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Digital image-based modeling applied to the homogenization analysis of intermetallic composites

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Abstract

Image processing technology is utilized for numerical analysis by the homogenization method for intermetallic composites. While the asymptotic homogenization method characterizes thermo-mechanical properties of composites and localizes the deformation to the microscopic level, the digital image-based (DIB) modeling method appropriately defines a finite element (FE) model of a representative volume element (RVE), i.e., a unit cell, through the use of digitized images. The results in linear and nonlinear analyses reflect the effects of the geometric configuration of the microstructure.

1. Introduction

The asymptotic homogenization method enables not only the derivation of the effective properties from the micromechanical characteristics but also the evaluation of the micromechanical behaviors by localizing the overall structural response to a local one. These processes are called homogenization and localization, respectively. The global-local approach was successfully applied to the engineering problems in both linear elasticity and elastoplasticity with the help of the Finite Element Method (FEM) (see, e.g., Guedes and Kikuchi[1], Terada and Kikuchi[2]). However, the complex microstructural morphology of intermetallic composites tend to be simplified in most of the developments. Then the specific effects of the heterogeneity cannot be taken into account in evaluating the microscopic variables such as characteristic deformation of the composite and microscopic stress obtained in the localization process. It is, therefore, necessary to construct the an appropriate unit cell model for the homogenization and the localization analyses. This is achieved though DIB modeling (see Hollister and Kikuchi[3] or Terada, Miura and Kikuchi[4]).

In this paper, we shall utilize the DIB geometric modeling technique to make a FE geometry model of the microstructure and interpret the micromechanical response of the intermetallic composites. The results are strongly influenced by the heterogeneous microstructure. After describing the analysis tools, examples in both linear thermoelasticity and elastoplasticity will be presented in order to illustrate the capability of the present method.

2. The Homogenization Method for Linear Thermoelasticity

In this section we shall briefly review the homogenization formulae for linear thermoelasticity. We recall that the theory concerns statistically homogeneous or periodic composite media of domain Ω^ε and the representative volume element (RVE) occupying a microscopic region V with characteristic length ε. Identifying the size of the RVE with ε, we introduce two different scales: one of these is a macroscopic scale denoted by $\boldsymbol{x}$, in the domain Ω^ε, at which the heterogeneities are invisible and the other is an microscopic one, denoted by $\boldsymbol{y}=\boldsymbol{x}/\varepsilon$ which enlarges the RVE region by ε such that $V=\varepsilon Y$. Thus, the superscripts introduced in variables indicate their orders as well as their dependency on $\boldsymbol{x}$ and/or $\boldsymbol{y}$.

Let the structure be subjected to a surface traction, $\hat{\boldsymbol{t}}$, and prescribed homogeneous displacement boundary conditions on Γ_t and Γ_u, respectively, with temperature change ΔT. Then, the displacement, $\boldsymbol{u}^\varepsilon$, is the solution of the following variational problem defined in the domain Ω^ε:

$$\int_{\Omega^\varepsilon} \boldsymbol{\varepsilon}(\boldsymbol{v}^\varepsilon) : \boldsymbol{D}^\varepsilon(\boldsymbol{x}) : \boldsymbol{\varepsilon}(\boldsymbol{u}^\varepsilon) dx = \int_{\Omega^\varepsilon} \left(\Delta T \boldsymbol{\varepsilon}(\boldsymbol{v}^\varepsilon) : \boldsymbol{D}^\varepsilon : \boldsymbol{\alpha}^\varepsilon + \boldsymbol{b}^\varepsilon \cdot \boldsymbol{v}^\varepsilon\right) dx + \int_{\Gamma_t} \hat{\boldsymbol{t}}(\boldsymbol{x}) \cdot \boldsymbol{v}^\varepsilon dx \qquad \forall \boldsymbol{v}^\varepsilon \tag{1}$$

with the constitutive relation

$$\boldsymbol{\sigma}^\varepsilon = \boldsymbol{D}^\varepsilon(\boldsymbol{x}) : \left(\boldsymbol{\varepsilon}(\boldsymbol{u}^\varepsilon) - \Delta T \boldsymbol{\alpha}^\varepsilon(\boldsymbol{x})\right) = \boldsymbol{D}^\varepsilon(\boldsymbol{x}) : \boldsymbol{\varepsilon}(\boldsymbol{u}^\varepsilon) - \Delta T \boldsymbol{\beta}^\varepsilon(\boldsymbol{x}) \tag{2}$$

