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# Homogenization of the average thermo-elastoplastic properties of particle reinforced metal matrix composites: The minimum representative volume element size

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ABSTRACT

The average thermo-elastoplastic properties of particle reinforced metal matrix composites (PRMMC) including the average coefficient of thermal expansion (CTE), Young's modulus, Poisson's ratio and isotropic hardening function are investigated. Computational homogenization method based on 3D realistic microstructures (RMs) is employed. Unit cell microstructure (UCM) based model and analytical models are also employed for comparison. As an illustration, 17 vol.%SiCp (3 μm)/2124Al composite is studied. Compared to RMs, UCM underestimates the average CTE and Poisson's ratio, while it overestimates the average Young's modulus and isotropic hardening function. The minimum representative volume element (RVE) size for determining the average CTE, Young's modulus and Poisson' ratio is $\delta = 15$, $\delta = 20$ and $\delta = 20$, respectively, where $\delta$ is the size ratio of microstructure model, which is defined by the ratio of the side length of the RVE to the nominal mean radius of reinforcement. The minimum size of RVE for estimating average isotropic hardening function of plastic deformation is dependent on both the temperature and the plastic deformation condition.

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## 1. Introduction

Particle reinforced metal matrix composites (PRMMC) are widely used due to their enhanced properties, e.g. strength, stiffness and toughness, which depend on many factors such as the content of reinforcements, the constituents' physical and morphological natures. Traditionally PRMMC is modeled as homogeneous medium in classic continuum medium. Such a modeling method does not take into account the intra-phase field fluctuations which appear in PRMMC and affect the properties significantly, especially the nonlinear properties. Multi-scale simulation methods permit to estimate the average properties of heterogeneous materials (e.g. composites) and calculate the intra-phase fields such as temperature, strain and stress fields when loads act on heterogeneous materials. Therefore, the multi-scale method provides a powerful tool for researching PRMMC and can be employed for the optimal design of PRMMC components/structures and for ensuring the safety of industrial applications of PRMMC.

An efficient and well-known multi-scale simulation method proposed by Ghosh et al. [1] is presented to compute a classical continuum mechanics problem at the macro-scale which is coupled with a micromechanical problem at the micro-scale. In this method, the average thermo-elastoplastic properties of PRMMC for describing its macroscopic thermo-elastoplastic constitutive model including the average coefficient of thermal expansion (CTE), Young's modulus, Poisson's ratio and isotropic hardening function are required. The objective of this work is to develop an integrated micromechanical model to determine the average thermo-elastoplastic properties of PRMMC and to discuss the required minimum size of the representative volume element (RVE).

The well-known concept of RVE was firstly defined by Hill [2] and usually used for determining the average properties of heterogeneous materials. For this purpose, the size of the considered microstructure domain for the homogenization must be large enough to ensure that the averaged properties are 'representative' and still small enough compared to the typical size of the macroscopic component or structure. Therefore, it is important to find out the minimum size of RVE to estimate the average properties of PRMMC.

In the past two decades, many researchers [3–13] have studied the minimum RVE size for estimating the average properties of composites. However, most previous studies focused on the elastic

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properties (e.g. Young's modulus and Poisson's ratio) or the thermal properties (e.g. thermal conductivity, CTE). Besides, most existent numerical models use idealized geometry models, e.g. unit cell model, which usually have regular shape and periodic structure. Such models do not reflect the true intra-phase field fluctuations which have a major impact on the average properties of composites, especially the plastic properties [14]. Recently, Galli et al. [15] investigated the minimum RVE size for average stress–strain of PRMMC based on a three-dimensional (3D) microstructure model with multi-irregular polyhedral particles. They showed that the minimum RVE size for average stress–strain depended on the volume fraction of particles. Nevertheless, no literature has systematically investigated the minimum RVE size to determine average thermo-elastoplastic properties of PRMMC in 3D realistic microstructure model.

In this study, the average thermo-elastoplastic properties of PRMMC are estimated via computational homogenization based on 3D realistic microstructures (RMs). The detailed methodology for constructing a 3D realistic microstructure (RM) is proposed in Reference [16]. In order to determine the minimum RVE size, 3D RMs with different domain sizes are employed. The unit cell microstructure (UCM) based homogenization model and classical analytical models of average properties of PRMMC are also studied for comparison. As an illustration of the computational homogenization, a 17 vol.%SiCp (3 μm)/2124Al composite is studied.

## 2. Homogenization theory

The average thermo-elastoplastic properties of PRMMC studied in the present work include the coefficient of thermal expansion (CTE), the elastic properties (include the Young's modulus and the Poisson' ratio) and the plastic yield property (the isotropic hardening function). With these properties, the average constitutive model of PRMMC can be formulated. In this integrated model, the damage effects of PRMMC such as the particle breaking, the matrix damage and the interfacial debonding are not considered.

