

NUMERICAL ANALYSIS OF THE EFFECT OF PARTICLE ARRANGEMENT ON MECHANICAL BEHAVIOR AND PARTICLE DAMAGE IN METAL MATRIX NANOCOMPOSITES

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1 Introduction

The spatial distribution of reinforcement particles has a significant effect on the mechanical response and damage evolution of metal matrix composites (MMCs). It is observed that particle clustering leads to higher flow stress, quicker and earlier particle damage, as well as lower overall failure strain. On the other hand, regular microstructure results in the highest strength [1, 2]. In recent years, experimental studies have shown that reducing the size of particles to the nanoscale dramatically increases the mechanical strength of MMCs even at low particle volume fractions. This is due to the higher plastic constraint in the matrix as well as activation of strengthening mechanisms operating at the nanoscale [3]. However, the effect of particle distribution on the mechanical response and particle damage in these metal matrix nanocomposites (MMNCs), which may be different from that observed in normal MMCs, has not been widely explored. In this paper, this effect will be investigated numerically using discrete dislocation simulations because size effects must be considered in the modeling of MMNCs [4].

2 Discrete Dislocation Formulation

The discrete dislocation plasticity framework used in this study follows closely the formulation developed by Van der Giessen and Needleman [5]. The nanocomposite is considered as a linear elastic body which contains elastic particles, with a distribution of dislocations which glide along pre-determined slip planes in the matrix. 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 modeled 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.

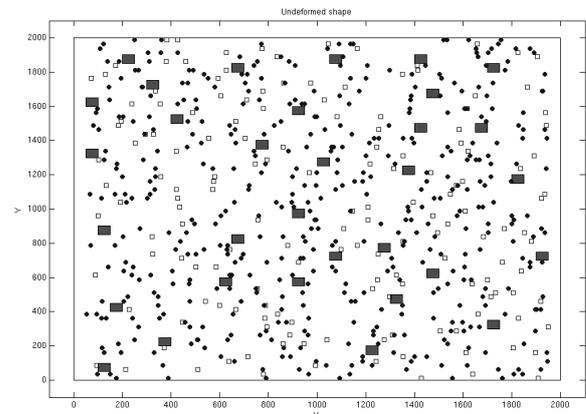


Fig. 1. Unit cell showing the locations of the particles (shaded boxes), dislocation sources (white rectangular markers) and impurities represented by point obstacles (small dark spots).

The discrete dislocation formulation is implemented in a $2 \mu\text{m} \times 2 \mu\text{m}$ plane strain unit cell model as shown in Fig. 1, which contains 80 equally spaced horizontal slip planes with 2 per cent particle volume fraction and particle size of 25 nm. Simple shear deformation is applied incrementally on the unit cell through prescribed displacements along the top and bottom edges, along which the average shear strain γ_{ave} and average shear stress τ_{ave} of the nanocomposite are also calculated. The numerical results presented in this study are obtained using representative elastic properties for aluminum matrix

and silicon carbide reinforcement nanoparticles; these material properties and various parameters used to describe dislocation processes in the constitutive relations follow that in Law *et al.* [6]. The mean overall response is computed using many different realizations of dislocation source, impurities and particle distributions since the overall response is highly dependent on these distributions.

3 Effect of Particle Arrangement on Overall Response of MMNCs with Undamaged Particles

Fig. 2 shows that regular rectangular and non-clustered random particle arrangements result in the lowest and highest flow stress, respectively. This is because the number of slip planes blocked by the particles is minimized for the rectangular arrangement and there are many large veins of unreinforced matrix as shown in Fig. 3(a). Dislocations can move relatively easily with little hindrance on the many unobstructed slip planes. On the other hand, most slip planes are blocked by particles when the arrangement is well-dispersed as shown in Fig. 3(b). Dislocations unable to bypass the particles will form many dislocation pile-ups, which retard the generation of new dislocations and hinder the motion of existing dislocations. Impediment to dislocation motion increases the flow stress of the metallic nanocomposite. Fig. 2 also shows that a highly clustered particle arrangement (the degree of clustering is measured using the nearest-neighbor index (NNI), with smaller NNI indicating greater degree of clustering) produces lower flow stress compared to non-clustered random arrangement because there are more unobstructed slip planes in the matrix, as shown in Fig. 3(c). On the other hand, a mildly clustered particle arrangement only results in minor reduction in the flow stress since most slip planes are still blocked by the particles as shown in Fig. 3(d).

