Some Factors Affected on Structure, Mechanical of Ni Bulk

Nguyen Trong Dung*, Nguyen Chinh Cuong

Faculty of Physics, Hanoi National University of Education, Hanoi, Vietnam
Email: *dungntsphn@gmail.com

Abstract

The article examines the effect of atomic number, temperature and tempering time on microstructure and mechanical of Ni bulk by molecular dynamics simulation and deformation z-axis. Samples Ni with \( N = 4000, 5324, 6912, \) and 8788 atoms at 300 K, 6912 atoms at \( T = 1100, 900, 700, 500, 300 \) K and 6912 atoms at 900 K after different annealing time. The samples were incubated with the same heating rate \( \Delta T/\Delta t = 4 \times 10^{12} \) K/s. Combined with common neighborhood analysis method shown in sample is always existing four types structure: FCC, HCP, BCC, and Amor. In particular, structural units FCC, HCP and Amor always prevail and BCC are very small and appear only at 300, 500 K and 6912 atoms. When increasing atomic number, lowering temperature or increasing tempering time will facilitate crystallization process leading to increased FCC and HCP units number. The increasing FCC, HCP units number and additional appearance BCC structure led to change microstructure and mechanical of material: When increasing atom, lowering temperature and increasing incubation time lead to an increase in density of atoms that increase mechanical properties of the material.

Keywords

Atoms Number, Temperature, Microstructure, Mechanical, Ni Bulk

1. Introduction

Nowadays, materials Ni bulk are always used in industries: Microelectronics [1] [2] [3] [4], photocatalyst [5] [6], photovoltaics [7], and solar energy [8]. In that, they have great influence on microstructure, surface morphology and crystallization state on microstructure, mechanical. To research and manufacture, materials have many methods: experimental [9]-[13] and theoretical [14] [15] [16]. The results do not always give the desired results. Phase transitions, heteroge-
uneous dynamic s, surface shape, size, and crystallization lead to changes structures: BCC, FCC, HCP, [17]-[24]. Cause when size material limited led to appearance quantum effects (Size effects, surface effects), materials appear much different natures [25] [26] [27] [28].

To get a better understanding of the factors that influence on microstructure and mechanical of material. Molecular dynamics simulation is considered an effective tool for empirical research to study the microstructure of metals [29]-[38], deformation of z-axis to determine mechanical properties of metal have structured FCC (Al, Cu và Ni) and BCC (Fe, Cr, W). Macmillan, Kelley [39] and Parrinello, Rahman found [40] that: With Ni bulk, deformation of material depends greatly on the direction of strain and the intensity of applied pressure. Komandari et al. [41] [42], Park et al. [43] [44] stretched nanowires in different directions and Wu [45] [46], Golovnev [47] studied the mechanical properties of Cu nanowires and determined relationship between temperatures. Dimensions are always proportional to deformation, and Lin Yuan and colleagues [48] examined monoclinic mechanics at different temperatures. The results show, we cannot predict the deformation of materials at high temperatures and high heating rates [49] [50] [51] [52]. Therefore, study a number of factors affecting the microstructure, and mechanics of nano-sized nanomaterials, will contribute to the fabrication of new materials [53]. In this paper, we focus on the influence of factors such as atomic number, temperature, microstructure and mechanical properties and termination; and the relationship among size, stress and number of structural units FCC, HCP, BCC, and Amor.

2. Research Methodology

Ni samples with $N = 4000, 5324, 6912$ và $8778$ atoms (respectively Ni4000, Ni5324, Ni6912, Ni8778) is placed in cubic with FCC structure at 0 K temperature and interruption radius 3.0 Å. After that increase temperature from 0 K up 2000 K and lower temperature from 2000 K down 1100, 900, 700, 500 and 300 K with heating rate is $4 \times 10^{12}$ K/s and process of thermal annealing with 0.0, 6 $\times$ 10$^4$, 12 $\times$ 10$^4$, 20 $\times$ 10$^4$ moving step, displacement time is 2fs (corresponding with 0.0, 120, 240, 400 fs) break initial state to study microstructure in new states. In particular, the process of increasing temperature (lower temperature) the follows Nosé-Hoover relation [54] [55] [56]. To perform this process, we used molecular dynamics (MD) simulations with interactive embedding Sutton-Chen (1) and periodic boundary conditions [57]-[62].

