INFLUENCE OF THE PARTICLE NUMBER ON THE MICROSTRUCTURE OF THE NiAl MODEL

Nguyen Trong Dung*, Nguyen Chinh Cuong
Faculty of Physics, Hanoi National University of Education

Abstract: This paper studies the influence of the number of particles on the microstructure of the NiAl bulk model and the NiAl nanoparticle model using Molecular Dynamics (MD) method with the Sutton-Chen embedded interaction potential and appropriate boundary conditions. The bulk model was studied with periodic boundary conditions, and the nanoparticle model was studied with aperiodic boundary conditions. The studies of NiAl models with 5,324 particles, 6,912 particles and 8,788 particles at increasing in temperatures from 0 K to 2,000 K, then at decreasing temperatures from 2,000 K to 300 K with a moving step $dr = 0.01$ gave consistent results with experiments. The microstructure characteristics were analyzed using the radial distribution function (RDF), the coordination number, the energy, the size of particles and the common neighborhood analysis method (CNA). The results showed that the structure phases fcc, hcp and bcc appeared in the models with 5,324 particles; 6,912 particles and 8,788 particles at 300 K. The research results also confirmed that there was an influence of the number of particles on the microstructure of the models.

Keywords: Microstructure, particle number, NiAl model, Molecular Dynamics method

1 Introduction

Today, the CoAl alloy, NiAl alloy, etc. have been used intensively in science and technology [13]. NiAl materials play an important role because they are the essential parts in electronic equipment and industrial products. NiAl can increase the conductivity [7, 11, 17] of the electronic equipment. For industrial products, NiAl serves as a ceramic coat that reduces the temperature effects on the materials surface and increases the adhesion on materials. In addition, NiAl is also a material with a high melting temperature from 750 °C to 850 °C and high capacity of heat conduction and antioxidation. NiAl, therefore, has been applied in the aerospace industries, as in jet engines [4, 5, 14]. In recent years, NiAl material has also been of interest due to their compression resistance, high antioxidant resistance and small mass density [1-3]. Experimental studies of NiAl showed that the distance between atoms (molecules) in the NiAl model is 2,2 Å [6], and studies of NiAl using the simulation method revealed that the distance between Al-Al atoms (molecules) and Ni-Ni is 2,7 Å and 2,25 Å, respectively.

Our study has not only given a new understanding about the NiAl material but also proved that when the number of particles is increased, the atom (molecule) density will increase, and the crystallization of atoms (molecules) occurs when the temperature is decreased. In this paper, we focus on a detailed study of the influence of the number of particles on the microstructure of the NiAl bulk model and the NiAl nanoparticles model using the Molecular Dynamics method and the Sutton-Chen embedded interaction potential with appropriate boundary conditions. The data were analyzed in Part 2. The obtained results were compared
with related experimental as well as simulation results which are presented in Part 3, and the
conclusions are shown in Part 4.

2 Method of calculation

Initially, the NiAl bulk models with 5,324 particles, 6,912 particles and 8,788 particles were put
randomly in a cubic box. These models were studied using the Molecular Dynamics (MD) [15]
method with the Sutton-Chen embedded (2.1) [9, 12, 16] interaction potential and periodic
boundary conditions. The NiAl nanoparticle models with 5,324 particles, 6,912 particles and
8,788 particles were put randomly in a spherical box. These models were studied using the
Molecular Dynamics (MD) method with the Sutton-Chen embedded interaction potential with
aperiodic boundary conditions.

\[
E_{\text{tot}} = \sum_{i=1}^{N} \frac{1}{2} \sum_{j=1, j\neq i}^{N} \Phi(r_{ij}) + F(\rho_i) \tag{2.1}
\]

\[
\Phi(r_{ij}) = \varepsilon \left( \frac{a}{r_{ij}} \right)^n, \quad \rho_i = \sum_{j=1, j\neq i}^{N} \rho(r_{ij}), \quad \rho(r_{ij}) = \left( \frac{a}{r_{ij}} \right)^n, \quad F(\rho_i) = -\varepsilon C \sum_{i=1}^{N} \sqrt{\rho_i}.
\]

where \( r_{ij} \) is the distance between two atoms \( i, j \); \( a \) is the lattice constant; \( \rho_i \) is the atomic density \( i \);
\( E_{\text{tot}} \) is the energy of the system; \( \Phi(r_{ij}) \) is the energy between two atoms \( i, j \); \( F(\rho_i) \) is the interaction
force of atom \( i \); \( r_c \) is the disconnect radius, \( \varepsilon \) is the energy; \( C, M, n, N \) are parameters of the
model. In which, parameters of the NiAl model were calculated as follows:

