Research Article

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Microstructure and finite element analysis of Mo$_2$C-diamond/Cu composites by spark plasma sintering

Abstract: Mo$_2$C layer was generated on the diamond surface via vacuum micro-evaporating, which was used as the reinforcement particles to fabricate diamond/Cu composites by spark plasma sintering (SPS). The effect of evaporation parameters on the forming of Mo$_2$C, and the holding time on diamond/Cu composites fabrication is studied. Combined with the experiment and finite element analysis (FEA), the holding time on diamond/Cu composites influence on the thermal conductivity (TC) of composites is further discussed. The results show that the Mo$_2$C area on the diamond surface would gradually enlarge and cover the diamond surface evenly with the increment in evaporation time and temperature, better vacuum micro-evaporating parameters were given as 1,000°C for 60 min. The fractures in the diamond/Cu composites are mainly ductile fractures on copper and diamond falling out from the Mo$_2$C interface. It was found that sintering time would significantly influence the dissipation property of diamond/Cu composites. A comprehensive parameter for SPS was obtained at 900°C, 80 MPa for 10 min, the relative density (RD) and TC of the composites obtained under the parameter were 96.13% and 511 W/(m K). A longer sintering time would damage the Mo$_2$C interlayer and further decrease the bonding between copper matrix and diamond particles, which would lower the RD and TC of composites. It can be obtained from the comparison of simulation results and experimental results that the FEA result is closer to the experimental results due to the gaps with low heat conduction, and the air in the gaps is added in the simulation process.

1 Introduction

Heat sink materials nowadays are becoming widely used in electronic packaging and other related fields. As the fast developments in electronics and communication, the demand for higher-integrated microchips and miniaturized electronics is highly increasing. Therefore, a higher requirement for heat dissipation is urgently needed. However, the first and second generations of heat sink materials available like Al$_2$O$_3$, SiC, etc., with a thermal conductivity (TC) of 210–300 W/(m K) [1], cannot meet the increasing heat dissipation demands. Fortunately, the interdisciplinary developments between materials and electronics have made it possible to build functional materials or composites with high thermal-conducting ability. In this context, an ideal composite with appropriate thermal properties is expected to be massively needed. Diamond/Cu composites are considered an ideal heat sink material because it is designed to combine TC of diamond and Cu. The TC of synthesized diamond can range from 1,500 to 2,000 W/(m K), while the Cu has an average TC of 398 W/(m K). However, the TC of the composites fabricated is far lower than expected [2–4]. Diamond and copper determines neither to react with nor solute to each other. Holes, gaps, cracks, and other defects existing in the diamond/Cu composites are mainly caused by the non-wettability and will significantly influence not only its mechanical properties but also the thermal conducting ability [5].

Compared with mere mechanical interfacial bonding, the bonding created through chemical reaction and solid solution can be more effective in improving interfacial bonding qualities [6,7]. Quantities of pores and holes in the composites can be reduced and the mechanical properties could be developed through the strong-bonded interfaces, and these are the reasons why the researchers are...
eager to find out the interface modifying methods between diamond and Cu matrix. Pre-alloying of Cu matrix [8] is one method that can obtain a better combination between Cu and diamond. Ti [9,10], B [11,12], Sn [13], Zr [14], Ag [15], carbides [16], and rare earth oxides like Sc₂O₃ [17] are added in the Cu matrix to strengthen the interface bonding because the additional elements can react or form solid solution in Cu matrix. It is an effective method of developing mechanical and thermal properties. Another method of modifying the interface is to deposit a coating on the diamond surface, and the coating can act as a medium that connects the two phases with chemical bonding by either reaction or solid solution [18]. Different elements, such as W [19–21], Cr [6,7,22–24], Nb [25], Ni [20,26], Ti and its carbides [27–30], and Mo and its carbide [31–36], are coated on the diamond surface to improve the interface properties. The coating methods are considered as the most direct method to strengthen the interface bonding. Several coating methods have been used to coat on diamond surfaces. Magnetron sputtering is an effective way that can obtain a smooth, even, and thickness-adjustable interface [33], but the coating is deposited under a relatively low temperature like room temperature, where the temperature is too low to react on diamond. Electrocoating is also used for depositing metal on the diamond surface to strengthen better the interface bonding between diamond and copper matrix [25,37–40]. In addition, a new manufacturing routine of vacuum-assisted material extrusion, a sandwich structure, and interleaving of the low-temperature issue of the composites is performed to eliminate matrix voids and improve the bonding quality of deposited layers [41–43]. Based on the above, vacuum micro-evaporating deposition is one of the physical vapor deposition methods that deposit the metal elements in a high vacuum and high temperature condition at a relatively low cost. Energy from a high vacuum and temperature environment could be provided to highly activate metal surface atoms, which makes the elements react with the diamond to generate compounds.

