Calculation of the Mechanical Properties of Cu-Ni Nanocluster

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Abstract:
The aim of this research is to calculate the elastic constants and Bulk modulus of Cu-20 wt% Ni random Nanoalloy. The molecular dynamics simulation technique was used to calculate the mechanical properties in NPT ensemble. The interaction between atoms as well as cohesive energy in the Nanoalloy modeled systems was calculated by Morse et al. two body potential. Also the temperature of the system was controlled by Nose-Hoover thermostat and the pressure was controlled by using the Berendsen barostat. The effects of the temperature and Nanoalloy size on the elastics constants as well as bulk modulus were studied. The obtained results show that the variation in the size and temperature of Cu, Ni as well as Cu-Ni Nano cluster causes some changes on the mechanical properties. Moreover, the effect of Ni concentration on the mechanical properties of Cu-Ni random Nanoalloy was investigated.
Keywords: *Cu-Ni Nanoalloy, Bulk Modulus, Elastic constants, Molecular Dynamics simulation.*

1- INTRODUCTION

The Copper alloys such as Copper-Nickel alloy are well known because of their resistance to corrosion and to stress-corrosion cracking. They are used in condensers and heat exchangers; therefore calculation of thermal and mechanical properties of these alloys is very important in industrial applications. The elastic stiffness constants, as well as bulk modulus of solids are intrinsically related to lattice stability. These properties depend on the composition and temperature.

Shen et al. studied Young's modulus of Nanocrystalline Fe, Cu, Ni, and Cu-Ni alloy by the nano-indentation technique and observed that Young's modulus depend on grain size [1]. In another study Zhang et al. conducted a comparative study of compressibility (i.e. inverse bulk modulus) between nanocrystalliane and bulk nickel using synchrotron X-ray diffraction at pressure up to 7.4 GPa. Their results showed elastic softening in nanocrystalline nickel as compared with the bulk nickel [2]. E. Iguchi and K. Udagawa in another research measured elastic constants as well as Young's modulus as a function of the atomic fraction of Cu by the use of the average cellular potential [3]. The elastic properties of bulk Cu, and Cu-Ni alloy were determined in different temperature by H. M. Ledbetter and W. F. Weston [4], but there aren't any results from size dependence of elastic properties of Copper-Nickel alloy.

The molecular Dynamics (MD) simulation technique used to study mechanical properties of materials in nano as well as macro scale [5]. In this study, elastic constants (C_{11}, C_{12}), as well as bulk modulus of Copper, Nickel, and Cu-20 wt% Ni in Nano scale is reported. The temperature dependence as well as size dependence of mechanical properties of Cu, Ni and Cu-20 wt% Ni was calculated by molecular dynamics simulation techniques. The obtained results compared with available experimental data. Moreover the Ni concentration effect on the

mechanical properties of Cu-Ni alloy was studied in this research.

This paper is organized as follows. Section 2 details our simulation methodology that was used for equilibrium molecular dynamics simulation. In section 3, the simulation results for the materials under investigation are reported. Finally, section 4 provides our concluding remarks.

2. SIMULATION DETAILS

The molecular dynamics simulations for this work were performed in the Isothermal-Isobaric (NPT) ensemble at zero pressure. The simulations were done in different size of nano clusters at different temperatures. Therefore, the temperature and size dependence of mechanical properties of Cu, Ni, as well as Cu-Ni alloy were obtained. The simulation time step, δt, was set between 0.1 to 0.5 ps for different simulations. The clusters were first equilibrated for 100000 time steps at T=20 K, then the temperature was raised by 1K at each time step, reaching 400 K after 2000000 Time steps. At each time step during arising the temperature, the system was re-equilibrated for 5000 Time steps. Periodic boundary conditions were imposed in all directions.

