Simulation on the Factors Affecting the Crystallization Process of FeNi Alloy by Molecular Dynamics

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1. INTRODUCTION

Nowadays, FePt, CoPt3, CoPt, CoRh, and NiFe alloys are being used in many application fields such as biology, adsorption, data storage, high-density storage, photocatalysts, chemical sensors, and biomedicine. FeNi alloys have received great attention from scientists thanks to their interesting properties: magnetic, antioxidative, and biomedical. This material is suitable for biomedical applications because they exhibit magnetic superparamagnetic properties and thus can be used for various applications dealing with drug delivery, hyperthermia, and magnetic resonance imaging. Experimental, theoretical, and simulation methods are used to investigate the structure of FeNi alloys. With the experimental method, FeNi alloys were successfully fabricated by the evaporation method at temperature \( T = 1823 \text{ K} \) with Fe concentrations of 36%, and the size (\( D \)) varies from 20 nm to 100 nm; the hydrogenation reaction gives spherical nanoparticles with size smaller than 35 nm, and the plasma treatment in the mixture of \( H_2 \) and Ar leads to nanoparticles with nanoscale size. The latter depends on the temperature and air flow rate, pyrolysis conditions, and preparative methods. Fe\(_{1-x}\)Ni\(_x\) alloys with size 10–25 nm are being implemented very little by the experimental method, whereas the simulation method is considered the most interesting method because of its ability to study at the atomic level without the consumption of energy as in the experimental methods. They were built by molecular dynamics (MD) method, Monte-Carlo method, combined with interaction potentials, such as the average effective field theory, atomic method, Finnis and Sinclair, and embedded interaction Sutton–Chen (SC). The obtained results are highly accurate. To study the structure of FeNi materials, Daw and Nguyen have used the MD method with the embedded interaction SC in combination with the parameters of Meyer and Entel. The experimental method and simulation method can be combined to obtain high-precision results. Ni has a face-centered cubic (FCC) structure and Fe has a blocked cubic center (BCC) structure; however, hybridization leads to new structures. The change of alloy structure depends on various factors including solute concentration, atomic number, temperature, annealing time, and so forth. The solute concentration (\( x \)) of Fe in Ni\(_{1-x}\)Fe\(_x\) alloy can reach 100% at high temperatures, ranging from \( T = 1183 \text{ K} \) to \( T = 1665 \text{ K} \) whereas at low temperatures, the impurity concentration can reach a maximum of \( x = 66\% \). In addition, scientists used the electron model to study the defect buttons, defects, and surface properties of materials. To study the structure and phase transition temperature of CuNi and CuAu, energy alignment method, the ability method of Blaha et al., and the network constants.
of the material are used. With the MD simulation method, Grujicic et al. have successfully studied the effect of impurity concentration and have established the relationship between the FCC and BCC structural phases. Lavrentiev et al. determined the effect of concentration of Ni impurities in Fe$_{1-x}$Ni$_x$ from $x = 5\%$ to $x = 75\%$ on the phase transition temperature ($T_m$) = 800 K; in the FCC structure, the crystallization temperature, $T_c = 600$ K. Recently, we have successfully studied the effect of the impurity concentration of Fe in Ni$_{1-x}$Fe$_x$ nanoparticles, with $x = 10$, 30, and 50%, on the radial distribution function (RDF) structural unit numbers, FCC, hexagonal close-packed (HCP), and amorphous (Amor). In addition, with the concentration of Cu solids of 33% in AlCu, the transition temperature ($T_m$) is found to be 821 K, whereas an increase in the number of CuNi atoms leads to an increase in the concentration of solute Ni and Ag increases in CuAg. As previously mentioned that FeNi is a promising material, however, the molecular structure is not reported in the literature. Moreover, the effect of inlet conditions such as heating rate, impurity concentration, and annealing time at a molecular level is investigated by using the MD method with the embedded interaction potential SC and recirculation boundary conditions. Various molecular parameters are calculated for these alloys, which will be useful for a better understanding of the behavior of these alloys at a molecular level.