\[
\varepsilon_{\text{NiAl}} = \sqrt{\varepsilon_{\text{Ni}} \cdot \varepsilon_{\text{Al}}}; \quad a_{\text{NiAl}} = \frac{a_{\text{Ni}} + a_{\text{Al}}}{2}; \quad n_{\text{NiAl}} = \frac{n_{\text{Ni}} + n_{\text{Al}}}{2};
\]

\[
m_{\text{NiAl}} = \frac{m_{\text{Ni}} + m_{\text{Al}}}{2}; \quad C_{\text{NiAl}} = \sqrt{C_{\text{Ni}} \cdot C_{\text{Al}}}; \quad r_{\text{NiAl}} = \frac{r_{\text{Ni}} + r_{\text{Al}}}{2}.
\]

The main parameters of the models are shown in Table 1.

| Model | \( \varepsilon \) (eV) | \( a \) (Å) | \( n \) | \( m \) | \( C \) | \( r_c \) (Å) |
|-------|----------------------|-------------|------|-----|------|-------------|
| Ni    | 0.000271083          | 3.52        | 10   | 5   | 84,745 | 6,643712784 |
| Al    | 0.001218102          | 4.05        | 7    | 6   | 16,399 | 7,653393855 |
| NiAl  | 0.000574636          | 3.785       | 8.5  | 5.5 | 37,279 | 7,148553319 |

Then, the temperature was increased to 2,000 K with a moving step \( dr = 0.01 \) in these
models to break their initial crystalline structure and turn to the liquid state. At the liquid state
with the temperature of 2,000 K, the temperature of the models was lowered to 300 K with a
moving step \( dr = 0.01 \). At 300 K, we obtained the samples with the crystalline state for studying
in this paper. The microstructure characteristics of these samples were studied using the radial
distribution functions (RDF), the coordination number, the energy, the size of particles and the common neighbourhood analysis method (CNA) [8, 10].

3 Results

The NiAl samples with 5,324 particles, 6,912 particles and 8,788 particles were studied in the same conditions of temperature, pressure, number of running steps, etc. We obtained their shapes as shown in Fig. 1 and Table 2.

![Fig. 1. The shape of the NiAl bulk samples (a) and the NiAl nanoparticle samples (b) with 5,324 particles](image)

| Number of particle | 5,324 | 6,912 | 8,788 |
|--------------------|-------|-------|-------|
| The size of the bulk model (nm) | 7,798 | 8,516 | 9,285 |
| The size of the nano model (nm) | 15,735 | 17,166 | 18,596 |

The results in Tables 3 and Table 4 showed that the NiAl bulk sample with 5,324 particles had the cubic shape (Fig.1a), and the NiAl nanoparticle sample with 5,324 particles had the spherical shape (Fig. 1b). The samples had a nanoscale size, and they were formed with two types of atoms: the Ni atoms which were blue and the Al atoms which were red. There appeared two distinct areas in the samples: the Al atoms density was large in the left area of the NiAl bulk sample, while the Ni atoms density was large in the right area; the Ni atoms density was large in the core area of the NiAl nanoparticle sample, while the Al atoms density was large in the surface area. This result showed that there were mainly couplings of the Al-Al and Ni-Ni atomic pairs, while there were a few couplings of the Ni-Al atomic pairs. The results also showed that when the number of particles in the NiAl samples increased, the size of the samples would be increased (Table 2).

To confirm this, we studied the radial distribution functions (RDF) of the NiAl samples. The results are shown in Fig. 2 and Table 2.
Fig. 2. The radial distribution functions of the NiAl bulk sample and the NiAl nanoparticle sample with 5,324 particles.

Table 3. The distance between atoms and the height of the radial distribution functions of the NiAl samples with different number of particles.

| Bulk sample      | The distance between atoms r(Å) | The height of the radial distribution functions g(r) |
|------------------|---------------------------------|---------------------------------------------------|
|                  | r_{11}  | r_{12}  | r_{13}  | g_{11}   | g_{12}   | g_{13}   |
| 5,324 particles  | 2.24    | 3.2     | 3.9     | 8.60     | 1.91     | 3.95     |
| 6,912 particles  | 2.24    | 3.2     | 3.9     | 7.87     | 1.58     | 3.41     |
| 8,788 particles  | 2.24    | 3.18    | 3.9     | 8.24     | 2.03     | 3.84     |
| Nanoparticle     | r_{11}  | r_{12}  | r_{13}  | g_{11}   | g_{12}   | g_{13}   |
| sample           |         |         |         |          |          |          |
| 5,324 particles  | 2.24    | 3.2     | 3.9     | 7.11     | 1.46     | 3.15     |
| 6,912 particles  | 2.24    | 3.2     | 3.9     | 7.50     | 1.49     | 3.38     |
| 8,788 particles  | 2.24    | 3.2     | 3.88    | 14.88    | 2.07     | 5.19     |
| experiment results [6] | 2.2 | | | | | |

