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## Molecular Dynamics Simulations on Nanocomposites Formed by Intermetallic Dispersoids of $L1_2$ Type and Aluminum Matrices

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### ABSTRACT

Molecular dynamics simulations were performed to characterize the lattice morphology in the region adjacent to the interfaces in nanocomposite systems of a  $Ni_3Al$  dispersoid embedded in Al matrix ( $Ni_3Al/Al$ ) and an  $Al_3Nb$  dispersoid embedded in aluminum matrix ( $Al_3Nb/Al$ ). A nearly perfect coherent interface is obtained in the  $Al_3Nb/Al$  system with the lattice planes of dispersoid and matrix aligned parallel in all directions. The simulation results show the presence of the matrix atom-depleted regions near the dispersoid boundary for most cases. Detailed analysis revealed that certain sites immediately next to the dispersoid are energetically favored for the matrix atoms to occupy. The matrix atoms occupying these sites attract other atoms producing the depleted regions. In certain specific situations of  $Al_3Nb/Al$  system, however, the wetting of a rotated dispersoid is overwhelmingly complete prompting the need of further study for better understanding. The order parameters of dispersoids calculated for  $Ni_3Al$  in aluminum is nearly constant while that for  $Al_3Nb$  in aluminum is rapidly decreasing function of temperature in the range of 300 to 1800K.

### INTRODUCTION

Second phase particles that are mixed and uniformly distributed within a matrix are called dispersoids. By selecting appropriate type, size, morphology, and concentration of these dispersoids in a matrix, it may be possible to develop structural components that are capable of actively indicating their physical/chemical states and are optimized for best performance based on given application purpose. For example, the magnetic properties of  $Ni_3Al$  particles can be affected by the local stress states that may be indicative of the changes in other material states. At the same time, when mixed with a substantial volume fraction, the small nearest neighbor distance between such densely populated dispersoids may prevent the dislocation loop formation while being highly resistant to cutting by dislocations [1]. The current series of investigation concentrates on the morphology of such composites to establish a foundation for systematic study on nanocomposite systems of damage indicating capabilities and prolonged service lives.

Our previous study clearly showed that a  $Ni_3Al$  dispersoid, which is coherent with the aluminum matrix, causes a substantial degree of local lattice distortion in the vicinity of matrix/dispersoid interface [2] that is known to enhance the strength of alloys [1]. An unresolved problem of the study was the appearance of lattice atom-depleted regions near the interface in the composite system with a rotated dispersoid and its origin was not well understood. Therefore, the purpose of the present study is to find ways of minimizing the

regions of matrix atom depletion near the interface and closely investigate the nature of these regions.

The lattice structure of  $\text{Ni}_3\text{Al}$  is known as  $\text{L}_{12}$  which possesses a cubic symmetry. Being paramagnetic in nanosize [3], the magnetic field effects of  $\text{Ni}_3\text{Al}$  particles are not considered in the present simulation. The stable phase of  $\text{Al}_3\text{Nb}$  is known to be  $\text{D0}_{22}$  structure which is tetragonal instead of cubic  $\text{L}_{12}$  [4]. Nevertheless, we choose the metastable  $\text{L}_{12}$  phase of  $\text{Al}_3\text{Nb}$  in the present study for two reasons. First, maintaining the cubic symmetry of the system, the simulation results can be directly compared between the two systems of  $\text{Ni}_3\text{Al}/\text{Al}$  and  $\text{Al}_3\text{Nb}/\text{Al}$ . Second, by varying the physical and chemical states of the metastable system, some unexpected but interesting facts may be found.

