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MOLECULAR DYNAMICS SIMULATIONS OF STRUCTURAL PROPERTIES OF CuNi ALLOYS DURING THE COOLING PROCESS AT HIGH PRESSURE

Nguyen Thi Thao, Bui Thi Ha Giang, Tran Phan Thuy Linh, Nguyen Van Hop, Pham Do Chung, Pham Van Hai and Nguyen Thi Huyen Trang
Faculty of Physics, Hanoi National University of Education

Abstract. Molecular dynamics simulations of $Cu_{80}Ni_{20}$ (Cu:Ni = 8:2) model with the size of 8788 atoms have been carried out to study the structure and mechanical behavior at high pressure of 45 GPa. The interactions between atoms of the system were calculated by the Quantum Sutton-Chen embedded-atom potentials. The crystallization has occurred during the cooling process with a cooling rate of 0.01 K/ps. The temperature range of the phase transition is determined based on the sudden change of atomic potential during the cooling process. There is also a sudden change in the number of individual atoms in the sample. At a temperature of 300 K, both Ni and Cu atoms are crystallized into the face-centered cubic (FCC) and the hexagonal close-packed (HCP) phases, respectively. The mechanical characteristics of the sample at 300 K were also analyzed in detail through the determination of elastic modulus, number of atoms, and void distribution during the tensile process.

Keywords: molecular dynamics simulations, CuNi alloy, crystalization, deformation.

1. Introduction

An increasing number of scientists are working on CuNi because it has many special properties that lead to many practical applications. Copper-nickel alloys are widely used for marine applications due to their excellent resistance to seawater corrosion, good fabricability, and their effectiveness in lowering macrofouling levels. They are also used in non-marine applications due to their durability, appearance, and antimicrobial properties [1]. CuNi alloys are typical solid solutions because of the infinite solubility [2]. CuNi alloy excels in the durability, hardness, thermoelectric properties, and corrosion resistance of seawater compared to pure copper [3, 4]. Research works often focus on

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Contact Nguyen Thi Thao, e-mail address: ntthao.hnue@gmail.com

crystallization in liquid CuNi alloys, pressure effects on CuNi rapid solidified alloy model systems. Based on lots of studies in the CuNi model, during the cooling process, a liquid metal has transitioned from amorphous atoms to crystalline atoms. When cooling to a lower temperature (approximately 300 K to 400 K), there is a big drop of energy in transition, atoms will move closer to the equilibrium position, from disorder to order crystalline [5-9]. The main thing that has an important role in the form of structure is the cooling rate [9]. With a high cooling rate, the alloy will have an amorphous structure; in contrast, with a slow cooling rate enough, it will have a crystalline structure [8, 9]. In particular, pressures also contribute to the stabilization of alloy. Investigating with a short-range from 0 GPa to 5 GPa, the increase of pressure will lead to an increase in crystalline temperature, density, and reduced interatomic distance between atoms. At high pressures, CuNi alloy easily forms a crystal structure when cooled and the resulting crystal structure is an FCC structure with all cooling rates [8]. The crystallization temperature of CuNi alloys was determined and depends on factors such as the cooling rate, the concentration of atoms in the sample, and the pressure [8, 10].

The mechanical properties of CuNi alloys have been studied with different concentrations of Ni atoms by the uniaxial deformation method [11]. The results indicated that with increasing Ni content the yield strength and ultimate tensile strength of CuNi alloys continue to increase and the instantaneous strain-hardening rate is improved gradually over the entire strain range. However, there are very few studies on the correlation between mechanical and structural properties of the CuNi alloys at high pressures.

In the present work, the structural and mechanical properties of the CuNi alloy at high pressures were studied by using molecular dynamics simulation, structural and mechanical analysis.

2. Content

2.1. Computational methods

CuNi alloy model with the size of 8788 atoms is constructed by molecular dynamics simulation, Cu and Ni atomic concentrations of 80% and 20%, respectively. The total energy of the system in quantum Sutton-Chen (Q-SC) type many-body FF given by ref. [7]. In the Q-SC interaction model, energy is defined in terms of surface energies, vacancy energies, and stacking-fault energies. The sample was heated at 2000 K and a high pressure of 45 GPa. Then these samples were cooled down to 300 K at a cooling rate of 0.01 $K.ps^{-1}$. The structural characteristics of this sample during the cooling process and at a temperature of 300 K were analyzed through PRDF (Pair radial distribution function), CNA (The Common Neighbor Analysis) methods, and visualization. The tensile strain is carried out at 300 K with a strain rate of $0.512ps^{-1}$. This deformation method was described in detail in previous work [12].