The results in Fig. 2 and Table 3 show that the first peak position of the radial distribution function prevailed in the NiAl samples with 5,324 particles at 300 K; the first peak height of the radial distribution function of the bulk sample was higher than that of the nanoparticle sample. When the number of particles in the samples increased to 6,912 particles and 8,788 particles, we saw that the first peak position of the radial distribution functions had unchanged value. This
proved that there only existed the near range interaction in the NiAl samples. The height of the remaining peaks of the radial distribution functions changed insignificantly.

When the number of particles increased, the first peak height of the radial distribution functions of all samples increased; it only decreased in the bulk sample with 6,912 particles. This proved that when the number of particles of the bulk samples increased, the increase and decrease in the particle density were due to the transformation of their microstructure. In the nanoparticle sample, when the number of particles increased, the first peak height of the radial distribution functions increased, leading to the increase of the particle density.

To confirm that, we continued to study the couplings of Al-Al, Al-Ni and Ni-Ni atomic pairs. The results are shown in Fig. 3 and Table 4.

![Fig. 3](image)

**Fig. 3.** The radial distribution functions of the couplings of Al-Al, Al-Ni and Ni-Ni atomic pairs in the NiAl bulk sample (a) and the NiAl nanoparticle sample (b) at 300 K

**Table 4.** The distance between atoms and the height of radial distribution functions of the couplings of Al-Al, Ni-Al and Ni-Ni atomic pairs in the NiAl nanoparticle samples with different number of particles at 300 K

| Bulk sample | The distance between atoms r(Å) | The height of the radial distribution functions g(r) |
|-------------|---------------------------------|-----------------------------------------------|
|             | r_{Al-Al}  | r_{Ni-Al}  | r_{Ni-Ni}  | g_{Al-Al}  | g_{Ni-Al}  | g_{Ni-Ni}  |
| 5,324 particles | 2.75        | 2.67        | 2.25        | 9.91       | 0.50       | 68.21       |
| 6,912 particles | 2.79        | 2.61        | 2.25        | 10.02      | 0.52       | 62.33       |
| 8,788 particles | 2.81        | 2.61        | 2.25        | 9.04       | 0.37       | 65.34       |
| Nanoparticle sample | | | | | | |
| 5,324 particles | 2.77        | 2.59        | 2.25        | 8.01       | 0.55       | 56.27       |
| 6,912 particles | 2.71        | 2.59        | 2.25        | 8.47       | 0.51       | 59.47       |
| 8,788 particles | 2.73        | 2.65        | 2.25        | 15.04      | 1.17       | 119.36      |
| Simulation results | 2.7         | 2.25        | | | | |

The results in Fig. 3 and Table 4 showed that the first peak position of the radial distribution functions of the couplings of Al-Al, Al-Ni and Ni-Ni atomic pairs prevailed in the NiAl samples with 5,324 particles at 300 K (Fig. 3). The length of the couplings changed insignificantly: the length of the couplings of Al-Al atomic pairs in the bulk sample was smaller
than that of the nanoparticle sample; the length of the couplings of Ni-Al atomic pairs in the bulk sample was larger than that of the nanoparticle sample; the length of the couplings of Ni-Ni atomic pairs was the same in both samples. The results in Table 4 were consistent with the simulation results.

The first peak height of the radial distribution functions of the couplings of Al-Al and Ni-Ni atomic pairs prevailed, while it was small with the couplings of Ni-Al atomic pairs. This showed that the atoms (molecules) density of the couplings of Al-Al and Ni-Ni atomic pairs was very large, while it was very small with the couplings of Al-Ni atomic pairs. However, the first peak height of the radial distribution functions of the couplings of Al-Al and Ni-Ni atomic pairs in the bulk sample was higher than that of the nanoparticle sample, while the first peak height of the radial distribution functions of the couplings of Ni-Al atomic pairs in the bulk sample was lower than that of the nanoparticle sample. This result showed that the atoms (molecules) density of the couplings of Al-Al and Ni-Ni atomic pairs in the bulk sample was larger than that of the nanoparticle sample, but the atoms (molecules) density of the coupling of Ni-Al atomic pairs in the bulk sample was smaller than that of the nanoparticle sample.

