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Multi-scale design of novel materials for emerging challenges in active thermal management: Open-pore magnesium-diamond composite foams with nano-engineered interfaces

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ABSTRACT

Open-pore Mg foams, which have been traditionally discarded for heat dissipation applications given their low thermal conductivity values, can prove appealing materials for active thermal management if they incorporate diamond particles coated with a nano-dimensioned layer of TiC. These composite foam materials can be manufactured by the replication method, conveniently adapted to Mg, that requires a strict multi-scale control: correct distribution of structural constituents (pores, diamond and Mg) on the meso-/micro-scale ensures homogeneity and complete pore connectivity, while a proper nanoscale control of the TiC coating on diamond particles achieves high thermal conductance at the interface between diamond particles and Mg. The manufactured Mg-diamond foam materials attain outstanding thermal conductivity values (up to 82 W/m K) and maximum heat dissipation performance, tested on active convective cooling, almost two times higher than their equivalent magnesium foams and twenty per cent superior to that of conventional aluminium foams.

1. Introduction

Thermal management has become a critical issue that often slows down, or even hinders, the progress of emerging technologies in power electronics [1–3]. Increasing power densities and diminishing transistor dimensions are hallmarks of modern electronics that demand an accelerating research progress in novel materials that allow heat dissipation [1]. Passive (or phase change material) thermal management is being extensively explored by developing novel composite materials with high thermal conductivity. Among this class of materials, those based on metal matrices and diamond particles with nano-engineered interfaces are noteworthy for their excellent thermal conductivity values (see [4–6] for aluminium-matrix and [7] for Mg-matrix composite materials). Despite the main disadvantage of active (air- or liquid-cooling) thermal management sometimes needing equipment overdesign, it has proven to be advantageous to enhance heat transfer efficiency in electronic devices. For those applications, the use of foam materials in which air or cooling liquids are forced to pass through their porous structure to remove heat by convection has been extensively evaluated [8–15] (research includes aluminium [9–11] and copper foams [12,13], among those of a metallic nature, and carbon/graphite foams [14,15], which have lately attracted much attention given their low density). These materials, which generally outperform similar dense material configurations [8], must combine high solid-phase thermal conductivity to entrain heat deep into the solid structure of foam and a suitable heat transfer coefficient with the coolant in order to sweep away heat by passing fluid. The heat transfer behaviour of several tested foams (with porosities generally over 85%) is strongly related with pore geometry characteristics [11,16] and performs better as the number of pores lowers [10], as does the thermal conductivity [16]. For the forthcoming generation of materials for active thermal management, it seems consequently necessary to work in two directions: (i) on the one hand, we must consider denser foam materials capable of combining a high heat transfer coefficient, while maintaining sound thermal conductivity (in [11] it was demonstrated the good performance in the active cooling of aluminium foams with porosities within the 66–69% range); (ii) on the other hand, the foamability of monolithic materials needs to move on to new complex materials based on developments of multiphase and multiscale designs with improved thermal properties.

Mg and its alloys have always been overlooked or discarded for thermal management because their thermal conductivity values are much lower than aluminium, silver or copper metals. However, a recent publication has shown that the combination of pure Mg and diamond particles coated with TiC generates composites of

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high thermal conductivity [7] capable of attracting candidates for passive thermal management (TiC coatings on diamond particles have also proven to enhance the metal–diamond interface thermal conductance for metals such as Al [17] and Cu [18,19]). Another issue that can be a disadvantage of Mg-based materials is their relatively easy degradation under corrosive environments. Nevertheless the authors of [20], in the aim of fabricating Mg foams for bioimplants, demonstrated that a coating of magnesium oxide successfully enhances the corrosion performance of these materials.

In this paper, we produced and characterised new foam materials whose skeleton consisted of a Mg-diamond composite with a nano-dimensioned TiC interface. To manufacture these materials the replication method, traditionally used for metal foaming, was followed. A porous preform made by the compaction of a mixture of large NaCl particles that touch one another and TiC-coated small diamond particles, located at the voids of NaCl particles, was infiltrated with pure Mg. Subsequently, NaCl particles were removed by dissolution in an aqueous solution of NaOH at pH 13. The resultant materials attained high thermal conductivity values (up to 82 W/m K) and a heat dissipation capacity, which was tested on active convective cooling, that was almost two times higher than their equivalent Mg foams and twenty per cent superior to that of conventional aluminium foams.

2. Predictive schemes

A set of analytical models was used to predict the following items of interest: (i) the volume fraction of bimodal mixtures of particles; (ii) the heat thermal conductance of nanodimensioned interfaces; (iii) the thermal conductivity of Mg-diamond composite foams. Details of each predictive scheme are provided below.

