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Computational and analytical prediction of the elastic modulus and yield stress in particulate-reinforced metal matrix composites

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In this work, three-dimensional finite-element analysis (FEA) simulations based on the representative volume element approach have been performed to determine the elastic modulus and yield stress of spherical particle-reinforced metal matrix composites. These simulations take into consideration of the degree of bonding between the matrix and the reinforcement. An analytical model has been developed using the FEA computations, and the results agree well with experimental findings reported in the literature for strongly bonded Al-2080/SiC and poorly bonded Al-2024/Al_2O_3 materials.

Keywords: Finite-element analysis; Mechanical properties; Modeling; Metal matrix composites

Predicting the mechanical properties of metal matrix composites (MMCs) has posed a considerable challenge throughout their history. The elastic modulus and yield stress have received the most attention; models of elastic modulus are typically derived from continuum mechanics considerations, whereas predictions of yield stress depend on the type of strengthening mechanism that is thought to be active in the composite. To determine which, if any, of the mutually incompatible models is correct, the change in properties due to the addition of the reinforcement must be compared to the properties of the unreinforced matrix, where the unreinforced matrix is in the same "condition" as it is in the composite. Regarding yield stress, the most important property requiring consistency is the matrix grain size. This is because the matrix yield strength is often significantly influenced by grain boundary strengthening, as described by the Hall–Petch relation. Since the incorporation of reinforcements has been shown to reduce the grain size in metal matrix micro- and nanocomposites [1], simply synthesizing material with and without reinforcement and performing a direct comparison between the two materials can lead to inaccurate results. It is also difficult to control particle distribution and the degree of matrix/reinforcement bonding in experiments, which are factors that can also greatly affect the performance.

In this study, in silico 3-D finite-element analysis (FEA) simulations were performed using regular, random, and clustered array of $N \times N \times N$ spherical reinforcement particles embedded in a cube of matrix metal, where N is the number of reinforcement particles in one direction ($1 \leqslant N \leqslant 5$). Throughout this study, ABAQUS FEA software (Dassault Systèmes Simulia Corp., Providence, Rhode Island) was employed, and a 3-D representative volume element (RVE) was used to embody a continuum. MMC systems of Al-2024 matrix reinforced with SiC particles were selected. Periodic constraint boundary conditions were applied for all of the computations. Inputs were (i) stress–strain curve of the matrix (Al-2024 [2] where the 0.2% offset $\sigma_{y_m} = 420$ MPa), (ii) elastic moduli of matrix ($Y_m = 72.4$ GPa) and reinforcement ($Y_r = 410$ GPa) and (iii) Poisson's ratios of matrix ($\nu_m = 0.33$) and reinforcement ($\nu_r = 0.14, 0.33$ and 0.50 were tested). The size and quantity of the reinforcement spheres were varied to produce the desired volume fractions, and simulations were run using differing reinforcement Poisson's ratios to isolate any effects of this parameter. To study the effect of incomplete bonding between the matrix and the reinforcement particles, six spherical caps were uniformly distributed across the rein-

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forcement sphere's surface such that the total surface area of the caps would constitute a certain percentage of the total sphere surface area. While the caps were unbonded and represented only a contact condition, perfect bonding was used for the remaining sphere surfaces. As it is not trivial to model the partial coherency of particles to the matrix, the geometric separation scheme employed in this work was intended to tailor the averaged impacts of the degree of bonding. This scheme allows for the isolation of changes in elastic modulus and yield strength due to (i) volume fraction, (ii) size of particle, (iii) particle distribution, (iv) differences in Poisson's ratio and (v) degree of bonding. Figure 1(a) presents an example FEA model with $N = 5$. In the enlarged images, yellow and gray surfaces represent the bonded and unbonded interface areas between the matrix and particles, respectively. Varying degrees of bonding (f_{Bond}) was modeled, including $f_{\mathrm{Bond}} = 0, 0.5, 0.75$ and 1. In Figure 1(b), examples of models with different particle distributions ($N = 3$) are shown. The solid spheres indicate the positions of reinforcement particles.

To predict the elastic modulus, the rule of mixtures is often used in the case of aligned continuous fiber-reinforced composites [3], but more sophisticated models have also been proposed that may be applied to particulate-reinforced materials [4,5]. We first tested the impacts of particle distributions on the modulus and yield strength, and it was found that all of the results from the systems with different particle distributions (i.e. regular, random and clustered as illustrated in Figure 1(b)) were nearly identical. This is consistent with results obtained by Deng and Chawla [6] that showed clustering of reinforcement particles has little effect on elastic modulus and yield stress, though it has a significant effect on work-hardening behavior and ductility. Therefore, in this work, we present the computational results based on the models with regular particle arrangements.