$$E_{tot} = \varepsilon \sum_{ij} \left[ \frac{1}{2} \sum_{j\neq i} \Phi(r_{ij}) - C \sqrt{\rho_i} \right]; \quad \Phi(r_{ij}) = \left( \frac{a_i}{r_{ij}} \right)^n, \quad \rho_i = \sum_{j\neq i} \left( \frac{a_i}{r_{ij}} \right)^n \quad (1)$$

With: $r_{ij}$ is distance between two atoms $i, j; a$ is parameter with dimension of length; $\rho_i$ is atomic density $i; E_{tot}$ is total energy of the system; $\Phi(r_{ij})$ is interaction force on atom $i, r_{ij}$ is radius discon-nect, $\varepsilon$ is energy; $C, m, n, N$ is constant. With $\varepsilon = 7.3767 \text{meV}, C = 84.745, n = 10,$
m = 5 và a = 3.52 Å selected for accurate results on microstructure of materials at different temperatures.

Previously, interactive embedding Sutton-Chen has been used extensively to study phase transition in metals [63] [64] [65] [66] [67]. In addition, study microstructure of materials we use Common Neighbor Analysis methods (CNA) [68] [69] [70]. To study mechanical properties of Ni, we used z-axis deformation method (2) to determine the relationship between stress and strain.

\[ \varepsilon_{zz} = \frac{l_{zz}(t) - l_{zz}(0)}{l_{zz}(0)} = \alpha \sigma_{zz}; \quad \alpha = \frac{1}{E} \quad \text{and} \quad \sigma_{zz} = \sigma_{zz} - \mu \left( \sigma_{xx} + \sigma_{yy} \right) \]

\[ G = \frac{E}{2(1+\mu)} \]

\[ \sigma_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{V_i} \left[ m_i v_{i\alpha} v_{i\beta} + \frac{1}{2} \sum_{j=1}^{N} F_{ij} r_{ij}^\alpha r_{ij}^\beta \right], \quad \mu = 0.31 \]

Here, \( m_i \) is mass of atom \( i \), \( v_{i\alpha} \) is velocity of atom \( i \) along axis \( \alpha \) and \( F_{ij} \) is interaction force between atom \( i \) and atom \( j \), \( r_{ij} \) is distance between atom \( i \) and \( j \), and \( r_{ij}^\alpha \) is vector in \( \alpha \) axis from atom \( i \) to atom \( j \). Where \( E \) is stress, \( G \) is slipping and \( \mu \) is deformation coefficient, \( \alpha \) is factor deformation, \( \varepsilon_{zz} \) is deformation z-axis; \( \sigma_{xx} \), \( \sigma_{yy} \), \( \sigma_{zz} \) is stress according to \( x, y, z \), and \( \sigma_{\alpha\beta} \) is stress model. Deformation is determined by the work [71] [72].

3. Results and Discussion

3.1. The Influence of the Atomic Number

The microstructure of Ni4000, Ni5324, Ni6912, Ni8788 at temperature 300 K, determined by radial distribution function (RDF), resulting in Figure 1.

The Ni4000 has the first peak of RDF prevail with valuable is 2.45 Å that shows sample Ni bulk do not far order exist that always exist near order (Figure 1(a)) and have average coordination number is 12 (Figure 1(b)). When increasing atoms number then first peak height of RDF decreased from 7.35 (Ni4000) down 5.76 (Ni6912) and increased 7.61 (Ni8788) leading to increased atomic density. The first peak of RDF increases and decreases do not follow specific rules. The minimum value at Ni6912, due to in material has microstructural units existence, results show in the second peak of RDF. The second position peak varies of RDF from 3.45 to 3.55Å reaching and a maximum value at 3.55Å. The first peak height RDF Ni bulk sample smaller nanoparticles, second peak position Ni bulk larger nanoparticles. These results are entirely consistent with Ni nanoparticles [73]. Confirm this, we use simulation method, resulting in Figure 2 and Table 1.

