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Molecular Dynamics Simulation of Thermal Properties of Au_3Ni Nanowire

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Abstract**—**The aim of this research was to calculate the thermal properties of Au_3Ni Nanowire. The molecular dynamics (MD) simulation technique was used to obtain the effect of radius size on the energy, the melting temperature and the latent heat of fusion at the isobaric-isothermal (NPT) ensemble. The Quantum Sutton-Chen (Q-SC) many body interatomic potentials energy have been used for Gold (Au) and Nickel (Ni) elements and a mixing rule has been devised to obtain the parameters of these potentials for nanowire stats. Our MD simulation results show the melting temperature and latent heat of fusion increase upon increasing diameter of nanowire. Moreover, the cohesive energy decreased with increasing diameter of nanowire.

Keywords**—**Au_3Ni Nanowire, Thermal properties, Molecular dynamics simulation

I. Introduction

A nanowire is an extremely thin wire with a diameter on the order of a few nanometers. Recently, nanowires and nanorods of metallic and semiconductor materials have drawn a lot of research interest because of their unique physical properties, which are interesting from the view point of different device applications such as nanoelectronic devices and sensors for environmental, medical etc [1]-[4]. One-dimensional nanowires possess unique electrical, electronic, thermoelectrical, optical, magnetic and chemical properties, which are different from that of their macroscale size [5]-[8]. Metallic nanowires are of great interest from a fundamental point of view as well as for future applications [9], [10]. The Au-based nanowires have been studied for more than 10 years in both fundamental and application aspects. Especially, in the last five years thermodynamic and mechanical properties of Au-based nanowires were studied by molecular dynamics simulation technique. Among the Au-based nanowire, the Au-Ni nanowire is of special interest owing to their magnetic properties. Very few experimental data are available for the thermal properties of Au_3Ni ordered nanowire. Therefore, the study of this nanowire is necessary for industrial application.

A facile and economic approach has been developed for the synthesis of coaxial nanocables with AuNi alloy nanowires as inner solid cores and NiO as outer shells by Q. Xu and co-workers [11]. E. Anglada et al. presented first-principles molecular dynamics simulations of the formation of monatomic gold nanowires with different impurities (H, C, O, S) [12].

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In the other investigation, X. Y. Zhang et al. reported the electrochemical fabrication of highly ordered Au nanowire arrays within hexagonal close-packed nanochannel alumina templates with pore diameters ranging from 35 nm to 100 nm. Also, the growth mechanism of the single crystal Au nanowires was studied by them [13].

In this investigation, we have performed molecular dynamics (MD) simulation under constant pressure, constant temperature (NPT) ensemble [14], [15] to calculate the thermal properties including, cohesive energy, melting temperature, and latent heat of fusion of Au_3Ni nanowire. The quantum Sutton-Chen Q-SC potential [16], [17] parameters of the pure Au and Ni metals were used as interatomic potential parameters to calculate the cohesive energy as well as the thermal properties of Au, Ni pure metals and Au_3Ni nanowire.

II. Details of MD simulation

A. Interatomic potential

The force experienced by individual atom i in an N-atom cluster was obtained from Q-SC interatomic potential energy function. The potential energy of the pure metals and alloys in Sutton-Chen formalism for the systems of N atoms is given as follows [16], [17]

$$U_{tot}=\sum_{i=1}^{N}\left[\sum_{j\neq i}\varepsilon_{ij}\frac{1}{2}\left(\frac{a_{ij}}{r_{ij}}\right)^{n_{ij}}-c_i\varepsilon_{ii}\left(\sum_{j\neq i}\left(\frac{a_{ij}}{r_{ij}}\right)^{m_{ij}}\right)^{1/2}\right] \tag{1}$$

The first term in equation (1) is a two body interaction between the atoms i and j, the second term represents the many-body cohesion term associated with atom i, a is the length parameter scaling to the lattice spacing of the crystal, c is a dimensionless parameter scaling the attractive terms, ε is an energy parameter determined from experiment, and n, m are integer parameter with $n>m$ which determine the range of the two component of the potential (Table I).

TABLE I
THE Q-SC POTENTIAL PARAMETERS FOR AU-NI MODEL NANOWIRE

Interaction	ε(eV)	a(Å)	C	n	m
Au-Au	0.0078052	4.0651	53.581	11	8
Ni-Ni	0.0073767	3.5157	84.745	10	5
Au-Ni	0.007584	3.7804	------	10.5	6.5

To construct the potential for the binary alloy state, Au-Ni, from the corresponding Q-SC potentials for the elemental state, we used the following mixing rule

$$\varepsilon_{ij} = (\varepsilon_i \varepsilon_j)^{1/2}, \quad a_{ij} = (a_i a_j)^{1/2} \tag{2}$$

$$m_{ij} = \frac{(m_i + m_j)}{2}, \quad n_{ij} = \frac{(n_i + n_j)}{2} \tag{3}$$

B. Temperature and pressure control

The temperature control was implemented via the Nose-Hoover heat bath [18], [19] whose introduction modifies the standard velocity Verlet equation of motion [15, 20].