Figure 2(a) shows the variations of calculated elastic modulus with number of particles for different volume fractions (f_r) with $f_{\mathrm{Bond}} = 1$ and demonstrates that the

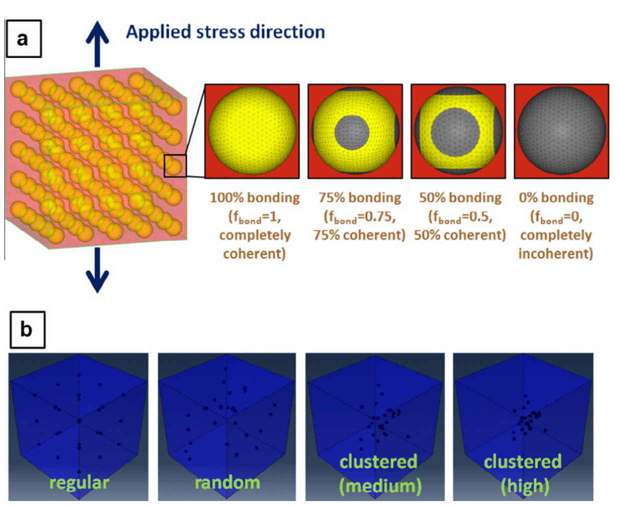

Figure 1. Example of 3-D FEA models (a) with regularly arranged reinforcement particles ($N = 5$) and (b) with different particle distributions ($N = 3$). In the enlarged images of (a), the surfaces in yellow and gray represent the bonded and unbonded interface areas between the matrix and particles, respectively.

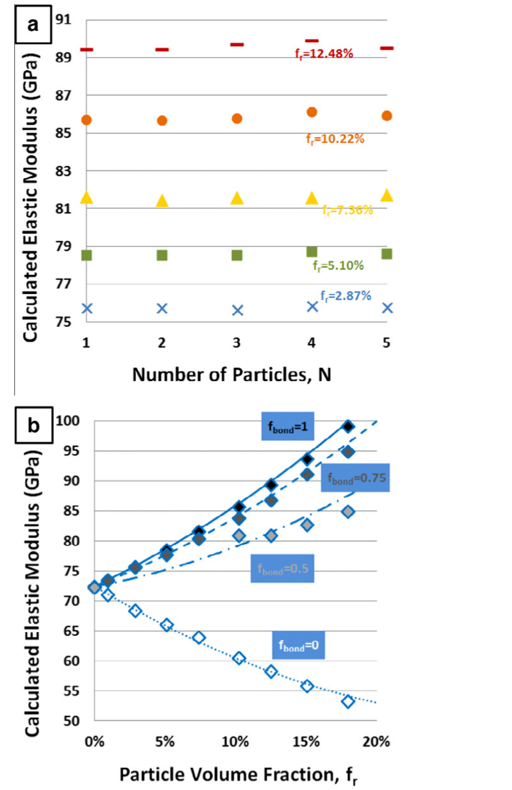

Figure 2. Variations of calculated elastic modulus with (a) number of particles for different volume fractions when $f_{\mathrm{Bond}} = 1$ and (b) particle volume fraction for different degrees of bonding when $N = 1$.

modulus depends primarily on f_r of reinforcement. For a fixed f_r, there were negligible differences between modulus values regardless of the number of particles incorporated. Small differences are likely the result of the limited size of the RVE model, where values are affected by particle/edge and particle/particle interactions. By varying the Poisson's ratio for the reinforcement, it was found that an increase in elastic modulus results as the difference between the Poisson's ratio of the matrix and reinforcement increases (data not shown). This effect also increases with increasing f_r; however, the effect is minor with a few percent difference in modulus values, which can be considered as negligible. Eqs. (1)–(5) were developed to predict the elastic modulus (Y_c) of the Al-2024/SiC composite (c), which is a modified rule of mixtures relation with adjustments for the shape (sphere) of the reinforcement (F_{sphere}), the second-order effects of reinforcement concentration (F_{f_r}), the Poisson's ratio effect ($F_{\Delta\nu}$) and the degree of bonding, f_{Bond} ($F_{\mathrm{bond}_{Y-\mathrm{SA}}}$ for surface area (SA) effect and $F_{\mathrm{bond}_{Y-\mathrm{concentration}}}$ for concentration effect, respectively). In Eq. (1), Y_m and Y_r denote the yield strength of matrix (m) and reinforcement particles (r), respectively.

$$Y_c = Y_m + (Y_r - Y_m) f_r F_{\mathrm{sphere}} (F_{f_r} + F_{\Delta\nu} - F_{\mathrm{bond}_{y-\mathrm{SA}}} F_{\mathrm{bond}_{y-\mathrm{concentration}}}) \text{ with } F_{\Delta\nu} \cong 0 \quad (1)$$

Because the rule of mixtures is strictly applicable to a cylindrical reinforcement aligned with the direction of applied stress, several adjustments must be made for