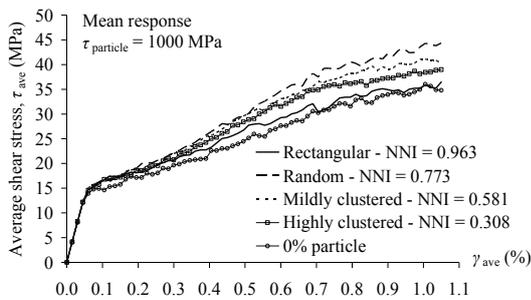


Fig. 2. Mean overall response of MMNC with undamaged particles for different particle arrangements.

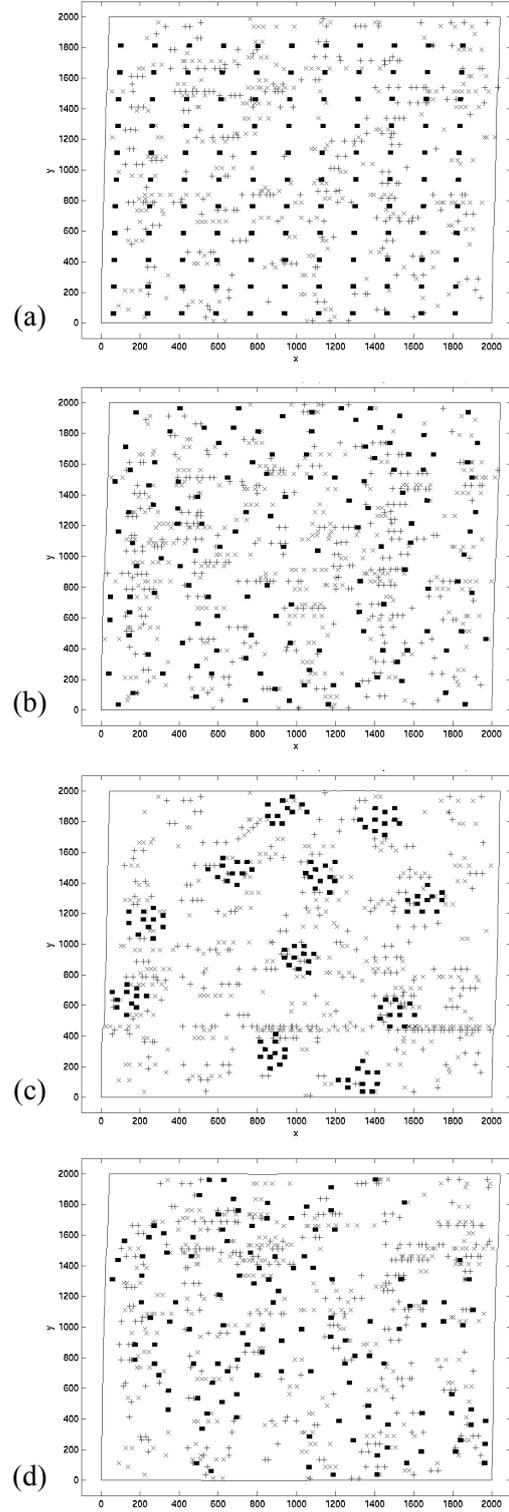


Fig. 3. Distribution of dislocations (+ and \times) and particles (shaded boxes) at $\gamma_{ave} = 1.05\%$ for (a) regular rectangular, (b) non-clustered random, (c) highly clustered (NNI = 0.308), and (d) mildly clustered (NNI = 0.581) particle arrangements.