Here $\boldsymbol{v}^\varepsilon$ is the virtual displacement, $\boldsymbol{b}^\varepsilon(\boldsymbol{x})$ the body force, $\boldsymbol{D}^\varepsilon(\boldsymbol{x})$ the elasticity tensor, $\boldsymbol{\alpha}^\varepsilon(\boldsymbol{x})$ the coefficient of thermal expansion (CTE) with $\boldsymbol{\beta}^\varepsilon = \boldsymbol{a}^\varepsilon : \boldsymbol{\alpha}^\varepsilon$.

With the help of the method of two-scale asymptotic expansion (see, e.g., Sanchez-Palsencia[5]), the theory shows that if the selected RVE is periodic and infinitesimally small, the actual displacement, $\boldsymbol{u}^\varepsilon$, tends to the homogenized one, $\boldsymbol{u}^0$, which is the solution of the following macroscopic equations whose coefficients have been homogenized.

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$$\int_{\Omega} \boldsymbol{\varepsilon}_x(\boldsymbol{v}) : \boldsymbol{D}^H : \boldsymbol{\varepsilon}_x(\boldsymbol{u}^0) dx = \int_{\Omega} \Delta T \boldsymbol{\varepsilon}_x(\boldsymbol{v}) : \boldsymbol{D}^H : \boldsymbol{\alpha}^H dx + \int_{\Omega} \boldsymbol{b}^H \cdot \boldsymbol{v} dx + \int_{\Gamma_t} \boldsymbol{t} \cdot \boldsymbol{v} d\Gamma \qquad \forall \boldsymbol{v} \tag{3}$$

and that the Y-periodic characteristic deformations $\boldsymbol{\chi}^{kh}$ and $\boldsymbol{\psi}$ can be obtained by solving the following microscopic equations, respectively:

$$\int_Y \boldsymbol{\varepsilon}_y(\boldsymbol{w}) : \boldsymbol{D} : \boldsymbol{\varepsilon}_y(\boldsymbol{\chi}^{kh}) dy = \int_Y \boldsymbol{D} : \boldsymbol{\varepsilon}_y(\boldsymbol{w}) dy \qquad \forall \boldsymbol{w};\ \text{Y-periodic} \tag{4}$$

$$\int_Y \boldsymbol{\varepsilon}_y(\boldsymbol{w}) : \boldsymbol{D} : \boldsymbol{\varepsilon}_y(\boldsymbol{\psi}) dy = \int_Y \boldsymbol{\beta} : \boldsymbol{\varepsilon}_y(\boldsymbol{w}) dy \qquad \forall \boldsymbol{w};\ \text{Y-periodic} \tag{5}$$

Here, the homogenized quantities in eqn.(2) are calculated by averaging over the unit cell:

$$\boldsymbol{D}^H = \frac{1}{|Y|} \int_Y \boldsymbol{D} : \boldsymbol{s} dy, \ \boldsymbol{\beta}^H = \frac{1}{|Y|} \int_Y \left(\boldsymbol{\beta} - \boldsymbol{D} : \boldsymbol{\varepsilon}_y(\boldsymbol{\psi}) \right) dy, \text{ and } \boldsymbol{b}^H = \frac{1}{|Y|} \int_Y \boldsymbol{b} dy \tag{6}$$

Also, the tensors of localization have been defined as (in component form)

$$s_{ij}^{kh} = I_{ij}^{kh} - \varepsilon_{y,ij}\left(\boldsymbol{\chi}^{kh}(y)\right) \tag{7}$$

where I_{ij}^{kh} indicates the forth order identity tensor. Once the macroscopic displacement $\boldsymbol{u}^0$ and ΔT are obtained in the macroscopic region by

$$\boldsymbol{\sigma}^0(y) = \left[\boldsymbol{D}(y) : \boldsymbol{s}(y) \right] : \boldsymbol{\varepsilon}_x(\boldsymbol{u}^0) - \Delta T \left(\boldsymbol{\beta}(y) - \boldsymbol{\varepsilon}_y(\boldsymbol{\psi}) \right) \tag{8}$$

Thus, the effective properties can be derived from the micromechanical characteristics and the micromechanical behaviors can be obtained by localizing the overall structural response to the local one. These processes are called the homogenization and the localization, respectively.