Despite Mo and its carbide having the ability to significantly improve the wettability between Cu matrix and diamond as an effective interlayer [32], it still causes a reduction in the TC of the composites with an inappropriate interlayer thickness, which ignored the negative effect from the Mo carbide or Mo itself [35]. Meanwhile, combined finite element simulation to analyze the effect of different coating thicknesses on the TC of the composites is rare. Based on the fact, the forming mechanism and optimization processing of Mo₂C coating on the diamond surface and finite element analysis (FEA) of the composites for the thermal properties need to be studied for the prediction and development.

In this work, the diamond particles with Mo₂C coating were fabricated by vacuum micro-deposition method, the microstructure of Mo₂C-coated diamond is presented and analyzed, and the formation mechanism of Mo₂C on diamond surfaces is discussed. Spark plasma sintering (SPS) is an effective way of producing diamond/Cu composites, thus, the prediction and heat dissipation properties of Mo₂C-coated diamond/Cu composites by SPS are researched as well in this work. The thickness of the Mo₂C interlayer on the microstructure and the thermal performance of the diamond/Cu composites were studied by simulation and experiment.

2 Experimental method

Commercially synthesized MBD-8 diamond particles with average particle sizes of 100 μm were purchased from Whirlwind Diamond Powder Co., Ltd, Henan, China. And Mo powder with a size of 2 μm (Shanghai Chaowei Nano Co., Ltd) was used for powder coating. The diamond particles were cleaned in 10 wt% NaOH solution and 20 wt% HCl, respectively, to remove the oil and coarsen the diamond surfaces, and the diamond particles were dried after being cleaned to neutral with distilled water. Diamond particles and Mo powders with a molar ratio of 10:1 was mixed evenly at a rotating speed of 300 rpm for 2 h by planetary ball mill.

The tube furnace (TL1200, Nanjing Boyuntong Co., Ltd) was used for vacuum micro-evaporating. The ceramic crucible including the mixed powder with a molar ratio of 10:1 was put in the tube furnace, vacuumed to a pressure of s10⁻³ Pa, and heated up to gradually reach the target temperature of 1,000°C, and this temperature is held for 50–60 min. Then, the coating is plated at 980–1,020°C for 60 min. The holding procedure is then stopped and the furnace is cooled to room temperature. The Mo₂C-coated diamond particles are cleaned with distilled water in the ultrasonic cleaner to wash away the Mo powder that might get exited on the surface of the diamond when heating. The coated diamond particles are then dried up.

The high-resolution transmission scanning electronic microscope (SEM, SU8220) was used to observe the further microstructure of the Mo₂C-coated diamond. X-Ray diffraction (XRD, SmartLab, Rigaku UltimaIII) with a scanning range of 20–90° at a scanning speed of 4°/min was used for analyzing the phase composition of the Mo₂C-coated diamond and the composites. Atomic force microscope (AFM, BRUKER) was used to study the differences in surface roughness between the original and coated diamonds. The TC of the composites was measured by laser flash TC
measurement apparatus (TC-7000H, Sinku-Riko Inc., Japan). The Mo$_2$C-coated diamonds were sent to mix with copper powder and sintered via spark plasma to make diamond/Cu composites for 10, 20, and 40 min. The process diagram of preparation of Mo$_2$C-diamond/Cu composites is shown in Figure 1.

3 Results and discussion

3.1 Microstructure analysis of Mo-coated diamond

Figure 2 displays the morphologies of as-received diamond and Mo-coated ones deposited at 1,000°C with different deposition time. The as-received diamond particle has a cubic octahedral shape, which has an intact and smooth surface as a perfect crystal, as shown in Figure 2(a) and (b). Mo was deposited on the have surface at the deposition time of 50 min, as shown in Figure 2(c) and (d), the deposited areas have a grain shape, and the grain shape connects and finally covers the diamond surface uniformly. The reason this phenomenon occurs is because of the reaction between carbon and Mo. As the deposition time increases to 60 min, more Mo gas mass gathered and reacted with carbon, Mo particles are gathering on the Mo carbide surface due to the increased deposition period. Meanwhile, Mo diffuses into diamond and bonds with carbon, the grain shape expands and joins others until it became a whole which covers the diamond surface. As shown in the SEM results, the Mo-coated diamond particles at 1,000°C for 60 min are better for the surface to be nearly covered with Mo$_2$C.

