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Ceramics International 41 (2015) 2706–2713

CERAMICS INTERNATIONAL

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Representation of thermal expansion coefficient of solid material with particulate inclusion

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Received 16 September 2014; received in revised form 8 October 2014; accepted 14 October 2014
Available online 29 October 2014

Abstract

This paper analyzed a Young's modulus (E) and a thermal expansion coefficient (TEC, β) of the material with simple cubic particulate inclusion using two model structures: a parallel structure and a series structure of laminated layers. The derived β equations were applied to calculate the β value of the W–MgO system. Both the models provided a good agreement for the measured and calculated β values. The accuracy was higher for the series model structure than for the parallel model structure.

Keywords: B. Composite; C. Thermal expansion; D. MgO

1. Introduction

A thermal expansion coefficient (TEC) is an important property of material, which affects thermal shock resistance or joining of two materials at a high temperature. Fortunately many TEC values of metals and ceramics are listed on a chemical handbook [1] or a metal handbook [2]. These available data are used to calculate the residual stress of the interphase between a mullite matrix and incorporated long fibers [3] at a low temperature or the critical temperature difference required for crack instability upon quenching of heated ceramics [4]. In a previous paper [5], we succeeded in relating a TEC to a heat capacity at a constant pressure and a Young's modulus of a material, or representing a TEC by the ratio of a heat capacity at a constant volume to a heat capacity at a constant pressure, the Poisson's ratio and heating temperature. The calculated TEC values agreed well with the reported TEC values for Al, Ag, Au, Be, Bi, C(diamond), Cu, Hf, In, Mo, Nb, Pb, Ta, Ti, V, W, Zr, $BaTiO_3$, $3Al_2O_3\cdot 2SiO_2$, SiO_2, SiC and TiN.

Our next challenge is to derive a mixing rule of TEC of a composite material. In text books of ceramics [6,7], some theoretical or empirical mixing rules are presented. Table 1 shows the theoretical equations of volume expansion coefficients of composite materials with particulate inclusion developed by Turner and Kerner [6,8]. The volume expansion coefficient of multiphase composite material by Turner's equation is composed of the weight fraction, the volume expansion coefficient, and the bulk modulus of each phase included [6,8]. The volume expansion coefficient by Kerner's equation for two phase composite is also related to the bulk modulus, the shear modulus, the fractional volume and the volume expansion coefficient of each phase [6]. The desirable mixing rule is to be expressed by less available well known parameters. In this paper, a model structure of material with simple cubic inclusion, which was used in the calculation of the thermal conductivity of composite [9], was applied to the derivation of a mixing rule of TEC of a composite material. The derived mixing rule was compared with the reported data of the W–MgO system presented in the text book [6]. A very good agreement was shown between the reported and calculated TECs. The newly derived mixing rule was also compared with the reported Turner's equation and Kerner's equation. As compared with the previously developed two equations, the

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http://dx.doi.org/10.1016/j.ceramint.2014.10.085

Table 1
Theoretical equations of volume expansion coefficients of composite materials with particulate inclusion developed by Turner and Kerner.

Turner's equation	
$\alpha_c = \frac{\alpha_1 K_1 W_1/\rho_1 + \alpha_2 K_2 W_2/\rho_2}{K_1 W_1/\rho_1 + K_2 W_2/\rho_2}$	(A)
Kerner's equation	
$\alpha_c = \alpha_1 + V_2(\alpha_2 - \alpha_1)\frac{K_1(3K_2+4G_1)^2 + (K_2-K_1)\left(16G_1^2+12G_1K_2\right)}{(4G_1+3K_2)[4V_2G_1(K_2-K_1)+3K_1K_2+4G_1K_1]}$	(B)
α_c: Volume expansion coefficient of composite material	
α_i: Volume expansion coefficient of phase i	
K_i: Bulk modulus of phase i	
W_i: Weight fraction of phase i	
ρ_i: Density of phase i	
V_i: Volume fraction of phase i	
G_i: Shear modulus of phase i	

mixing rule in this paper was closer to the measured TEC of the W–MgO system.

2. A model structure

Fig. 1 shows a simple cubic inclusion model with length a in one cubic box with length $1/p$ [9]. The number (n) and the volume fraction (V) of cubic inclusion in unit volume of the composite are related by Eq. (1),

$$V = a^3 n \tag{1}$$

The number (p) of inclusion along one direction of cubic composite is equal to $n^{1/3}(=V^{1/3}/a)$ and the distance between two inclusion is given by $(1/p-a)$. The structure surrounded by dotted lines (Fig. 1(b)) represents the linear connection of inclusion and matrix. This structure of Fig. 1(b) is sandwiched by two layers of a continuous matrix phase as shown in Fig. 1(c) (unit cell structure). At first, the Young's modulus of the composite (Fig. 1(a)) with particulate inclusion is calculated.

