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The influence of thermal residual stresses and thermal generated dislocation on the mechanical response of particulate-reinforced metal matrix nanocomposites

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Due to thermal expansion mismatch between reinforcing particles and matrix, thermal induced dislocations are generated in metal matrix nanocomposites (MMNCs) during cooling down from the processing temperature. These dislocations have been identified as an important strengthening mechanism in particulate-reinforced MMNCs. In this study, the development of thermal residual stresses and thermal induced dislocations in MMNCs are predicted using discrete dislocation simulation, assuming the whole material is under uniform temperature change. Shear deformation is applied after the composites are cooled down to room temperature and the influence of thermal residual stresses and thermal generated dislocation on the overall response of particulate-reinforced MMNCs are investigated. The results show that the thermal residual stresses are high enough to generate dislocations and the dislocation density is higher in the interfacial region than the rest of the matrix. The predicted mechanical behavior of the MMNCs matches the experimental results better when thermal residual stresses are included in the simulations.

1. Introduction

Metal matrix nanocomposites (MMNCs), which can be defined as metal matrix composites (MMCs) reinforced with nano-sized fillers, show significant promise for use in the aerospace and automotive industries [1]. This is substantiated by many experiments which show that reducing the size of particles to the nanoscale dramatically increases the mechanical strength of MMCs while preserving good ductility [2]. While extensive experimental studies have been conducted on MMNCs [3], only a handful of numerical studies have been performed for MMNCs.

Recently, Law et al. [4,5] conducted a two-dimensional multi-particle representative volume element simulation using discrete dislocation method to investigate the mechanical properties of MMNCs. These numerical investigations have successfully simulated the trend of increasing flow stress and degree of hardening with decreasing size of nano-particles and increasing particle volume fraction [4,5]. However, the improvements in flow stress and degree of hardening with increasing particle volume fraction and decreasing particle size as reported in experiments are more significant than those shown in simulations especially at very low particle volume fractions [6], which strongly suggests that there are other strengthening mechanisms to be considered in the simulations.

Current discrete dislocation dynamics simulations have ignored the presence of thermal residual stress which is an important and inevitable consequence arising from the fabrication process. During fabrication and subsequent heat treatment processes, MMCs initially behave in a stress-free state at the solution treatment temperature; significant thermal residual stresses develop upon cooling to the room temperature due to the difference of the coefficients of thermal expansion (CTE) between the matrix (e.g. CTE of Al is 23.2×10^{-6}/K) and the reinforcement (e.g. CTE of Al_2O_3 is 7.4×10^{-6}/K) [7,8]. To relieve stresses due to the mismatch in CTEs with the matrix, reinforcements in MMCs generate (1) rows of prismatic loops and/or (2) tangles of dislocations, forming a well-defined plastic zone [9]. It is believed that the density of thermal induced dislocation will increase with a decrease in particle size; thus nanoparticle which has extremely high surface area to volume

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ratio can induce high dislocation density in the MMNCs system even with low volume percentages [10]. Indeed, thermal-generated dislocations in MMNCs have been observed by experiments [11–13]. These dislocations play important roles on the mechanical properties of the composite material. When the material is subsequently deformed or work hardened, thermal residual stresses and thermal-generated dislocations may essentially alter the rate at which dislocations bypass the particle, the yield stress, and the continued work hardening of the material [14]. The high density of thermal-generated dislocations results in the improvement of hardness [11] and yield strength [13] of the composites.

As with any composite models, before any imposed loadings, one must first assess the current material state to predict accurately the material's actual response [15]. The existing numerical models of MMNCs have assumed that the material is initially stress and dislocation free [4,16,17]. It seems natural to conclude that more realistic models should include the effect of thermal residual stresses and thermal-generated dislocations. Hence, an influential step towards understanding the mechanical properties of MMNCs would be a quantitative description of thermal residual stresses as well as thermal induced dislocations.

In this work, we performed numerical simulations to investigate the effect of thermal residual stress and thermal induced dislocation on the mechanical response of MMNCs. Numerical simulation will be carried out in discrete dislocation framework. For the sake of simplification and computational cost, only two-dimensional plane strain models based on the unit cell approach will be used in this study. Metal matrix – ceramic reinforcement systems will be used and the host material could be lightweight metals such as aluminum and magnesium, while the particle reinforcements could be common ceramics such as silicon carbide and alumina. Matrix, reinforcements, as well as interphases, are assumed to be isotropic. Shear deformation is applied after the composites are cooled down uniformly to room temperature. The influence of thermal residual stresses and thermal generated dislocation on the shear response of particulate-reinforced MMNCs will be investigated.

2. Problem formulation

The discrete dislocation plasticity framework, which is briefly outlined here, followed closely the formulation developed by Van der Giessen and Needleman [18]; further details and references are given in Ref. [18] and their subsequent works [18–21].

