Molecular Dynamics Simulation on Characteristics of Nano-sized Nickel Aluminide Dispersoids in Aluminum Matrix

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ABSTRACT

Molecular dynamics simulations were performed on the morphology of the interfaces between intermetallic nano-sized dispersoids of Ni_3Al and $NiAl$, and a pure aluminum matrix. The lattice constants of dispersoids were initially set to be identical to that of pure aluminum. The results with the Ni_3Al dispersoid demonstrate the presence of strong strain fields in the vicinity of coherent interface as the lattice constant of Ni_3Al is smaller than that of pure aluminum. It is also seen that a noticeable degree of disorder is introduced in the aluminum matrix near the incoherent Ni_3Al/Al interface. Hence, Ni_3Al is expected to be an effective strengthener for the nanocomposite system of Ni_3Al/Al. Having eight nearest neighbors, the atoms in $NiAl$ are not as strongly bonded as in Ni_3Al, where each atom is surrounded by twelve nearest neighbors, a $NiAl$ dispersoid disintegrates by interacting with the matrix while attempting to decrease its lattice spacing during the simulation.

Keywords; molecular dynamics, EAM potential, inter-metallic compounds, dispersoids

1. INTRODUCTION

Small second phase particles dispersed uniformly through out the bulk of an alloy enhance its strength by impeding dislocation motion. Such is accomplished by either mechanically mixing these particles with the matrix material or precipitating second phase particles from a supersaturated solution. The former provides independent controls of the size, type, morphology, and volume fraction of the particles called as dispersoids. For the present study, we selected Ni_3Al and $NiAl$ dispersoids and embedded them in pure aluminum matrix to form nanocomposites.

It is expected that the characteristics of the interface between the dispersoid and matrix play a critical role on the overall mechanical properties of a nanocomposite system.

The particular concern of the present study is the morphology of the lattice in the vicinity of the dispersoid/matrix interface. It is expected that the lattice will be distorted near a coherent interface due to the difference in the lattice constants of dispersoid and matrix. Also expected is a certain degree of disorder present in the aluminum matrix near the region of incoherent interface due to the formation of dangling bonds at the surface.

The following section presents the details of the molecular dynamics simulation processes involved in the current study. The simulation results are presented and discussed in section 3 followed by summary and conclusion.

2. DETAILS OF SIMULATION

Dispersoids were constructed at the center of an aluminum block consisting of 10 x 10 x 10 face-centered unit cells by modifying the atomic arrangements within a given radius. The lattice structure of Ni_3Al is known as Ll_2 which has an aluminum atom at each cube corner and a nickel atom at the each face-center [1]. On the other hand, the lattice structure of $NiAl$, known as B2, has an aluminum atom at each cube corner and a nickel atom at the body-center [1]. For simplicity, the rotation of dispersoid was limited to about the z-axis.

The modified embedded atom (EAM) potential by Baskes [2] was selected for this study since it provides an explicit expression for binary systems and all the necessary parameter values for a range of atoms. The lattice constants of the dispersoids were initially set to be identical to that of the pure aluminum leaving the task of finding the proper lattice constants of the dispersoid up to the system. The interaction among the atoms was limited to those of nearest neighbors for the present work. For the main simulation of this study, the radius of dispersoid was kept 2.88 times the cube edge of aluminum, i. e., about 1.3 nm.

Fig. 1 shows initial arrangement of lattices of the Ni_3Al/Al composite system containing a fully coherent interface, i. e., no rotation of dispersoid with respect to that of matrix is involved at all. The shape of dispersoid shown here is rather close to an octagon instead of a circle. A simple test shows that the radius has to increase by two

orders of magnitude to obtain a reasonably round dispersoid.

Simulations were performed by increasing the temperature from 300K to 1100K for the Ni₃Al/Al composite and the extent of disorder was calculated for the case of forming a coherent interface. As shown in the following section, unexpected but interesting results were obtained for other cases.

3. RESULTS AND DISCUSSION

Fig. 2 shows the results of a simulation for Ni₃Al/Al with a coherent interface at T = 300K. The aluminum matrix in this figure is seen to be distorted in region close to the interface as well as that of dispersoid. To provide a more clear view of distortion of the lattice planes, the atoms in Fig. 2 were connected by lines as show in the next figure. The results of Fig. 3 are a classic case of lattice strain field due to a second phase particle embedded in a matrix with a larger lattice constant [3, 4].