3. Digital Image-Based Geometric Modeling

The microstructure of a composite material usually reveals a more or less random distribution of inclusions (reinforcement). For example, Figure 1 shows an intermetallic composite which is composed of a $MoSi_2$-matrix and SiC-inclusions. In order to accurately evaluate the microscopic stress given in Eqn. (8), we shall utilize the DIB modeling technique, which was originally developed by Hollister and Kikuchi [3]) for micromechanical study of bone tissues. Since the FE model obtained by this method is the direct interpretation of the scanned image using two dimensional micrographs of the real composite materials along with image-processing software, the homogenization analyses

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can reflect the effects of the real geometric configuration.

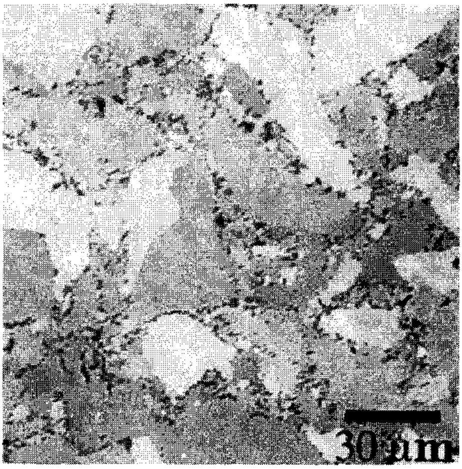

Figure 1: Micrograph of SiC-reinforced $MoSi_2$

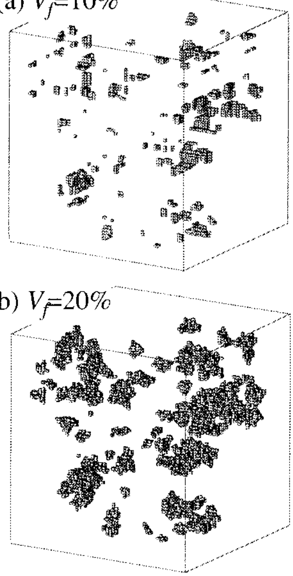

Figure 2: Unit cell models of different volume fractions

The whole procedure can be divided into the following major four parts: 1. *Capturing* and *Sampling* by taking a picture and storing it in a digital computer; 2. *Selecting* and *Thresholding* which determine the unit cell size, its FE model size and the microstructural configuration by giving the thresholding pixel value; 3. *Exporting* (and *Adjusting*, if necessary) which provides the prototype for the FE model; 4. *Stacking* which uses the exported data to construct the three-dimensional (3D) structure prior to or during the FEA. In order to construct 3D FE model in DIB modeling, two dimensional digital images have to be combined. The fourth process, namely stacking, corresponds to such a data operation. In 3D FE modeling, each pixel in a 2D image is recognized as a voxel, which is identified as a finite element in FEA.

This method involves image processing which fully utilizes both newest hardware and software capability available. For later use, the process of changing the volume fraction of a constituent is readily done by manipulating the voxel values of the digitized unit cell model. Combined with the 3D realization of images, digital image processing provides several FE geometric models of the composite microstructure, each of which has a different volume fraction of the inclusion. Figure 2 shows the virtually-represented 3D models with volume fractions of 10% and 20%, both of which keep the original morphology. More details of the modeling procedure, the related image processing and some applications of the homogenization analyses are found in Terada, Miura and

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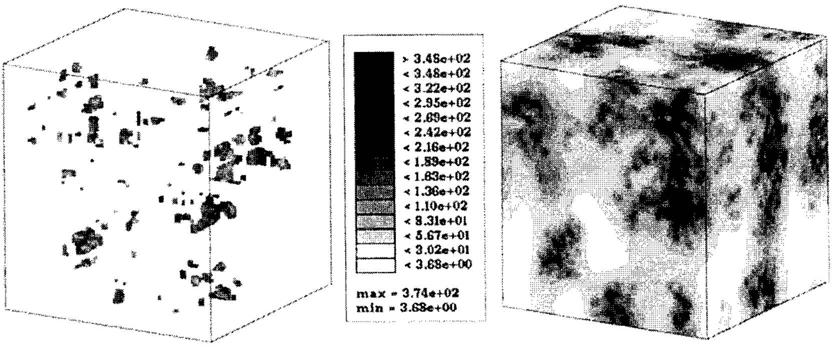
Kikuchi[4].