2.2. Results and discussions

In the cooling process, we investigate the dependence of potential energy on temperature. In Figure 1, when temperature increased, potential energy increased too. It seems to be a linear function until at range T_2 to T_1, potential energy went high suddenly.

This signal showed that the sample had a phase transition at that range. Therefore, we analysis the temperature range of these samples.

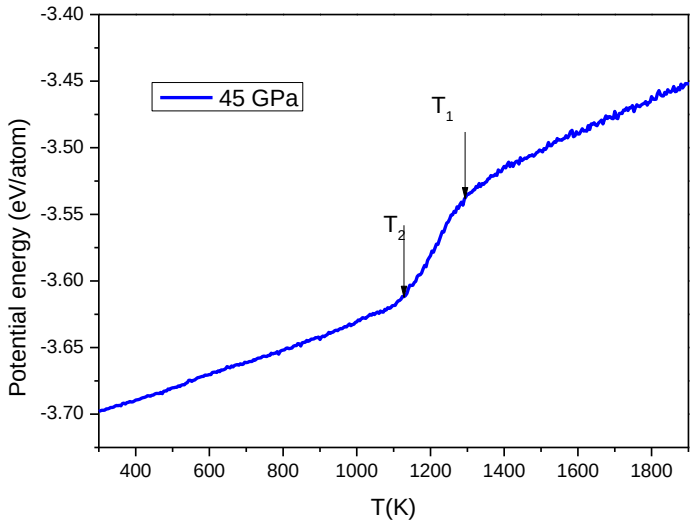


Figure 1. Dependence on the temperature of potential energy under the cooling process at the pressure of 45 GPa

The temperature range of crystallization can be evaluated in a range of (1320, 1150) K. This result is larger than the calculated result of [10] (1016, 1000) K because of the difference in atomic concentration, cooling rate, and interaction potential.

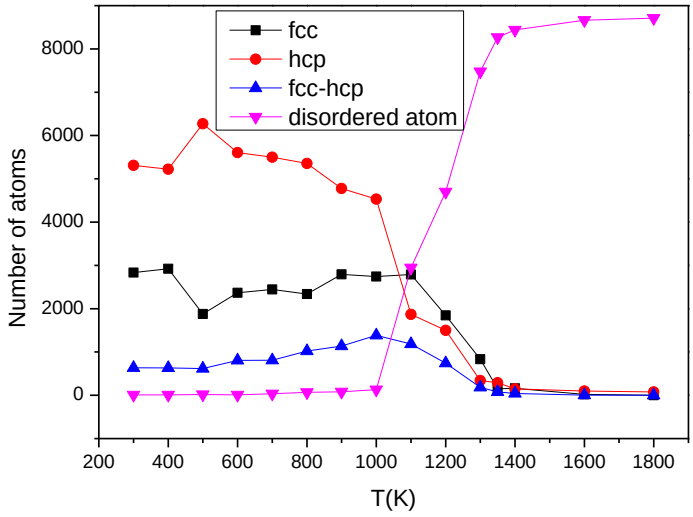


Figure 2. Variations of FCC, HCP, HCP-FCC, and disordered atoms upon the cooling process at the pressure of 45GPa

To study the structural change during the cooling process, the number of each type of atoms present in the sample is determined at different temperatures from 1800 K to 300 K. The temperature dependence of the atom types is shown in Figure 2. At the temperature range of phase transition, there are both sudden changes in the number of different types of atoms and the transition from disordered atoms to HCP atoms. In the crystal phase, the atomic number of each type is virtually unchanged. At 500 K, there is a relative number of HCP atoms that change to the FCC structure.

