Molecular Dynamics Simulations on Nanocomposites Formed by Intermetallic Dispersoids of B_2 Structure and Aluminum Matrices

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ABSTRACT

Molecular dynamics simulations were performed in order to characterize the local lattice structure in the vicinity of the interfaces between nanosized aluminide dispersoids of B_2 structure and pure aluminum matrices. The dispersoid materials selected for the present study are NiAl and FeAl which have almost identical lattice constants. The formation of misfit-like dislocations at the interface is inevitable, due to the noticeable difference between the lattice constants of these aluminides and pure aluminum (about 0.29 versus 0.405 nanometers). The lattice disorder and matrix atom depletion regions appear near the interface regardless of the relative orientations between the lattices of dispersoid and matrix, which is partially due to the presence of the dislocations and intrinsic geometrical factors. However, elevated temperatures are seen to fill up these depletion regions closely simulating densification of compacts through sintering.

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

1. INTRODUCTION

One of the newly emerging technical areas of nondestructive materials testing is the development of composite systems with embedded damage-indicating agents as integrated structural components [1]. Such a scheme brings a number of major advantages. First, the health of critical components can be continuously monitored. Second, using sensing agents that actively respond to external fields, test procedures are simpler and the results can be more accurate compared with those in conventional testing methods. Third, by incorporating the sensor configuration at the design stage, the classical conflicts between the functionality and testability can be significantly reduced. Finally, through careful design of the system, it is even possible to enhance the material properties of the components by the presence of the sensor materials.

One potential method is to develop composites with metallic nanoparticles uniformly dispersed throughout the bulk. Small second phase particles of a considerable volume fraction are well known to strengthen alloys [2]. One of the factors governing the effectiveness of strengthening is the inter-particle distance; the strength of an alloy is a decreasing function of the inter-particle distance [2]. For a given total amount of the second phase per volume, the inter-particle distance is reduced as the average particle size is reduced, leading to the obvious choice of using nanoparticles.

One way to disperse nanoparticles in a matrix is to mechanically mix them with matrix particles. Then compact the mixture and sinter it for densification. The dispersoids, crystalline nanoparticles dispersed in a matrix, have a minimal chance of forming coherent interfaces with the matrix. Hence, the details of structural characteristics of semi or incoherent interface boundary of nano-composites need to be investigated.

The present study was performed on two intermetallic dispersoids, NiAl and FeAl, embedded in aluminum matrices. The former was one of the materials included in our previous study with incomplete results. The latter is known to be nonmagnetic when perfectly ordered but becomes ferromagnetic when disordered [3], and is a potential candidate material for damage indicating agents.

2. DETAILS OF SIMULATION

Each dispersoid was constructed at the center of an aluminum matrix. The lattice structure of NiAl and FeAl, at the stoichiometric composition, is known as B_2 in which nickel and aluminum atoms are arranged in a body-centered cubic-like structure, i.e., nickel atoms occupy the eight cube corners while an aluminum atom occupies the body-center, or vice-versa. The lattice constants of NiAl and FeAl are 0.289 and 0.291 nm, respectively, and are considerably smaller than that of pure aluminum which is 0.405 nm. Accordingly, the initial configuration was set by replacing a given volume at the center of aluminum block by a dispersoid with smaller lattice spacing. Therefore, the ratio between the number of aluminum

planes and that of dispersoid is roughly three to four. Hence, misfit-like dislocations are produced at the interface.

Simulations were performed with and without rotating the dispersoid lattice with respect to that of the matrix. The temperature range of investigation is 300K to 1800K. The modified embedded atom (EAM) potential by Baskes [4] was selected for this study since it provides an explicit expression for binary systems and all the necessary parameter values are available for a range of elements.