3. Young's modulus of composite of a parallel structure

When a tensile or compressive stress (σ) is applied to the cross section (area, a^2) of composite (b) in Fig. 1(b), the strain ($\varepsilon=\Delta L/L_0, L_0$: starting length) is related to the applied σ and the Young's moduli (E) of materials 1 and 2.

$$\sigma = E_1\varepsilon_1(for\ inclusion\ phase\ 1) = E_2\varepsilon_2(for\ matrix\ phase\ 2) \tag{2}$$

The above relation results in Eq. (3)

$$\varepsilon_2 = \left(\frac{E_1}{E_2}\right)\varepsilon_1 \tag{3}$$

The extended lengths for inclusion phase 1 and matrix phase 2 of the composite (b) shown in Fig. 1(b) are given by Eqs. (4) and (5), respectively.

$$\Delta a = a\ \varepsilon_1(for\ \ inclusion\ phase\ 1) \tag{4}$$

$$\Delta b = \left(\frac{1}{p}-a\right)\varepsilon_2(for\ matrix\ phase\ 2) \tag{5}$$

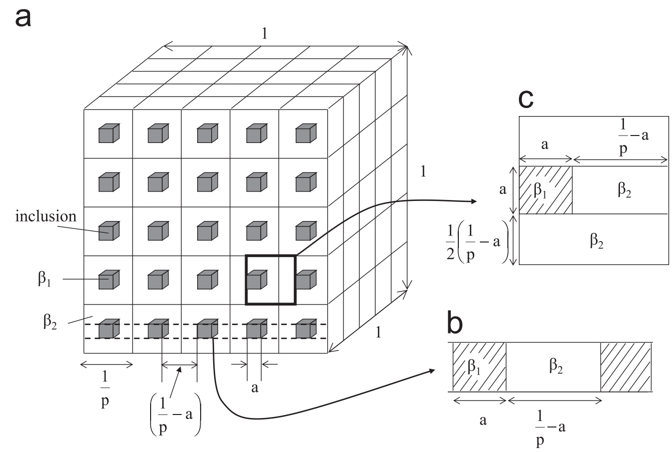

Fig. 1. A parallel structure model of material with simple cubic inclusion with length a. The geometrical features are shown in (b) and (c).

The strain (ε_b) for the composite (b) is expressed by Eq. (6) using Eqs. (3), (4) and (5).

$$\varepsilon_b = \frac{\Delta a + \Delta b}{a + ((1/p) - a)} = \varepsilon_1\left[p\ a + \left(\frac{E_1}{E_2}\right)(1-p\ a)\right] \tag{6}$$

When a tensile or compressive stress is applied along the direction of the length of the composite (b), the Young's modulus (E_b) of composite (b) is expressed by Eq. (7).

$$\sigma = E_b\varepsilon_b = E_1\varepsilon_1 \tag{7}$$

The substitution of Eq. (6) for Eq. (7) gives the Young's modulus, E_b, by Eq. (8) as functions of E_1 and E_2.

$$E_b = \frac{E_1\ E_2}{p\ a\ E_2 + (1-p\ a)\ E_1} \tag{8}$$

Since the product of pa is equal to $V^{1/3}$ (see Eq. (1)), Eq. (8) is expressed as a function V by Eq. (9).

$$E_b = \frac{E_1\ E_2}{E_2 V^{1/3} + E_1\ (1-V^{1/3})} \tag{9}$$

Next, we derive the Young's modulus (E_c) of the composite (c) shown in Fig. 1(c). When a tensile or compressive stress (σ_c) is applied to the cross section of composite (c), the force (F_b) applied to the cross section of composite (b) is given by Eq. (10).

$$F_b = E_b a^2 \varepsilon_c \tag{10}$$

The cross sectional area (S_m) of the matrix in Fig. 1(c) surrounding composite (b) is expressed by Eq. (11),

$$S_m = \left(\frac{1}{p}\right)^2 - a^2 \tag{11}$$

The force (F_m) applied to the cross section of the matrix phase 2 is given by Eq. (12)

$$F_m = E_2\varepsilon_c S_m = E_2\varepsilon_c\left\{\left(\frac{1}{p}\right)^2 - a^2\right\} \tag{12}$$