The composite material is assumed to be a linear elastic isotropic body which contains elastic particles and has a distribution of dislocations in the matrix material. Plasticity originates from the motion of the edge dislocations, which are regarded as line defects in the matrix material. The current state of the body in terms of the displacement, strain and stress fields can be written as the superposition of two fields:

$$\mathbf{u} = \tilde{\mathbf{u}} + \hat{\mathbf{u}}, \quad \boldsymbol{\varepsilon} = \tilde{\boldsymbol{\varepsilon}} + \hat{\boldsymbol{\varepsilon}}, \quad \boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} + \hat{\boldsymbol{\sigma}} \tag{1}$$

where the (~)-fields are associated to the dislocations in their current configuration but in an infinite medium. These fields are obtained by sum of the long-range fields of each individual dislocation

$$\tilde{\mathbf{u}} = \sum \tilde{\mathbf{u}}_i, \quad \tilde{\boldsymbol{\varepsilon}} = \sum \tilde{\boldsymbol{\varepsilon}}_i, \quad \tilde{\boldsymbol{\sigma}} = \sum \tilde{\boldsymbol{\sigma}}_i \quad (i = 1, \ldots, \mathrm{n}) \tag{2}$$

The solution for the dislocation field can be obtained from literature [22]. The (^)-fields are associated to the image fields which correct for the actual boundary conditions and the presence of particles, and can be solved as a linear elastic boundary value problem using finite element method with the appropriate boundary conditions, as detailed in Ref. [18].

The dislocations are evaluated through the following constitutive rules: (1) dislocation generation; (2) dislocation motion; (3) dislocation annihilation and (4) pinning at obstacles or particles. All these are governed by the Peach-Koehler force

$$f_{\mathrm{i}} = \boldsymbol{n}_{\mathrm{i}} \cdot \left(\hat{\boldsymbol{\sigma}} + \sum_{j \neq i} \tilde{\boldsymbol{\sigma}}_j \right) \cdot \boldsymbol{b}_{\mathrm{i}} \tag{3}$$

where $\boldsymbol{b}_{\mathrm{i}}$ is the Burgers vector of dislocation i and $\boldsymbol{n}_{\mathrm{i}}$ the unit tangent vector of the glide plane. The dislocations are generated through a distribution of Frank-Read sources. A dislocation dipole is created with a nucleation distance L_{nuc} when the Peach-Koehler force on the source exceeds the nucleation strength τ_{nuc} during a time span t_{nuc}. The dipole consists of two opposite dislocations which signs are determined by the direction of the Peach-Koehler force. Dislocation motion is taken to be drag controlled and the magnitude of the velocity v_i of dislocation i is directly proportional to the Peach-Koehler force $f_i = B \cdot v_i$. A moving dislocation will be pinned by a distribution of obstacles if the Peach-Koehler force acting on the dislocation is smaller than the obstacle strength τ_{obs}. The Frank-Read sources density ρ_{nuc} and obstacles density ρ_{obs} are prescribed according to different matrix materials. Two dislocations with opposite Burgers vector are annihilated when they approach each other within a material-dependent annihilation distance $L_e = 6b$, where b is the magnitude of the Burgers vector.

The deformation process is solved explicitly. At time t, the boundary conditions for the linear elastic boundary value problem are computed from the existing dislocation structure and the applied displacement. The Peach-Koehler forces are calculated according to Eq. (3). Then the dislocation positions are updated based on the constitutive rules. Following that, new dislocations are generated at the Frank-Read sources and opposing dislocations are annihilated if they are within L_e. Further details on the numerical implementation can be found in Ref. [18].

In this study, two-dimensional discrete dislocation analysis is performed on the investigation of thermal residual stress in MMNCs. A unit cell with randomly distributed multiple particles is used, assuming plane strain conditions. Both the width and height of the unit cell are taken to be 2000 nm and the element size is set as 50 nm, as shown in Fig. 1(a). A similar configuration has been used to study the mechanical properties of MMNCs [4,5]. Except otherwise stated, the matrix material is taken to be representative of aluminum, Young's modulus $E_m = 70$ GPa, Poisson's ratio $\nu_m = 0.3$ and the thermal expansion coefficient $\alpha_m = 23.2 \times 10^{-6}$ K. For the nanoparticles, the material properties are taken to be representative of silicon carbide, $E_p = 460$ GPa, Poisson's ratio $\nu_p = 0.3$ and the thermal expansion coefficient $\alpha_p = 4.1 \times 10^{-6}$ K. The drag coefficient is taken to be $B = 10^{-4}$ Pa·s and the magnitude of the Burgers vector is taken as $b = 0.25$ nm. The dislocation nucleation time span is $t_{\mathrm{nuc}} = 10$ ns. The Frank-Read sources density is $\rho_{\mathrm{nuc}} = 40\ \mu\mathrm{m}^{-2}$ with a mean strength $\tau_{\mathrm{nuc}} = 27$ MPa and coefficient of variation of 0.2. The obstacle density is taken to be $\rho_{\mathrm{obs}} = 120\ \mu\mathrm{m}^{-2}$ with strength $\tau_{\mathrm{obs}} = 300$ MPa. An applied shear deformation rate $\dot{\Gamma} = 10^3 s^{-1}$.

The simulation is divided into two stages: in stage one, the thermal residual stresses and thermal induced dislocations are developed by simulating a uniform temperature drop; in stage two, the unit cell is subsequently deformed by applying prescribed shear displacements along the top and bottom edges and the overall shear stress–strain response is computed. In this paper, shear deformation is considered due to the availability of test data for validation of approach and for comparison with other existing