

Dislocation-Based Strengthening Mechanisms in a Nano-Particle Reinforced Composite

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ABSTRACT

The present paper presents a 3D numerical analysis of a nanoparticle reinforced crystalline metal using a multi-scale simulation technique: the Multi-scale Discrete Dislocation Plasticity (MDDP). This model couples two length scales: discrete dislocation dynamics (meso) and finite element analysis (continuum). The crystalline metal considered is aluminum and nano-sized SiC particles are used for reinforcement. An attempt is made to understand the change in mechanical properties of metal reinforced with nanoparticles from the viewpoint of dislocation theory using the MDDP simulation model. The formation of prismatic loops is observed and the increase of tensile strength and decrease in percentage elongation is explained based on this observation.

INTRODUCTION

The development of nano-particle reinforced composites commonly referred to as nanocomposites is on the rise since the last decade. Such composites hold the promise of advanced materials tailored to specific intended use and service requirements. While nanoparticles can be used to reinforce any matrix material, light weight metals such as aluminum and magnesium are excellent candidates for matrix material due to their inherent good balance of strength and weight with applications especially in automobile and aerospace industry.

As mentioned, aluminum and magnesium are the most popular metals among researchers to be reinforced with nanoparticles. Several different nanoparticles have been used for reinforcement mainly of ceramic origin. Ferkel and Mordike (2001) used SiC nanoparticles to reinforce magnesium using powder metallurgy techniques and studied the mechanical

properties of the nanocomposite using tensile and creep tests. The results reveal that 3% volume fraction of SiC nanoparticles give larger flow stress and lower creep rate to the pure magnesium. Lan et al. (2004) fabricated magnesium nanocomposites by reinforcing magnesium with SiC nanoparticles using ultrasonic method and reported that ultrasonication improved the dispersion of nanoparticles in the matrix and the microhardness of the nanocomposite. Wang et al. (2010) also used ultrasonic method to prepare SiC nanoparticles reinforced magnesium nanocomposites and investigated the effect of nanoparticles' mass fraction. It is noted that the improvement in mechanical properties is due to both grain refinement and strengthening effects by SiC nanoparticles. Sun et al. (2012) employed friction stir processing to prepare SiC nanoparticles reinforced magnesium alloy and reported a uniform dispersion of nanoparticles both inside the grain and along grain boundaries. An investigation into the effects of SiC nanoparticles showed significant increase in Vicker hardness (28%) and ultimate tensile strength (19%). Various aluminum alloys have also been used to nanoparticles' reinforcement and subsequent analysis. Yar et al. (2009) studied the effect of adding MgO nanoparticles to aluminum alloy (A356) with respect to the nanoparticles volume percent and casting temperature. They concluded that 1.5vol% MgO nanoparticles reinforcement and fabrication at 850°C provides uniformly dispersed nanoparticles and improved mechanical properties. Jiang and Wang (2015) and Jiang et al. (2016) investigated the mechanical properties of 7075 aluminum reinforced with SiC nanoparticles undergoing semisolid processing and concluded that the SiC nanoparticles volume fraction of more than 1% leads to degradation of yield and ultimate tensile strength. Jamalain et al. (2016) investigated SiC nanoparticles reinforced aluminum alloy prepared by friction stir welding. They reported results on parameters related to friction stir welding such as traverse speed/passes done for each weld and reported that single passes cause agglomeration of nanoparticles and therefore a reduction in percentage elongation and tensile strength. Multiple passes help to remove the agglomeration and percentage elongation is increased by as much as 71% after six passes. Harichandran and Selvakumar (2016) compared the effect of adding micro and nano B₄C particles to

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aluminum matrix and concluded that B₄C nanoparticles provide a better improvement to mechanical properties as compared to B₄C microparticles. A high-volume fraction of nanoparticle can help in improving properties like wear resistance, if desired.