2.1. Volume fraction of the bimodal particle compacts

The volume fraction of the compacts conformed by particles of two different sizes of any average size ratio (bimodal mixtures) has been proved to well account for using the well-known Yu and Standish model [21]. This predictive scheme has proven to accurately fit different sets of experimental data [5,7,21,22] and is described by the following equation:

$$\left(\frac{v-v_cX_c}{v_s}\right)^2+2G\left(\frac{v-v_cX_c}{v_s}\right)\left(\frac{v-X_c-v_sX_s}{v_c-1}\right)+\left(\frac{v-X_c-v_sX_s}{v_c-1}\right)^2=1 \quad (1)$$

where v is the apparent volume occupied by the unit solid volume of particles (i.e., the reciprocal of the particle packing volume fraction V) and X is the fraction of an inclusion type in the bimodal particle mixture. Subscripts c and s refer to coarse and small particles, respectively, and G is a parameter that relates to the particle size ratio, which can be accounted for with the following empirical formula [23]:

$$G=1-(1-v_l)^{0.63}\left(\frac{v_c}{v_s-v_cv_s}\right)^{-0.63}+\left(\frac{1}{R}\right)^{-1.89} \quad (2)$$

where R is the ratio coarse-to-small particle radius.

2.2. Thermal conductance of nanodimensioned interfaces

The thermal conductance (h) of Mg-TiC-diamond interfaces can be estimated by the following equation, derived from an electrical analogy model [7]:

$$\frac{1}{h_{Mg-TiC-D}}=\frac{1}{h_{Mg-TiC}}+\frac{TiC\ thickness}{K_{TiC}}+\frac{1}{h_{TiC-D}} \quad (3)$$

To use Eq. (3), the data in Table 1 are necessary (the qualities of the Mg metal and diamond particles used in this work are the same as those used in the cited references). Table 1 also contains information on the Mg-diamond interface, which is necessary for predictive purposes on composites that contain uncoated diamond particles.

2.3. Thermal conductivity of magnesium-diamond composite foams

The thermal conductivity of Mg-diamond composite foam materials can be predicted with the Generalised Differential Effective Medium Scheme (GDEMS), which has been applied successfully to model and interpret thermal conduction in different composite materials [5,7,26,27]. The leading integral equation of the GDEMS approach for a multi-phase composite material is

$$\int_{K_m}^{K_c}\frac{dK}{K\sum_i X_i\frac{-(K-K_r^{eff})}{(K-K_r^{eff})P-K}}=-\ln(1-V) \quad (4)$$

where K is thermal conductivity and subscripts c and m refer to composite and matrix, respectively. X_i is the fraction of the i inclusion type in the total amount of inclusions of the composite (in these materials we consider two types of inclusions: diamond particles (D) and pores (P); hence $X_D + X_P = 1$). V is the total volume fraction of inclusions and P is the polarisation factor of an inclusion (equal to 0.33 for spheres, as modelled in this study). K_r^{eff} is the effective thermal conductivity of an inclusion which, for spherical geometries, is related to its intrinsic thermal conductivity, K_r^{in}, the matrix-inclusion interface thermal conductance h, and the radius of the inclusion r, by

$$K_r^{eff}=\frac{K_r^{in}}{1+\frac{K_r^{in}}{hr}} \quad (5)$$

In general, the integral on the left-hand side of Eq. (1) has no analytical solution and needs to be solved numerically with appropriate mathematical software.

3. Experimental procedures

3.1. Materials

High purity magnesium (>99.9 wt%) was purchased from Goodfellow Metals, Cambridge, UK, with nominal major impurities shown in Table 2. Two sets of particles were used: diamond particles of MBD4 quality and two different average sizes of 36 μm and

Table 1
Thermal conductivity K and interface thermal conductance h for different phases and interfaces.

		K (W/m K)	h (W/m^2 K)
Phases	Mg (99.99%)	156 [24]	–
	$Diamond_{MBD4}$	1450 [5,7]	–
	TiC	17–31 [25]	–
Interfaces	$Mg\text{-}Diamond_{MDB4}$	–	1.41×10^6 [7]
	Mg-TiC	–	1.34×10^8 [7]
	$TiC\text{-}Diamond_{MBD4}$	–	6.18×10^8 [7]

Table 2
Nominal major impurities of the magnesium metal (>99.9 wt%).

	Fe	Mn	Al	Si
Concentration (ppm)	<280	<170	<70	<50