Available online at www.sciencedirect.com
SciVerse ScienceDirect
Acta Materialia 60 (2012) 8–21
Acta MATERIALIA
www.elsevier.com/locate/actamat

Effects of particle arrangement and particle damage on the mechanical response of metal matrix nanocomposites: A numerical analysis

Elliot Law, Sze Dai Pang *, Ser Tong Quek

Department of Civil and Environmental Engineering, National University of Singapore, Block E1A, #07-03, 1 Engineering Drive 2, Singapore 117576, Singapore

Received 25 July 2011; received in revised form 21 September 2011; accepted 21 September 2011
Available online 28 October 2011

Abstract

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, earlier particle damage, as well as lower overall failure strain. 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. However, the effects of particle distribution and particle damage on the mechanical response of these metal matrix nanocomposites, which may be different from that observed in normal MMCs, has not been widely explored. In this paper, these effects are investigated numerically using plane strain discrete dislocation simulations. The results show that non-clustered random and highly clustered particle arrangements result in the highest and lowest flow stress, respectively. The effect of particle fracture on the overall response of the nanocomposite is also more significant for non-clustered random and mildly clustered particle arrangements, in which particle damage begins earlier and the fraction of damaged particles is higher, compared to regular rectangular and highly clustered arrangements.

Keywords: Metal matrix composites (MMCs); Nanoparticles; Discrete dislocation dynamics; Plasticity; Particle clustering

1. Introduction

The spatial distribution of reinforcement particles has been known to have a significant effect on the mechanical properties and damage evolution of metal matrix composites (MMCs). Mishnaevsky [1] found that the flow stress and degree of hardening of the composite material is lowest for a highly graded particle arrangement but highest for a regular microstructure. Composites with clustered particles show higher flow stress due to more severely strain-hardened matrix compared with composites with uniformly distributed particles [2]. However, the overall failure strain is significantly lower for composites with clustered particles [3]. In addition, numerical computations show that the effective stresses and local stress and strain fields are much higher in microstructures with random particle distribution compared to a regular distribution. Nevertheless, particle arrangement does not influence the effective response of MMCs in the elastic and small plastic deformation regimes but is significant only at loads at which a significant number of particles begin to fail [1].

The effect of particle damage on the mechanical properties of MMCs has been discussed rather extensively in the literature [4–7]. Results from numerical simulations show that particle damage reduces the flow stress and degree of hardening considerably and the effect of particle damage is influenced by the spatial distribution of the reinforcement particles. Segurado et al. [8] reported that the fraction of damaged particles increases dramatically in a clustered particle arrangement compared to that of a uniform

* Corresponding author. Tel.: +65 6516 2799; fax: +65 6779 1635.
E-mail address: ceepsd@nus.edu.sg (S.D. Pang).

1359-6454/$36.00
doi:10.1016/j.actamat.2011.09.033

distribution due to higher average maximum principle stress and its standard deviation in composites with non-homogeneous particle distribution. In addition, Ayyar et al. [9] showed that MMCs with an ordered distribution of particles and uniform particle fracture strength have the highest strength to failure, but a uniform distribution of particles having fracture strength that follows a Weibull distribution results in the lowest strength to failure.

In recent years, many experimental results have shown that reducing the size of particles to the nanoscale dramatically improves the mechanical properties of MMCs such as tensile strength, hardness and creep resistance even at very low particle volume fractions while preserving good ductility [10–12]. This is due to the activation of strengthening mechanisms operating at the nanoscale within the metallic matrix such as Orowan strengthening [13,14]. However, the effects of particle arrangement and particle damage on the mechanical response of these metal matrix nanocomposites (MMNCs), which may be different from that observed in conventional MMCs due to the different dominant strengthening mechanisms in both types of material, have not been widely explored even though experimental studies have reported that agglomeration of nanoparticles (i.e. formation into coarse clusters) has detrimental effects on the mechanical properties of MMNCs.

In this paper, the effects of particle arrangement and particle damage on the mechanical response of MMNCs will be investigated numerically using discrete dislocation simulations. This is because the size effect must be considered for MMNCs as the size of the particles is at the nanoscale and distance between particles approaches the mean free path of dislocations [15]. It is well known that classical plasticity laws are unable to capture the size effect and are only useful at characteristic sizes greater than 10 μm where the effect of individual dislocation processes is insignificant and the material can be viewed as homogeneous. At the nanoscale, dislocations should be accounted for in a discrete manner. For a range of characteristic size between tens to hundreds of nanometers, the discrete dislocation approach is one of the most suitable methods for investigating the mechanical response of a plastic material due to the collective motion of dislocations [16,17].

2. Discrete dislocation formulation

The discrete dislocation plasticity framework used in this study follows closely the formulation developed by Van der Giessen and Needleman [18] which is outlined here; further details and references are given in Ref. [18] and their subsequent works [19–21]. The nanocomposite is considered as 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: the dislocation field and the image field. The dislocation field is associated with the dislocations in their current configuration but in an infinite medium of the homogeneous matrix material; the solution for the dislocation field can be obtained from literature [22]. The image field corrects for the actual boundary conditions and the presence of particles, and can be solved as a linear elastic boundary value problem using the finite-element method.

Constitutive relations are used to describe the nucleation, motion and annihilation of dislocations. Firstly, assuming dislocation glide only, the force f which acts on a dislocation with Burgers vector magnitude b and causes it to move with velocity v along its slip plane is directly proportional to the resolved shear stress τ_{rss} acting on the dislocation. This can be expressed as $f = \tau_{rss} b = Bv$ where B is the drag coefficient. Furthermore, 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 and dislocations on other slip systems in blocking slip. A dislocation moving towards an obstacle or impurity will initially be pinned at the obstacle and can only bypass the obstacle when the resolved shear stress on the dislocation exceeds the strength of the obstacle or impurity τ_{obs}. Secondly, new dislocation pairs are generated by simulating Frank–Read sources: a point source located on a slip plane will generate a pair of opposite dislocations when the magnitude of the resolved shear stress at the source exceeds the nucleation strength τ_{nuc} during a period of time t_{nuc}. Thirdly, annihilation of two opposite dislocations occurs when they are within a material-dependent, critical annihilation distance $L_e = 6b$ [18]. However, in the present study, dislocation motion on every slip plane will be tracked to determine whether annihilation of dislocation occurs; once a pair of opposite dislocations has crossed paths, they will be considered as annihilated. This tracking method allows for the use of greater timesteps in the discrete dislocation simulations.

The discrete dislocation formulation is implemented in a two-dimensional plane strain unit cell model with periodic boundary conditions shown in Fig. 1. The unit cell contains equally spaced horizontal slip planes with the spacing between slip planes $d = 100b$. Due to the periodicity of the unit cell, dislocations exiting the unit cell through one side will re-enter through the opposite side. Simple shear deformation is applied on the unit cell through prescribed displacements along the top and bottom edges and the overall shear stress–strain response is computed. The overall or average shear stress τ_{ave} and average shear strain γ_{ave} of the nanocomposite are calculated, respectively, from the traction and displacement along the top and bottom edges of the unit cell. Computation of the deformation history, assuming small strain kinematics, is carried out in an incremental manner.

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