When the number of particles increased to 6,912 particles and 8,788 particles, the distance between the two atoms in the couplings of Al-Al atomic pairs in bulk sample increased, but it decreased in the nanoparticle sample; the distance between the two atoms in the couplings of Al-Ni atomic pairs in the bulk sample decreased, but it increased in the nanoparticle sample; the distance between the two atoms in the couplings of Ni-Ni atomic pairs was the same in both samples. In the bulk sample, the first peak height of the radial distribution functions of the couplings of Al-Al and Al-Ni atomic pairs first increased then decreased, but it was in the reverse order in the couplings of Ni-Ni atomic pairs. In the nanoparticle sample, the first peak height of the radial distribution functions of the couplings of Al-Al and Al-Ni atomic pairs increased (Table 4). This result showed that when the number of particles increased in the model, the particle density would be increased, leading to the increase in the couplings of Al-Al, Ni-Al and Ni-Ni atomic pairs density. This confirmed that the influence of the number of particles on the microstructure was significant.

To simulate shape microstructure of crystal NiAl at 300 K, we used the methods common neighbourhood analytical (CNA). The results are shown in Fig. 4, Table 5a and Table 5b.

![BCC Structure](image1)

![HCP Structure](image2)

![FCC Structure](image3)

Fig. 4. The shape microstructure of the crystal NiAl at 300 K
Table 5a. The crystalline states of the NiAl bulk model with different number of particles

| Model  | Nicken Aluminum bulk |
|--------|----------------------|
|        | fcc  | hcp  | bcc  | crystal | Amorphous |
| 5324   | 2240 | 384  | 0    | 2624    | 2700      |
| 6912   | 2575 | 796  | 0    | 3371    | 3541      |
| 8788   | 3793 | 588  | 0    | 4381    | 4407      |

Table 5b. The crystalline states of the Al, Ni, NiAl nanoparticle models with different number of particles

| Model  | Aluminum nano | Nicken nano | Nicken Aluminum nano |
|--------|---------------|-------------|----------------------|
|        | fcc  | hcp  | fcc  | hcp  | bcc  | ico | crystal | Amorphous |
| 5324   | 37   | 47   | 0    | 1593 | 89   | 0   | 2384    | 2940      |
| 6912   | 74   | 45   | 15   | 2618 | 15   | 0   | 3303    | 3609      |
| 8788   | 71   | 52   | 35   | 2842 | 35   | 42  | 3820    | 4926      |

We can see from Fig. 4, Table 5a and Table 5b that there primarily existed two main types of structure fcc and hcp in the NiAl models at the temperature of 300 K, and particularly there appeared two types of structure bcc and ico in the NiAl nanoparticle model. When the number of particles in the bulk model increased, the number of structure states fcc and hcp first tended to increase then decrease (Table 5a). When the number of particles in the nanoparticle model increased, the number of structure states fcc, hcp and ico increased, except for the fact that the structure state bcc first decreased then increased (Table 5b). This result confirmed that there was a significant influence of the number of particles on the microstructure and the formation of the microstructure states fcc, hcp, bcc and ico. The main reason for that formation was the size effect. When the number of particles increased, the atoms (molecules) density increased, and this made the atoms (molecules) in the surface layer tend to be clotted. As the result, this led to the formation of the microstructure states fcc, hcp, bcc and ico in the surface layer and core layer of the model.

4 Conclusion

Studying the influence of the number of particles on the microstructure of NiAl samples with 5,324 particles, 6,912 particles and 8,788 particles at 300 K, we have drawn some conclusions on the NiAl bulk model and the NiAl nanoparticle model as follows:

- The Sutton-Chen embedded interaction potential, the chosen boundary conditions (periodic or fixed) and parameters gave consistent results with experiments.

- The NiAl models have the nano-size, and the atoms (molecules) focus more in the core layer than in the surface layer. The existence of the two areas with large Ni and Al density leads to the different structures of the surface layer.
Two types of structure hcp and fcc mainly exist in the NiAl models, and particularly the structure bcc and ico appear only in the nanoparticle model.

The influence of the number of particles on the microstructure is due to the size effect. When the number of particles is increased, the atoms (molecules) density increases, while the energy of the model decreases. This leads to the increase in the coordination number both in the surface layer and in the core layer.

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