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Molecular Dynamics (MD) Simulation of FCC Metallic Ni_3Al Alloy at High Temperature

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Abstract: *The unique properties of nanowires compared with their bulk counterparts can be attributed to their large surface-area-to-volume ratio. The mechanical properties of Ni_3Al alloys nanowires have been studied at high temperatures using molecular dynamics simulations. MD simulations have been carried out on Ni_3Al metallic alloy with face-centered cubic (FCC) lattice upon application of uniaxial tension at Nano-scale. A many-body interatomic potential within the second-moment approximation of the tight-binding model (the Cleri and Rosato potentials) was employed to carry out. MD simulation used to investigate the effect of temperature of Ni_3Al nanowire on the feature of deformation and fracture. Temperature effect on the extension property of metal nanowire is discussed in detail. The mechanical strengths and the mechanical strain of the nanowires decrease linearly with the increasing temperature. The feature of deformation energy can be divided into four regions: quasi-elastic, plastic, flow and failure. Experiments have shown that when the temperature increases the first stage of deformation was narrowed, and the second stage was widened. The results showed that breaking position depended on temperature. The simulation results at Nano-scale play an important role on the mechanical behaviors of nanostructure. The yield stress of Ni_3Al metallic alloy is found to be 100 times higher than that of the corresponding bulk metals. The yield strain and fracture stress of Ni_3Al metallic alloy are also found to be significantly higher compared with those of the bulk metals. The influence of deformation mechanisms on the mechanical properties of FCC Ni_3Al metallic alloy was discussed.*

Keywords: *Nano-scale, FCC, Ni_3Al, metallic, alloy, strain and fracture.*

1. INTRODUCTION

Nanowires are considered one-dimensional (1D) structures that have drawn a great deal of interest as a result of their remarkable physical mechanical, electronic, optical and magnetic properties. The behavior of surface atoms differs from those inside the bulk because the surface atoms have a coordination number deficiency and are subjected to surface stresses. The surface stresses vary based on the nanowire material and crystal structure. For example, surface stresses in Face-centered cubic (FCC) metals are typically tensile, leading to the contraction of nanowires are typically compressive leading to an increase in length of semiconductor nanowires. Metallic nanowires (MNWs) have been given extensive attention in recent years as a result of their widespread application in myriad areas such as optoelectronic applications, Nano-electronic and Nano-mechanical devices, catalysis, Nano-pipette probes, superconductors, and reinforcement in high-strength/light-weight composite materials. They have also been explored as tips for scanning tunneling and atomic force microscopes. MNWs are attracting strengths and modulus compared with the bulk metals. Molecular dynamics (MD) Simulation has become an invaluable technique to study a variety of complex physical, chemical and biochemical systems. The Ability of MD to build observations across length scales based on the data at atomic level gas enhanced its spectrum of applications. MD techniques have been applied to analyze structural and dynamical response of polymers, drug delivery and diffusion of small molecules through biological membranes, physical properties of nanowires and properties of Nano-composites in the present work, the results of MD simulations on FCC MNWs are summarized. Recent MD Studies have identified two distinct mechanisms that mediate the structural response in FCC MNWs: novel phase transformations and lattice reorientation. Associated with reversibility and temperature dependence of these structural changes, pseudo elastic behavior and shape memory effect

(SME) are also discovered. The following sections discuss MD simulation methodology, properties of FCC nanowires, and comparison of their properties with body-centered cubic (BCC) and hexagonal closed-packed (HCP) nanowires. The mechanical properties of Ni nanowires dependence on size, shape, as well as the temperature have been studied [1-7]. Characterization of strain-induced structural transformations in CdSe nanowires using molecular dynamics simulation also studied [8].

