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Thermal conductivity of metal matrix composites with coated inclusions: A new modelling approach for interface engineering design in thermal management

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ABSTRACT

Despite the importance of interface engineering in technological metal matrix composites, both systematic experimental studies and modelling approaches are still lacking to predict some of their properties. This paper presents an insight into experimental results and modelling of the thermal conductivity in metal matrix composite materials with coated inclusions. Two types of composites of technological importance, Al/diamond and Mg/cobalt, have been interfacially engineered either by deposition of a 0-14.6 µm TiC layer on the diamond particles or by oxidative formation of a 0-21.4 µm Co_3O_4 layer on the cobalt particles, respectively. The experimental results of thermal conductivity can be properly accounted for by a new modelling approach that consists in a multi-step application of the GDEMS model. This modelling scheme demonstrates a predictive capacity far superior to the few current models available in the literature and allows an accurate calculation of the critical interface thickness, such that it outlines a proper interface engineering tool to design high thermally conductive composite materials.

1. Introduction

Predictive schemes for the physical thermal conductivity property in metal matrix composite materials are an essential tool to assess their potential use in thermal management for electronics, aeronautics or aerospace applications. Among the different modelling schemes developed for two-phase composite materials, the Maxwell mean-field (MMF) scheme and the Generalized Differential Effective Medium Scheme (GDEMS) are two approaches that take into account a finite value of the interface thermal conductance (h) between the two solid phases [1–3]. When comparing these two models, MMF displays an inferior predictive capacity to that of GDEMS for both high inclusion volume fractions and phase contrasts (the ratio between the effective thermal conductivity of the inclusion and that of the matrix) higher than 4 [4].

The composite materials that incorporate other phases located at the interface (the so-called interfacial-engineered composite materials) have opened up new possibilities in their thermal applications, but their modelling still remains an unresolved challenge. In this regard, there are some pioneering works that have followed mainly two modelling approaches. One approach is to consider the interface as a third phase material and to then derive exact solutions based on a mean-field scheme [5,6]. This approach uses plausible yet no rigorous assumptions. For the physical limit of there being no third phases present, the modelling solutions reduce to those of the MMF scheme, with consequently clear limitations in their predictive capacities. Another approach is that adopted by Tan et al. [7], in which the different materials located at the interface can be simplified by considering a single zero-thickness interface with an equivalent h. This model is based on an electrical resistance analogy (referred to as the ER model from this point onwards), by which the overall interfacial thermal conductance h can be calculated by considering a series arrangement of thermal resistances with the following equation:

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

where h_i stands for the interface thermal conductance of the i_{th} interface, and $l_{(i-1)\to i}$ and $K_{(i-1)\to i}$ are the thickness and thermal conductivity of the layer from the $(i-1)_{th}$ to the i_{th} interface,

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respectively. h_i can be either obtained experimentally or be calculated by the acoustic mismatch model (AMM) [8] and can be later implemented into any available modelling scheme (e.g. MMF or GDEMS) to predict thermal conductivity. Tan et al. [7] used the ER model in combination with the GDEMS scheme for theoretical purposes. The ER model has been applied with relative success to various experimental systems in combination with both MMF [9,10] and GDEMS [11,12] schemes.

Nevertheless, the simplification of the ER model, which converts a certain multi-phase interface into an equivalent single zero-thickness interface, might be reasonably good for certain cases, but does present a clear drawback in those cases where the thickness of the whole interface is not negligible. Hence it represents a volume fraction that is far from being approximately zero in the overall composite material.

This work presents a new modelling approach based on a multi-step application of the GDEMS scheme and compares its predictive capacity to that of the ER-GDEMS modelling approach. Both were tested against the experimental results obtained for composites with coated inclusions. The new modelling approach accounted for the volume fraction of the coating in the composite material and proved to be accurate enough to be a good predictive tool from which important conclusions can be drawn to design interfaces in high thermally conductive composites.

2. New generalized modelling approach

The manuscript is intended to offer a generalized modelling scheme to calculate the thermal conductivity of composite materials with multi-coated inclusions. This modelling is based on the assumption that any thermal inclusion-coating couple can be modelled with the GDEMS scheme by considering that the coating acts as the surrounding matrix of the thermal inclusion. Then, for multi-coated thermal inclusions with n different concentric coatings (we assume for simplicity spherical geometry) in a matrix m, the i coating can be treated as the matrix of pseudo-inclusion materials that consist of the inner i-1 materials (Fig. 1). Such modelling considers the subsequent coatings of the original thermal inclusions in an m-step procedure to calculate in each step the thermal conductivity of equivalent pseudo-inclusions PI_i. The final step consists in considering a composite material with a certain volume fraction (V_r) of the PI_n pseudo-inclusion surrounded by matrix m (Fig. 1).