3. RESULTS AND DISCUSSION

Fig. 1 shows the simulation results for NiAl/Al system at 300K without rotating the dispersoid. In this figure, the atomic arrangement in the x-y planes is viewed along the z-axis. The small dots represent the aluminum atoms while the open circles represent the nickel atoms. The plot range in the z-axis is $\pm a/2$, where a is the length of cubic edge and the atoms in three planes are shown. The dispersoid boundary in Fig. 1 consists of four edges having nickel atoms only, and four others having a mixture of nickel and aluminum atoms. It is seen that three matrix aluminum atoms appear immediately next to each of four nickel-only edges. Such appearance of aluminum atoms is found to be persistent under other conditions as well and the possible reason for this is explained in the next figure

Fig. 2 shows four nickel atoms (open circles) at the dispersoid boundary along with six aluminum atoms (closed circles) within the dispersoid. The matrix lattice near the interface tends to be locally disordered. The matrix aluminum atoms in the disordered region execute

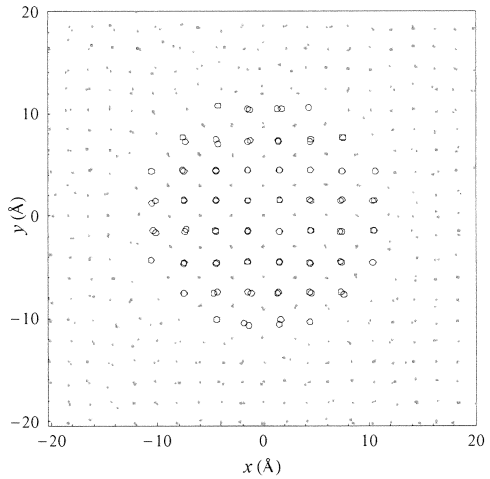

Fig. 1: Simulation results with a NiAl/Al composite system at 300K without rotating the dispersoid. Open circles represent Ni atoms and dots represent Al atoms.

random motion and reach sites denoted x and remain there to form B_2 unit cells to lower the total energy of the system. A similar process can occur along the other edges but the probability is lower since these sites lack the four nickel-atom environment.

When two crystals of substantially different lattice constants meet to form a flat two-dimensional interface, misfit dislocations with a well defined spatial periodicity are produced if their atomic planes are appropriately aligned [5]. Such, however, is not the case in the interface shown in Fig. 1. Upon a close inspection, one can see the presence of a reasonable four-fold symmetry in the system. One possible way of defining the rows and columns of extra atoms, highlighted by shades, and the related lattice distortion while preserving the four fold symmetry are shown in Fig. 3. Detailed analysis of such a dislocation structure, however, is beyond the current scope of investigation.

Fig. 4 shows the simulation results for the FeAl/Al system at 300K without dispersoid rotation. These results are virtually identical to the results of Fig. 1 for the NiAl/Al system. The lattice constant of FeAl is very close to that of NiAl. This indicates that the lattice constant dispersoid may be a factor governing the of the outcome of the simulation results.

The simulation results with 15° rotation are shown in Fig. 5 for NiAl/Al system at 300K. To make the situation more tractable the rotations are limited in the x-y plane. One can readily notice that matrix aluminum atoms are depleted near the edges that consist of nickel and aluminum atoms. This is easy to explain. The degree of

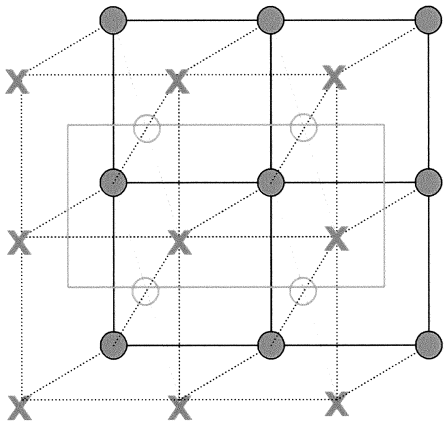

Fig. 2: A simple model explaining the reason for the persistent appearance of matrix atom immediately near the nickel-only dispersoid boundary. Open and closed circles denote nickel and aluminum atoms, respectively. The plane in the middle represents the dispersoid boundary and the symbol **X** denotes the energetically favored sites by the matrix aluminum atoms.

