro/nanodevices. In this paper, the non-equilibrium molecular dynamics method was used to study the effect of amorphization of the diamond surface layer on the thermal conductance of the Cu/C-diamond interface with different heat treatment temperatures and different thicknesses. The reasons for the TBC enhancement of the Cu/C-diamond interface were analyzed through theVDOS, overlap energy and PPR. The conclusions were as follows:

Amphorous diamond film improves the vibration matching degree with Cu in the range of 0-10 THz, while VDOS is significantly improved in the range of 10-20 THz due to the influence of inelastic scattering. When the heat treatment temperature makes the atoms in the amorphous diamond film completely disordered, the vibration matching degree with Cu reaches the maximum, and the TBC increases the maximum.

For the complete disordered diamond film, Cu/C-diamond TBC increases with the film thickness (< 4.5 nm). The results of overlap energy and PPR show that the improvement of vibration coupling of an amorphous diamond is superior to the decrease of heat transfer performance with the increase of thickness, thus increasing the TBC.

This study shows that diamond surface amorphization can significantly enhance the heat transfer between Cu/C-diamond, which provides a new idea for the design of Cu/C-diamond composites with high thermal conductance

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