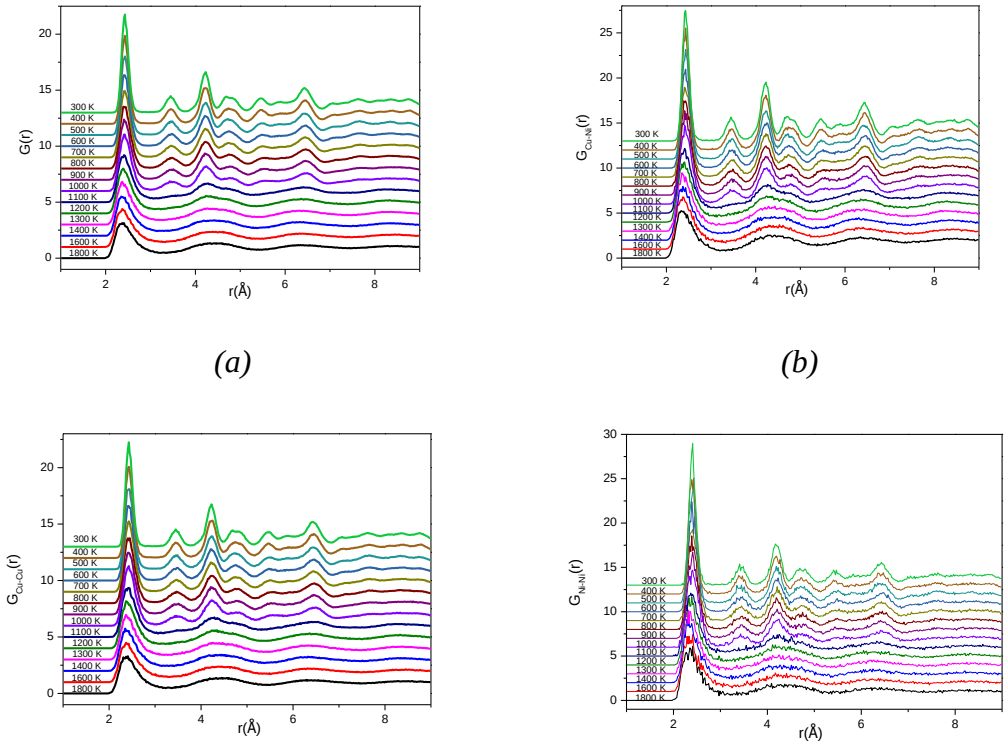


Figure 3. The RDF of $Cu_{80}Ni_{20}$ samples at the pressure of 45GPa: a) The total radial distribution function G(r) of CuNi samples; b) The pair RDF $G_{Cu\text{-}Ni}(r)$ for Cu-Ni pair; c) The pair RDF $G_{Cu\text{-}Cu}(r)$ for Cu-Cu pair; d) The pair RDF $G_{Ni\text{-}Ni}(r)$ for Ni-Ni pair

The structural change of samples is illustrated through the transformation of RDF during the cooling process. Figure 3 shows the RDF of CuNi samples at the pressure of 45 GPa at different temperatures from 1800 K down to 300 K. The results in Figure 3 indicate that samples at a temperature below 1100 K show a crystal structure because of the appearance of multiple peaks.

Table 1. Variation of the Total number of crystal atoms upon the cooling process at the pressure of 45GPa

T(K)	300	400	500	600	700	800	900	1000	1100	1200	1300	1400	1600	1800
Total number crystal atoms	8778	8778	8769	8778	8753	8716	8707	8658	5843	4088	1355	350	124	78

The variation of the total number of crystal atoms upon the cooling process is indicated in Table 1. When the temperature was less than 1100 K, the total number of crystal atoms insignificant change. The spatial distribution of crystal atoms of $Cu_{80}Ni_{20}$ samples during the cooling process is shown in Figure 4.

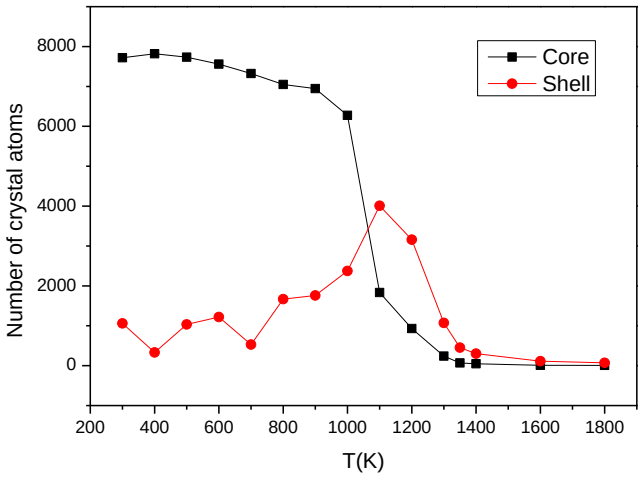


Figure 4. Spatial distribution of crystal atoms of $Cu_{80}Ni_{20}$ samples during the cooling process

Figure 4 shows that, in the temperature range of phase transition, there is a sudden change in the number of crystal atoms, the crystal atoms increase faster in the shell of the sample. In the temperature range from 1100 K to 1000 K, the crystalline atoms strongly transfer the shell particles into the cores of the samples. Below 1000 K, the crystalline atoms in the core increase slightly in proportion to the slight decrease in the crystalline atoms in the shell of the sample.