The standard Berendsen barostat [14] was used for pressure control of the system. The Berendsen barostat uses a scale factor, μ, which is a function of instantaneous pressure, P, to scale lengths in the system

$$\begin{aligned} x(i) &\to \mu x(i) \\ y(i) &\to \mu y(i) \\ z(i) &\to \mu z(i) \\ L &\to \mu L \end{aligned} \tag{4}$$

where μ is given by

$$\mu = \left[1 + \frac{\delta t}{\tau_p}(P - P_0) \right]^{1/3} \tag{5}$$

Here, τ_p is the rise time of the barostat, and P_0 is the set point pressure. The system pressure is set toward a desired value by changing the dimensions of the simulation cell size during the simulation.

C. Simulation data

Our MD simulations were carried out using Q-SC interatomic potential energy function. The simulations involved nanowires of Au_3Ni which have face center cubic structure. The Nickel atoms occupy the corner cites, and gold atoms occupy the face centers of the basis cube. The radius of nanowire changed between 3 to 7 nm to observe the effect of nanowire diameter on the physical properties. The simulation time step was set to 0.7 fs. The periodic boundary conditions were employed in nanowire axis only. The clusters were first equilibrated for 140 ps at T=250 K, and then the temperature was raised by 1 K at each temperature step. At each step that the temperature was increased, the system was re-equilibrated for 0.7 ps. Fig. 1 shows the variation of temperature and pressure in order to obtain the equilibrium state. Also, the variation of volume and energy with time step plotted in the fig. 2. The fluctuations of physical properties such as cohesive energy, pressure, temperature as well as volume around constant value show equilibration of the nanowire.

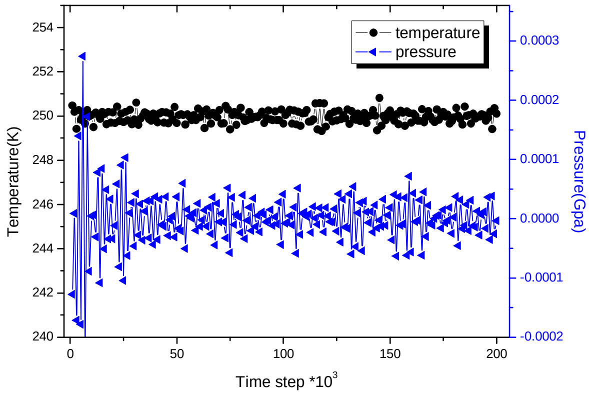

Fig. 1 Time variation of the temperature and pressure for Au_3Ni during equilibration phase

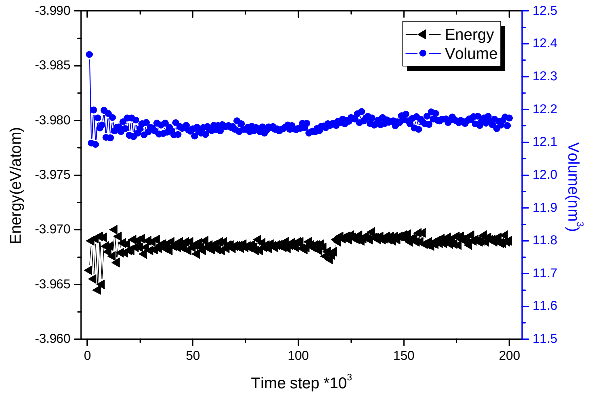

Fig. 2 Time variation of the cohesive energy and volume for Au_3Ni during equilibration phase

III. Results and Discussion

In these MD simulations, we calculated the effect of nanowire radius on the thermal properties including the cohesive energy, the melting temperature and latent heat of fusion. The cohesive energy for different radius, which plotted in the fig. 3, obtained from Q-SC interatomic potential. The cohesive energy was used for determining solid-liquid phase transition. The transition from solid to liquid can be identified by a jump in the potential energy curve. The variation of the energy with temperature for Au_3Ni nanowire was computed in the MD simulation under different diameters conditions. The results from this simulation are shown in fig. 4. The variation of melting points as well as cohesive energy with radius of nanowire were plotted in fig. 5. This plot shows that melting temperature increase upon radius increase in a nonlinear manner and approach to constant value. Inversely, the cohesive energy decrease upon radius increase in a nonlinear manner and approach to constant value. This is a typical behavior of nanoscopic systems in which the physical properties change with size and then reach a constant value, characteristic of the bulk.

