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A predictive model for interfacial thermal conductance in surface metallized diamond aluminum matrix composites

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ABSTRACT

As promising thermal management materials with tailored thermal expansion and light weight, diamond/aluminum composites have not exhibited desirable thermal conductivity (TC) yet, due to poor interfacial thermal conductance (ITC) between diamond and aluminum. Although some experimental studies have been made to improve the ITC by means of diamond surface metallization, there are no systematic theoretical evaluations of the influences of interface layers' structures on the ITC yet. In terms of the components of diamond/Al interface layer, a carbide–metal–intermetallic, multi-layered interface model was established in this work, and the effects of different components and structures of interface layers on the ITC and TC of the surface metallized diamond/Al composites were predicted. The calculated results indicate that, basically, an interface layer of nanoscale thickness with high TC and large sound velocity is desirable to achieve high ITC. Under this premise, W and Mo interface layers are proposed to be the most promising candidates to improve the thermal performance of diamond/Al composites.

1. Introduction

Diamond/aluminum composites have drawn much more attentions than ever before as promising candidate materials for thermal management, due to the perfect combination of high thermal conductivity (TC), tailored coefficient of thermal expansion (CTE) and light weight [1–5]. For a given quality and volume fraction of diamond, the interfacial thermal conductance (ITC) is one of the most crucial factors that determines the TC of diamond/Al composites. It is well known that a direct contact of diamond with Al at elevated temperatures will inevitably lead to the formation of aluminum carbide (Al_4C_3), which helps enhancing the interfacial bonding to some extent. However, excessive Al_4C_3 may also greatly deteriorate the ITC due to its rather low TC. Since the kinetics of Al_4C_3 formation is too fast to be controlled at elevated temperatures, both alloying of metal matrix [6–8] and surface metallization of diamond particles [4,9–11] were adopted to form an interface layer between diamond and Al, aiming to impede the formation of Al_4C_3 and/or facilitate the formation of favorable carbides other than Al_4C_3, such as TiC [4,10,12], Cr_7C_3 [11,12], and WC [13,14]. However, alloying will cause a large degradation of TC for the Al matrix, and thus results in rather lower TC of the diamond/Al composites as made than expected [6–9]. In contrast, surface metallization of diamond particles provides the possibility to achieve high ITC without the deterioration of TC for the matrix, which makes it the focus discussed in the following parts.

In the fabrication of diamond/Al composites by liquid infiltration and powder metallurgy, when surface metallization is applied to the diamond particles, the coated metal layer may react with diamond and matrix metal on each side, and thus form a multi-layered interface composed of carbide, metal and intermetallic sublayers. Such an interface is supposed to be able to enable good bonding with the metal matrix by the metal/intermetallic sublayer, and with the diamond by the carbide sublayer [13]. Based on this point, some carbide-forming elements, such as Ti [4,10], Cr [11,12], W [13,14] and Mo [15], had been studied as interface layers to strengthen the interfacial bonding, most of which were reported to be effective. However, good interfacial bonding is just a prerequisite but not the sufficient condition for desirable ITC, for the incorporated additional interface layers will probably also act as thermal boundary barriers, which is more significant for the layer with a rather large thickness and low TC. Moreover, although both the carbide-forming metals and some non-carbide-forming metals, such as Cu [16], Ni [17], and Ag [18] , were investigated experimentally as interface layers to improve interfacial bonding, there is no quantitative evaluation and comparison of their influences on the thermal properties yet.

This work aims to theoretically evaluate the effects of several categories of interface layer on the ITC and TC of diamond/Al composites using a carbide–metal–intermetallic, multi-layered interface model. The effects of thickness and formation of interface

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layers of carbides as well as intermetallics on the ITC and TC of diamond/Al composites were quantitatively investigated, which could be used as guidance for the design and fabrication of the composites. To the best of our knowledge, it is the first study that considers the effect of an intermetallic layer, and gives such an overall, theoretical evaluation of the effect of a series of metals (Cr, W, Ni, Mo, Ti, Cu, Ag) and their carbides as interface layers on the thermal performance of diamond/Al composites.

2. Modelling

Generally, the metal interface layer in the composites originating from the surface metallized diamond particles may diffuse into the matrix, forming an alloy layer first and then probably producing some intermetallics in the alloy layer at elevated temperatures [10]. Thus, the interface layer in the surface metallized diamond composites usually consists of metal, carbide and/or intermetallic layers, depending on the heat treatment of diamond metallization and the consolidation of the composites, of which a single metal or carbide layer was most considered in Refs. [4,9–11]. For lack of data, in this study, the intermetallic layer instead of the alloy layer is considered for the calculation. Fig. 1 shows the schematic and physical model of the diamond/Al composites with a carbide–metal–intermetallic, multi-layered interface.