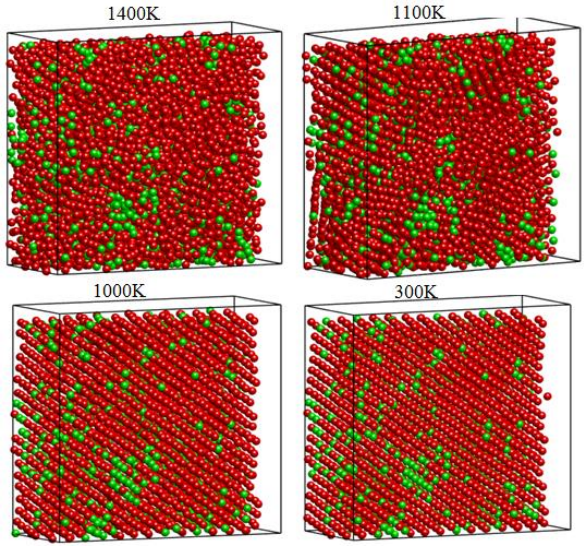


Figure 5. Cross-sectional $Cu_{80}Ni_{20}$ samples during the cooling process

The structures of samples at different temperatures are visualized in Figure 5. This result is consistent with the total number and distribution of crystal atoms as shown above.

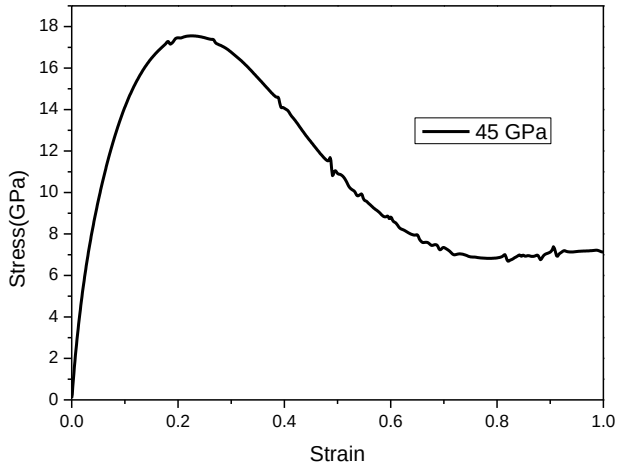


Figure 6. The stress-strain curve of $Cu_{80}Ni_{20}$ sample with the size of 8788 atoms at 300 K upon uniaxial tension

The mechanical behavior of CuNi alloy at 300 K is studied by applied uniaxial tension tests. Figure 6 shows the stress-strain curves at a strain rate of 0.052 ps^{1}. The stress increases linearly to the maximum value of 17 GPa at a strain of 0.2. As the strain continues to increase, the stress decreases to 7 GPa at a strain value of 0.7 and then remains constant. So CuNi sample exhibits both elastic and plastic deformations under the uniaxial tension test. The elastic regions correspond to the strain below 0.2 and the plastic regions correspond to the strain. The value of Young's modulus which is determined from the slopes of the stress-strain curves in the linear region is 291GPa.