### 2. RESULTS AND DISCUSSION

#### 2.1. Effect of Impurity Concentration.

The effect of Ni concentration in the alloys on the shape and RDF of samples Fe$_{90}$Ni$_{10}$, Fe$_{80}$Ni$_{20}$, Fe$_{70}$Ni$_{30}$, Fe$_{60}$Ni$_{40}$ (FeNi), and Fe$_{60}$Ni$_{40}$ is shown in Figure 1. Figure 1a shows that Fe$_{90}$Ni$_{10}$ at $T = 300$ K has a cube shape, created by two types of atoms, Fe and Ni, in which Fe atoms are in red color and Ni atoms are in blue color. The first peak position of RDF has a value, $r = 2.45$ Å, height $g(r)$ of 5.03 (Figure 1b), size $(l) = 7.46$ nm, and the total energy of the system $(E_{tot}) = -2188.47$ eV. An increase in the impurity concentrations ($x$) of Ni in FeNi alloys from Fe$_{90}$Ni$_{10}$ to Fe$_{80}$Ni$_{20}$, Fe$_{70}$Ni$_{30}$, Fe$_{60}$Ni$_{40}$, and FeNi leads to an increase in the $r$ value from 2.45 Å to 2.45, 2.48, 2.60, and 2.60 Å; $g(r)$

### Table 1. Size, Total Energy of the System, Position, and Height of RDF FeNi Alloys with Different Ni Impurity Concentrations

| FeNi alloys | Fe$_{90}$Ni$_{10}$ | Fe$_{80}$Ni$_{20}$ | Fe$_{70}$Ni$_{30}$ | Fe$_{60}$Ni$_{40}$ | FeNi | results |
|-------------|-------------------|-------------------|-------------------|-------------------|------|---------|
| $r$ (Å)     | 2.45              | 2.45              | 2.48              | 2.60              | 2.60 | experiment 2.53 Å$^{21}$ |
| $g(r)$      | 5.03              | 4.73              | 4.46              | 4.28              | 4.71 | simulation 2.49 Å$^{1}$ |
| $l$ (nm)    | 7.46              | 7.50              | 7.54              | 7.59              | 7.63 |          |
| $E_{tot}$ (eV) | $-2188.47$      | $-3437.55$      | $-4703.88$      | $-5929.33$      | $-7175.27$ |          |

Figure 2. Relationship between the size ($l$) and the solute concentration of Ni (a) and that between the total energy of the system ($E_{tot}$) and the solute concentration of Ni (b).
Figure 3. Structural unit number shapes of FeNi alloys: FCC structure (a), HCP structure (b), BCC structure (c), and Amor structure (d).

Table 2. Structural Unit Numbers of FeNi Alloys with Different Ni Impurity Concentrations

| Ni doped concentration | FCC | HCP | BCC | Amor |
|------------------------|-----|-----|-----|-----|
| Fe90Ni10               | 2168| 1425| 43 | 1688|
| Fe90Ni20               | 3274| 1310| 109| 811 |
| Fe90Ni30               | 3547| 1290| 53 | 434 |
| Fe90Ni40               | 1777| 852 | 32 | 2663|
| Fe90Ni50               | 1722| 1080| 25 | 2497|

The results show that the size \( l \) of FeNi alloys is always directly proportional to the solute concentration of Ni and satisfies the formula: \( l = 7.415 + 0.43x \) (Figure 2a); the energy of the system \( E_{\text{tot}} \) is directly proportional with the solute concentration of Ni \(-x\) and satisfies the formula: \( E_{\text{tot}} = -947.28 - 12.465x \). Figure 2b shows that the solute concentration \( x \) has a significant influence on \( l \) and \( E_{\text{tot}} \) of FeNi alloys. The obtained results show that \( l \) is directly proportional with \( x \) and \( E_{\text{tot}} \) is directly proportional with \(-x\). The results are in line with those recently reported by the simulation method\(^5\) and the experiment method\(^7\). To confirm the accuracy of the obtained results, the visualization method and common neighborhood analysis (CNA) method have been used, and the results are shown in Figure 3, Table 2.

2.2. Effect of Heating Rate. Several molecular parameters of the sample Fe70Ni30 at \( T = 300 \) K as a function of heating rate \( (4 \times 10^{12}, 4 \times 10^{13}, \) and \( 4 \times 10^{14} \) K/s) are shown in Table 3.

Table 3. Size, Energy, First Peak Position, and First Peak Position Height of RDF with Different Heating Rates

| FeNi alloys | heating rate (K/s) | 4 \( \times \) 10^{12} | 4 \( \times \) 10^{13} | 4 \( \times \) 10^{14} | results (Å) |
|-------------|-------------------|---------------------|---------------------|---------------------|-------------|
|             | \( r \) (Å)       | 2.48                | 2.50                | 2.6                | 2.53\(^1\) |
|             | \( g(r) \)        | 4.46                | 3.92                | 3.90               | 3.90        |
|             | \( l \) (nm)       | 7.54                | 7.59                | 7.56               | 7.56        |
|             | \( E_{\text{tot}} \) (eV) | -4703.88           | -4688.11            | -4685.93           | -4685.93   |