2. MD SIMULATION METHODOLOGY

MD is a simulation technique where the time evolution of interacting atoms is followed by integrating their equation of motion. It consists of integrating Newton's second law for each atom present in the system by discretization of time. In general, it is difficult to obtain an analytical solution that precisely describes the atoms' trajectories. Therefore, the equations of motion are solved numerically using a time-discredited finite difference methodology such as the Verlet method or the velocity Verlet method, which incorporate the velocities explicitly into the integration scheme. The initial atomic positions for metallic systems are defined on the crystal lattice of the metal, while the initial velocities are assigned according to the Boltzmann distribution at the given simulation temperature. The validity and accuracy of MD simulation results depend on the accuracy of the interatomic forces used as inputs, which rely on the selection of an efficient underlying interatomic force-field potential. For modeling metallic systems, the most commonly used potential is the semi-empirical embedded atom method (EAM) potential. The parameters of EAM potential are generally obtained by fitting cohesive energy, equilibrium lattice constant, elastic constants, bond length, and diatomic bond strength. Since its introduction, the ability and viability of EAM in modeling metals have been extensively analyzed and tested The classic EAM method is not suitable for describing systems in which covalent bonds are present, such as carbon (in diamond or graphite structures), because the EAM description does not account for the angular dependence of the interatomic interactions. To account for angular dependence, as in the case of the BCC lattice where it is important, a modified embedded atom method (MEAM) was proposed. The total energy U in a system of N atoms in the EAM framework

$$U = \sum_i (E_b^i + E_r^i), Where, E_r^i = \sum_j A.\exp[-p(\frac{r_{ij}}{r_0} - 1)],$$

Is the two-body term, and

$$E_b^i = -\sqrt{\rho_i}$$

$$\rho_i = \sum_{j \neq 1} \zeta^2 . \exp[2q(\frac{r_{ij}}{r_0} - 1)]$$

Is the many-body term.

can be written as:

Where r_0 is the equilibrium distance between atoms, r_{ij} is the distance between the i^{th} and j^{th} atoms, and A, ξ, p and q are fitted parameters these parameters were taken directly from [9, 10]. The potentials proposed by Cleri and Rosato [9, 10] have already worked well in cluster studies.

Fig. 1(a) shows the MD simulation model of Ni_3Al alloy. Let x, y, and z coordinate axes represent the [100], [010] and [001] crystallographic directions, respectively. The initial lengths of the MD models are denoted by Lx, Ly, and Lz, respectively, with z denoting the length direction of the lattice. Fig. 1 (b) shows the MD Simulation plot of XZ plan at the start of the experiment for Metallic Ni_3Al alloy.

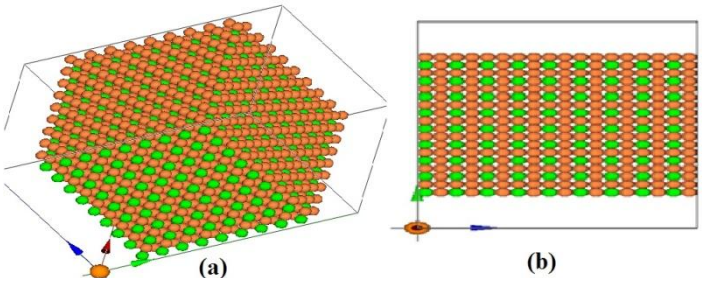

Fig1. *(a) 3D plot for Ni_3Al and (b) MD Simulation plot of XZ plane at the start of the experiment for Metallic Ni_3Al alloy.*

3. Results And Discussion

A computer experiment is performed at different temperature, the deformation involving the possibility of chilling calculation unit for detailed analysis of the structural changes occurring in it. The estimated size of the crystal unit was for various experiments of 6912 atoms (12 atoms along the edges at the bottom and 72 - in height (12 x 12 x 72 atomic plane). Simulation cell of one side the XZ plane which contain 872 surface atoms as in fig.2.

Fig.3. Show the stress-Strain relation for Ni3Al nanowires. Where the stress–strain diagram is essentially smooth with a linear slope in the elastic region, in Nano-tensile testing, a series of steps of rise and fall in the stress values with engineering strain occurs in the initial elastic region. This is followed by a plastic region up to the maximum stress. Animation of the tensile tests indicated considerable reorganization of the atoms followed by rapid movement due to the generation of dislocations. Also, neither clear demarcation of linear elastic range nor the yield point is visible.