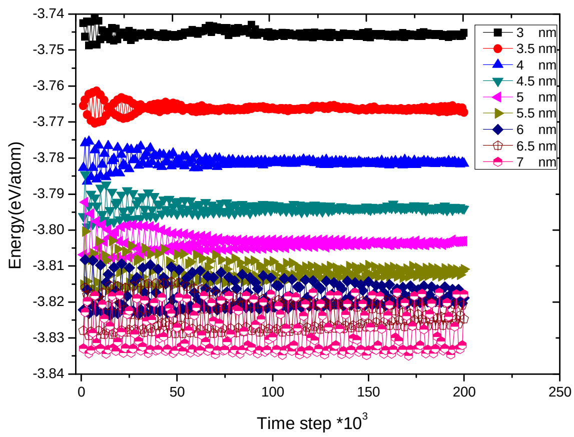

Fig. 3 Time variation of the cohesive energy for Au_3Ni during equilibration phase

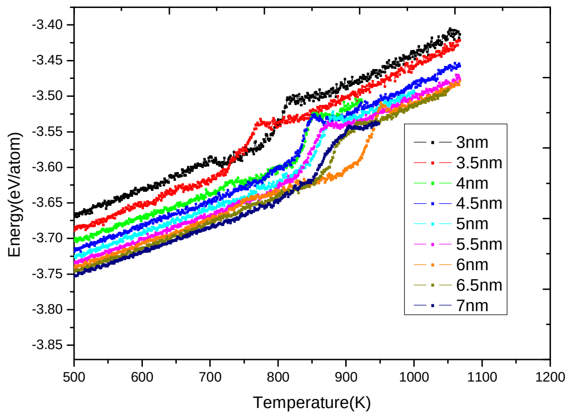

Fig. 4 Variation of energy of Au_3Ni with temperature

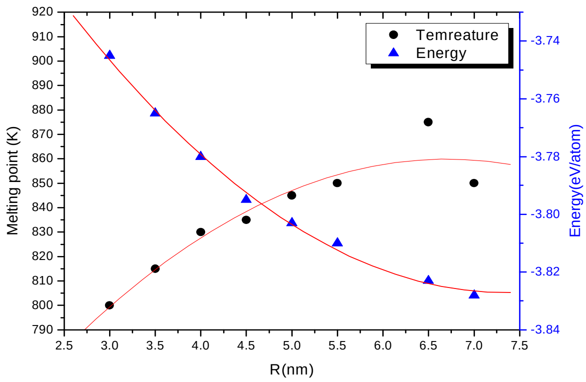

Fig. 5 Variation of melting point and cohesive energy of Au_3Ni nanowire with radius

The latent heat of fusion obtained from the change in enthalpy resulting from heating of a nanowire to change its state from solid to liquid phase. In term of enthalpy, this quantity can be expressed as

$$L = H_l - H_s \tag{6}$$

Where, H_l and H_s are enthalpy of system in the liquid and solid phase respectively. The enthalpy obtain to the following equation

$$H = E + PV \tag{7}$$

Where, E is total energy. The calculated results of latent heat of fusion are plotted in the fig. 6. From This figure we see that there is an initial change in the mechanical properties with the size of the cluster, following which the latent heat remain unchanged as the cluster grows in size.

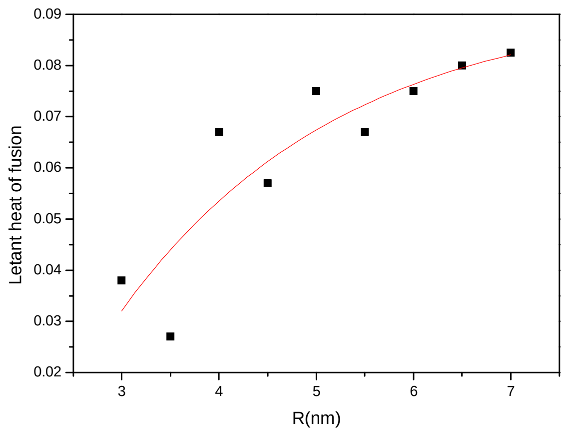

Fig. 6 Variation of latent heat of fusion of Au_3Ni nanowire with radius

IV. Conclusion

In this investigation, we have performed molecular dynamics simulations, based on Q-SC potential, to study the thermal properties of Au_3Ni nanowire. The size dependence of the energy, the melting temperature and the latent heat of fusion were obtained from these simulations. This research shows the melting point and latent heat of fusion increase with diameter of nanowire. Moreover, the cohesive energy decreases with the increased diameter in a nonlinear manner. Summing up the results of our MD-based simulations, we see that thermal properties of the Au_3Ni nanowire depend on radius of nanowire which has to consider in the industrial application.

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