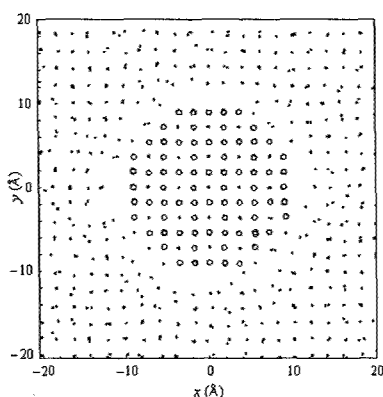
## DETAILS OF SIMULATIONS

For each system of  $\text{Ni}_3\text{Al}/\text{Al}$  and  $\text{Al}_3\text{Nb}/\text{Al}$ , a dispersoid is constructed at the center of a cubic block of pure aluminum. Simulations are first performed by arranging the lattice planes of dispersoid and matrix parallel in all three axes of Cartesian coordinates. Then the dispersoid lattice is rotated with respect to that of the matrix. As an initial investigation of a systematic study on nanocomposites, the rotation of the dispersoids in the present study is limited to the x-y plane and three angles of rotation, i. e.,  $15^\circ$ ,  $30^\circ$  and  $45^\circ$ . Also in this study, the dispersoid lattice spacings are initially set to be very close to their real values, i. e., 0.357 nm for  $\text{Ni}_3\text{Al}$  and 0.384 nm for  $\text{Al}_3\text{Nb}$  compared to 0.405 nm for pure aluminum. The inner radius of matrix and the outer radius of dispersoid are chosen to allow partial overlap between two lattices. The overlapping lattice points are removed to ensure a minimum separation among the atoms in the interface region. With further adjustment of these radii, the two-dimensional dispersoid boundaries in the x-y planes are selected to be Ni-only edges for  $\text{Ni}_3\text{Al}/\text{Al}$  and Al-only for  $\text{Al}_3\text{Nb}$ . The simulations are performed in the temperature range of 300 -1800K based on the temperature-independent parameter values for a modified embedded atom method (EAM) potential given by Baskes [5].

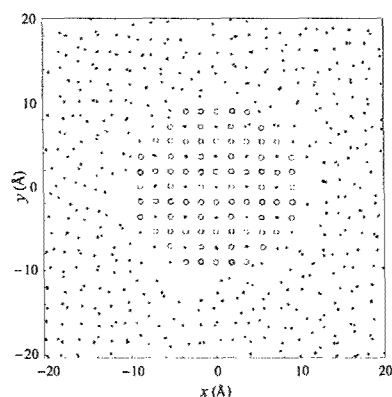
## RESULTS AND DISCUSSION

Fig. 1 shows the results of simulations performed at 300 K on the  $\text{Ni}_3\text{Al}/\text{Al}$  system with their lattice planes arranged parallel in all three directions. Shown are the atoms in three planes of (001) centered at  $z = 0$ . The hexagons and tiny dots in this figure represent Ni and Al atoms, respectively. Similar results obtained at 900 K are shown in Fig. 2. The presence of the matrix atom-depleted regions around the dispersoid is clear in the results of these two figures. One of the goals of the present study is to find the origin of such matrix atom-depleted regions at the interface, and a simple model has been established and applied to the results of Figs. 1 and 2, as explained in the following.

The dispersoids shown in Figs. 1 and 2 are almost octagons and two types of edges are found in their boundaries; those consisting of four nickel atoms and the others consisting of five nickel atoms, which we call the four-atom edges and five-atom edges, respectively, for brevity. Upon a close inspection, one finds that three matrix aluminum atoms are lined up immediately next to the four-atom edges.



**Figure 1.** Simulation results of the  $\text{Ni}_3\text{Al}/\text{Al}$  composite system at 300K without rotating the dispersoid.



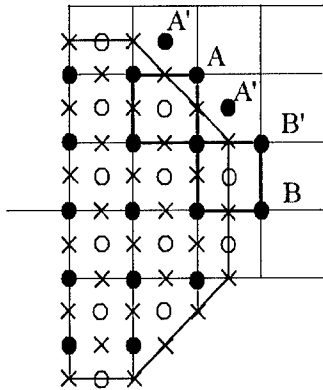
**Figure 2.** Simulation results of the  $\text{Ni}_3\text{Al}/\text{Al}$  composite system at 900K without rotating the dispersoid.

Fig. 3 shows lattice sites near the interface for the matrix aluminum atoms to occupy. Referring the results of Figs. 1 and 2, it is clear that the sites A and A' next to a four-atom edge are energetically more favored than B and B' which are next to a five-atom edge. In Fig. 3, one can see that an aluminum atom in site A has four dispersoid Ni atoms, denoted by x, at the nearest neighbor distance. The same applies to an aluminum atom occupying site B. The important difference is that a complete two-dimensional unit cell is formed when an aluminum atom occupies site A. Once this occurs, A' is the next favorite site for occupation since there are four nickel atoms at the nearest neighbor distance and there exists an aluminum atom at site A to lower the energy of site A'. Along the other edge, however, both B and B' sites have to be occupied by two aluminum atoms simultaneously to form a unit cell and such an occurrence has a much lower probability than that of occupying sites A and A' in sequence. In addition, site B' has only two Ni atoms at the nearest neighbor distance and the probability of occupation is even lower for this site. Hence, the matrix aluminum atoms tend to occupy the sites immediately next to the four-atom edges. This argument is based on a two-dimensional picture but it is trivial to extend the logic to a three-dimensional situation.