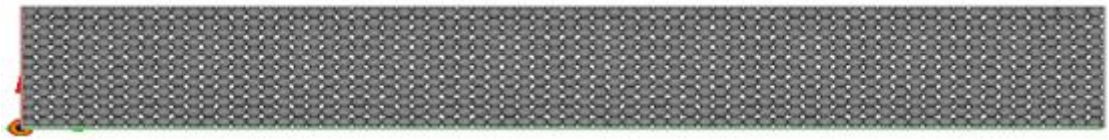

Fig2. *XZ plane of Ni_3Al nanowire at the start of the experiment.*

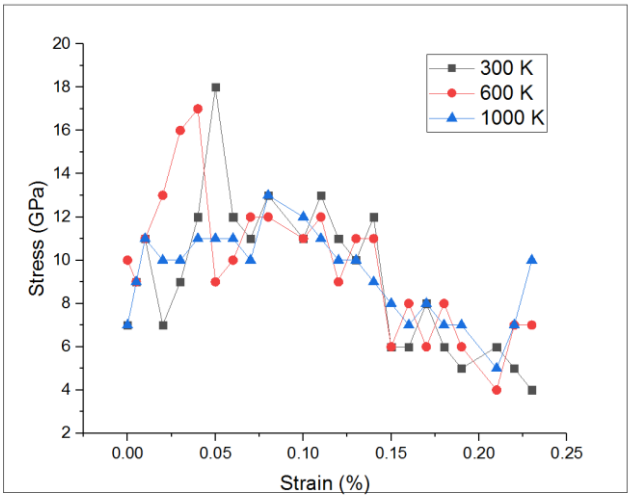

Fig3. *Stress-strain curve for three 12x 12 x 24 nanowire of Ni3Al at different temperature.*

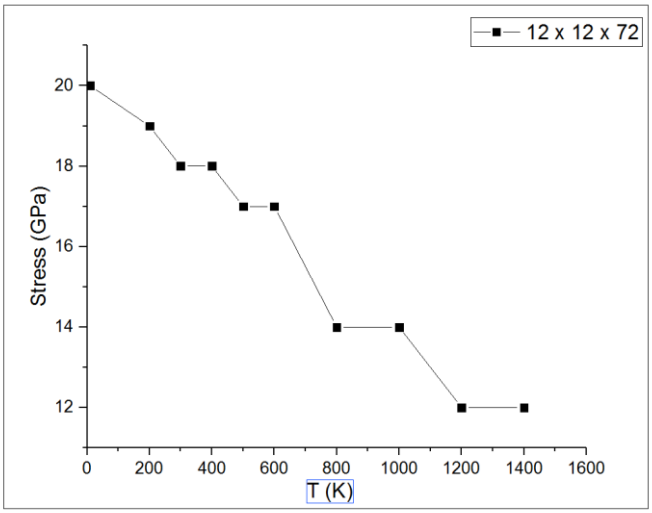

Fig4. *The relation of stress with temperature for Ni3Al-12x12x72*

It is observed that the first yield stress decreases as the temperature increases (Fig. 4). When the plastic deformation of the nanowire begins, the drop of the first yield stress also decreases. In order to

clearly study these characters, in Fig. 4, we show the average statistical results of the first yield strain (Ɛ), the first yield stress (σ) at different temperatures. The average result is from 150 samples at each temperature, and temperatures from 0 to 1600 K. The MD simulation plots of the XZ plane of the tensile specimens are for the FCC Ni_3Al alloy, are shown in Figs. 5 and 6 at 300 K and 1200K respectively it may be noted that the discussion of the results presented here is based not only on the MD simulation plots of the various stages presented here but also on the detailed study of the animation of the process which was accomplished using a special computer program developed for this purpose [10].

