MECHANICAL RESPONSE OF METAL MATRIX NANOCOMPOSITES USING DICRETE DISLOCATION APPROACH

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Introduction

Experimental studies have shown that reducing the size of reinforcement particles to nanoscale dramatically increases the mechanical strength of metal matrix composites (MMCs) even at low particle volume fractions [1-2]. While numerical simulations have also been used in recent years to investigate the mechanical properties of conventional MMCs, relatively few numerical studies have been done for metal matrix nanocomposites (MMNCs). Size effects must be considered in the modeling of MMNCs as particle size is in the nanoscale and distance between particles approaches the mean free path of dislocations [3-4]. At the nanoscale, dislocations should be accounted for in a discrete manner. This paper presents the use of the discrete dislocation approach on MMNCs to investigate the effects of particle volume fraction and particle size on the overall response of the composite material.

Discrete dislocation formulation

The discrete dislocation plasticity framework used in this study follows closely the formulation developed by Van der Giessen & Needleman [5] which is outlined here. The composite material is considered as a linear elastic body which contains elastic inclusions or particles with a distribution of dislocations in the matrix material. Constitutive relations are used to describe the motion, nucleation and annihilation of dislocations. Firstly, a dislocation will glide along its slip plane with its velocity directly proportional to the resolved shear stress acting on the dislocation. Obstacles to dislocation motion modelled as fixed points on a slip plane are distributed randomly in the matrix to account for the effects of small precipitates or impurities in blocking slip. A dislocation moving towards an obstacle or impurity will initially be pinned at the obstacle, after which it will be released when the resolved shear stress on the dislocation exceeds the strength of the obstacle τ_{obs}. Secondly, new dislocation pairs are generated by simulating Frank-Read sources. Thirdly, annihilation of two opposite dislocations occurs when they are within a material-dependent, critical annihilation distance. The discrete dislocation formulation is implemented in a 2D plane strain unit cell model as shown in Fig. 1. Simple shear deformation is applied on the unit cell through prescribed displacements along the top and bottom edges.

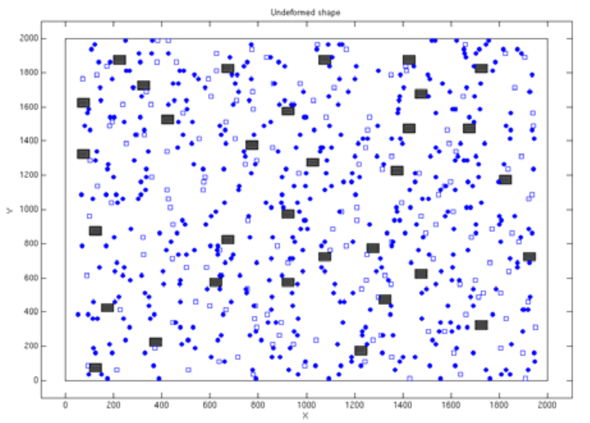

Fig. 1. 2D unit cell model showing the locations of the particles (shaded boxes), dislocation sources (white rectangular markers) and impurities represented by point obstacles (small dark spots).

Numerical results and discussion

The numerical results presented in this paper are obtained using representative elastic properties for aluminum matrix and silicon carbide nanoparticles. The composite material is deformed at an applied shear strain rate of 1000 s^{-1}, using 30000 equal time increments for an imposed shear strain of 1.5 per cent. The size of the unit cell is 2 μm × 2 μm and contains 80 equally spaced horizontal slip planes. The density of dislocation sources ρ_{nuc} is 40 μm^{-2}, with the strength of dislocation sources randomly chosen from a Gaussian distribution with mean strength τ^*_{nuc} of 26.92 MPa (0.1% of the matrix's shear modulus G) and coefficient of variation of 0.2. The density of impurities on the slip planes is set at ρ_{obs} = 120 μm^{-2} with the strength of impurities τ_{obs} = 0.2692 GPa (0.1% of G) [6]. The mean overall response is computed using three different realizations of random dislocation source, impurity and particle distributions for every case studied as the overall response is highly dependent on the random distribution of these features.