The Berendsen barostat method and Nose-Hoover thermostat were used to control the pressure [6] and the temperature [7, 8] of the system respectively. One of the well-known approaches to implement the temperature control in an MD simulation is the use of Nose-Hoover (N-H) heat bath (thermostat). The introduction of this mechanism modifies the standard velocity Verlet equations of motion to the following forms [10].

(1)

$$\vec{r}_i(t+\delta t)=\vec{r}_i(t)+\delta t\vec{v}_i(t)+\frac{1}{2}\delta t^2\left[\frac{\vec{f}_i(t)}{m_i}-\zeta(t)\vec{v}_i(t)\right]$$

$$\vec{v}_i(t+\frac{\delta t}{2})=\vec{v}_i(t)+\frac{\delta t}{2}\left[\frac{\vec{f}_i(t)}{m_i}-\zeta(t)\vec{v}_i(t)\right]$$

$$\zeta(t+\tfrac{1}{2}\delta t)=\zeta(t)+\frac{\delta t}{2Q}\left[\sum_i^N m_i\vec{v}_i^{\,2}(t)-gk_bT\right]$$

$$\zeta(t+\delta t)=\zeta(t+\tfrac{1}{2}\delta t)+\frac{\delta t}{2Q}\left[\sum_i^N m_i\vec{v}_i^{\,2}(t+\tfrac{1}{2}\delta t)-gk_bT\right]$$

$$\vec{v}_i(t+\delta t)=\frac{2}{2+\delta t\zeta(t+\delta t)}\left[\vec{v}_i(t+\tfrac{1}{2}\delta t)+\frac{1}{2}\delta t\frac{\vec{f}_i(t+\delta t)}{m_i}\right]$$

Where ζ is the dynamic friction coefficient of the bath. This coefficient is not a constant and can take on both positive and negative values, leading to the deceleration or acceleration of the atoms respectively, if their total kinetic energy is greater or smaller than $gk_BT/2$. A particular parameterization of Q is given by

$$Q = gk_BT\tau^2 \qquad (2)$$

Where τ is the relaxation time of the thermostat, normally of the same order of magnitude as the simulation time step, $\delta\tau$. This controls the speed with which the thermostat damps down the fluctuations in the temperature. The number of degrees of freedom, g, is given by g=3(N-1).

In the classical MD simulation, the force experienced by an individual atom i in an N-atom nano scale cluster is obtained from the force equation

$$\vec{f}_i = -\sum_{j\neq i}\nabla_{r_i}U(r_{ij}) \qquad (3)$$

Where $U(r_{ij})$ is the prescribed interatomic potential energy function, and r_{ij} represents the separation distance between two atoms i and j. the potential employed in MD simulation reported in this paper is the Morse et al. two body potential [11], which is expressed as follow

(4)

$$U(r_{ij}) = D\{\exp(-2\alpha(r_{ij}-r_0))-2\exp(-\alpha(r_{ij}-r_0))\}$$

To construct the potentials for the binary alloy state, Cu-Ni, from the corresponding Morse potential for the elemental states, Lorentz-Berthelot rules were followed [12,13]. An arithmetic average were used

for the r_0 as well as α_i, while a geometric average is used for the D_i

$$D_{ij} = (D_i D_j)^{1/2}$$
$$\alpha_{ij} = \frac{1}{2}(\alpha_i + \alpha_j) \quad (5)$$
$$r_{0ij} = \frac{1}{2}(r_{0i} + r_{0j})$$

The potential parameters for the pure Cu, Ni and Cu-Ni alloy are listed in table 1.

The quantities calculated in these MD simulations are the mechanical properties including of Elastic constants C_{11}, C_{12}, and bulk modulus B of Pure Cu and Ni as well as Cu-Ni alloy in Nano scale.