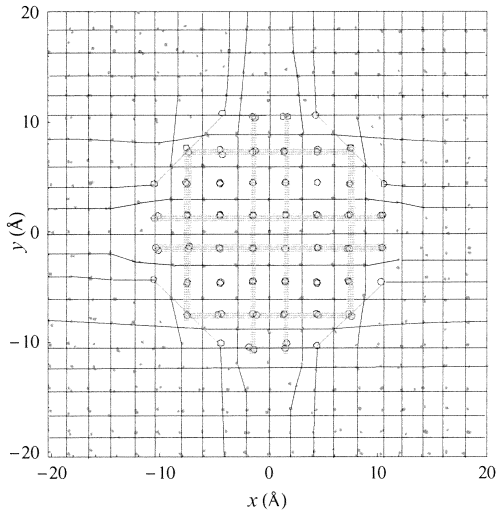

Fig. 3: Extra rows of atoms in the NiAl dispersoid as highlighted with shading and related lattice distortion in the matrix.

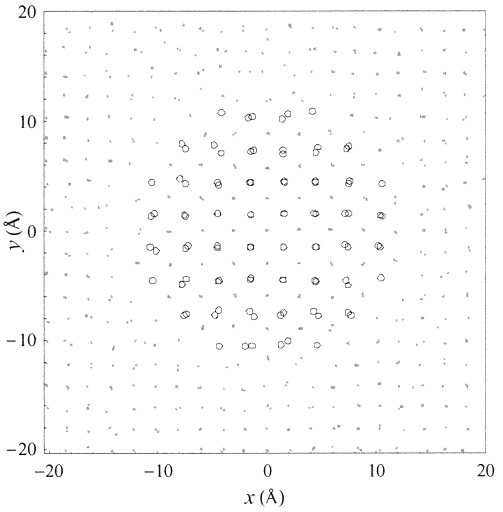

Fig. 4: Simulation results with an FeAl/Al composite system at 300K without rotating the disepersoid. These results are nearly identical to those in Fig. 1.

local lattice disorder increases with the rotation of the dispersoid and more aluminum atoms execute random motions. More matrix aluminum atoms will then have chances of moving near those already occupied in the sites next to nickel-only edges shown in Fig. 2 creating depleted regions. Fig. 6 shows the simulation results with the FeAl/Al system with the dispersoid rotated by 15° which are almost identical with that in Fig. 5 obtained for the NiAl/Al system.

Fig. 7 shows the results of FeAl at 700K

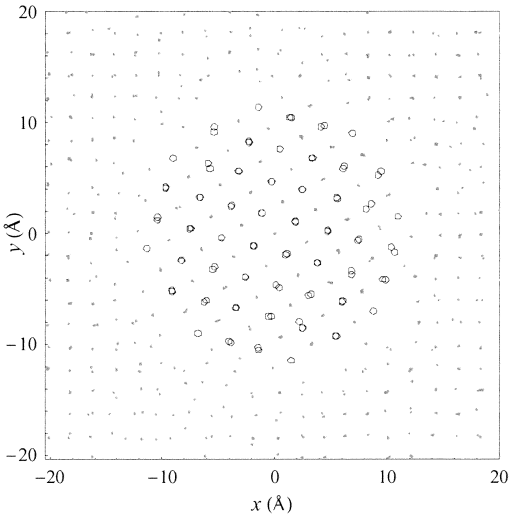

Fig. 5: Simulation results with the NiAl/Al system at 300K with the dispersoid rotated in the x-y plane by 15°.

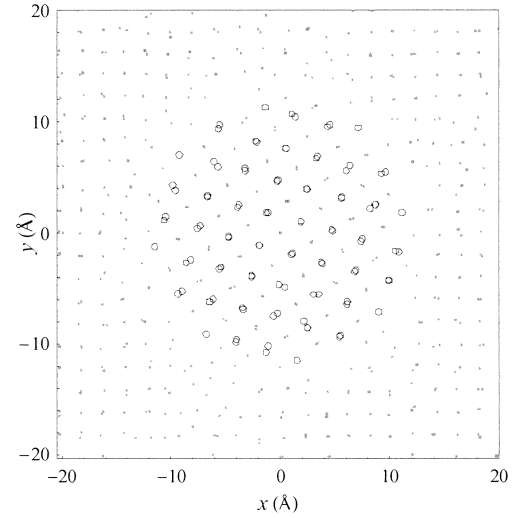

Fig. 6: Simulation results with the FeAl/Al system at 300K with the dispersoid rotated in the x-y plane by 15°.

demonstrating the filling of the matrix atom-depleted regions. As far as filling up the aluminum depleted regions near the interface is concerned, increasing the temperature beyond 700K does not seem to change anything even though the order in the aluminum matrix is continuously decreased.