The results show that Ni4000 at 300 K has three types of structures: FCC, HCP, Amor (Figure 2(e), Figure 2(g), Figure 2(i)). When increasing \( N \) from 4000 to 5324, 6912 and 8788 atoms then number units of FCC, HCP increased, Amor decrease (Figures 2(a)-(c)) and Table 1. However, with Ni8788 sample shows has four types structures of FCC, HCP, BCC, Amor (Figure 2(e), Figure 2(g), Figure 2(h), Figure 2(i)). When increases atoms number lead to a density of atoms
increases, increasing units number of FCC, HCP, BCC and decrease units number Amor in the sample. The main cause leading to the appearance of number units structural of BCC is due to the size effect. The appearance of structural

| Samp (atom) | 4000   | 5324   | 6912   | 8788   |
|-------------|--------|--------|--------|--------|
| FCC         | 2044   | 3154   | 4017   | 4886   |
| HCP         | 1943   | 1816   | 2025   | 3887   |
| BCC         | 0      | 0      | 14     | 0      |
| Amor        | 13     | 354    | 8      | 15     |

**Figure 1.** Radial distribution function (a); average coordination number (b) with different atomic numbers at temperature 300 K.

**Figure 2.** New state of sample 4000 atoms (a); 5324 atoms (b); 6912 atoms (c); 8788 atoms (d) at temperature 300 K and structural shape in the sample (e); (g); (h); (i).
units FCC, HCP, Amor consistent with the results [74] [75] [76] [77], unit number of BCC structure fit with Brewer [78]. With the emergence of BCC structure units, number at sample Ni_{4912} is astonished by scientists. However, these results should be checked and assessed for accuracy by results of Centrosymmetry Parameters [79] [80], Bond Angle Analysis [81], Bond Order [82] and another method to solve this problem. To study the influence of atomic number up mechanical properties of sample Ni bulk we used z-axis distortion method to determine the relationship between stress and strain of sample. The results are shown in **Figure 3** and **Table 2**.

The results show, with Ni_{4000} sample has stress value of $E = 173.04$ GPa. When N increases from 4000 to 5324, 6912, 8788 atoms then E increases from 173.04 to 194.76 GPa and decreases to 189.83 GPa and reaches a maximum value of 194.76

![Figure 3](image)

**Figure 3.** Relationship between deformation and stress of samples with different atomic numbers.

**Table 2.** Characteristics mechanical properties of Ni bulk samples at temperature 300 K.

| sample (atoms) | Deformation coefficient | Stress Young module E (GPa) | Slipping module G (GPa) | Experimental results at 20°C E (GPa) |
|---------------|-------------------------|-----------------------------|------------------------|------------------------------------|
| 4000          | 0.9454                  | 173.04                      | 66.04                  | 200 [83]                           |
| 5324          | 0.0069                  | 181.07                      | 69.11                  |                                    |
| 6912          | 0.03237                 | 194.76                      | 74.33                  |                                    |
| 8788          | 0.2004                  | 189.83                      | 72.45                  |                                    |
GPa at Ni₆₉₁₂ (Figure 3(b)). This result is consistent with influence atoms number on microstructure and number structural units. With Ni₆₉₁₂ structure appears BCC and increase structure number FCC, HCP, BCC is greatest. That raises the question: Is there a link between atoms number, structural units number and stress value of the material. To answer this question, previous studies have examined the effect of porosity on mechanical properties of materials by equation Voigt [84], Spriggs [85] and correlation function Hashin–Strikman [84]. Besides, under influence of external forces leading to change of shape when the structural units number in crystal lattice changes: Ito and est [86] assume that size of empty hole increases when deformation increases lead to stress decreases. The results were consistent with experimental results, at 293 K with \( E = 200 \) GPa [56], Slipping \( G = 79.6 \) GPa, deformation coefficient \( \alpha = 0.31 \). This shows that influence of atoms number on microstructure leads to appearance BCC structure at Ni₆₉₁₂ to increase stress \( E \).

### 3.2. Effect of Temperature

The microstructural, mechanical properties of Ni₆₉₁₂ bulk at 1100, 900, 700, 500 and 300 K are shown in Figure 4.