As shown in Fig. 2(a), the flow stress τ_{flow} and degree of hardening n increase significantly with particle volume fraction when 50 nm size particles are used. The particles act as impenetrable barriers to dislocation motion, resulting in the formation of dislocation pile-ups. The number of dislocations in these pile-ups increases with imposed deformation. The dislocations impeded by the particles are unable to glide pass the particles even when the glide force on the dislocations is high. As the number of particles in the matrix increases with particle volume fraction, a greater proportion of the dislocations are also impeded and more dislocation pile-ups are formed, generating a greater back-stress which results in a larger applied load or deformation required to generate new dislocations and move existing dislocations. Consequently, τ_{flow} and n increase with particle volume fraction since the number of slip planes blocked by the particles is also increased. Improvement in τ_{flow} with increasing particle volume fraction is also observed for cases with larger particle sizes, as shown in Fig. 2(b) for particle size of 200 nm. However, the improvement in τ_{flow} with increasing particle volume fraction is much less significant for cases with large particles compared to small ones. As shown in Fig. 3, τ_{flow} and n decrease with increasing particle size. This is because the number of particles reduces when the particle size is increased at the same particle volume fraction. As less slip planes are blocked by particles, it will be easier for dislocations to form and propagate within the material, resulting in fewer impediments to dislocation motion and formation of fewer dislocation pile-ups. Therefore, improvement to the material's mechanical resistance can be achieved by reducing the particle size as small particles are most effective in blocking dislocation motion, which is the dominant mechanism of plastic deformation in metallic materials.

Conclusions

2D discrete dislocation simulations used to study the mechanical response of MMNCs are able to capture the trend of increasing flow stress and degree of hardening with increasing particle volume fraction and decreasing particle size, which is due to the greater number of particles blocking dislocation motion. The simulations show that dislocation motion and the formation of dislocation pile-ups are the dominant mechanisms which govern plastic deformation in metallic nanocomposites, which agrees well with experimental observations.

References

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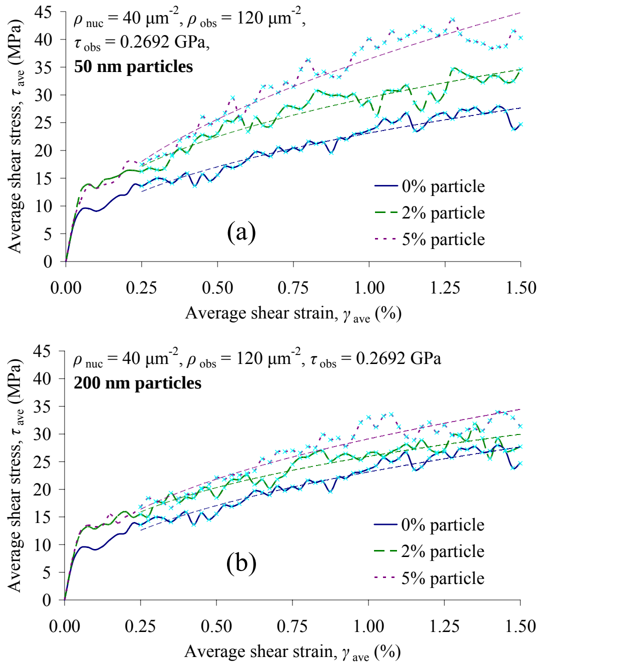

Fig. 2. Mean overall response of composite material for different particle volume fraction with uniform particle size of (a) 50, and (b) 200 nm.

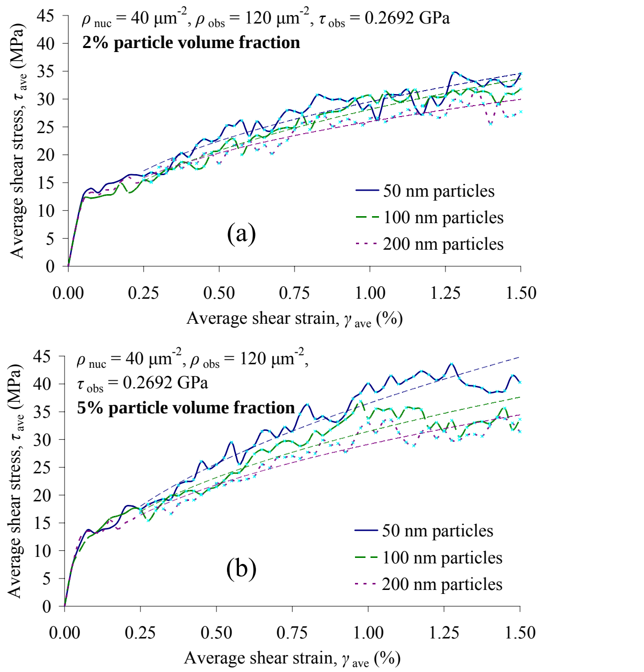

Fig. 3. Mean overall response of composite material for different uniform particle size with particle volume fraction of (a) 2, and (b) 5 per cent.