For each introduced interface layer, one more new interface and thermal barrier zone will be added. Then, from the concept of an electrical resistance analogy [9], the ITC, h can be expressed by equation:

$$\frac{1}{h} = \sum \left(\frac{1}{h_i} + \frac{l_{(i-1)\to i}}{K_{(i-1)\to i}} \right) (i \geqslant 1) \tag{1}$$

where h_i stands for the ITC of the ith interface, $l_{(i-1)\to i}$ and $K_{(i-1)\to i}$ stand for the thickness and TC of the layer from the $(i-1)$th to the i th interface, respectively. h_i can be calculated by the acoustic mismatch model (AMM) [9,12]:

$$h \approx \frac{1}{4}\rho c v \eta = \frac{1}{2}\rho_m c_m \frac{v_m^3}{v_r^2} \frac{\rho_m v_m \rho_r v_r}{(\rho_m v_m + \rho_r v_r)^2} \tag{2}$$

where ρ, c, v and η are the mass density, specific heat capacity, sound velocity and the average probability for the transmission of the phonon across the interface of the materials, respectively, and

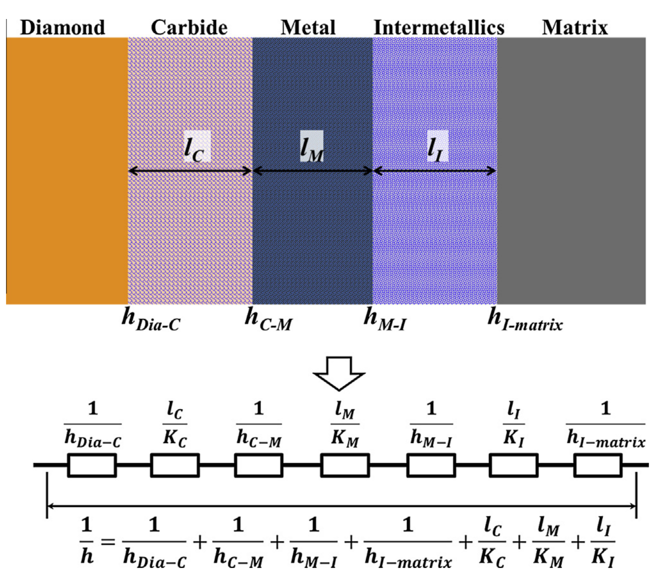

Fig. 1. Schematics and physical model of diamond/Al composites with interface layers. *Dia*, *C*, *M* and *I* stand for diamond, carbide, metal and intermetallic, respectively.

m and r denote the matrix and reinforcement. v can be established from the longitudinal (v_l) and transverse (v_t) velocities by [19–22]:

$$v = \left(\frac{3(v_l v_t)^3}{2v_l^3 + v_t^3} \right)^{\frac{1}{3}}. \tag{3}$$

The sound velocities of some materials were also calculated from equations [20]: $v_l = \sqrt{\frac{B+\frac{4}{3}G}{\rho}}$ and $v_t = \sqrt{\frac{G}{\rho}}$, where B and G are the bulk and shear moduli, respectively. Then the ITC of the (diamond/carbide/metal/intermetallic/matrix) interface layer can be expressed as:

$$\frac{1}{h} = \frac{1}{h_{Dia-C}} + \frac{1}{h_{C-M}} + \frac{1}{h_{M-I}} + \frac{1}{h_{I-\text{matrix}}} + \frac{l_C}{K_C} + \frac{l_M}{K_M} + \frac{l_I}{K_I} \tag{4}$$

where *Dia*, *C*, *M*, *I* and *m* stand for diamond, carbide, metal, intermetallic and matrix, respectively. Specifically, for diamond/Al interface without an incorporated interface layer (designated as "pure diamond/Al" hereafter), the ITC can be expressed as: $\frac{1}{h} = \frac{1}{h_{Dia/Al}}$. Table 1 shows the parameters of materials for the calculation in this work.

As an effective model in TC prediction for the composites with high phase contrast, e.g. diamond/Al, the differential effective medium (DEM) scheme was applied in this study, which can be expressed as [5,31]:

$$(1 - V_r)\left(\frac{K_c}{K_m}\right)^{\frac{1}{3}} = \frac{K_r^{eff} - K_c}{K_r^{eff} - K_m} \tag{5}$$

where K_c and K_m are TC of the composite and metal matrix, respectively, and V_r is the volume fraction of reinforcement. Considering the average size of reinforcement, a, and the ITC between the reinforcement and matrix, h, the effective TC of reinforcement, K_r^{eff}, can be expressed as [5,31]: $K_r^{eff} = \frac{K_r}{1+\frac{K_r}{ha}}$.

3. Results and discussion

As concluded from the equations for h in section 2, thermal boundary resistance will increase with each layer introduced in the interface. From this point of view, the pure diamond/Al interface should be most favorable if sufficient wettability or bonding occurs at interfaces. Therefore, a diffusion bonding layer is rather feasible to obtain high thermal property [32], since it contributes to the perfect interfacial bonding and the maximal ITC ($\frac{1}{h} \approx 0$), and thus the TC can be calculated directly by the DEM scheme with $K_r^{eff} = K_r$.

However, it is difficult to prepare diamond/Al composites with such diffusion bonding by the conventional methods, such as liquid infiltration [33–35] or spark plasma sintering (SPS) [4,36], because the former often leads to excessive formation of Al_4C_3, a detrimental phase to the thermal and chemical properties [9], while the latter causes severe interfacial debonding. Therefore, it is more feasible and necessary to improve interfacial bonding and ITC by introducing additional interface layers by surface metallization of diamond particles. In the following parts, the effects of various metals, and the corresponding carbides and intermetallic layers on the ITC and TC of diamond/Al composites are evaluated using the developed multi-layered interface model.

3.1. Effect of the metal layers

The effects of some mostly used carbide-forming metals, Cr, Ti, W and Mo, as interface layers in improving the ITC and TC of diamond/Al composites were compared with those of some popular non-carbide-forming metals, i.e. Cu, Ni and Ag. Fig. 2 shows the ITC and TC of 50 vol.% diamond/Al composites with various metal