The diamond surface under different parameters was observed by AFM, as shown in Figure 3. As seen from

![Figure 1: The process diagram of preparation of Mo$_2$C-Diamond/Cu composites.](image-url)
Figure 3(a), the initial diamond particle is relatively flat as a whole, but there are also some micron level protrusions which are mainly caused by the preparation process of the diamond, it increases the surface area of the diamond and is conducive to the deposition of coating elements during vacuum micro-evaporating. Figure 3(b) is the AFM result of Mo$_2$C-coated diamond surface with a peak height of 349.8 nm at 1,000°C for 50 min, and the diamond surface roughness changes more rapidly, the rough Mo$_2$C-coated surface is obtained due to the irregular movement of Mo gas groups and the microscale Mo powder size. The diamond surface at 1,000°C for 60 min with obvious changes in surface morphology and numerous surface fluctuations with the peak height of 236.4 nm at the highest point, is shown in Figure 3(c).

Compared to the former, the coating on the diamond surface becomes relatively flat and uniform. According to the work of Pan et al. [36], the rough and dense Mo$_2$C surface would be easier for copper to bond and increase the shearing force between copper and Mo$_2$C to prevent the Mo$_2$C-coated diamonds from desquamating and debonding from the copper matrix.

Figure 4 is an EDS analysis of Mo$_2$C-coated diamonds at 1,000°C for different deposition time. Mo coating is completely plated on the whole diamond surface, but the surface is rugged and rough, as shown in Figure 4(a) and (b). The reason for the local agglomeration of Mo is that during the coating process, the part is too much in contact with Mo powder resulting in the aggregation of Mo molecular
Figure 3: AFM morphology of diamond at 1,000°C for different deposition time: (a) as-received, (b) 50 min, and (c) 60 min.

Figure 4: EDS analysis of Mo$_2$C-coated diamonds at 1,000°C for different deposition time: (a) 50 min, (b) mapping of (a), (c) 60 min, and (d) mapping of (c).
groups around them at the high temperature and connected as a whole. Figure 4(c) shows that the Mo coating on the diamond surface is more even and smooth. The EDS surface scanning results with a coating time of 60 min are shown in Figure 4(d), it can be seen that Mo is evenly distributed on the surface of diamond, which shows that the process parameters are conducive to the uniform preparation of Mo coating, and provides a basis for obtaining good surface quality and interface adhesion.

Figure 5 shows the surface morphology of Mo coated diamond deposited at different temperatures for 60 min. It is observed that the surface of diamond is in the form of gullies and rough at 980°C, the coating degree of the surface is not high, and the microstructure with transverse growth trend diffuses on the diamond surface, as shown in Figure 5(a) and (b). When the deposition temperature elevates to 1,020°C, as seen from Figure 5(c) and (d), almost all diamond surfaces have grown a coating layer, the surface massive structure of diamond continues to expand, Mo groups adhere on the coating layer, and the transverse growth between the groups is before the longitudinal growth. From the above SEM results, it can be concluded that the surface coating preferentially grows laterally under different coating temperatures, that is, a uniform and dense coating layer is preferentially obtained on the diamond. As the temperature increases, Mo preferentially combines with the diamond that is more prone to react to obtain the Mo2C interface faster, various parts of Mo groups combine to form a denser caking layer, which makes the transverse diffusion of the coating.

Figure 6(a) shows the AFM morphology of diamond after coating at 980°C for 60 min. The surface is very flat, and the highest peak is 749.4 nm. The surface at 1,020°C gathers thicker Mo molecular groups, as shown in Figure 6(b). The maximum difference between the groups and the formed coating surface is 317.2 nm. The Mo molecular groups have fused, which is consistent with Figure 5 results. It is proved that the relatively flat coating surface will be combined with Mo particles again at 1,020°C. The reason for the phenomenon is that as the ambient temperature increases, the energy supply increases, and the Mo on the surface of diamond obtains enough energy to form Mo coating. Compared with the micro-evaporating temperature of 1,000°C, the coating at 980 and 1,020°C is not relatively dense enough. Therefore, the optimum process parameters for coating Mo on the diamond surface is 1,000°C for 60 min.