4. Numerical Examples

4.1. Application in Thermoelasticity

Using the material constants (SiC: Young's modulus; E_f=450 GPa, Poisson's ratio; ν_f=0.2, CTE; $\alpha_f=5.0\times10^{-6}$/C° and $MoSi_2$: E_m=400 GPa, ν_m=0.25, $\alpha_m=8.1\times10^{-6}$/C°), the homogenization and localization are readily carried out for all the unit cell models. Figure 3 shows the microscopic von-Mises stress distribution by applying the temperature change at ΔT=-300C° and no global strain. It should also be noted that the simulation is reliable enough in the sense that we had a similar geometric configuration, i.e., a similar pattern of inclusion scattering.



(a) Without matrix phase (a) Whole unit cell

Figure 3: Microscopic von-Mises stress distribution

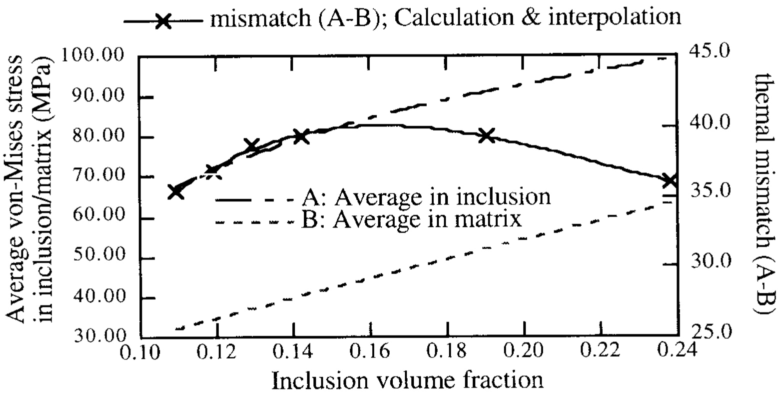


Figure 4: Variation of thermal stress mismatch with volume fraction of inclusion (SiC)

After carrying out several homogenization and localization computations for prepared unit cell models of different inclusion volume fractions, the variation of thermal stress mismatch can be evaluated as shown in Figure 4. Here, the mismatch can be an indicator of interfacial damage and is defined as $F = \left|\langle\overline{\sigma}_f\rangle - \langle\overline{\sigma}_m\rangle\right|$, where $\overline{\sigma}_f$ and $\overline{\sigma}_m$ are the equivalent stresses of the inclusion and matrix respectively computed from eqn.(8). Once the desired intervals of the homogenized elasticity constants as well as the homogenized CTE are decided, the optimal volume fraction can be determined by this figure.

4.2 Effects of Microstructure in the Nonlinear Homogenization Method

The evaluation of microscopic stress is critical in nonlinear problems such as elastoplasticity. When the nonlinear deformation of the overall structure is computed by the incremental solution method (see Terada and Kikuchi[2]), the values of microscopic stress within a certain increment are used as initial values in the next increment. Therefore, the microstructural geometry must be modelled correctly so that the microscopic stress and hence the macroscopic deformation are evaluated accurately. In the present example, the dependence of the global-local nonlinear mechanical behavior on the RVE geometric modeling will be examined.

The same intermetallic composite as in Figure 1 is used to obtain the overall mechanical response to unidirectional tensile force. Elastoplasticity with large deformation is assumed as the mechanical behavior of matrix phase. In addition to the same elastic constants as before, the yield stress and hardening parameter of matrix phase are respectively given as 300 MPa and 0.2. In order to illustrate the potential of DIB modeling, we shall compare the result with that of the idealized unit cell model by usual FE meshing presented in Figure 6 (a), while both models reveal isotropy in linear elasticity.