The results show that Fe70Ni30 at \( T = 300 \) K with a heating rate of \( 4 \times 10^{12} \) K/s has \( r = 2.48 \) Å, \( g(r) = 4.46 \), \( l = 7.54 \) nm, and \( E_{\text{tot}} = -4703.88 \) eV. An increase in the heating rate from \( 4 \times 10^{12} \) to \( 4 \times 10^{13} \) and \( 4 \times 10^{14} \) K/s leads to an increase of \( r \) from 2.48 Å to 2.60 Å and a decrease of \( g(r) \) from 4.46 to 3.90; \( l \) changes in the range from 7.54 to 7.59 nm; and \( E_{\text{tot}} \) increases from -4703.88 eV to -4685.93 eV. These results show that the increase of the heating rate leads to the transfer of Fe70Ni30 from the crystalline state to amorphous state. To confirm the accuracy of the results, the visualization method and the CNA method are used, and the results are shown in Figure 4.

2.3. Influence of Temperature. The relationship between the energy of the system \( E_{\text{tot}} \) and temperature \( T = 300, 400, 500, 600, 700, 900, 1100, \) and 1300 K is also investigated, and the results are shown in Figure 5.

Figure 5 shows that Fe70Ni30 at \( T = 300 \) K has \( E_{\text{tot}} = -4703.88 \) eV. When \( T \) is increased from 300 K to 400, 500, 600, 700, 900, 1100, and 1300 K, the \( E_{\text{tot}} \) value increases from 75.41 nm to 75.47, 75.57, 75.64, 75.75, 75.93, 76.32, and 76.79 nm, and \( E_{\text{tot}} \) increases from -4703.88 eV to -4699.06, -4691.34, -4685.80, -4677.88, -4689.81, -4665.10, -4647.32, and -4631.61 eV (Figure 5). The results show that an increase of \( T \) leads to an increase of \( l \) and \( E_{\text{tot}} \). When \( T \) increases from 300 K to 600 K and from 600 K to 1300 K, \( E_{\text{tot}} \) decreases from 5.03 to 4.73, 4.46, 4.28, and 4.71; \( l \) increases from 7.46 nm to 7.50, 7.54, 7.59, and 7.63 nm, and \( E_{\text{tot}} \) decreases from -2188.47 eV to -3437.55, -4703.88, -5929.33, and -7175.27 eV (Table 1).
increases linearly, and an interrupting point at $T = 600$ K, corresponding with $E_{\text{tot}} = -4685.80$ eV, is observed. This value is assigned to the crystallization temperature ($T_g$) 600 K. This seems to be consistent with the experimental results ($T_g = 593$ K). To confirm the accuracy of the obtained results, CNA and RDF methods are used, and the results are shown in Figure 6.

Figure 6 indicates that at $T = 300$ K, Fe$_{70}$Ni$_{30}$ has $r = 2.48$ Å and $g(r) = 4.46$. When $T$ is increased from 300 K to 1300 K, $r$ increases from 2.48 Å to 2.63 Å, and $g(r)$ changes in the range from 4.46 to 4.06 (Figure 6a); however, the structural unit number of FCC remains unchanged when the temperature varies from 300 K to 600 K. When $T > 600$ K, FCC declines rapidly; HCP decreases slowly in the range from 300 K to 600 K. When $T > 600$ K, HCP decreases rapidly; BCC changes; and Amor lightly increases in the temperature range from 300 K to 600 K.
K to 600 K, and then Amor increases rapidly when \( T > 600 \) K (Figure 6b). This asserts that Fe\(_{70}\)Ni\(_{30}\) has a thermal transition at \( T = 600 \) K.

2.4. Effect of Annealing Time. The results of Fe\(_{70}\)Ni\(_{30}\) after the annealing process are shown in Figure 7.

The results shows that Fe\(_{70}\)Ni\(_{30}\) at an annealing time (\( t_1 \)), \( t_1 = 0.0 \) ps has \( E_{\text{tot}} = -4685.80 \) eV. When annealing \( t \) increased from 0.0 ps to 450 ps, \( E_{\text{tot}} \) remains almost unchanged (Figure 7a1). This confirms that after annealing time, there is no structural change; a negligible change in the structural unit numbers is also observed (Figure 7b1); RDF has a negligible change with the annealing time (Figure 7c1). Similar tendency has been observed for structural shapes (Figure 7a2−d2). When \( x = 30\% \), the crystallization process reaches the maximum value. When the annealing time is increased, the crystallization process remains stable. In other words, the crystallization of these alloys is relatively rapid and is completed after a very short time, and thus annealing is not necessary to improve the crystallization degree.