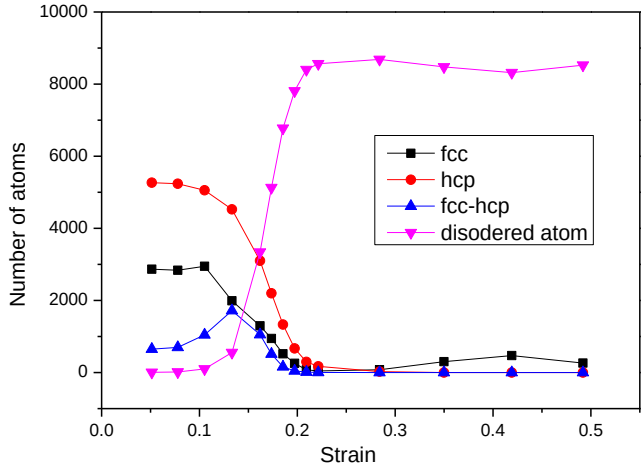
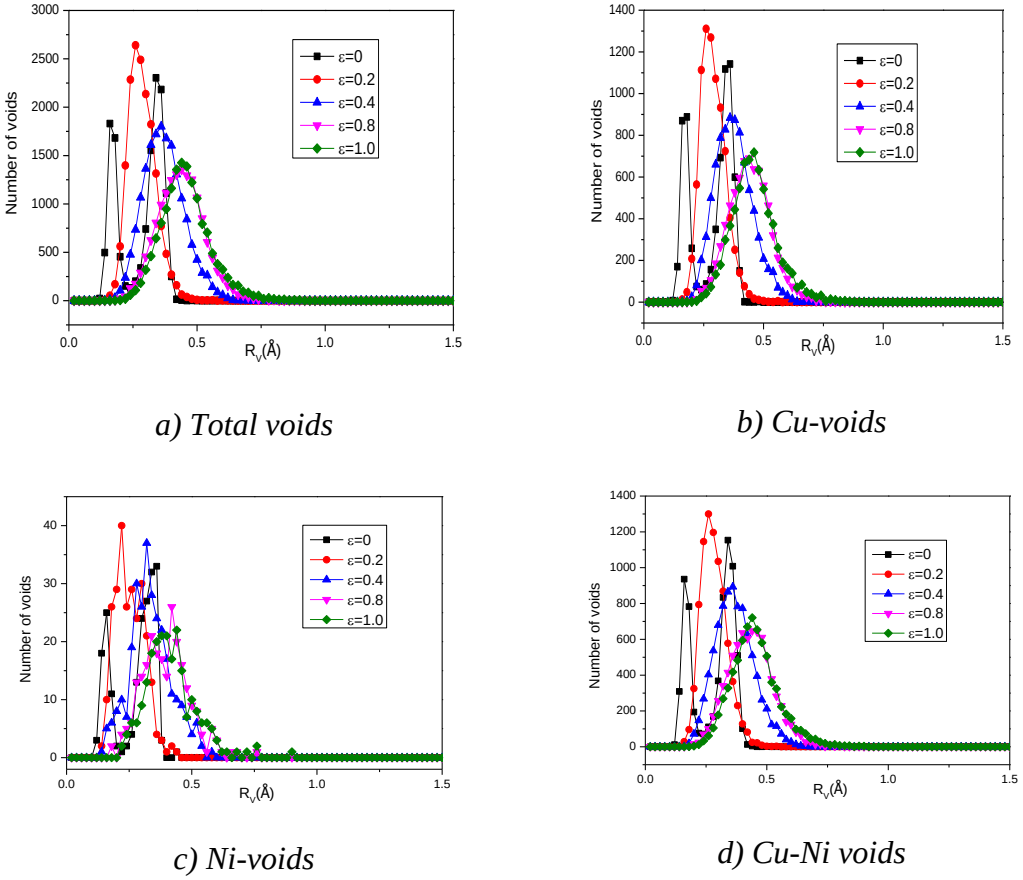


Figure 7. The change of different kinds of atoms upon the uniaxial tension process at a pressure of 45 GPa

Figure 7 shows the change of HCP, HCP-FCC, FCC, and disordered atoms under the uniaxial strain. The number of crystal atoms is almost unchanged in the elastic region. The number of crystal atoms decreases quickly while the number of disordered atoms increases in the plastic region.



a) Total voids *b) Cu-voids*

c) Ni-voids *d) Cu-Ni voids*

Figure 8. The radii distributions of voids under uniaxial tension: a) Totals voids of the sample, b) Cu-voids, c) Ni-voids, and d) Cu-Ni-voids

The radii distributions of the total voids, Cu-voids, Ni-voids, and Cu-Ni-voids in the sample upon uniaxial tension at different strain (ε) are shown in Figure 8a-d. Here R_v is the radius of the void. The peaks of these radii distributions shift to the right and become wider as the strain increases. These show that radii of these voids increase as the strain increase.

3. Conclusions

The structural transformation of the CuNi sample has been studied by molecular dynamics simulations upon the cooling process at a pressure of 45 GPa. The crystal transition temperature range of this sample is between 1320K and 1150K. The structural transformation to the crystalline phase is analyzed in detail through the radial distribution function and the common neighbor analysis method. The result shows both Ni and Cu atoms are crystallized into face-centered cubic and hexagonal close-packed phases. CuNi

samples exhibit both elastic and plastic deformations under the uniaxial tension test. The number of crystal atoms decreases quickly while the number of disordered atoms increases in the plastic region.

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