The results show that at 1100 K on sample there existed only 13 atoms has HCP structure (Figure 4(a1)). The first peak of radial distribution function \( g(r) \) is 3.4 Å (Figure 4(a2)) and stress \( E = 0 \) and slope \( G = 0 \) (Figure 4(a3)). When temperature lowered 900, 700, 500 and 300 K then structure units number FCC, HCP and BCC increased sharply lead to Amor structure units number decrease resulting (Figures 4(b1)-4(e1)), \( g(r) \) increased sharply from 3.4 Å up 5.82 Å (Figures 4(b2)-4(e2)) and \( E, G \) increased from 0.0 up 194.76 GPa, 74.33 Gpa (Figures 4(b3)-4(e3)). However, phase transition from liquid to amorphous states lead to structure units number of structural, \( g(r) \), \( E \) and \( G \) increased. The obtained results show that at 900 K is transition temperature (\( T_m \)) of Ni₆₉₁₂ bulk.

This result is consistent with Ni₄₀₀₀ bulk has crystalline temperature is 800 K [32], Ni₃₂₃₄ nanoparticles have \( T_m = 800 \) K [73] and when \( N \) increases then \( T_m \) increasing [30]. In addition, phase transition temperature depends not only on number of atoms but also on shape and size [35] such as: Wen et al. assume that melting temperature \( T_m \) of Ni nanowires is inversely proportional with size \( D \) [31] and Trong Dung Nguyen assumes that for Ni nanoparticles then \( D \) is proportional with \( N^{-1/3} \), \( E \) is inverse with \( N \) and confirm that transition temperature of sample is not applicable to nanoparticles [73]. The other side, when temperature decreases then \( E, G \) increase [87]-[91] as by deformation of z-axis, \( E = 171 \) GPa [92]. This confirms when temperature decreases then \( E \) increases and determination at 900K is phase transition temperature of Ni₆₉₁₂ bulk.

### 3.3. The Effect of Crystallization

The energy, size, number of structural units, radial distribution function, \( E \) and \( G \) of Ni₆₉₁₂ bulk after incubation time are shown in Table 3, Figure 5.
The results show that at 0.0 fs then energy of sample is −1097.37 eV, size is 8.209 nm, structural units number are 56 FCC, 75 HCP, g(r) = 3.59 Å, $E = G = 0$ GPa. When increases the heating time up 120, 240, 400 fs then energy, size decreases leading structural units number FCC, HCP increases, g(r) increases, E and G increase. This result is consistent with simulation results of Ni$_{5324}$ nanoparticles [73]. On the other hand, when increasing tempering time then E, G of sample increases. After 400 fs heating time then deformation coefficient $\alpha = 0.01299$ and stress $E = 200.31$ GPa, $G = 76.46$ GPa (Figure 5(d3)). These results simulation are consistent with results of the experiment [83]. This confirms that there is a great influence of atoms number, temperature and thermal time on microstructure and mechanical properties of Ni bulk.

### 4. Conclusion

The Ni$_{4000}$, Ni$_{5324}$, Ni$_{6912}$, Ni$_{8788}$ samples were prepared by molecular dynamics simulation and z-axis compression. The results showed that when increasing atomic number (decreasing temperature and increasing incubation time) then RDF height decreases (increasing) leading to structural unit number FCC, HCP, BCC, $E$, $G$, and mechanical properties increase. The influence of atomic number, temperature, tempering time on microstructure and mechanical properties in the material structure exists in FCC, HCP, and BCC. Based on results shown, sample Ni bulk with a higher atomic number, lower temperature, and higher thermal incubation time than sample Ni bulk will has more balanced and stable. With samples Ni bulk has an atomic number, temperature and different heating time then structural unit number FCC and HCP changes are still dominant mainly in FCC structure while structure units number BCC is very small. When increasing $N$
Figure 5. Structural unit number, radial distribution function, mechanical of Ni	extsubscript{6912} bulk after different heating time.

from 4000 to 8788 atoms then $g(r)$ decreases, structure units number FCC and HCP increase as $\alpha$, $E$, $G$ increase. At Ni	extsubscript{6912} add structure BCC lead to $E$ reach maximum value, this suggests that addition of BCC structure increases entropy. This is an indispensable basis for the balance of Ni bulk also when decreasing temperature and increasing incubation time lead to stress increases, is due to in structure units number FCC and HCP increase. The results are based on theoretical foundations of structural units number FCC, HCP, and BCC. Amors are unclear and should be encouraged in further studies.

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