3. CONCLUSIONS

In this study, the crystallization process of FeNi alloys by the MD method is investigated. We have successfully described and calculated various molecular parameters for these alloys by using the SC interaction potential and recirculating boundary conditions. We show that the increase of the solute concentration (x) of Ni in FeNi alloys leads to an increase of the crystallization process and that a maximum value is obtained at \( x = 30\% \). Our findings show that the crystallization temperature (\( T_g \)) is found to be about 600 K and that the annealing time (\( t \)) does not affect the crystallization state. We have successfully established the relationship of \( x \) with \( l \) and \( E_{\text{tot}} \): \( l \) is proportional with \( x \), whereas \( E_{\text{tot}} \) is directly proportional with \( -x \). These obtained results are supported by experimental and simulation results. Different types of structural unit numbers are found for these alloys including FCC, HCP, BCC, and Amor which are completely consistent with the experimental and theoretical results.

4. CALCULATION METHOD

Initially, FeNi alloys with 5324 atoms at different solute concentrations of Ni, heating rate, temperature, and annealing time were randomly planted into a cube and then studied by MD method with embedded interaction potential SC, Verlet algorithm, and recirculation boundary conditions.

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

where \( \Phi(r_{ij}) = \sum_{j \neq i} \rho(\rho_i) = \sum_{j \neq i} \rho(\rho_{ij}) \), \( \rho_i = \rho_{ij} = \rho_{ij} = \left( \frac{\alpha}{r_{ij}} \right)^n \),

and \( F(\rho_i) = -eC \sum_{j=1}^{N} \sqrt{r_i} \)

where \( r_{ij} \) is the distance between two atoms \( i \) and \( j \); \( \alpha \) is the network constant; \( \rho_i \) is the atomic density; \( E_{\text{tot}} \) is the total energy of the system; \( \Phi(r_{ij}) \) is the energy between two atoms \( i \) and \( j \); \( F(\rho_i) \) is the interaction force of atom \( i \); \( r_g = 3.15 \) Å is the interrupt radius; \( e \) is the energy; and \( C, m, n, \) and \( N \) are the parameters of FeNi alloys. The parameters of FeNi alloys are presented in Table 4.

After collecting the samples of FeNi alloys with different solute concentrations, \( x = 10\% (\text{Fe}_{90}\text{Ni}_{10}), 20\% (\text{Fe}_{80}\text{Ni}_{20}), 30\% (\text{Fe}_{70}\text{Ni}_{30}), 40\% (\text{Fe}_{60}\text{Ni}_{40}), \) and \( 50\% (\text{Fe}_{50}\text{Ni}_{50}) \), \( \text{Fe}_{50}\text{Ni}_{50} \) the heating rates are \( 4 \times 10^2 \), \( 4 \times 10^3 \), and \( 4 \times 10^4 \).
Table 4. Main Parameters of FeNi Alloys

| Material | \( a_{\text{FeNi}} \times 10^{-11}\, \text{eV} \)^a | \( m_{\text{FeNi}} \) | \( E_{\text{NiFe}} \) | \( C_{\text{FeNi}} \) |
|----------|---------------------------------|----------------|----------------|----------------|
| Fe       | 1.730                           | 3.471          | 8.137          | 4.787          | 24.939         |
| Ni       | 0.271                           | 3.520          | 10             | 5              | 84.745         |

\( a_{\text{FeNi}} = \sqrt{a_{\text{Fe}}a_{\text{Ni}}} \),

\( b_{\text{FeNi}} = \frac{(\eta_{\text{Fe}} + \eta_{\text{Ni}})}{2} \),

\( m_{\text{FeNi}} = m_{\text{Fe}}m_{\text{Ni}} \),

\( C_{\text{FeNi}} = C_{\text{Fe}}C_{\text{Ni}} \).

\( \times 10^4 \, \text{K/s} \) at \( T = 300 \, \text{K} \); for the Fe$_{33}$Ni$_{67}$ sample, \( T = 300, 400, 500, 600, 700, 900, 1100, \) and 1300 K; \( t = 450 \, \text{ps} \) (corresponding to the moving step number of \( 1.8 \times 10^4 \) steps; time of each step is of 2.5 fs) at \( T = 600 \, \text{K} \). The temperatures of all samples were increased from 0 K to 2500 K to break the initial crystalline structure state and moved to a liquid state. When the temperature is conducted to 2500 K, the samples were cooled to different temperatures of 1300, 1100, 900, 700, 600, 500, 400, and 300 K, with the same heating rate, to switch from the liquid to crystalline state. The crystallization process of FeNi alloys is investigated through RDF, size (\( l \)), total energy of the system (\( E_{\text{total}} \)), structure (through shape, size, and relationship between the temperature (\( T \) ) and \( E_{\text{total}} \)). CNA$^3$ is used to determine the structure unit number of FCC, HCP, BCC, and Amor structures, and the heating rate process of FeNi alloys is carried out by the Nosé–Hoover temperature regulator.$^4,5$

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