In Ni-Al alloys, Ni₃Al precipitates form in NiAl matrix. The former is known as the γ' phase and the latter is known as the γ phase. Both are face-centered cubic and their lattice constants differ by only about 0.5%. The yield strength of a solution heat treated, hence containing a considerable fraction of γ', Ni-14Al alloy is 40 ksi, which is twice that of pure γ'. Therefore, it is not the intrinsic strength of γ' but instead the lattice strain due to such a small mismatch is known to be the source of the noticeable increase in the yield strength [3].
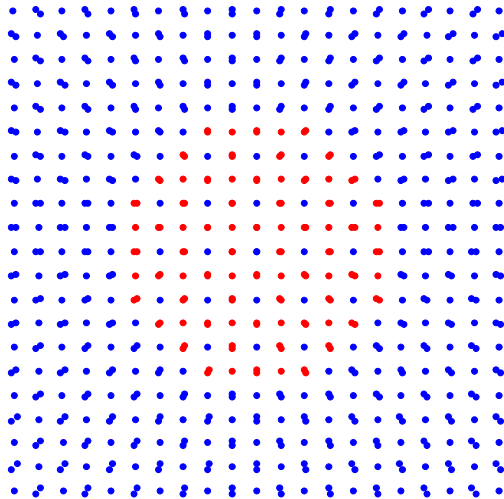
Therefore, a rather severe lattice strain field seen in Fig. 3 is expected to impede dislocation motion resulting in substantial increase in the strength of an aluminum alloy.

There exist other issues related to strengthening. Cutting dispersoids by dislocations creates extra interfaces and the cutting will be strongly resisted if the interface energy is high. Also important is the stability of dispersoids, i. e., they should not coarsen to lower the their density thereby increasing the
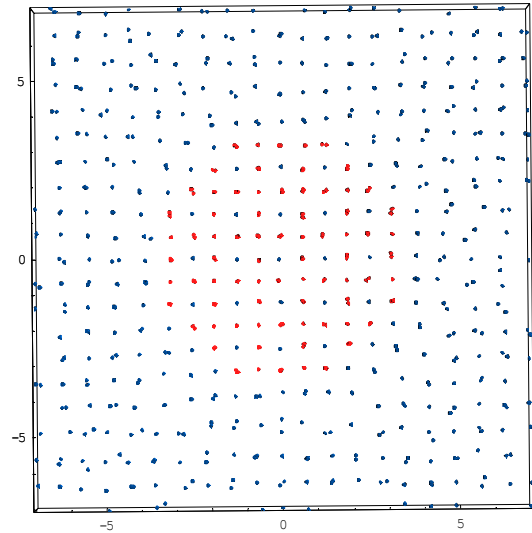

Fig. 2. Results of simulation with a Ni₃Al/Al composite system at T = 300K. A strong lattice strain field is seen in the matrix as well as in the dispersoid.
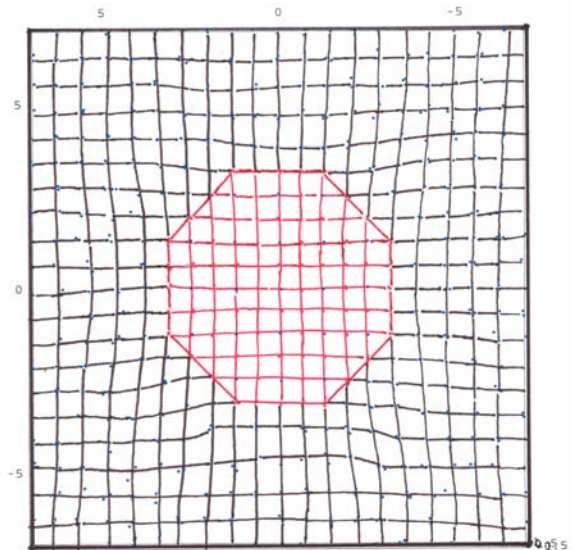

Fig. 3. Lattice planes in the Ni₃Al/Al composite system of Fig. 2. The strain fields both in the matrix and dispersoid can be seen more clearly in this figure.

Fig. 1. The initial atomic arrangements forming a coherent interface in a Ni₃Al/Al nano-composite. The atoms in the xy-planes are viewed for -0.5 a ≤ z ≤ 0.5 a, where a is the length of the FCC unit cell edge. Red dot represent nickel atoms and blue dots represent aluminum atoms.

average neighboring dispersoid distance allowing dislocations to pass by bowing. The former needs to be computed by an other means while latter is not a concern since, unlike precipitates, dispersoids are not created through a diffusion-induced phase transformation.