According to the Hooke's law, for sufficiently small deformations, the stress components σ_{ij} are directly proportional to the strain components ε_{kl} via [14]

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \quad (6)$$

Where C_{ijkl} are the elastic stiffness constants, with dimensions of force per area or energy per volume. Due to symmetry conditions, the number of independent elastic constants can be reduced. For example, for cubic crystals, there are three independent constants C_{11}, C_{12}, and C_{44}. In terms of interatomic potentials, these constants can be expressed by [15]

$$C_{11} = \frac{1}{\Omega}\frac{\partial^2 U}{\partial \varepsilon_{11}^2}$$
$$C_{12} = \frac{1}{\Omega}\frac{\partial^2 U}{\partial \varepsilon_{11}\partial \varepsilon_{22}} \quad (7)$$
$$C_{44} = \frac{1}{4\Omega}\frac{\partial^2 U}{\partial \varepsilon_{12}^2}$$

Where ε_{11}, ε_{12} and ε_{22} are the components of the strain tensor, Ω is the atomic volume, and U is the total energy, is given by (4), per atom.

The bulk modulus, which measures how the volume of a solid changes with hydrostatic pressure, is measured at constant temperature, and is referred to as isothermal bulk modulus, denoted by B_T. This is related to the interatomic potential energy function via [14]

$$B_T = \mathrm{v}\left(\frac{\partial^2 U}{\partial \mathrm{v}^2}\right)_{\mathrm{v}=\mathrm{v}_0} \quad (8)$$

Where V_0 is the equilibrium value of V.

3. RESULTS

3.1. Temperature dependence of mechanical properties

The variation of the elastic properties with temperature for elemental materials Cu, Ni and the Cu-20 wt% Ni was computed using molecular dynamics simulations. Our motivation to compute these properties for the elemental materials was to obtain an estimate of the Morse potential accuracy. The results which were obtained from these simulations are plotted in figures 1 to 3. Elastic constants were calculated in the temperature ranges between 10 up to 400 K. Figures show that the elastic constants (C_{11}, C_{12}), as well as bulk modulus decrease with the increasing of the temperature. Our calculated values have the reasonable agreement with the available experimental data. This indicates the high quality of the alloy potential energy functions which were constructed on the basis of these elemental potentials. Therefore, it is reasonable to assume that the results which are obtained with the constructed alloy potentials provide good estimation of the experimental results. The percentage errors between the calculated values and experimental data for Cu, Ni and Cu-Ni are listed in table 2.

3.2. The composition dependence of mechanical properties

The composition dependence of C_{11}, C_{12}, and bulk modulus are shown in figure 4 between the pure elements. The results approximately show a liner trend in the mechanical properties. Also it is clear that the simulation results are in good agreement with available experimental values.

3.3. Size dependence of mechanical properties

The main goal of this research was to calculate the Size dependence of mechanical properties. The dependence of the mechanical properties of nano-sized cluster of Cu, Ni, and Cu-20 wt% Ni alloy was computed by changing the number of atoms in the clusters. The simulations were performed at constant pressure and temperature again. Results are plotted in figures 5-7. The effect of the cluster size on the mechanical properties can be seen from these profiles. All figures show that there is an initial change in the mechanical properties with the size of the cluster. These properties remain unchanged when the cluster size grows. This is a typical behavior of nanoscopic (or nanoscale) structures in which the mechanical and thermal properties change with size until reach a constant value which is the characteristic of the bulk or macroscopic dimension properties.

4. CONCLUSIONS

By using the molecular dynamics simulation it can be concluded that the mechanical properties of the studied system depend on the cluster temperature. Furthermore, the elastic constants as well as bulk modulus of CuNi have approximately a liner trend with the Nickel concentration. Finally, the mechanical properties of Cu, Ni and CuNi alloy depend on the cluster size in nano-scale which is a typical behavior for nanoscopic (or nanoscale) systems.