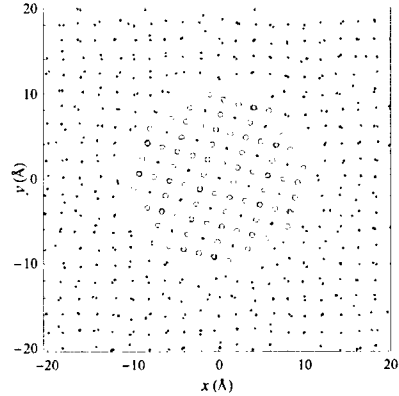
The aluminum atoms executing random motion in the interface region arrive at sites A and A'. Once the aluminum atoms occupy sites A and A', they attract other aluminum atoms causing matrix atom-depleted regions near the other edges of dispersoid boundary. The validity of this argument is supported by the absence of such unit cell formation activity by the matrix aluminum atoms when the symmetry of the system is reduced as shown in the results of Fig. 4 obtained with the dispersoid lattice rotated by  $15^\circ$  about the z-axis. Nevertheless, the strongest evidence for the above argument comes from the results of  $45^\circ$  rotation shown in Fig. 5. Here, the five-atom edges are compatible with matrix lattice and the unit cell formation along these edges is clearly seen. Such site preference vanishes at elevated temperature as shown in the simulation results of Fig. 6 for the  $\text{Ni}_3\text{Al}/\text{Al}$  system at 900K with the dispersoid rotated by  $30^\circ$  where a significant reduction of the matrix atom depletion is seen.

Fig. 7 shows the results of the  $\text{Al}_3\text{Nb}/\text{Al}$  system at 300K obtained without rotating the dispersoid. The system under this situation forms a perfect coherent interface without any noticeable lattice strain in the interface region. Fig. 8 shows the results with the dispersoid rotated by  $30^\circ$  about the z-axis. Here again, the matrix atoms are found to occupy the sites to form unit cells as discussed in the descriptions of the model shown in Fig. 3.

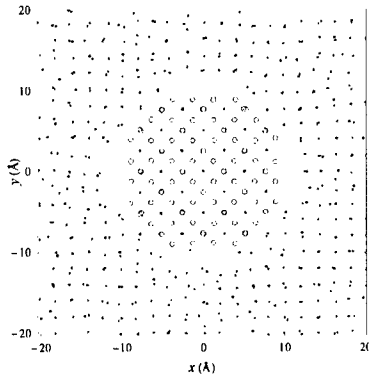
The most unexpected results are found for the  $15^\circ$  and  $45^\circ$  rotation cases as seen in Figs. 9 and 10. The two-dimensional shape of the dispersoid in these two figures is much different from that appeared in the results of Figs. 7 and 8. Here, the dispersoid/matrix bonding is



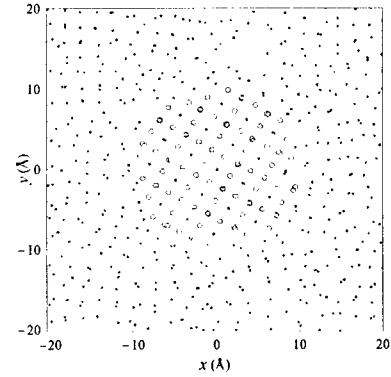
**Figure 3.** Sites favored (A & A') and less favored (B & B') by matrix atoms. X is for Ni at  $z = \pm a/2$ , O for Ni at  $z = 0$  and ● for Al at  $z = 0$ .



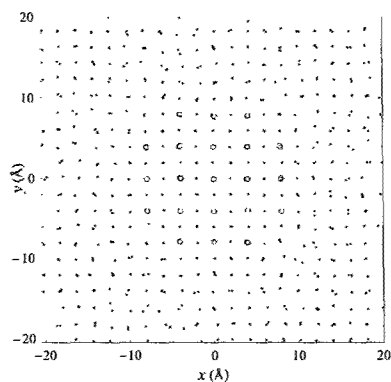
**Figure 4.** Simulation results of the  $\text{Ni}_3\text{Al}/\text{Al}$  system at 300K with the dispersoid rotated by  $15^\circ$  about the z-axis.



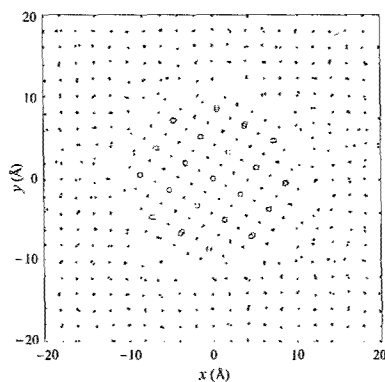
**Figure 5.** Simulation results of the  $\text{Ni}_3\text{Al}/\text{Al}$  system at 300K with the dispersoid rotated by  $45^\circ$  about the z-axis