As the temperature increases, the lattice strain relaxes. In order to present the degree of lattice strain systematically, an order parameter, as defined below, is evaluated for different regions of the Ni$_3$Al/Al nano-composite at different temperatures. The order parameter given by Verlet for an FCC lattice has the following expression [5]:

$$\lambda = \frac{1}{3}[\lambda_x + \lambda_y + \lambda_z]$$

where $\lambda_x = \frac{1}{N}\sum_i^N \cos\left(\frac{4\pi x_i}{a}\right)$ and a is the length of the cube edge of the FCC unit cell. It is obvious that the above expression concerns with the deviation of each atom from the lattice sites instead of the correlation between neighboring atoms. Hence, the lattice strain directly contributes to the parameter value.

Fig. 4 shows the variation of order over different regions over the temperatures. The curve in the bottom of this figure represents the order in a region in the immediate vicinity of the interface (R < r < 1.2R) where R is the radius of dispersoid. Obviously, in this region the major contribution to disorder comes from the lattice strain at 300 K. The upper two curves show the temperature dependence of the order parameter of the regions, i. e., the region beyond the dispersoid radius (■) and that beyond 1.2 R (▲). The similarity of two upper curves confirms that the lattice strain very localized to the area of the interface. Beyond T = 450K, the temperature dependence is essentially the same for the all three curves. However, the effect of lattice strain is seen to persist for all temperature as evidenced by the constant shift of the bottom curve from the other two.
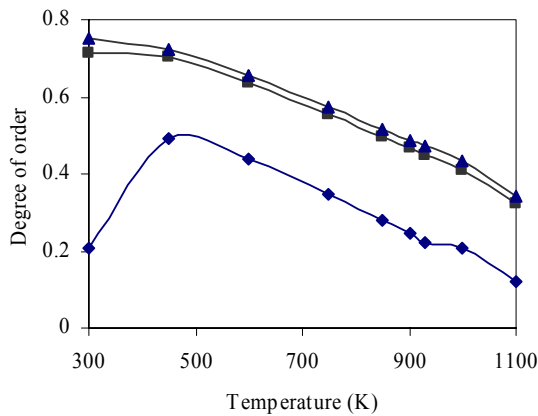
Fig. 5 shows the results of a simulation for the Ni$_3$Al dispersoid which is rotated about the z-axis 45° with respect to the matrix lattice. The rotation of the dispersoid inevitably creates some empty space between the dispersoid and matrix. Nevertheless, the fact to be emphasized is that a noticeable degree of disorder is introduced in the matrix lattice in the region where the matrix and dispersoid interact. The occurrence of such is, of course, expected since the matrix aluminum atoms at the interface do not have neighboring atoms of dispersoid to maintain the regularity in their positions.

It is expected that the disorder in the lattice near the interface impede dislocation motion. Nonetheless, the lattice orientation of dispersoid being different from that of the matrix, a dislocation moving in the slip plane of matrix will not easily find a proper slip plane in the dispersoid lattice to continue its motion. Therefore, such an incoherent dispoerosid itself can be an effective barrier impeding dislocations providing the alloy strength.

Fig. 6 presents the results of a simulation for a NiAl/Al nanocompostie system at 300 K. As in the case of Ni$_3$Al/Al, the lattice constant of the dispersoid was initially set to be the same as that of the matrix. During the simulation, NiAl tends to shrink but its interaction with martrix atoms also tends to maintain the original lattice size. Apparently, the atoms in the NiAl lattice are not bonded as strongly as those of Ni$_3$Al and the NiAl dispersoid destroys itself by interacting with the matrix. To demonstrate this point, simulations were repeated with a reduced interaction between the matrix and dispersopid. Fig. 7 shows the results obtained by reducing the NiAl lattice to 85% of the aluminum lattice constant. With a minimal interaction with the matrix, the NiAl lattice is seen fairly agitated even though it was not totally destroyed as in the results of Fig. 6.
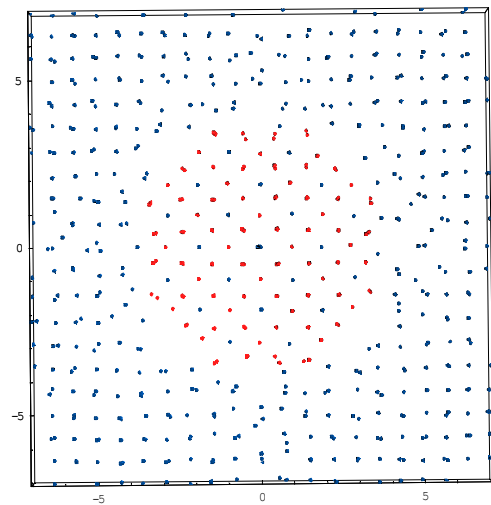

Fig. 4. Temperature dependence of the order parameter in selected regions in the Ni$_3$Al/Al nano-composite. See text for details.