Table 1: Morse potential parameters for the Cu, Ni, and Cu-Ni alloy

Material	D(ev)	α (A^{-1})	r_0(A)
Cu	0.3446	1.3921	2.838
Ni	0.4279	1.3917	2.793
Cu-Ni	0.3839	1.3919	2.815

Table 2: The percentage errors between the calculated and experimental values

Mechanical properties	C_{11}	C_{12}	Bulk modulus
Ni	9	7	10.9
Cu	0.9	14	5
Cu-20%Ni	14	1.7	3

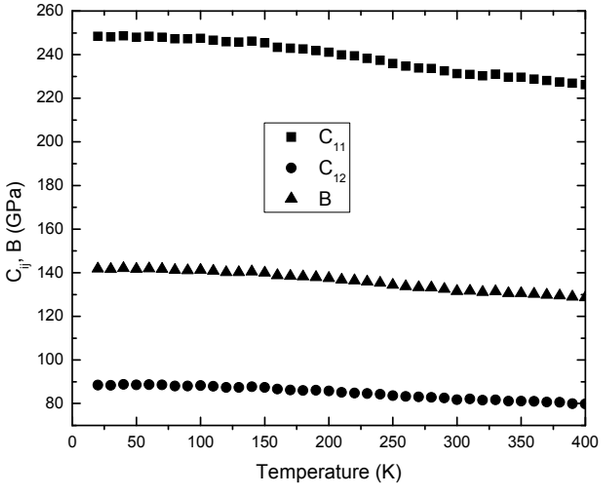

Figure 1: Variation of the elastic stiffness constants and bulk modulus versus the temperature for Cu consist of the 2048 atoms.

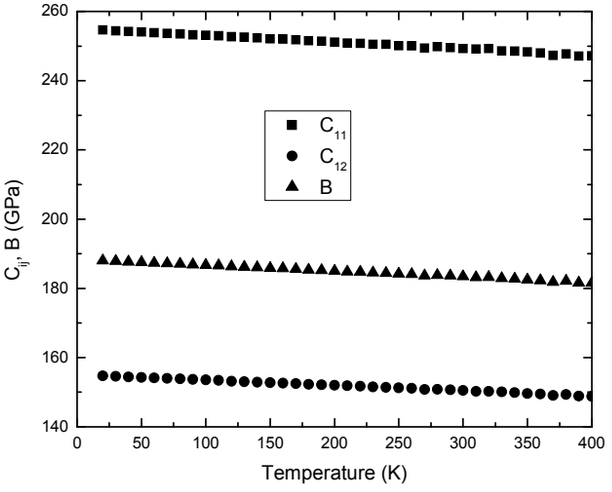

Figure 2: Variation of the elastic stiffness constants and bulk modulus versus the temperature for Ni consist of 2048 atoms.

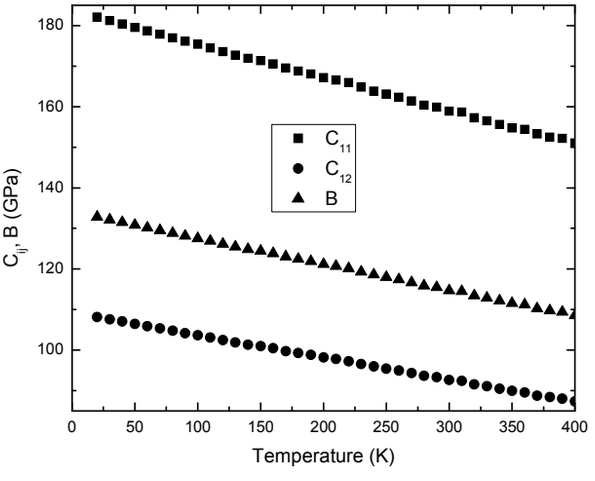

Figure 3: Variation of the elastic stiffness constants and bulk modulus versus the temperature for Cu-20 wt% Ni consist of 2048 atoms.