### 2.1. Governing equation

A bounded domain $V$ with the boundary $\partial V$ is considered. The macro-scale equilibrium equation of mechanical problem reads

$$\nabla \cdot \boldsymbol{\sigma} = 0, \tag{1}$$

where $\boldsymbol{\sigma}$ is the stress tensor.

### 2.2. Micro-constitutive models

The $J_2$ flow theory of plasticity is used for the metal matrix [17], according to which the von-Mises yield function of the matrix is

$$f(\boldsymbol{\sigma}, p_m) = \sqrt{3/2}\|dev(\boldsymbol{\sigma})\| - \sigma(p_m), \tag{2}$$

where $f$ denotes the yield function, $p$ indicates the accumulated plastic strain, subscript $m$ denotes the matrix, $\|\square\|$ denotes the norm of the indicated tensor, $dev(\square)$ denotes the deviator of the indicated tensor, $\sqrt{3/2}\|dev(\boldsymbol{\sigma})\|$ denotes the von-Mises equivalent stress and $\sigma(p_m)$ denotes the yield stress which is computed by the Voce type isotropic hardening rule [18]

$$\sigma(p_m) = \sigma_\infty + hp_m + (\sigma_0 - \sigma_\infty)\exp(lp_m), \tag{3}$$

where $\sigma_0$ is the initial yield strength, $\sigma_\infty$ is the ultimate strength, $h$ and $l$ are material constants.

Since the reinforcing particles in PRMMC are usually brittle ceramic particles, they seldom experience plastic deformation. The reinforcing particles are modeled as linear elastic materials in the present work.

### 2.3. Hill's condition and boundary condition

For a material with a perfectly bonded microstructure and in the absence of body forces, an identity is known as [2,19]

$$\langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle - \langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\varepsilon} \rangle = \frac{1}{|V|}\int_{\partial V} \{\boldsymbol{u} - \boldsymbol{x} \cdot \langle \nabla \otimes \boldsymbol{u} \rangle\} \cdot \{\boldsymbol{n} \cdot (\boldsymbol{\sigma} - \langle \boldsymbol{\sigma} \rangle)\} dS, \tag{4}$$

where $\langle \square \rangle$ denotes the volume average function with respect to the indicated argument, i.e.

$$\langle \square \rangle = \frac{1}{|V|}\int_V \square dV, \tag{5}$$

$|V|$ denotes the volume of the bounded domain $V$.

For two basic physically important types of boundary conditions, the right-hand side of Eq. (4) vanishes. They are pure linear displacement boundary condition

$$\boldsymbol{u}|_{\partial V} = \zeta \boldsymbol{x} \tag{6}$$

and pure traction boundary condition

$$\boldsymbol{t}|_{\partial V} = \xi \boldsymbol{n}, \tag{7}$$

where $\zeta$ and $\xi$ are specific second order tensors [20].

With these two special types of boundary conditions, the average of stress work equals the work of average stress

$$\langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle = \langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\varepsilon} \rangle. \tag{8}$$

This identity was obtained by Hill [2] and named after him as Hill's condition. In the present work, pure linear displacement boundary conditions are employed in finite element simulation based on RVEs for determination of homogenized composite properties. It is noteworthy that the tensor $\zeta$ may differ when computing different average properties.

### 2.4. Homogenization of CTE

To compute the average linear thermal expansion tensor $\langle \boldsymbol{\alpha} \rangle$, the tensor $\zeta$ is set as [10]

$$\zeta = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{9}$$

The relationship between the average elasto-plastic strain tensor $\langle \boldsymbol{\varepsilon}^{ep} \rangle$ and the average linear thermal expansion tensor can be written as

$$\langle \boldsymbol{\varepsilon}^{ep} \rangle = -\langle \boldsymbol{\alpha} \rangle (T - T_0). \tag{10}$$

Hence the average linear thermal expansion tensor is evaluated by

$$\langle \boldsymbol{\alpha} \rangle = -\langle \boldsymbol{\varepsilon}^{ep} \rangle / \Delta T. \tag{11}$$

If the employed microstructure is assumed to be isotropic, the average CTE can be estimated by

$$\langle \alpha \rangle = \frac{1}{3}(\langle \alpha_{11} \rangle + \langle \alpha_{22} \rangle + \langle \alpha_{33} \rangle), \tag{12}$$

where $\langle \alpha_{11} \rangle$, $\langle \alpha_{11} \rangle$ and $\langle \alpha_{11} \rangle$ are the three main diagonal components of $\langle \boldsymbol{\alpha} \rangle$.

Classical approaches for evaluating the average CTE of PRMMC includes the Turner, Kerner and Schapery models. The Turner model [21] is

$$\alpha = \frac{\alpha_1 C_1 K_1 + \alpha_2 C_2 K_2}{C_1 K_1 + C_2 K_2}, \tag{13}$$

where $\alpha$ is the CTE, subscripts 1 and 2 denote the matrix and the reinforcement, respectively, $C$ means the volume fraction, $C_1 + C_2 = 1$ and $K$ denotes the bulk modulus.

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