Based on dislocation theory, plastic deformation is believed to occur as a result of dislocation motion on certain crystallographic slip planes. This motion causes dislocations to arrange themselves into certain structures and patterns, which therefore hold valuable information about the characteristics of the plastic deformation history. Therefore, the mechanical properties of nanocomposites in the plastic regime primarily depend on the existing microstructure including any reinforcing nanoparticles and their properties. The current study investigates the effect of volume fraction of the nanoparticles on the mechanical properties of nanocomposite as predicted by dislocation motion mechanism using a 3D multi-scale discrete dislocation plasticity model that has been developed over several years. The novelty of current studies in the fact that 3D multi-scale discrete dislocation plasticity simulations are used to analysis SiC nanoparticles reinforced aluminum alloy, and to look closely at the mechanisms responsible for strengthening.

MULTI-SCALE DISCRETE DISLOCATION PLASTICITY

Multi-scale Discrete Dislocation Plasticity (*MDDP*) has emerged as a powerful tool to analyze various dislocation mechanisms including interaction with other microstructural features (Zbib et al., 2003). The core of *MDDP* lies in coupling two lengths scales: micro (discrete dislocation dynamics analysis) and macro (continuum elasto-viscoplasticity finite element analysis). The description of the *MDDP* code used in the present study is as follows.

Discrete Dislocation Dynamics

In *discrete dislocation dynamics (DD)* simulations, the plastic deformation of a single crystal is obtained by explicitly accounting for the evolution of a multitude of dislocation loops and curves. The dislocations are discretized into segments of mixed character. The Peach-Koehler force acting on a dislocation segment is calculated from the stress field of all other dislocations and the applied stress. For a dislocation segment bounded by j and $j+1$, the Peach-Koehler force $\mathbf{F}_{j,j+1}$ on the segment is obtained by integration over the entire segment length L , such that:

$$\mathbf{F}_{j,j+1} = \left(\sum_{i=1}^{N-1} \frac{1}{L} \int_L (\sigma_{i,i+1}^D(p) + \sigma^a(p)) \cdot \mathbf{b}_{j,j+1} \right) \times \boldsymbol{\xi}_{j,j+1} dl + \mathbf{F}_{j,j+1-self} \quad (1)$$

where p is a field point on the dislocation segment $j,j+1$, N is the total number of nodes, $\sigma_{i,i+1}^D(p)$ is the stress from a remote dislocation

segment bounded by i and $i+1$, $\sigma^a(p)$ is any other externally applied stress plus internal friction (if any) and stress induced by other defects, $\mathbf{b}_{j,j+1}$ is the Burgers vector, $\boldsymbol{\xi}_{j,j+1}$ is the line sense vector, and $\mathbf{F}_{j,j+1-self}$ is the Peach-Koehler force corresponding to local interaction between the segment adjacent to $j,j+1$. Then, following standard finite element procedure and using linear interpolation shape functions over the segment, the Peach-Koehler force per unit length $\mathbf{F}_{j,j+1}$ is distributed equally to the nodes j and $j+1$. Thus, once all the forces are assembled, the net force on each node would have contributions from all the segments connected to it. The N dislocation nodes move simultaneously in the glide direction over a characteristic time corresponding to the least time increment required for an interaction to take place. The governing equation of glide motion for each dislocation node is nonlinear and given as:

$$m_i^* \dot{\mathbf{v}}_i + \frac{1}{M_i(T,P)} \mathbf{v}_i = \mathbf{F}_{iglide-component} \quad (2)$$

where m^* is the effective mass per unit dislocation length, M is the dislocation mobility which could depend on both temperature T and pressure P , $\mathbf{v}_i$ is the velocity of node i , $\dot{\mathbf{v}}_i$ is the acceleration, and $\mathbf{F}_{iglide-component}$ is the glide component of the Peach-Koehler force. Thus, the motion and interaction of an ensemble of dislocations in a 3-D crystal is integrated over time yielding macroscopic plastic distortion, which is defined as:

$$\dot{\boldsymbol{\epsilon}}^p = \sum_{i=1}^K \frac{l_i v_{gi}}{2V} (\mathbf{n}_i \otimes \mathbf{b}_i + \mathbf{b}_i \otimes \mathbf{n}_i) \quad (3)$$

where l_i is the segment length, $\mathbf{n}_i$ is a unit normal to the slip plane, v_{gi} is the magnitude of the glide velocity, K is the total number of segments and V is the volume of the Representative Volume Element (*RVE*). For further details of the *DD* code, please see Zbib et al. (1996, 1998) and Rhee et al. (1998).

