Connection between diffusion coefficient and thermal conductivity of a metal matrix composite

M A Anisimova[1], A G Knyazeva[1,2] and I Sevostianov[3]

[1] Institute of High Technology Physics, National Research Tomsk Polytechnic University, 634050 Tomsk, Russia
[2] Institute of Strength Physics and Materials Science, 634055 Tomsk, Russia
[3] Department of Mechanical and Aerospace Engineering, New Mexico State University, Las Cruces, NM 88003, USA

E-mail: anisimova_mawa@mail.ru

Abstract. The paper discusses the calculation of the effective thermal and diffusion properties of metal matrix composites containing diamond particles. The effective properties are calculated using Maxwell homogenization scheme. We also establish cross-property connection between overall thermal conductivity and diffusion coefficient and illustrate it on example of Al\diamond composites.

1. Introduction

The paper focuses on the problem of the effective properties - thermal conductivity and diffusion coefficient - of metal matrix composites containing diamond particles. Composites of this kind are widely used for thermal management of electronic components and it is necessary to know their effective properties, such as thermal and electrical conductivity, thermal expansion coefficient, diffusivity etc. However, some effective properties, such as diffusion coefficient, are more difficult to measure experimentally than thermal or electrical properties. In this paper, we propose a method for evaluation of the effective diffusion coefficient through the thermal conductivity measurements.

2. Property contribution tensors

Property contribution tensors are used in the context of homogenization problems to describe contribution of a single inhomogeneity into the property of interest – it may be elastic compliance or stiffness, thermal or electrical conductivity, or diffusion coefficient [1].

2.1. Thermal conductivity problem

In the thermal conductivity problem, the key quantity is the conductivity contribution tensor that gives the extra heat flux produced by introduction of the inhomogeneity into a material subjected to otherwise uniform field of temperature gradient. We assume that the background material of volume V having the isotropic thermal conductivity k^0 contains an isolated inhomogeneity of volume V^1 of the isotropic thermal conductivity k^1. The limiting cases $k^1 = 0$ and $k^1 = \infty$ corresponds to an insulating and a superconducting inhomogeneities. Assuming linear relation between temperature gradient ∇T and the heat flux vector $\boldsymbol{q}$ per reference volume (Fourier law), for both constituents, the change in $\boldsymbol{q}$ in response to the presence of the inhomogeneity is given by

$$\Delta \boldsymbol{q} = \frac{V^1}{V} \boldsymbol{K} \cdot (\nabla T) \tag{1}$$

where the symmetric second-rank tensor $\boldsymbol{K}$ is the *conductivity contribution tensor* of the inhomogeneity.

This tensor for a spherical inhomogeneity is given by Sevostianov and Kachanov [2]

$$\boldsymbol{K} = 3\frac{k^0\left(k^1 - k^0\right)}{2k^0 + k^1}\boldsymbol{I} \ . \tag{2}$$

2.2. Diffusion problem

Diffusivity contribution tensor can be introduced by analogy with conductivity contribution tensors [3]. The homogeneous boundary conditions are assumed: the "remotely applied" concentration gradient, or flux of particles, would be uniform in absence of the inhomogeneity. Let, for example, the concentration gradient $\nabla c = \boldsymbol{G}^0$ be prescribed at the boundary of V. Then, the average over $V = V^0 \cup V^1$ flux and concentration gradient are

$$\langle \boldsymbol{J} \rangle_V = \frac{V^1}{V}\langle \boldsymbol{J} \rangle_{V^1} + \left(1 - \frac{V^1}{V}\right)\langle \boldsymbol{J} \rangle_{V^0}, \tag{3}$$

$$\langle \nabla c \rangle_V = \boldsymbol{G}^0 = \frac{V^1}{V}\langle \nabla c \rangle_{V^1} + \left(1 - \frac{V^1}{V}\right)\langle \nabla c \rangle_{V^0}. \tag{4}$$

Taking into account that $D^1\langle \nabla c \rangle_{V^1} = \backslash\langle \boldsymbol{J} \rangle_{V^1}$ and $D^0\langle \nabla c \rangle_{V^0} = \backslash\langle \boldsymbol{J} \rangle_{V^0}$, one can write

$$\langle \boldsymbol{J} \rangle_V = \frac{V^1}{V} D^1\langle \nabla c \rangle_{V^1} + \left(1 - \frac{V^1}{V}\right) D^0\langle \nabla c \rangle_{V^0} = \frac{1}{D^0}\boldsymbol{G}^0 + \frac{V^1}{V}\left(D^1 - D^0\right)\langle \nabla c \rangle_{V^1}. \tag{5}$$

Introducing tensor $\boldsymbol{A}$ that expresses $\langle \nabla c \rangle_{V^1}$ in terms of $\boldsymbol{G^0}$:

$$\langle \nabla c \rangle_{V^1} = \boldsymbol{A} \cdot \boldsymbol{G}^0 \tag{6}$$

the latter expression can be rewritten as

$$\langle \boldsymbol{J} \rangle_V = \left[D^0 \boldsymbol{I} + \frac{V^1}{V}\left(D^1 - D^0\right)\boldsymbol{A} \right] \cdot \boldsymbol{G}^0 . \equiv \left[D^0 \boldsymbol{I} + \frac{V^1}{V} \boldsymbol{H}^D \right] \cdot \boldsymbol{G}^0 . \tag{7}$$

The second term in the brackets represents the contribution of the inhomogeneity into overall diffusivity of the volume V and tensor $\boldsymbol{H}^D$ can be called the diffusivity contribution tensor.