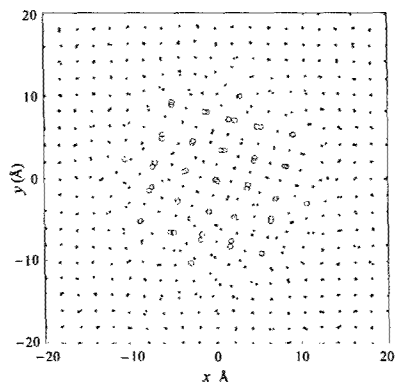
**Figure 6.** Simulation results of the  $\text{Ni}_3\text{Al}/\text{Al}$  system at 900K with the dispersoid rotated by  $30^\circ$  about the z-axis



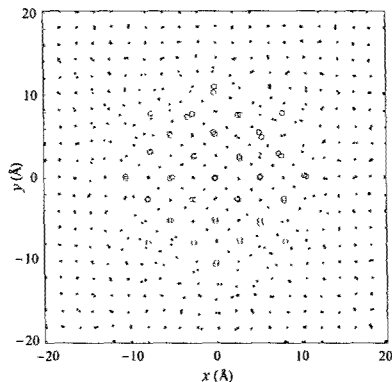
**Figure 7.** Simulation results of the  $\text{Al}_3\text{Nb}/\text{Al}$  system at 300K without rotating the dispersoid.



**Figure 8.** Simulation results of the  $\text{Al}_3\text{Nb}/\text{Al}$  system at 300K with the dispersoid rotated by  $30^\circ$  about the z-axis.

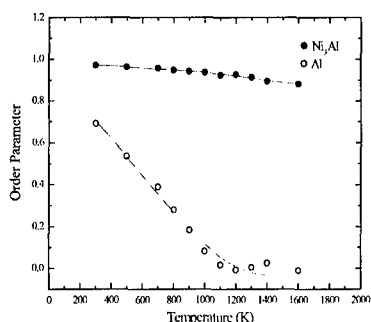


**Figure 9.** Simulation results of the  $\text{Al}_3\text{Nb}/\text{Al}$  composite system at 300K with the dispersoid rotated by  $15^\circ$  about the z-axis.

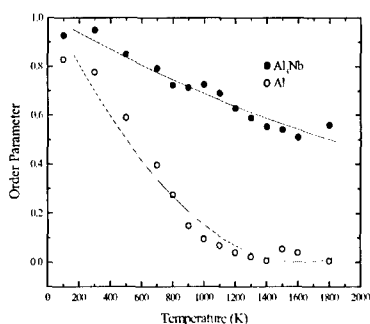


**Figure 10.** Simulation results of the  $\text{Al}_3\text{Nb}/\text{Al}$  composite system at 300K with the dispersoid rotated by  $45^\circ$  about the z-axis.

complete as if they were interdiffused into each other. Such a change in the dispersoid geometry may or may not be related to the fact that the currently assumed  $\text{L1}_2$  structure of  $\text{Al}_3\text{Ni}$  is a metastable phase. No explanation is available at the moment and systematic study is needed to understand the results of these figures. Finally, the order parameters calculated for systems with unrotated dispersoids over a range of temperature are shown in Figs. 11 and 12 for  $\text{Ni}_3\text{Al}/\text{Al}$  and  $\text{Al}_3\text{Nb}/\text{Al}$ , respectively. It is seen that the  $\text{Ni}_3\text{Al}$  dispersoid is thermally stable while  $\text{Al}_3\text{Nb}$  is not. This is puzzling since the melting temperature is considerably higher in  $\text{Al}_3\text{Nb}$  than  $\text{Ni}_3\text{Al}$  (1953K vs. 1673K). The melting behavior of a particle embedded in a matrix can be strongly



**Figure 11.** Temperature dependence of order parameters of the unrotated dispersoid and matrix in the  $\text{Ni}_3\text{Al}/\text{Al}$  system.



**Figure 12.** Temperature dependence of order parameters of the unrotated dispersoid and matrix in the  $\text{Al}_3\text{Nb}/\text{Al}$  system.

dependent on the surrounding environment and the temperature dependence of the order parameter needs to be evaluated under various situations to make a general statement.

## SUMMARY AND CONCLUSION

The simulation results of the present study show the general trend of unit-cell formation in the matrix if the lattice planes of the matrix and dispersoid are appropriately aligned. The case of  $15^\circ$  and  $45^\circ$  rotations of the dispersoid atoms produce matrix atom-concentrated and depleted regions near the dispersoid. It was found that a perfectly coherent interface forms between  $\text{Al}_3\text{Nb}$  and aluminum matrix under appropriate conditions. Also in the  $\text{Al}_3\text{Nb}/\text{Al}$  system, the dispersoid geometry is significantly changed while its wetting with the matrix remains perfect for particular dispersoid orientations. The underlying mechanism for such perfect wetting needs further systematic study along with the temperature effects and stability of the composite systems.

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