Analysis of mechanical properties of nanocrystalline Al+α-Al₂O₃ composites using molecular dynamics simulation

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Abstract. In this article, mechanical properties of nanocrystalline Al+α-Al₂O₃ composites are investigated using molecular dynamics simulations. The configurations of matrix and volume fraction of α-Al₂O₃ may affect the mechanical properties of the particle reinforced metal-matrix composites and are taken into account. The potentials for the Al+α-Al₂O₃ system developed by Xin Lai et al. are adopted to depict the interactions between Al and α-Al₂O₃. Monocrystal Al and Bicrystal Al based α-Al₂O₃ particle reinforced nanocomposites are modelled respectively. Results show that: (1) volume fraction of the particles has no explicit effects on the elastic modulus and ultimate strength in both monocrystal Al and bicrystal Al based matrix nanocomposites, (2) disappearance of valley in the stress-strain curve of bicrystal Al results from existence of dislocation in matrix of various orientations.

1. Introduction
Over past decades, particle reinforced metal-matrix composites (PRMMCs) have became an important class of materials for their high specific modulus, high specific strength and good wear resistance [1]. The characteristics of mechanical properties of composites results from strengthening effect caused by ceramic particle embedding. To dominate mechanical properties of composites for application, investigation of strengthening effect on composites is necessary.

In PRMMCs, strengthening effects of ceramic particles mainly include following aspects [2]: (1) constrained plastic flow (dislocation) in the matrix, (2) load transferred to particles, (3) thermal history, (4) material texture, (5) grain size, and (6) volume fraction. The aspects (1), (2), and (3) construct the primitive mechanisms for strengthening PRMMCs directly. The last three aspects are relatively easier than the first three to be investigated and can provide specific parameters for further studying the first three aspects. In addition, they are convenient to realize in experiment and simulation.

Actually, to investigate strengthening effects of composites caused by the last three aspects, large amount of experimental and numerical simulations have been carried out [2-9]. However, results of experiments are mostly affected by more than three factors. Therefore, the relationship between single aspect and mechanical properties of material cannot be inferred. In simulation by FEM, although

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influence factor is contracted to texture of particles, but the results are unreasonable because of ignorance of affect of the interface between particle and matrix.

Nowadays, a simulation method named molecular dynamics (MD) which is based on atomistic system can remedy it by capturing the effect of interface accurately. Vikas Tomar et al. [10] investigate the impacts of volume fractions and grain sizes on mechanical properties of PRMMCs by MD. However, original GBs in their models are destroyed by particles. Three factors that consist of the interface between particle and matrix, GBs between metal and volume fraction of particles are considered.

To investigate strengthening effect accurately, we focus on the way to contract the number of factors from three to two by removing variable on GBs in metal. The present study is devoted to explore the effect of matrix texture configuration and volume fraction effect on composites properties by MD without any operation on GBs. Particle of \(\alpha\)-Al\(_2\)O\(_3\) reinforced matrix of Al composites, which are abundant in nature, are employed. The material properties of composites with alteration of matrix configuration and various volume fractions with the same particle are performed.

2. Computational Methods

2.1. Potential

In MD, the potential functions, which describe the interaction between atoms, are determinant factors for the reasonable results. The potentials, which are adopted in this article, are cited from previous work by the authors [11]. It consists of three parts: a. pure Al adopts EAM potential which is proposed by Mishin [12]; b. Buckingham potential proposed by Matsui for pure \(\alpha\)-Al\(_2\)O\(_3\); c. Interfacial interactions between Al and \(\alpha\)-Al\(_2\)O\(_3\) are given by the following formulas, which are divided into two parts: Al-Al interactions(2.1) and Al-O interactions(2.2).