![Figure 5](image-url)  
Figure 5: Microstructure of Mo2C-coated diamond at 60 min for different temperatures: (a) 980°C, (b) magnified view of the region in (a), (c) 1,020°C, and (d) magnified view of the region in (c).
3.2 Phase composition of Mo-coated diamond

Based on the above discussion results, the optimum parameters of Mo coated on the diamond surface is 1,000°C for 60 min, the next work only analyzes the effect of different deposition time on the phase composition of Mo coated diamond at 1,000°C. Mo will react with carbon to form carbide at a temperature of 600°C.

\[
\text{Mo(s) + C(diamond) \rightarrow MoC(s)}, \quad (1)
\]

\[
2\text{Mo(s) + C(diamond) \rightarrow Mo}_2\text{C(s)}.
\]

Figure 7 is the XRD analysis of Mo coated diamond at 1,000°C for different deposition time. The XRD pattern shows that the graphite phase was not detected. The high peak near 2\(\theta\) = 45° specifies that this matter is diamond, which means the diamond graphitization is not an obvious phenomenon in vacuum micro-evaporating, and the Mo-C is more likely to be the main product compared with MoC through this processing under this condition according to formulas (1) and (2). MoC is successfully produced through deposited Mo by vacuum micro-evaporating, as shown by the MoC peak in Figure 7, which indicates the successful generation of MoC on the diamond surfaces at the deposition time of 50 min; this is due to the reaction between Mo and carbon in diamond when the reacting temperature between Mo and carbon is above 650°C as reported by Liu et al. [31].

Figure 8 is the forming process of Mo\(_2\)C. Mo reacts with carbon in the diamond surface, as shown in Figure 8(a). Figure 8(b) is the ideal structure of Mo\(_2\)C after reacting for the structure is similar to the structure of the original diamond, which means Mo would react with carbon to form this structure with less energy. Although Mo\(_2\)C has different space groups, it can be defined by comparing the experimental XRD pattern with the calculated diffraction patterns of different Mo\(_2\)C structures. The crystal structure of diamond is referred to the structure of Pm\(_3\)m shown in Figure 8(b) as the calculated diffraction pattern fits the experimental XRD pattern shown in Figure 7, the XRD pattern of the space structure shown in 8(b) when the sweeping angle ranges from 20–90°. The peaks of Figure 8(b) show when 2\(\theta\) is 33.676, 38.707, 38.989, 52.227, 60.228, 70.247°, which can fit the experimental XRD pattern shown in Figure 8. Therefore, it can basically be ensured from the experimental XRD pattern that most Mo\(_2\)C space group generated on the diamond surface is in a structure of P\(_3\)m\(_1\), which makes the Mo\(_2\)C interlayer properties more specific.

Mo\(_2\)C coating thickness is calculated through the simplified model referred to in the work of Chang et al. [34] presented in Figure 9. \(\Delta m\) is the additional weight of diamond after being coated with Mo\(_2\)C, which is measured by the gravimetric method. The measured additional weight statistics are listed in Table 1. The calculating expression is shown in formula (3).

\[
\delta = [r^3 + 3\Delta m \times \rho_{\text{dia}} \times r^3/\rho_{\text{coating}}]^{1/3} - r, \quad (3)
\]

where \(r\) stands for the average diamond radius, which could be presented by diamond particle size, \(\Delta m\) is measured as additional weight, which is given in Table 1. \(\rho_{\text{dia}}\) and \(\rho_{\text{coating}}\) are the densities of diamond and Mo\(_2\)C coating, respectively.

According to the morphology of Mo\(_2\)C-coated diamond in Figure 2 and theoretical thickness values at different evaporating time, the amount of Mo deposited at 1,000°C for 50 min is not dense. Therefore, the Mo\(_2\)C-coated diamonds at 1,000°C for 60 min are more suitable to be selected to fabricate diamond/Cu composites by SPS.

3.3 Compactness analysis of Mo\(_2\)C-coated diamond/Cu composites

Based on the above research results, the Mo\(_2\)C-coated diamond particles at 1,000°C deposited for 60 min were selected to fabricate diamond/Cu composites. The composites were
Figure 7: XRD analysis of Mo coated diamond at 1,000°C for different deposition time: (a) as-received diamond, (b) 50 min, and (c) 60 min.