Integrating Multi-scale Approach

Using *DD* for infinite domain problems, the computational cell as a whole is considered as an *RVE*, with either reflection boundary conditions (ensuring the continuity of the dislocation curve) or periodic boundary conditions (ensuring conservation of the dislocation flux across boundaries as well as continuity). However, for the simulation of a unit cell representing, say a grain or for finite domain problems, these models are no longer valid, and a more rigorous treatment of boundary conditions is required to account for dislocation image stresses. This issue has been addressed by developing a *3-D multi-scale model* that couples the microscale *DD* analysis with the continuum scale via a viscoplasticity model. In this model, the governing equations for the continuum scale are based on an *RVE* over which the deformation field is assumed to be homogeneous. On the macroscale, the material obeys the law of conservation of linear momentum:

$$\text{div} \mathbf{S} = \ddot{\mathbf{u}} \rho \quad (4)$$

and the energy equation:

$$\rho c_v \dot{T} = k \nabla^2 T + \mathbf{S} \cdot \dot{\boldsymbol{\epsilon}}^p \quad (5)$$

where $\mathbf{S}$ is the stress tensor, $\mathbf{u}$ is the particle displacement, ρ , c_v and k are the mass density, specific heat and thermal conductivity respectively. For elastoviscoplastic behavior, the strain rate tensor $\dot{\boldsymbol{\epsilon}}$ is decomposed into an elastic part $\dot{\boldsymbol{\epsilon}}^e$ and a plastic part $\dot{\boldsymbol{\epsilon}}^p$ such that:

$$\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}^e + \dot{\boldsymbol{\epsilon}}^p \quad (6)$$

For most metals, the incremental form of Hooke's law can be used to express the elastic response for large deformation and material rotation such that:

$$\overset{o}{\mathbf{S}} = [\mathbf{C}^e] \overset{o}{\boldsymbol{\epsilon}}^e, \overset{o}{\mathbf{S}} = \dot{\mathbf{S}} - \boldsymbol{\omega} \mathbf{S} + \mathbf{S} \boldsymbol{\omega}, \boldsymbol{\omega} = \mathbf{W} - \mathbf{W}^p \quad (7)$$

where $\mathbf{C}^e$ is a fourth order tensor, $\boldsymbol{\omega}$ is the spin of the substructure and is given as the difference between the material spin $\mathbf{W}$ and plastic spin $\mathbf{W}^p$. Combining Eqs. 11 and 12 leads to:

$$\overset{o}{\mathbf{S}} = [\mathbf{C}^e][\dot{\boldsymbol{\epsilon}} - \dot{\boldsymbol{\epsilon}}^p] \quad (8)$$

When coupling *DD* with *FE*, the principle of superposition is employed to correct for the actual boundary conditions, for both finite domain and homogeneous materials. The dislocations contained within the *RVE* give rise to an internal stress $\mathbf{S}^D$ (homogenized over the element) and the effective total stress within the *RVE* is the sum of the stresses by all external agencies and the internal stress $\mathbf{S}^D$. This way, the long-range stress is treated as internal variables, yielding an efficient numerical scheme. $\mathbf{S}^D$ is responsible for the energy stored in the material by virtue of presence of dislocations. With this approach, one can deal with mixed boundary conditions of cells containing complex dislocation structures. Details of the *MDDP* code can be found in Zbib and de la Rubia (2002). Please note that the *MDDP* code cannot simulate at atomic or molecular length scale and it can only simulate single crystals.