4 Effect of Particle Arrangement on Overall Response of MMNCs with Damaged Particles

Fig. 4(a) shows that the effect of particle damage on the mean overall response of the nanocomposite is insignificant for a rectangular arrangement of particles. This is because few dislocations are impeded by the particles, hence only a small fraction of particles is damaged and there is little change to the sequence of dislocation processes and the final distribution of dislocations in the matrix as shown in Figs. 3(a) and 5(a). The same trend is observed for the nanocomposite with highly clustered particle arrangement, in which particle damage results in only a minor reduction in the flow stress and degree of hardening as shown in Fig. 4(b). On the other hand, the effect of particle damage on the mean overall response is more significant for mildly clustered and random particle arrangements as shown in Figs. 4(c) and 4(d), respectively. As these particle arrangements are more effective in blocking the motion of dislocations, many impeded dislocations are suddenly released upon particle failure. Hence, particle damage results in fewer dislocation pile-ups in the matrix which is evident when comparing Fig. 3(b) with Fig. 5(b). This leads to lower flow stress and degree of hardening when particle failure occurs. Figs. 4(b) and 4(c) show that the flow stress at applied shear strain $\gamma_{ave} = 1.0\%$ for the case with particle fracture strength 200 MPa is approximately 5 and 15 per cent lower, respectively, compared to the case with no particle damage (in which fracture strength is 1000 MPa) for highly clustered and mildly clustered particle arrangements.

Due to the increased efficiency in impeding the motion of dislocations, the average stresses within the particles in non-clustered random and mildly clustered particle arrangements are also higher compared to that in regular rectangular and highly clustered arrangements. Consequently, particle damage begins earlier and the fraction of damaged particles is also higher in these cases as shown in Fig. 6. A greater fraction of particle damage must be reached in these particle arrangements before the weakest path for localization of dislocation activity can be found. Also, as shown in Figs. 5(c) and 5(d) not all particles in a cluster will be damaged. The outermost particles will tend to fail first because they are under higher stresses due to the pile up of dislocations, whereas inner particles will be damaged later after the dislocations have bypassed the damaged periphery particles and begin to pile up against the inner particles.

The results here are in slight contrast to that observed in conventional MMCs in which the flow stress and fraction of damaged particles increase with degree of clustering [1]. This is because the dominant strengthening mechanism in MMNCs is impediment of dislocation motion, while load transfer from matrix to particles (i.e. constraint on deformation of the matrix surrounding the particles) governs the response of conventional MMCs.

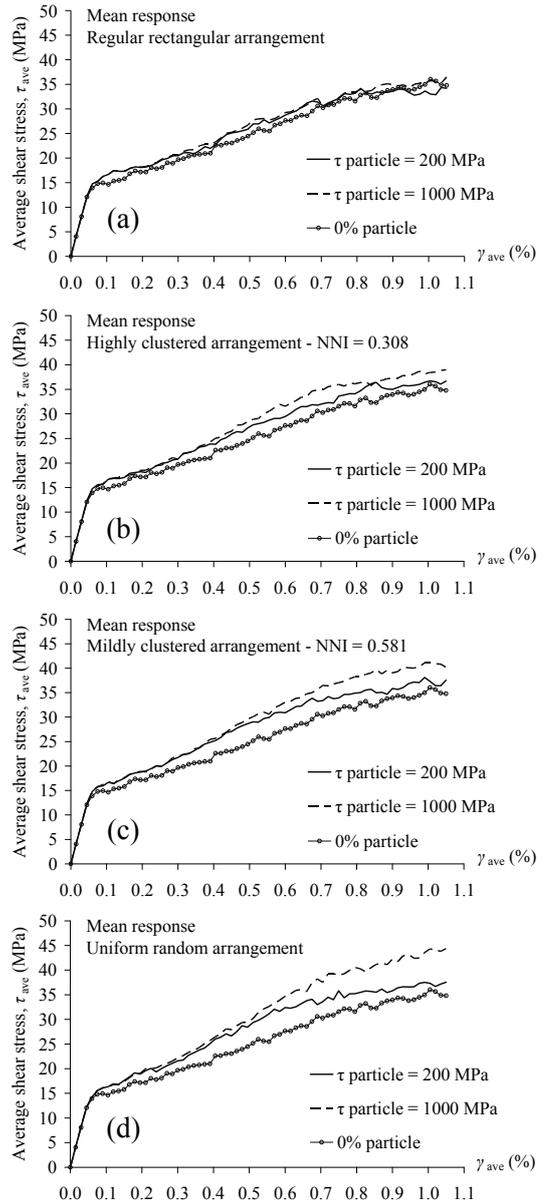


Fig. 4. Mean overall response of MMNC with different particle fracture strength for (a) regular rectangular, (b) highly clustered (NNI = 0.308), (c) mildly clustered (NNI = 0.581), and (d) non-clustered random particle arrangements.