Figure 8: The forming process of Mo$_2$C: (a) diamond combining with Mo, and (b) combining product Mo$_2$C.
fabricated with 50 vol% Mo2C-coated diamonds by SPS at 80 MPa, 900°C for 10, 20, and 40 min, respectively. Figure 10 shows the relative density (RD) of Mo2C-coated diamond/Cu composites. The highest RD of Mo2C-coated diamond/Cu composites is 96.13% at the holding time of 10 min, the two main fracture types of diamond/Cu composites are ductile and diamond falling out from the surface, some diamond faces are bonded with copper compactly where there are fewer cracks inside, while the RD of Mo2C-coated diamond/Cu composites decreases at the holding time of 10 and 20 min, it can be seen that cracks and gaps exist between diamond surfaces and copper. Meanwhile, more voids and gaps appear between copper and Mo2C-coated diamond composites as the sintering time is prolong. Due to the SPS period going up, the spark pulse would produce instantaneous high temperature, which will damage the interlayer between copper matrix and diamond, the same effect as diamond/Cu composites with non-coated diamond. Therefore, the RD of composites is consistent with the morphology, because the lower the RD is, the more voids and gaps will appear in the composites. The decrease in RD can also prove that the bonding between copper and the Mo2C interlayer is weakened with the increase in sintering time, which causes the increase in voids and cracks as seen in Figure 10. The morphologies of the fracture show that there is better interfacial bonding in diamond/Cu composites fabricating under 900°C, 80 MPa sintering for 10 min.

**Table 1: Additional weight percentage of Mo2C-coated diamond**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Molar ratio</th>
<th>Time (min)</th>
<th>Additional weight (%)</th>
<th>Theoretical coating thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,000</td>
<td>10:1</td>
<td>50</td>
<td>2.7690</td>
<td>176.30</td>
</tr>
<tr>
<td></td>
<td></td>
<td>60</td>
<td>4.2055</td>
<td>267.30</td>
</tr>
</tbody>
</table>

**Figure 9: Simplified model of coating thickness on the diamond surface.**

**Figure 10: RD of Mo2C-coated diamond/Cu composites at different holding time.**

**Figure 11: XRD pattern of Mo2C-coated diamond/Cu composites with different sintering parameters.**
Figure 12: Finite element model of Mo2C-coated diamond/Cu composites: (a) 3D model, (b) mesh generation, and (c) temperature field model.

Figure 13: 3D model of Mo2C-coated diamond/Cu composites with different porosities: (a) 4.87%, (b) 9.45%, and (c) 14.68%.

Figure 14: FEA result of Mo2C-coated diamond/Cu composites with different porosities: (a) 4.87%, (b) 9.45%, and (c) 14.68%.
Figure 11 is the XRD pattern of Mo2C-coated diamond/Cu composites at different sintering parameters. The XRD result shows that there is no other phase generated when fabricating the composites, which is in agreement with that in the study by Li et al. [44]. And Cu and Mo2C still exist after sintering. The diamond phase is detected means there would be no graphite phase generated by SPS, which also indicates that 900°C would be a suitable temperature for fabricating diamond/Cu composites.

3.4 FEA and experiment analysis on TC of Mo2C-coated diamond/Cu composites

The representative volume element (RVE) model of Mo2C-coated diamond/Cu composites is established by using Digimat and ABAQUS simulation software. Voxel mesh generation for 3D models can be chosen due to its stable mesh quality, high accuracy, low consumption of computing power, and a high degree of customization for the number of meshes. Due to the isotropic nature of diamond/Cu composites, the thermal field can be loaded in a specific direction. The simulation field is set as heat exchange, the right side of its X-axis is set as the heat source contact surface, the peak temperature is 100°C, and the unidirectional heat transfer along the X-axis of RVE is carried out, as shown in Figure 12, and the parameters for FEA of the composites is displayed in Table 2.

It can be seen from Figure 10 that the RD of the composites under different holding time is 96.13, 90.55, and 85.32%, respectively, in other words, the porosity of the composites is 4.87, 9.45, and 14.68%. Since porosity has a great influence on the TC of diamond/Cu composites, the effect of porosity on TC is mainly discussed, which is based on the 3D model with the Mo2C coating thickness of 267 nm. The 3D model of Mo2C-coated diamond/Cu composites with different porosities is shown in Figure 13. In the image, the blue portion is Mo2C continuous coating and the green portion is randomly distributed pores.

The FEA TC results of Mo2C-coated diamond/Cu composites at different parameters are shown in Figure 14 and Table 3. It is seen that the pores have a completely negative effect on the TC of the composites, and the heat could not be effectively conducted when it is accumulated in the pores. As the porosity increases, the surface heat flux of the composites gradually decreases due to the large scattering range and high degree of air in the pores, where high thermal resistance is formed and the TC is only 0.026 W/(m K). Therefore, the heat flux density at the pores is much lower than that in other parts.