The analytical expression for the modelling approach was based on that of the GDEMS scheme, which was conveniently adapted for multi-coated inclusions:

$$\int_{K_{PI_{i-1}}}^{K_{PI_i}} \frac{dK}{K\cdot V_{PI_{i-1}}^{\frac{-\left(K-K^{eff}_{PI_{i-1}}\right)}{\left(K-K^{eff}_{PI_{i-1}}\right)S_{PI_{i-1}}-K}}} = -ln\left(1-V_{PI_{i-1}}\right) \quad \forall i=[1,m] \tag{2}$$

where K_{PI_i} refers to the thermal conductivity of the PI_i pseudo-inclusion, K_i is the thermal conductivity of material i and $V_{PI_{i-1}}$ and $K^{eff}_{PI_{i-1}}$ are respectively the volume fraction and effective thermal conductivity of the PI_{i-1} pseudo-inclusion. In turn, $K^{eff}_{PI_{i-1}}$ and $V_{PI_{i-1}}$ can be respectively calculated by the following expressions:

$$K^{eff}_{PI_{i-1}} = \frac{K_{PI_{i-1}}}{1+\frac{K_{PI_{i-1}}}{h_{i-1/i}\cdot\left(r_0+\sum_1^{i-1}\varepsilon_i\right)}} \quad \forall i=[1,m] \tag{3}$$

$$V_{PI_{i-1}} = \frac{\left(r_0+\sum_1^{i-1}\varepsilon_i\right)^3}{\left(r_0+\sum_1^{i}\varepsilon_i\right)^3} \quad \forall i=[1,n]; V_{PI_{i-1}}=V_r \quad \forall i=m \tag{4}$$

where $h_{i-1/i}$ is the thermal conductance of interface i-$1/i$, r_0 is the radius of the original thermal inclusion and ε_i is the thickness of coating i. $S_{PI_{i-1}}$ is the polarization factor of the pseudo-inclusion PI_{i-1}, taken as being spherical for simplicity reasons; hence $S_{PI_{i-1}}=1/3$. Notice that for composites where i = m (there being no coatings on original inclusions), Equation (2) reduces to the well-known expression of the GDEMS model.

The interface thermal conductance h for any solid–solid interface can be accurately estimated with the acoustic mismatch model (AMM) [8]:

$$h=\frac{1}{4}\rho_{in}C_{in}v'_{in}\eta \tag{5}$$

where ρ is the density of the material, C is the specific heat, v' is the

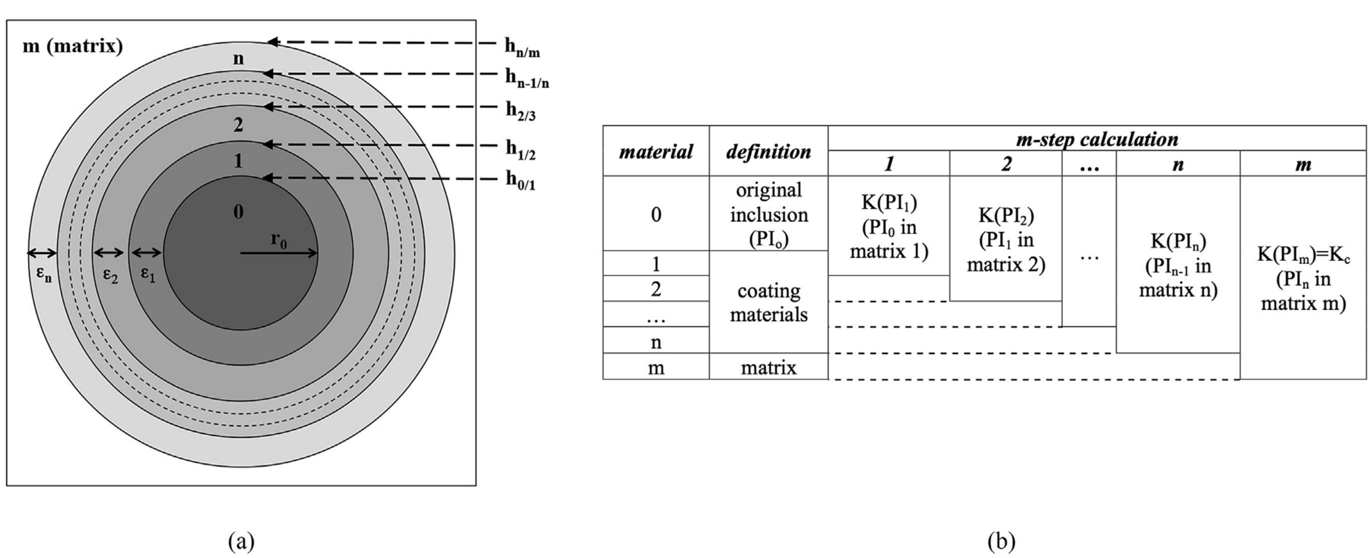

Fig. 1. Schematic view of a composite material formed by matrix m and multi-coated inclusions (a), and a diagram showing the calculation procedure proposed in the present work.