\[
E_{\text{Al,Al}}(r) = 2\gamma f_0/b_{\text{Al}} b_{\text{Al}} c_{\text{Al}} \exp\left(\frac{-2\gamma}{b_{\text{Al}} c_{\text{Al}} - r} \right)
\]

\[
E_{\text{Al,O}}(r) = \gamma f_0/b_{\text{Al}} b_{\text{O}} c_{\text{Al}} \exp\left(\frac{-\alpha_{\text{Al,O}}}{b_{\text{Al}} c_{\text{Al}} c_{\text{O}} - r} \right) + \gamma \beta_0 D_{\text{Al,O}} c_{\text{Al}} \exp\left(-2\alpha_{\text{Al,O}}(r - r_{\text{Al,O}})\right) - 2c_{\text{Al}} \exp\left(-\alpha_{\text{Al,O}}(r - r_{\text{Al,O}})\right)
\]

In which, \(\gamma = 1.65\), \(\beta_0 = 0.4\) and \(\beta_{\text{Al}} = 1\), while some relevant potential parameters can get from table 1.

| Table 1. Potential parameters |
|-----------------------------|
| \(f_0(b_i + b_j)\) (kcal/mol\(^{-1}\)) | \(a_i + a_j\) (0.1 nm\(^{-1}\)) | \(1/(b_i + b_j)\) (10/1 nm) | \(D_{ij}\) (kcal/mol\(^{-1}\)) | \(\alpha_{ij}\) | \(r_{ij}\) (0.1 nm) |
|-----------------------------|
| Al-O 0.2903 3.0493 3.4445 21.6893 2.0 1.8 |
| O-O 0.3604 3.7766 2.7775 0 - - |

2.2. Modeling

As illustrated in Figure 1, two groups of models are employed for the MD simulations. A few particles that are depicted by yellow balls with the same radius (23.736 Å) and the same orientation are embedded in monocrystal Al in uniform simulation box (129.6 Å×129.6 Å×129.6 Å), as shown in Figure 1(a). We mark them 1-1 for one particle, 1-2 two particles, 1-3 four particles and 1-4 eight particles, volume fraction of \(\alpha\)-Al\(_2\)O\(_3\) in them are 2.57%, 5.14%, 10.28% and 20.56% respectively. The other parts of the box excluding the particle(s) are filled by monocrystal Al with the orientation of [100]Al//X-axis, and [001]Al//Z-axis. To demonstrate the details of the orientation relationship between matrix and particles, sketch of model 1-1 in Figure 1(a) are shown in Figure 2. The mid cross-section in Figure 1(a) is shown in Figure 2(b), in which Al and \(\alpha\)-Al\(_2\)O\(_3\) have an orientation relationship of [100] Al // [210] \(\alpha\)-Al\(_2\)O\(_3\) and {020} Al // {100} \(\alpha\)-Al\(_2\)O\(_3\).

Models of bicrystal Al based composites are constructed as displayed in Figure 1(b). Different from monocrystal models, the same box as Figure 1(a) is divided into eight sections, in which, Al in part two, three, five and eight have the same orientation with first four models, while remain parts being
rotated about the Y axis compared to monocrystal models that leads orientation of X-axis varied from [100] Al to [10] Al.

Four particles which are the same as particles in Figure 1(a) are embedded into part three, two, five and eight one by one, we mark them 2-1, 2-2, 2-3 and 2-4 respectively, volume fraction of $\alpha$-Al$_2$O$_3$ in them are 2.57%, 5.14%, 7.71% and 10.28% respectively.

![Image](a) ![Image](b)

**Figure 1.** Two group models which are adopted for (a) monocrystal Al based and (b) bircrystal based composites respectively.

![Image](a) ![Image](b)

**Figure 2.** (a) Sketch of model 1-1 in Figure 1(a), the mid cross-section which is highlighted by black line in (a) is re-drawn at (b).

2.3. Simulation Methods

The simulations in this paper are carried out on conditions of periodic boundary conditions (PBCs) in three dimensions at room temperature (300K). A time step is set to 0.0005ps and pressure is 0Pa. To get a reasonable model configuration, equilibration is performed 30000 time steps with isothermal-isobaric (NPT) ensemble. After model configuration gets a steady condition, tension is applied to models along X-axis. In addition, for convenience and saving of calculation cost, the strain rate is set to 109/s.