PROBLEM SETUP

The problem setup is shown in Fig. 1. The size of the *RVE* is the same in all directions, i.e., $L_x = L_y = L_z = 1.41 \mu\text{m}$. The origin of the reference frame coincides with the geometric center of the *RVE*. A set of five Frank-Read (FR) sources at each of the uniformly placed nine locations in the *RVE* are used as the initial dislocation configuration. FCC crystal structure is used to simulate aluminum, and the FR sources are randomly distributed on all slip planes. In addition, SiC particles of 30 nm size are randomly distributed in the *RVE* with three different volume fractions: 1%SiC, 2%SiC and 3%SiC. Several simulations are run to investigate the interaction of dislocations with nanoparticles and the effect of nanoparticles fraction on the mechanical properties. SiC nanoparticles are shown in blue colored dots while

the dislocations are shown in red colored lines in Fig. 1.

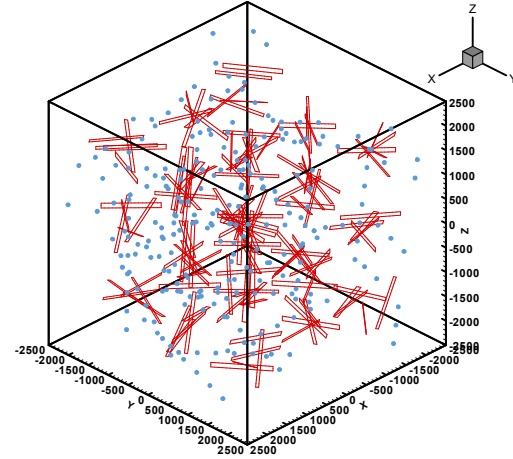


Figure 1: Problem configuration

RESULTS AND DISCUSSION

Figure 2a shows the configuration of the dislocations and nanoparticles after several steps. The SiC nanoparticles act as a hindrance to dislocation motion, which are multiplying and expanding due to the applied load. This hindrance may result in enough resistance to stop a dislocation from further motion thus effectively making it sessile or causing it to cross-slip to another slip plane.

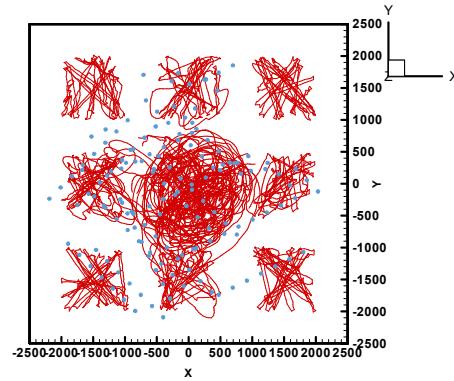


Figure 2a: Interaction between dislocations and nanoparticles

Of particular importance is the formation of prismatic loops as captured in the close-up shown in Fig. 2b. Such prismatic loops are sources of further hindrance to dislocation motion and thus reduce plastic deformation. Please note that Figs. 1 & 2 show problem configuration and results for 1%SiC nanocomposite. As obvious, the results with 2%SiC and 3%SiC will showcase more obstacles to dislocation motion and the odds of forming prismatic loops will also increase.

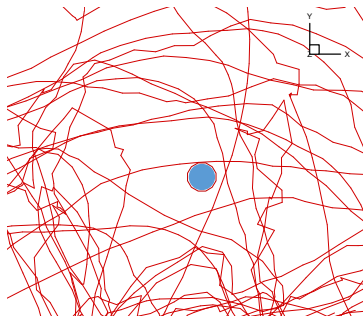


Figure 2b: Close-up from Fig. 2a: Formation of prismatic loop

Presumably, both of these factors should affect the stress-strain curve. Therefore, the stress-strain curves for non-reinforced aluminum and aluminum with 1%, 2% and 3% SiC nanoparticles were generated using the *MDDP* code, which are shown in Fig. 3.