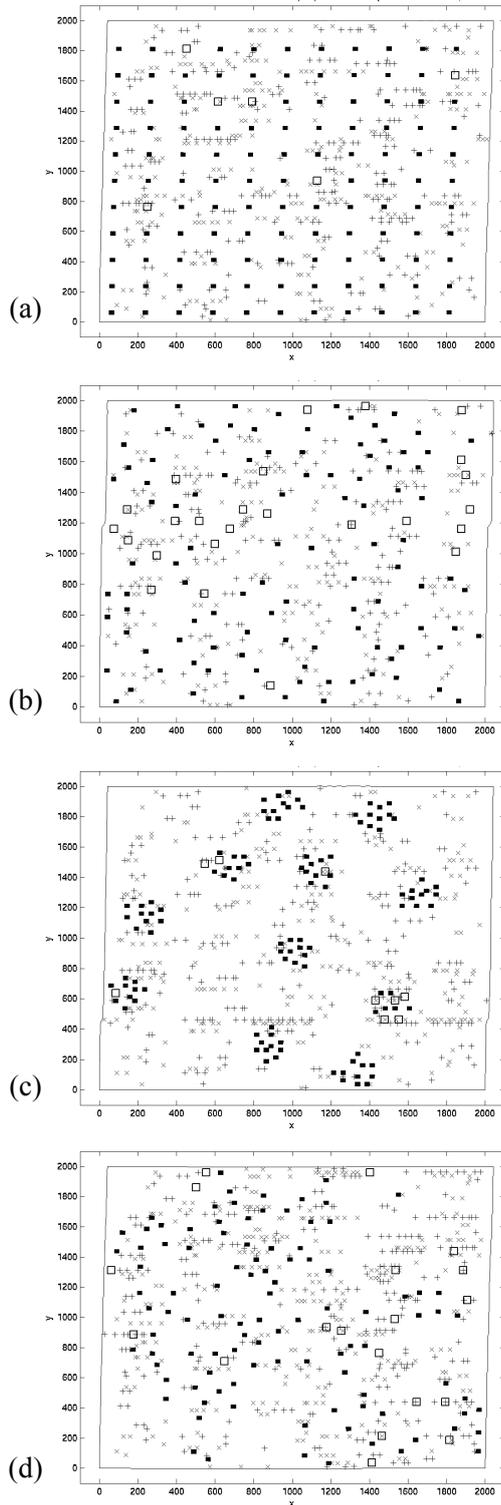


Fig. 5. Distribution of dislocations and particles at $\gamma_{ave} = 1.05\%$ for (a) regular rectangular, (b) non-clustered random, (c) highly clustered (NNI = 0.308), and (d) mildly clustered (NNI = 0.581) particle arrangements. Intact particles are denoted by shaded boxes while damaged particles are represented by blanks; fracture strength of particles is 200 MPa.

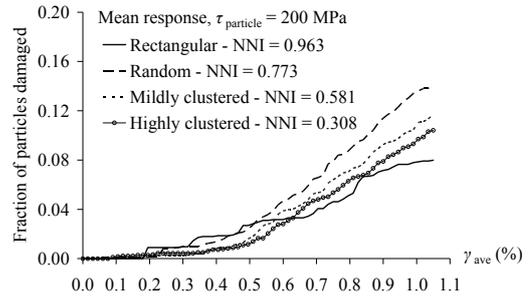


Fig. 6. Fraction of damaged particles in MMNC with particle fracture strength $\tau_{particle} = 200$ MPa for different particle arrangements.

5 Conclusions

The flow stress for metallic nanocomposites with undamaged particles is lowest for rectangular and highly clustered particle arrangements while non-clustered random and mildly clustered arrangements result in higher flow stress. The effect of particle damage on the overall response of the nanocomposite is also more significant for random and mildly clustered particle arrangements, in which particle damage begins earlier and the fraction of damaged particles is higher, compared to rectangular and highly clustered arrangements.

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