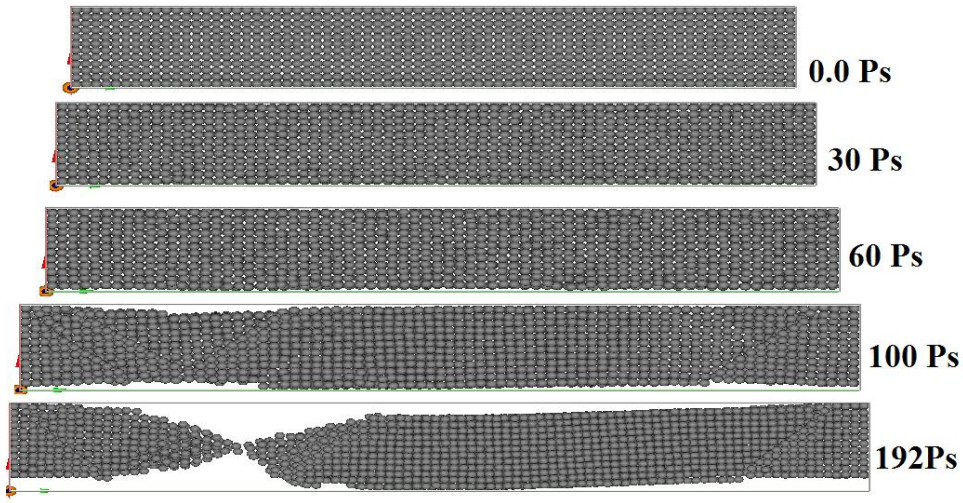

Fig5. *Atomic configurations of 12x12x72 Ni3Al alloy under extension loading at T=300 K, at different period of time.*

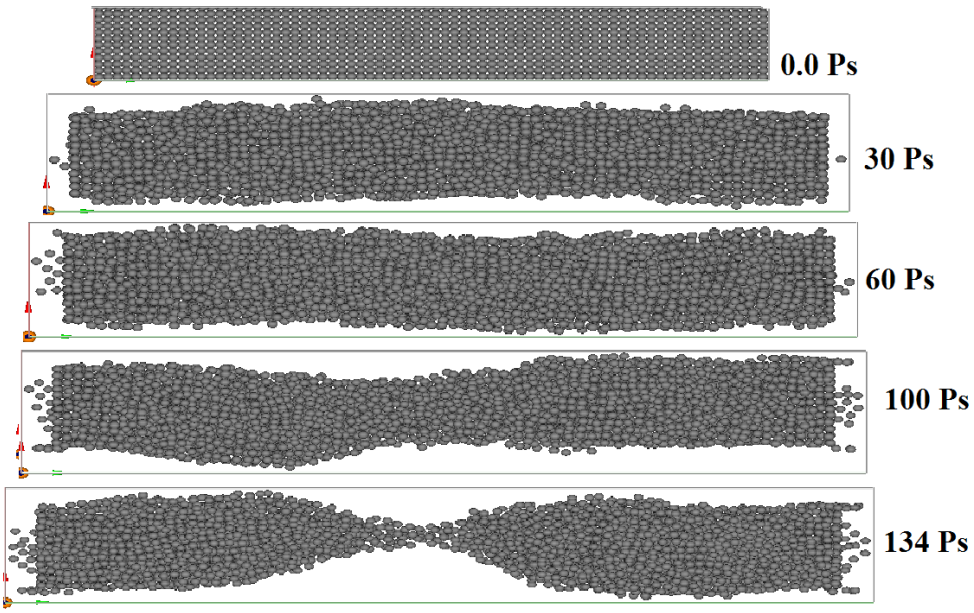

Fig6. *Atomic configurations of 12x12x72 Ni3Al alloy under extension loading at T=1600 K, at different period of time.*

The experiments were obtained plots of the stored energy of deformation with the time, reflecting the processes in the nanowire during deformation. There are four stages of deformation: the quasi-elastic deformation (I), plastic deformation (II), the breaking (flow) (III), and failure (IV). At all temperatures, in the first stage there was almost linear increase in stress. The initial stage quasi-elastic area there is only relative displacement of atoms and there are no defects. Therefore, in this region the energy stored varies periodically. This stage is completed in 23 Ps for 12 x 12 x 72 Ni3Al nanowire at 100K and 27 Ps for 12 x 12 x 72 Ni3Al nanowire at 1000K. The sharp fall takes place only at the point of transition from the first to second stages of deformation (Fig. 7 a and 7 b). Experiments have shown that when the temperature increases the second stage of deformation was narrowed. When the strain rate is small for the nanowire, keeps its crystalline structure during the tensile process, the

necking occurs in the last part of deformation. Quasi-elastic deformation takes place at that region. Then nanowire transforms from a FCC crystal to amorphous state, and the other part still keeps its ordered structure during the tensile process. Several necks can be observed after certain strain. This is the plastic deformation of nanowire during the deformation process beyond the elastic limit. This is the flow deformation of nanowire. Therefore stress goes to zero. This is the failure deformation of nanowire.