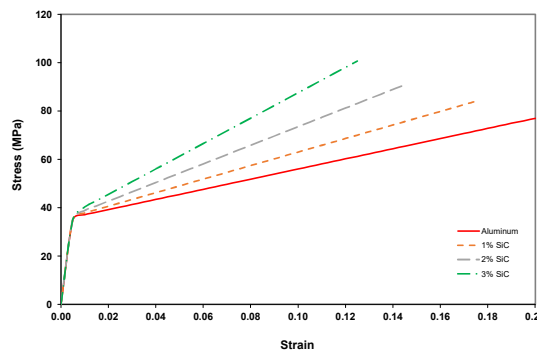


Figure 3: Stress-strain behavior

With increasing SiC nanoparticles fraction, it is observed that the tensile strength increases with a corresponding reduction in ductility. This is in accordance with the experimental observations and provides a plausible explanation for the observed phenomenon. Wang et al. (2010) has attributed the improvement in mechanical properties to both grain refinement and strengthening effects of nanoparticles. Though *MDDP* cannot simulate grain refinement, the mechanism of strengthening can be explained by the impedance caused by harder SiC nanoparticles and further through the formation of prismatic loops forming as a result of interaction between the expanding dislocations and nanoparticles. Figure 4 summarizes the effect on tensile strength and percentage elongation in each case. The relationship between the volume fraction of strengthening nanoparticles and mechanical properties appears to be linear, however a critical limit to the volume fraction of nanoparticles must exist at which the dislocations may not be able to interact with the nanoparticles or contribute to further plasticity. Jiang and Wang (2015) and Jiang et al. (2016) have predicted this to happen at 1% nanoparticles but they have worked on a different

aluminum alloy. This will be studied in further detail in future endeavors.

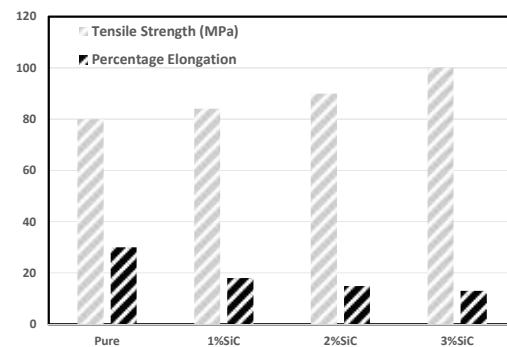


Figure 4: Effect of nanoparticles on mechanical properties

CONCLUSIONS

An attempt is made to understand the underlying strengthening mechanisms responsible for material behavior when nanoparticles are added to a crystalline metal. The formation of prismatic loops is observed along with stress-strain behavior indicative of experimental results. Further comprehensive results are needed to quantify the effect of nanoparticle addition to a crystalline metal while considering the dislocation multiplication and motion. The current study highlights the effectiveness of 3D multi-scale discrete dislocation modeling in understanding the underlying mechanisms contributing to the enhanced mechanical properties of nanoparticles reinforced metal matrix composites. Future studies will be performed to comprehensively and statistically quantify the strengthening mechanisms in nanocomposites.

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NOMENCLATURE

Symbol	Definition
$\mathbf{F}_{j,j+1}$	Peach-Koehler force on the dislocation segment bounded by j and $j+1$ nodes
N	Total number of nodes
$\sigma_{i,i+1}^D(p)$	Stress from a remote dislocation segment bounded by i and $i+1$ nodes
$\sigma^a(p)$	Externally applied stress and stress induced by other defects
P	Field point on the dislocation segment
$\mathbf{b}$	Burgers vector
$\mathbf{N}$	Unit normal to the slip plane
$\xi_{j,j+1}$	Line sense vector
$\mathbf{F}_{j,j+1-self}$	Peach-Koehler force on the dislocation segment bounded by j and $j+1$ due to local interaction with adjacent segments
m^*	Effective mass per unit dislocation length
v_i	Velocity of node i
v_{gi}	Glide component of velocity of node i
M	Dislocation mobility
$\mathbf{F}_{i\text{ glide-component}}$	Glide component of Peach-Koehler force
$\dot{\epsilon}^p$	Plastic strain rate tensor
$\dot{\epsilon}^e$	Elastic strain rate tensor
$\dot{\epsilon}$	Total strain rate tensor
l_i	Segment length
V	Volume of the representative volume element
K	Total number of segments
ρ	Mass density
c_v	Specific heat
k	Thermal conductivity
u	Particle displacement
$\mathbf{S}$	Stress tensor
T	Temperature
P	Pressure
C^e	Compliance
W	Material spin
W^p	Plastic spin
ω	Difference between material and plastic spin
$\cdot$	Represents time rate change of the quantity