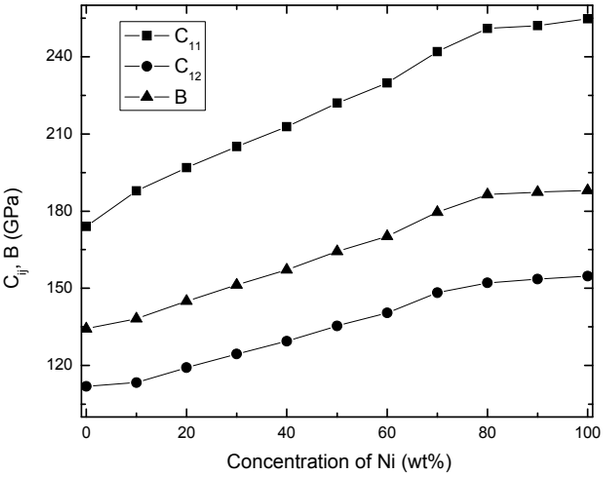

Figure 4: Variation of the elastic stiffness constants and bulk modulus of Cu-Ni alloy versus the concentration of Ni. The total number of atoms which were used is 2048.

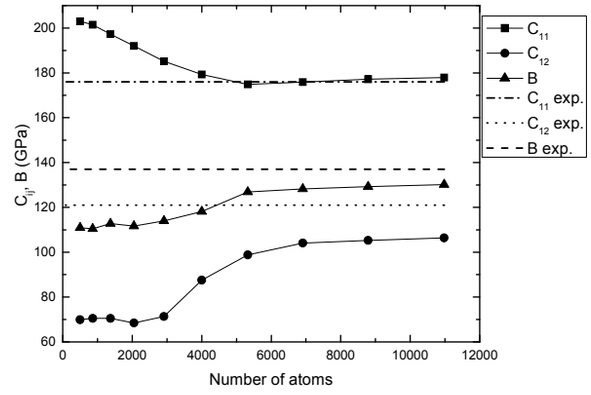

Figure 5: Variation of the elastic stiffness constants and bulk modulus of Cu versus the cluster size and bulk experimental values at room temperature.

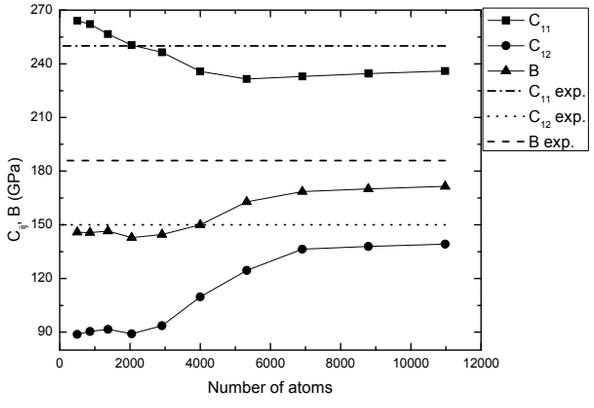

Figure 6: Variation of the elastic stiffness constants and bulk modulus of Ni versus the cluster size and bulk experimental values at room temperature.

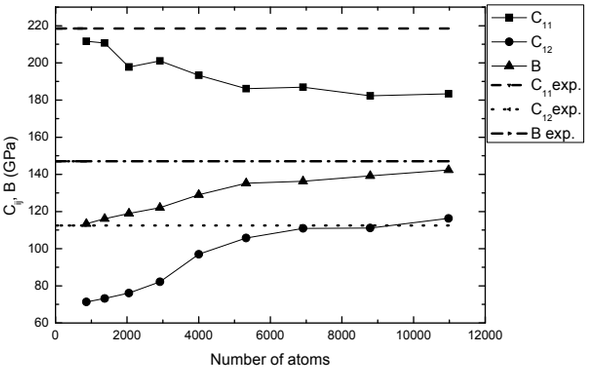

Figure 7: Variation of the elastic stiffness constants and bulk modulus of Cu-20 wt% Ni versus the cluster size at room temperature.

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