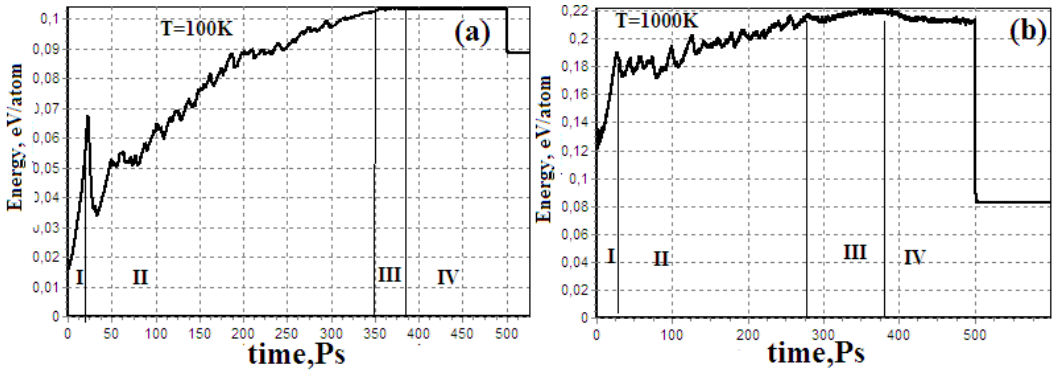

Fig7. *The dependence of the stored energy of deformation of the experiment for Ni_3Al 12 x 12 x 72, (a) at 100K and (b) 1000K.*

Figure 8 presents the breaking for Ni_3Al nanowires. The breaking position depends on temperature of the experiment. Surface atoms play an important role in the mechanical behaviors of Nano structures, and the temperature effect commonly found in small-scale systems is the surface effect. If the breaking position is predictable, the nanowire can be strengthened near the breaking position to avoid failure. Although the single breaking case is not predictable, many breaking cases show a statistic feature. Figure 8 presents the representative snapshots of Ni_3Al nanowires with different temperature at the breaking moment.

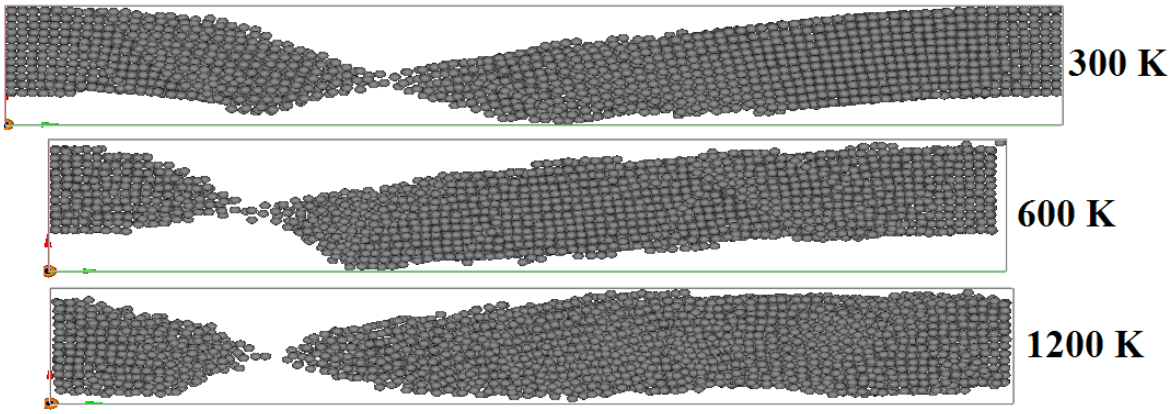

Fig8. *Atomic configurations of 12 x 12 x 72 Ni3Al nanoalloy at different Temperature under extension loading at breaking time.*

4. Conclusion

Molecular dynamics simulations have been carried out to investigate the mechanical behaviors of 12 x 12 x 72 Ni_3Al Nano-alloy at different Temperature under extension loading. The effect of temperature was successfully studied; the elastic modulus and the yield stress were linearly decreased. The stress–strain relation of nanowire is obtained. The temperature effect on the extension properties is discussed in detail. Temperature exhibited a great effect on the mechanical properties of nanowires. Study on the mechanical properties of metal nanowires can give us more fundamental understanding of Nano-scale machines from atomistic motions. The simulation results would be helpful to avoid the materials failure by predicting the breaking position. This study of mechanical properties of metal nanowires will be helpful to the design, manufacture and manipulation of nano-devices.

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