The central symmetry parameter (CSP) [14] proposed by Kelchner et al. is adopted to identify the dislocation nucleation and visualize dislocations, and usually, atom is identified as defective while value of CSP is higher than six.

3. Results and Discussion
3.1. Relaxation
To search nanocrystalline composites after equilibration, Figure 3 shows atom configuration of monocrystal Al (1-1) and bicrystal Al (2-1) based composites contain one particle with atom coloured by CSP approach. The α-Al2O3 in composites is found to have amorphous structural order after relaxation, which is impossible to identify defect atoms by CSP. Defect analysis will focus only on the Al phase.

![Atom configurations after equilibration: models (a) 1-1 and (b) 2-1.](image)

Figure 3. Atom configurations after equilibration: models (a) 1-1 and (b) 2-1.

To investigate the distribution of interior dislocation in Figure 3(b), the origin of coordinates is adjusted. The area, which red square enclosed, is the mid cross-section of part three while black line is the outline of mid cross-section of particle shell. According to CSP, the dislocation is only distributed at interface between matrix and particle in model 1-1, whereas the dislocation in model 2-1 exists at both interface and GBs. The particle and interface at GBs keep steady as original location that makes the models reliable.

3.2. Monocrystal Al+α-Al2O3

![Stress-strain curves for monocrystal Al based composites with various volume fractions of 0.57%, 5.14%, 10.28% an 20.56% respectively for models 1-1, 1-2, 1-3 and 1-4.](image)

Figure 4. Stress-strain curves for monocrystal Al based composites with various volume fractions of 0.57%, 5.14%, 10.28% an 20.56% respectively for models 1-1, 1-2, 1-3 and 1-4.
In Figure 4, stress-strain curves of tension along X-axis about monocrystal Al based composites are illustrated together. To investigate the relationship between stress-strain curves and material structure, atom configurations of model 1-1, which are coloured by CSP, are illustrated at three specific strains in Figure 5.

In the article, the stress in the simulation is calculated over current volume. Therefore, it corresponds to true stress. The strain is calculated based on the variation in the current volume of periodic simulation cell, and therefore corresponds true strain. Due to non-linear nature and insufficient equilibration, the elastic modulus necessitates a compromise between having enough data for a reliable fit and staying within the linear region. It is found that a reasonable compromise is to use strain of 0.1%–1% for all models. Results show that, all of materials have the same elastic modulus (116GPa) which are calculated from the slope of line AB (0.1% strain to 1% strain). The range of strain is different from the traditional strain, which is defined as 0%–0.2%. This perhaps results in a slightly misestimate of elastic modulus.

Strain hardening starts at strain of 3.44% (Point C) in Figure 4, from that on, more particles lead less stress at the same strain level, which is different from substitute of particles in macro-compositing, here particles bring composites more misfit dislocation (Figure 5(a)). Therefore, model 1-4 has the smallest slope in strain hardening stage. With the dislocation piling, the curve goes to the first peak. Then, with the dislocation loops emitting (Figure 5(b)), composites start to soften, while tendency of strengthening is covered by softening effect. The structure goes to another relative steady condition once dislocation loops encounter with former dislocation and structure (Figure 5(c)). At this stage, three in four models have explicit valley in curves, which results from emission and pile of dislocation. Model 1-4, which contain particles of volume fraction of 20.56%, have no valley because the dislocation is blocked by particle and large amount of dislocation.
In simulation, with particle embedding, the interface between particle and matrix is formed. Misfit dislocation caused by interface affects the material properties of composites greatly. Materials in experiment and manufacture contain large number of defect. Such nature decreases ultimate to a small level. Matrix is so weak that the embedded particles reinforce the matrix properties obviously. Compared with results using Finite Element Method (FEM) by Y.W. Yan et al. [4], the ideal interface of particle and matrix is perfect. They identify the ideal results ignoring misfit dislocation, which closely affects material properties. Compared with simulation by molecular dynamics (MD), Vikas Tomar et al. investigate the tensile deformation of PRMMCs [10]. They replace the original nanocrystalline with reinforced material. The interface of reinforced material coincides with original GBs. The weakening effect is confused by misfit dislocation caused by GBs. The results from experiments, simulations by FEM and MD previously contain many extra factors. The relationship between interface and material properties is buried in many factors.

