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Finite Element Simulation of Graphene Thermal Conductivity Framework

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Abstract. With the rapid development of electronic devices towards miniaturization and high integration, the problem of overheating and heat dissipation forces people to find thermal conductive materials with good comprehensive properties to meet the needs of development. Inspired by the three-dimensional boron nitride network, this paper creatively proposed the construction of a composite thermal conductive material with 3D graphene network structure and PDMS as filling matrix, and carried out finite element analysis and simulation with COMSOL. The results show that the thermal conductivity of the composite thermal conductive material with graphene 3D network structure is significantly better than that of the single thermal conductive material without graphene and the thermal conductive material with random distribution of graphene, and most of the heat flow forms a connected thermal conductive path along the heat transfer direction in the graphene of 3D network composite. It can be seen that the prepared composites with 3D thermal conduction network structure have excellent thermal conductivity, and will have broad market prospects in the fields of heat dissipation materials, computers, smart phones, laser weapons and so on.

1. Introduction

With the rapid development of technology and the continuous expansion of industrial demand, as well as the development of electronic devices towards miniaturization and high integration, the problem of overheating and heat dissipation has become a huge obstacle to the development of electronic devices[1]. At present, there are many kinds of high thermal conductivity materials studied, and they can be roughly divided into several categories. One is metal based thermal conductivity materials. Metal is one of the widely used heat conducting materials at present. However, due to its poor corrosion resistance and electrical insulation, it can not meet the heat dissipation requirements of electrical insulation and chemical corrosion. The second type is ceramic thermal conductive materials. Ceramics are inorganic materials with the advantages of high hardness, high temperature resistance and high pressure resistance among common engineering materials. Among them, ceramics such as aluminum nitride and silicon nitride have excellent thermal conductivity. However, their large-scale application is seriously limited due to their high processing cost and poor impact resistance [2].

Whether the thermal conductivity of thermal conductive materials is excellent is very important in industries with high requirements for heat dissipation performance. At present, there is an urgent need to research and develop new heat conducting materials with good comprehensive properties to meet the needs of the development of industry, science and technology and national defense, so people turn their attention to polymer materials. Polymer materials have excellent plasticity, electrical insulation, corrosion resistance and easy processing. They are widely used in many fields. However, most polymer materials have low thermal conductivity, which greatly limits their large-scale application, so polymer based thermal conductive materials came into being[3][4][5]. That is, some high thermal conductivity materials are compounded in the polymer matrix to improve its comprehensive properties, so as to promote the development of thermal conductivity materials in the industrial field.

Hexagonal boron nitride has the advantages of high thermal conductivity, good insulation performance, good chemical stability and industrial production. It is considered to be one of the most ideal thermal conductive fillers. However, hexagonal boron nitride polymer thermal conductive composites have not been applied yet. The two key factors causing this problem are the poor dispersion and serious viscosity increase of hexagonal boron nitride. Yu Kangkang [6] prepared a new spherical boron nitride silicone rubber thermal conductive composite with the advantages of uniform dispersion, dense microstructure and high thermal conductivity by high gravity deposition. Jiang Wenzheng et al. [7] and Jing et al. [8] introduced a polymer composite with three-dimensional boron nitride network structure. However, this polymer composite constructed by them still has some problems, such as easy agglomeration and difficult dispersion of boron nitride in the polymer matrix.

Graphene is composed of single or few layers of carbon atoms, with high strength and modulus, and its in-plane thermal conductivity is as high as 3500-5300 W / (m · K). It is the material with the highest thermal conductivity known at present. Its mechanical and thermal conductivity are far higher than ordinary thermal conductivity materials, and has been widely used in various fields [9]. Wang et al. [10] found that adding graphene oxide to epoxy resin can improve the thermal conductivity of composites. In terms of the material characteristics of graphene, some scholars have found that the random dispersion of graphene in the matrix will disrupt the unidirectional heat conduction mechanism in the composite and reduce the effective thermal conductivity of graphene [3] [11]. At present, some scholars use three-dimensional graphene preform as thermal conductive filler, and then composite it with polymer by vacuum impregnation to obtain composite thermal interface material, which effectively improves the thermal conductivity of polymer [12]. Qi et al. [13] prepared the phase change thermal interface material through CVD method, which increased the thermal conductivity from 0.27 W/ (m. K) to 1.22 W/ (m. K).