The simulated and experimental TC of Mo2C-coated diamond/Cu composites are shown in Figure 15. Compared with the experimental value, the simulation result is closer to the experimental results, since the gap with low heat conduction and the air in the gap is added in the simulation process, so that it can simulate in a more real heat conduction situation. Meanwhile, the simulation results considering pores and coatings can be used as a tool to predict TC, and the TC prediction database based on the simulation results can be established, but there exists a difference in them, as the coating on the diamond surface is uneven actually, while the simulation considers the uniform coating between diamond and Cu.

<table>
<thead>
<tr>
<th>Sintering temperature (°C)</th>
<th>Loading pressure (MPa)</th>
<th>Holding time (min)</th>
<th>Porosity (%)</th>
<th>Specific direction</th>
<th>TC (W/(m K))</th>
</tr>
</thead>
<tbody>
<tr>
<td>900</td>
<td>80</td>
<td>10</td>
<td>5</td>
<td>K11</td>
<td>574</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>K22</td>
<td>573</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>K33</td>
<td>574</td>
</tr>
<tr>
<td>20</td>
<td>10</td>
<td></td>
<td></td>
<td>K11</td>
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<td>K22</td>
<td>458</td>
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<td>K11</td>
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<td></td>
<td></td>
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<td>K33</td>
<td>364</td>
</tr>
</tbody>
</table>

Table 2: Parameters for finite simulation of the composites [45–47]

<table>
<thead>
<tr>
<th>Materials</th>
<th>Density (g/cm³)</th>
<th>Heat capacity (J/(kg K))</th>
<th>Debye sound velocity (m/s)</th>
<th>TC (W/m K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diamond</td>
<td>3.52</td>
<td>512</td>
<td>13,430</td>
<td>1,500</td>
</tr>
<tr>
<td>Mo2C</td>
<td>8.89</td>
<td>347</td>
<td>4,003</td>
<td>21</td>
</tr>
<tr>
<td>Porosity</td>
<td>1.205</td>
<td>1,002</td>
<td>—</td>
<td>0.026</td>
</tr>
<tr>
<td>Cu</td>
<td>8.96</td>
<td>386</td>
<td>2,801</td>
<td>398</td>
</tr>
</tbody>
</table>
4 Conclusion

Mo$_2$C layer was generated on the diamond surface via vacuum micro-evaporating, which was used as the reinforcement particles to fabricate diamond/Cu composites by SPS. The effect of evaporation parameters on the forming of Mo$_2$C, and the holding time on diamond/Cu composites fabrication is studied. Combined with the experiment and FEA, the holding time on diamond/Cu composites influence on TC of composites is further discussed.

But, in the work, the process parameters of diamond and diamond-copper composite materials are merely experimentally studied by using the principle of single variable. In the future, neural networks and other algorithms can be further used to construct the optimization design of process parameters under multi-factor and multi-coupling. The conclusion of the study is as follows:

1) As the evaporation of time and temperature increases, the Mo coating on diamonds surface becomes evenly, the optimum time and temperature of coated Mo$_2$C on diamond particles is 1,000°C for 60 min.

2) Diamond/Cu composites were fabricated by SPS at 900°C, 80 MPa, sintered for 10, 20, and 40 min, respectively, and high density of the composites with Mo$_2$C interlayer can be fabricated by SPS at 900°C, 80 MPa for 10 min. The fractures in the diamond/Cu composites are mainly ductile fractures on copper and diamond falling out from the Mo$_2$C interface. It was found that sintering time would significantly influence the dissipation property of diamond/Cu composites.

3) The comprehensive parameter for SPS was obtained as 900°C, 80 MPa for 10 min, the RD and TC of the composites obtained is 96.13% and 511 W/(m K). A longer sintering time would damage the Mo$_2$C interlayer and further decrease the bonding between copper matrix and diamond particles, which would lower the RD and TC of composites.

4) On comparison, the simulation result is closer to the experimental results, since the gap with low heat conduction and the air in the gap is added in the simulation process. Meanwhile, the simulation results considering pores and coatings can be used as a tool to predict TC, and the TC prediction database based on the simulation results can be established, but difference exist in them, as the coating on the diamond surface is uneven actually, while the simulation considers uniform coating between diamond and Cu.

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Conflict of interest: Authors state no conflict of interest.

Data availability statement: The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

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