For a spherical shape, tensor $\boldsymbol{A}$ can be written as

$$\langle \nabla c \rangle_{V^1} = \boldsymbol{A} \cdot \boldsymbol{G}^0 = \frac{3D^0}{D^1 + 2D^0}\boldsymbol{G}^0 \tag{8}$$

and the diffusivity contribution tensor for a spheroidal inhomogeneity has the following form:

$$\boldsymbol{H}^D = \frac{3D^0\left(D^1 - D^0\right)}{D^1 + 2D^0}\boldsymbol{I}. \tag{9}$$

3. Maxwell scheme

According to Maxwell's idea [4], we evaluate fields at far points in two different ways and equate the results. First, we evaluate this field as the one generated by a homogenized region Ω possessing the (yet unknown) effective properties. Secondly, we consider the sum of far fields generated by all the individual inhomogeneities within Ω (being considered as non-interacting ones). Equating the two quantities yields the desired effective property [5]. For the thermal conductivity problem, the result has the following form:

$$\boldsymbol{k}^{\boldsymbol{eff}} = \boldsymbol{k}^0 + \left\{ \left[\frac{1}{V^\Omega} \sum_i V_i \boldsymbol{K}_{\boldsymbol{i}} \right]^{-1} - \boldsymbol{P}^\Omega \right\}^{-1} . \tag{10}$$

where $\boldsymbol{P}^\Omega$ is the second-rank Hill's tensor for domain Ω [6]. For isotropic composite

$$P_{ij}^\Omega = \frac{1}{3k^0}\delta_{ij} , \ \frac{1}{V^\Omega}\sum_i V_i \boldsymbol{K}_{\boldsymbol{i}} = k^0 A \boldsymbol{I} . \tag{11}$$

where parameter A depends on the shape and properties of the individual inhomogeneities. Thus

$$k^{eff} = k^0 \left(\frac{1+2A\phi}{1-A\phi} \right), \ A = \frac{k^1 - k^0}{2k^0 + k^1} . \tag{12}$$

The effective diffusion coefficient is given by

$$\boldsymbol{D}^{\boldsymbol{eff}} = \boldsymbol{D}^0 + \left\{ \left[\frac{1}{V^\Omega} \sum_i V_i \boldsymbol{H}_i^D \right]^{-1} - \boldsymbol{Q}^\Omega \right\}^{-1} . \tag{13}$$

where $\boldsymbol{Q}^\Omega$ is second-rank tensor that reflects the shape of domain Ω. For a spherical shape of Ω

$$\boldsymbol{Q}^\Omega = \frac{1}{3D^0}\boldsymbol{I} \tag{14}$$

$$D_{eff} = D^0 \left[\frac{1+2B\phi}{1-B\phi} \right], B = \frac{D^1 - D^0}{D^1 + 2D^0} \tag{15}$$

4. Cross-property connections

Comparison of equations (12) and (15) shows their complete identity. We now consider aluminum matrix composite with diamond particles in the context of hydrogen diffusion. For this system $k^0 = 236W/mK$, $k^{1`} = 1500W/mK$, $D^0 = 10^{-7} m^2/s$, and $D^1 = 0$. Solving (12) for the volume fraction of inhomogeneities and substituting it into (15), we can write the effective diffusion coefficient as a function of the thermal conductivity:

$$D_{eff} = D_0 + D_0 \left[\frac{3B\left(k_{eff} - k_0\right)}{A\left(2k_0 + k_{eff}\right) - B\left(k_{eff} - k_0\right)} \right] \tag{16}$$

Figure 1 shows dependence of $\left(D^{eff} - D^0\right)/D^0$ on $\left(k^{eff} - k^0\right)/k^0$.

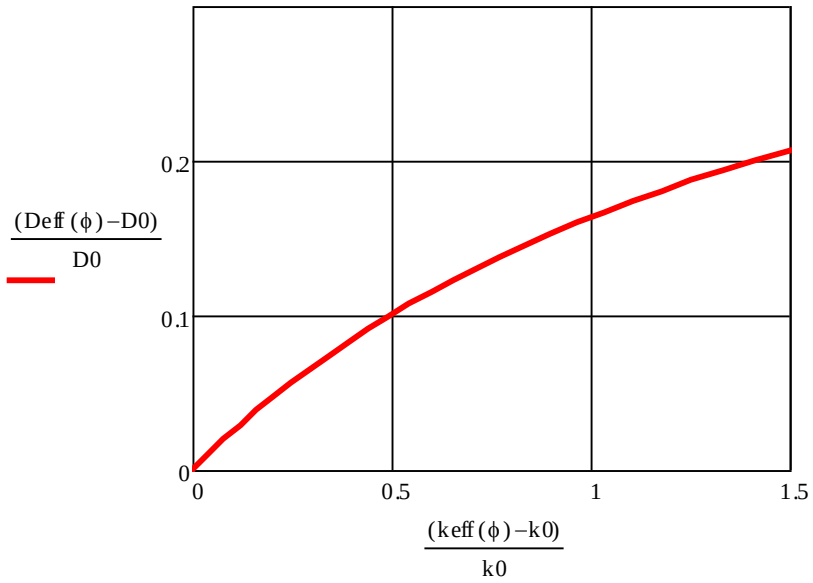

Figure 1. Cross-property connection between effective diffusion coefficient and effective thermal conductivity of Al/diamond composite

5. Concluding remarks

In this paper, we modelled effective thermal and diffusion properties of a particle reinforced composite. The effective properties are calculated using Maxwell homogenization scheme. We also established cross-property connection between effective thermal conductivity and diffusion coefficient and illustrate it on example of aluminum reinforced with diamond particles.

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