Inspired by the above, building a three-dimensional filler network in the polymer matrix can efficiently build a heat conduction path. Compared with the randomly dispersed filler system, the composites with three-dimensional heat conduction network structure show higher heat conduction properties. Therefore, the composites with three-dimensional graphene thermal conductive structure are simulated by finite element analysis.

2. Methods

In order to verify whether the existence of graphene and 3D network structure can promote the heat transfer ability of the material, we analyzed it through COMSOL finite element simulation, and revealed the total heat flux and temperature distribution of the material during heating. The boundary conditions are shown in the Figure 1. The outer walls on the left and right sides are thermally insulated, the temperature at one end of the upper and lower ends is 273K, the other end is 323K, and the inward heat flux from the hot end is 0.1W.

3. Results and discussion

The finite element model established in the Figure 2 shows three cases: one is that graphene is randomly dispersed in the PDMS matrix, the other is that graphene forms a 3D network structure in the PDMS matrix, and the other is that there is only PDMS matrix. Because graphene and PDMS are solid, solid heat transfer interface is selected. After the boundary setting is completed, the established model is meshed, and the physical field is selected to control the super refinement of the mesh, so as to improve the calculation accuracy and obtain more accurate results. We can see from the temperature distribution image that the top temperature of the composites with graphene 3D network structure is significantly higher than that of the composites with graphene random dispersion in Figure 2(a) compared with Figure 2(c), which indicates that the 3D network structure has better heat transfer ability, which is consistent with the simulation conclusion of Xu Xingxing [3] and the experimental conclusion of Wenzheng Jiang et al. [7]. Comparing Figure 2(a) with Figure 2(b), in the case of the same 3D network structure, it is obvious that the top temperature of the thermal conductive material with graphene is higher, which shows that the addition of graphene can well improve the thermal conductivity of the thermal conductive material. Moreover, in the heat flux distribution diagram, it is obvious from Figure 2(d) and Figure 2(f) that most of the heat flux is obviously located in graphene, indicating the super thermal conductivity of graphene. The comparison between Figure 2(d) and Figure 2(e) shows that the heat flow forms a connecting path along the heat transfer direction in the 3D network composite, while in the random composite, the random dispersion of graphene will hinder the heat flow conduction, which indirectly proves the super heat transfer ability of the 3D composite. This simulation result is consistent with the simulation conclusion of Jingchao Li et al. [8].

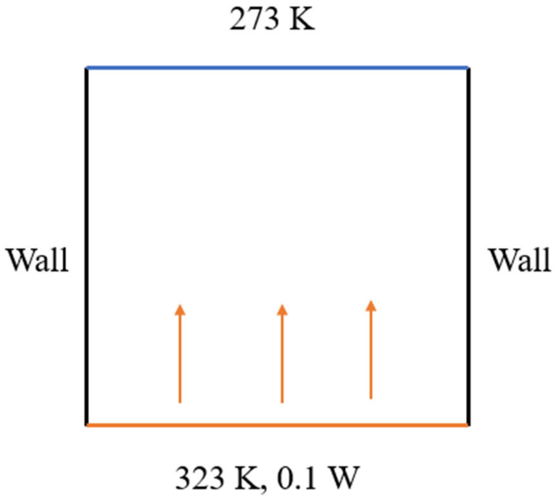
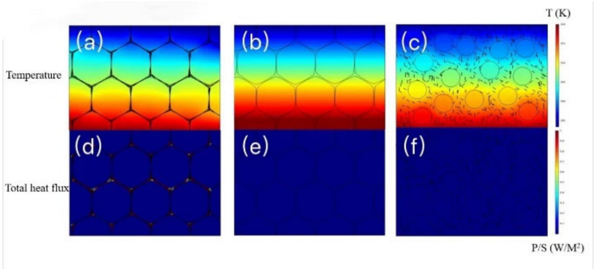


Figure 1. Boundary conditions.



Fifure 2. Simulate temperature distribution (a)(b)(c) and total heat flux distribution (d)(e)(f) as well as the thermal conductivity values of the 3D graphe-PDMS composites, the 3D PDMS and the random graphe-PDMS composites based on a heat source acquired by finite element analysis.

4. Conclusion

To sum up, adding graphene as filler into PDMS matrix can improve the thermal conductivity of graphene PDMS composites, and the 3D thermal conductivity network structure formed by graphene as filler also greatly improves the thermal conductivity of composites. This shows that 3D graphene PDMS has broad application prospects in the field of heat dissipation in the future.

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