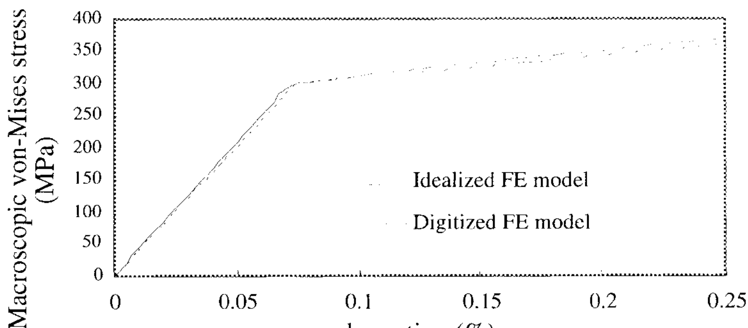


Figure 5: Unidirectional response of overall structure

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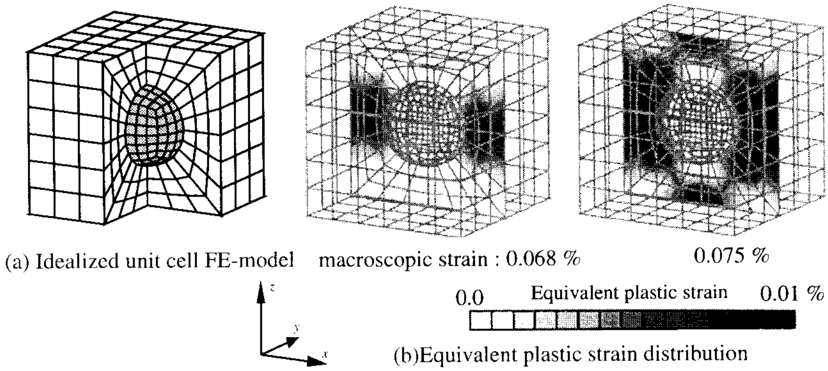

Figure 6: Finite element mesh and the onset of plastic yielding for idealized unit cell model

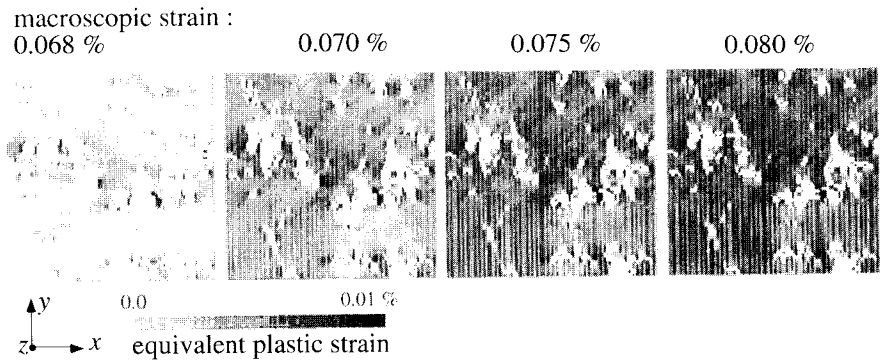

Figure 7: Onset of plastic yielding in the unit cell

The macroscopic stress-strain curves are shown in Figure 5 to illustrate the influence of the geometry of the unit cell model. It can be seen from the figure that the idealized model is slightly stiffer than the digitized one in the linear elastic range. Note that the number of elements for a single fiber in the idealized model is much larger than that of the digitized model. Therefore, while a direct comparison is difficult, a qualitative discussion seems possible. That is, if the digitized model has the same order of FE approximation as that of the idealized one to represent the heterogeneity, the elasticity response becomes more compliant. Then the onset of the microscopic plastic yielding will be delayed and therefore the slope of the strain hardening would be different. This is also confirmed from the equivalent plastic strain distribution when the plastic deformation begins (see Figure 6(b) and 7). The plastic yielding occurs in several local regions and propagates gradually within the unit cell. Thus, if the resolution of the original image were high, the actual stress-strain curve for the digitized unit cell model would probably be quite different from that of the idealized one.

In summary, the constitutive modeling of the asymptotic homogenization method cannot provide an accurate evaluation of the nonlinear global-local deformation of a composite material until the microstructural geometry of composites is appropriately modeled using DIB modeling.

5. Conclusions

Digital imaging technology was utilized to construct the geometric model of the microstructure of intermetallic composites. Then the homogenization analyses were carried out to see the specific effects of the complex geometry. It was found that the geometry modeling technique developed not only provided a unit cell model of real microstructure but also enabled us to characterize the mechanical response within the microstructure. It was also shown that the analysis results from the nonlinear homogenization method depended on the geometric configuration of the unit cell. In conclusion, in order to evaluate the nonlinear mechanical behavior of the intermetallic composite, we have to construct the geometry model as accurately as possible.

Acknowledgment

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