The authors have calculated tensile strength of pure monocrystal Al (9.03GPa) in orientation of [100] using the potential which is used here. In this article, we find that embedded particle lessen it to 6.5GPa–6.8GPa, and not changed with particle embedding and volume of particles. Accordingly, existence of original dislocation is a decisional factor inducing Al [100] to get a steady strength (6.6GPa) on average where dislocation distributes. Combination of monocrystal $\alpha$-Al$_2$O$_3$ and his interface have the strength of 6.6GPa and elastic modulus of 116GPa.

### 3.3. Bicrystal Al+$\alpha$-Al$_2$O$_3$

![Stress-strain curves for bicrystal Al based composites with various volume fractions](image)

**Figure 6.** Stress-strain curves for bicrystal Al based composites with various volume fractions, for convenience to investigate, we prepare (a) whole curves and (b) locally zoomed out curves of (a).

Figure 6 shows stress-strain curves of bicrystal Al based composites with various volume fractions and pure bicrystal. Figure 6(b) shows the locally magnified curve of Figure 6(a) by black dotted line. Figure 7 shows atom configuration of pure bicrystal Al and model 1-1 at specific strain. The orientation of figures is the same as Figure 3(b).

Results of pure bicrystal Al have the strength of 6.6GPa and elastic modulus of 107GPa which are both close to the properties of combination of monocrystal $\alpha$-Al$_2$O$_3$ and his interface. With particle embedding, elastic modulus and ultimate tension strength of composites are supposed to will not change greatly. In addition, it is verified by stress-strain curves.

Although results show that the same elastic modulus and strength which is a starting and ending at curves are almost the same in models, the processes of strain hardening are different, e.g. pure bicrystal Al. In pure bicrystal Al base composite, there is a small valley in a stress-strain curve which results from large amount of original dislocations caused by GBs in structure (Figure 7). The dislocation starts to emit at place, which is enclosed by red line in Figure 7. When dislocation reaches a steady condition (Figure 7), the curve gets to valley. The particles affect the GBs around (red line in
Figure 7). Once particles are embedded to matrix in bicrystal, the valley disappears, which results from import of dislocation in interface of particles.

According to Griffith’s theory [15], the theoretical strength should be a material constant, closely related to the energy of cohesive bone, with a value of order E/10 for all solids, where E is elastic modulus. In this article, the ratios between elastic modulus and strength in composites are all 6% which means the results are valid and reliable. The results are lower than ideal value (10%). That should result from calculation misestimate. Nevertheless, the ratios are at the same magnitude, which agree with the theory and verify it.

4. Conclusions
The present study is devoted to investigate the impact of matrix texture configuration and volume fraction on mechanical properties of PRMMCs by MD without any operation on GBs.

After equilibration, nanocomposites keep steady as original with the interface between metal and particle homogenized. Good stability on equilibration verifies the reliability of models. Volume fraction of particles has no explicit effect on elastic modulus and tensile strength of monocrystal Al[100] and bicrystal Al based composites since embedded particles are employed with interface dislocation. Strength of all the models has a value of 0.06E, which is slightly lower than E/10 in Griffith’s theory which may result from calculated misestimate. Existence of original dislocation is a decisional factor inducing pure monocrystal Al[100] to get a steady strength about 6.6GPa on average and elastic modulus of 107GPa. Dislocation emits from the interface between particle and matrix for
monocrystal Al based composites while start from GBs for bicrystal Al based composites. Disappearance of valley in the stress-strain curve of bicrystal Al results from import of dislocation in interface of particles.

The observations reported here provide important data and insights for further realization of strengthening effect.

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