Fig. 5. Results of simulation on the Ni$_3$Al/Al nano-composite with the dispersoid rotated about the z-axis by 45°.

By reducing the matrix/dispersoid interaction further, as seen in Fig. 7, the complete NiAl lattice is restored when the initial NiAl lattice constant is initially set to 75% of that of pure aluminum. The results of Fig. 6 and 7 are acceptable from the simulation point of view but these are not a possible scenario in actual material processes.

4. SUMMARY AND CONCLUSION

In the present study, molecular dynamics simulation was performed on nano-composite systems of Ni_3Al/Al and NiAl/Al with the intermetallic aluminide particles
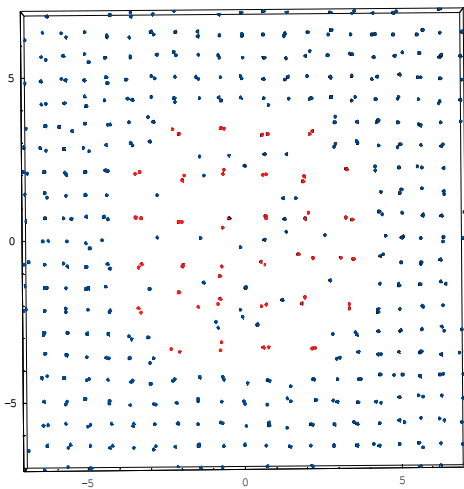

Fig. 6. Results of simulation on the NiAl/Al nano-composite at 300K. Due to the interaction with the matrix that tends to keep the original lattice constant of pure aluminum, the weakly bonded NiAl lattice self-disintegrates.
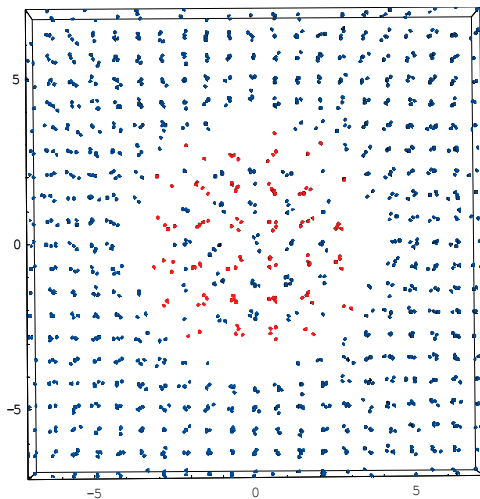

Fig. 7. Results of simulation at 300K with a minimal matrix/dispersoid interaction accomplished by reducing the initial NiAl lattice constant to 85% of that of pure aluminum.
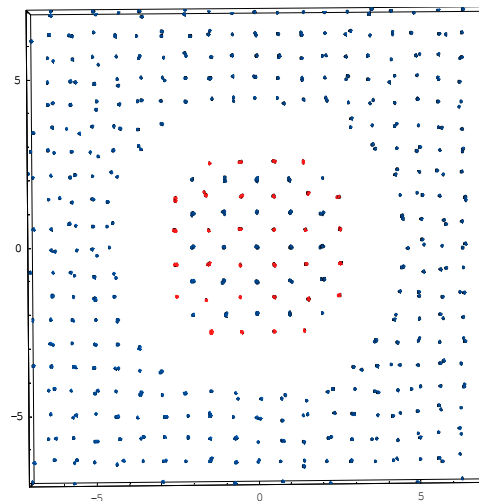

Fig. 8. Results of simulation at 300K without the matrix/dispersoid interaction by reducing the initial NiAl lattice constant to 75% of the pure aluminum lattice constant. The NiAl lattice is seen to preserve an undisturbed lattice structure.

embedded in the aluminum matrix. A severe lattice strain field is observed in the Ni_3Al/Al system forming a coherent interface while considerable disorder in the matrix is observed in the system forming an incoherent interface. The formation of a NiAl/Al system turned out to be a challenging task due to the insufficient bondimg among the atoms in the dispersoid.

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