Fig. 8 and 9 show the temperature dependence of the structural order of NiAl/Al and FeAl/Al systems, respectively. The bulk melting temperature of NiAl is 1911K and that for FeAl is 1583K. The results of Fig. 8, however, show that the dispersoid does not melt well over

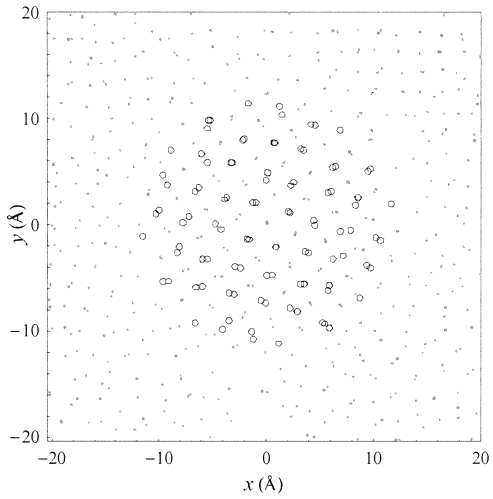

Fig. 7: Simulation results with a FeAl/Al composite system at 700K with the disersoid rotated by 15°. The matrix atom-depleted regions are all filled up.

the bulk melting temperature. It is well known that the melting temperature of nano-sized metallic particles under ambient air pressure can be reduced considerably from that for the bulk material [5]. The results in these figures, nonetheless, indicate that the melting temperatures, which directly depend on the pressure of surroundings, may be noticeably enhanced by embedding nanosized particles in matrices. However, detailed further study is needed to confirm these since the pressure of a system is sensitive to the conditions set for simulation.

4. SUMMARY AND CONCLUSION

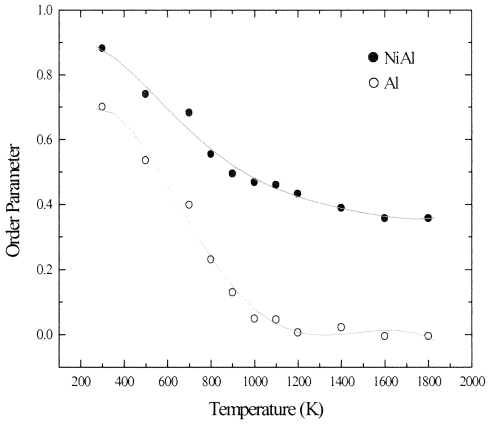

Fig. 8: Temperature dependence of the order parameter in selected regions in the NiAl /Al nano-composite.

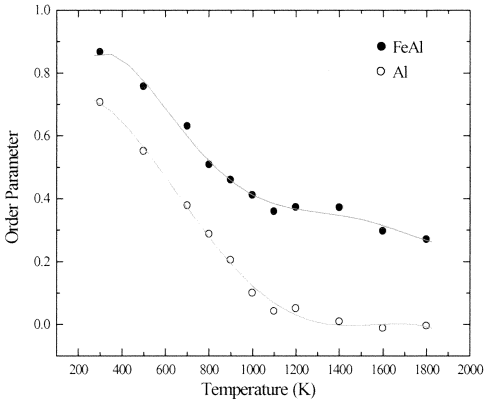

Fig. 9: Temperature dependence of the order parameter in selected regions in the FeAl /Al nano-composite.

Molecular dynamics simulations were performed with the nanocomposite systems of NiAl and FeAl dispersoids embedded in aluminum matrices. The lattice constants of these materials being substantially smaller than that of aluminum, the presence of misfit-like dislocations at the interfaces is inevitable in order to construct stable composite systems. It was also found that the melting temperatures of dispersoids are considerably increased by embedding. However, more systematic study is needed before general statements can be made on the melting behavior of nanosized dispersoids embedded in matrices.

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