Molecular Dynamics Simulations of Bauschinger Effects on a Defect- Free Single Crystal Nickel

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Abstract

In this study, the Bauschinger effect on a defect-free single crystal of Nickel is modeled implementing molecular dynamics simulations in nanoscale. The inter-atomic interactions are represented by employing embedded-atom potential. First, the stress-strain curves of tension and compression loading are simulated. The generated results show that the yield stress in compression is lower than the tensile yield stress. At the second stage, the tension-followed-by-compression process at a known strain rate is applied to the specimen. It is observed that the obtained yield stress in the reloading or reversed loading is substantially less than the compressive yield stress in the original direction which is known as Bauschinger effect. The reversed loading process is performed at different strain levels after tensile yield stress and the influence of strain levels on Bauschinger effect is studied. In this state the Bauschinger stress parameter (BP) is introduced to quantify the Bauschinger effects on Ni crystal.

I. INTRODUCTION

In recent years, researchers have become increasingly interested in nano science and technology. Utilizing the structure at the nanometer or micron level is a key technology in the development of electronic devices and elements of micro/nano electro-mechanical systems (MEMS/NEMS). Therefore, it is important to understand the mechanical properties not only for the sake of scientific interest, but also for engineering usefulness such as design of fabrication processes and reliability in service.

Over the last decades, computer simulation technique was developed to calculate the mechanical properties of nanoscale materials. Simulations using realistic molecular dynamics method are capable of unveiling some processes to explain the fundamental mechanisms of dislocation formation, plastic region and breaking of nanomaterial under stress. For this applications, it is required that the nanomaterial to be strained and relaxed at extremely high velocities and displacement amplitudes. In consequence, recently many researchers have studied the mechanical properties of single crystals under uniaxial loading using numerical methods such as molecular dynamics [1, 2].

In this paper, the Bauschinger effect is examined in nickel single crystals. The consequences of this phenomenon are important for the forming processes of materials at nanoscale. Fang et al. [3] studied Bauschinger effects in nickel single crystals and nickel containing arrays of high angle or low angle grain boundaries under shear deformation using molecular dynamics with embedded atom method (EAM) potentials.

However, very few researches have investigated the Bauschinger effect at the atomic scale and to the authors' knowledge, a study to understand this effect at the atomic scale in tension-followed-by-compression process has not been performed before.

II. BAUSCHINGER EFFECT

First in 1881, Bauschinger observed that in many metallic materials, after a plastic prestrain in tension (respectively in compression), the flow stress in the reverse direction is lower than the flow stress in the forward direction. This reduced reverse flow is known as the Bauschinger effect (BE).

Generally for metals that experience plastic deformation, the mechanical response depends on their deformation history and not just on their current stress

state. This history can manifest changes in the mechanical response, like a difference between the yield stress in tension and compression. A schematic stress–strain curve for a ductile material is illustrated in Figure 1.

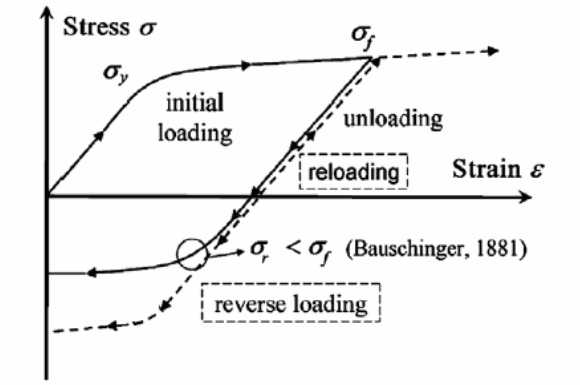

Figure 1. Schematic stress-strain curve that exhibits the Bauschinger effect for typical metallic alloys in macro scale [4]

The Bauschinger effect has been found to be a function of several parameters such as prestrain level. In nanoscale the hardening model such as kinematic hardening is not observed and stress-strain curve in plastic region is saw-shape. Thus, we cannot predict a specific hardening model for material in nanoscale. But if the tension-followed-by-compression loading is subjected to material, the yield stress in reversed direction is reduced in comparison with the original compressive yield. To clarify this effect, we introduce the Bauschinger parameter (BP) as follows:

$$BP = \frac{\sigma_y^c - \sigma_y^r}{\sigma_y^c} \tag{1}$$

Where σ_y^c, is the original compressive yield stress and σ_y^r is the compressive yield stress in the reversed direction. The definition of BP parameter indicates that the stronger Bauschinger effect leads to the larger value of the BP.

III. SIMULATION METHOD

In this paper, MD simulation has been performed using the EAM potential model reported by Johnson [5]. The total energy U for a system of atoms in the EAM model [6] can be written as,

$$U = \sum_i^N (F_i(\rho_i) + \frac{1}{2}\sum_{j\neq i}\phi_{ij}(r_{ij})) \tag{2}$$
$$\rho_i = \sum_j f(r_{ij})$$

where the summations in Eq. (2) extend over the total number of atoms N in the system, F_i is the embedding function, ρ_i is the electron density at atom i, ϕ_{ij} is a pair interaction function, f is the contribution to the electron density at atom i due to atom j and r_{ij} is the distance between atoms i and j.

In this model, the bulk stress tensor $\sigma_{\alpha\beta}$ of a single crystal is defined to be the strain derivative of the total energy per unit volume [7, 8],

$$\sigma_{\alpha\beta} = \frac{1}{V}\frac{\partial E}{\partial \varepsilon_{\alpha\beta}} = \frac{\Omega_0}{V}\sum_i \sigma_{\alpha\beta}^i \tag{3}$$

here E is the total energy of the single crystal, $\varepsilon_{\alpha\beta}$ is the strain tensors $(\alpha,\beta \in x,y,z)$, Ω_0 is the undeformed atomic volume in the perfect crystal and $\sigma_{\alpha\beta}^i$ is the local stress at atom site *i*. Using the embedded-atom potential, $\sigma_{\alpha\beta}^i$ can be expressed as,

$$\sigma_{\alpha\beta}^i = \frac{1}{\Omega_0}\frac{\partial E_i}{\partial \varepsilon_{\alpha\beta}} = \frac{1}{\Omega_0}(-m v_i^\alpha v_i^\beta + \sum_{j\neq i}(\frac{1}{2}\frac{\partial \varphi_{ij}}{\partial r_{ij}} + (\frac{\partial F_i}{\partial \rho_i} + \frac{\partial F_i}{\partial \rho_j})\frac{\partial f}{\partial r_{ij}})\frac{r_{ij}^\alpha r_{ij}^\beta}{r_{ij}}) \tag{4}$$

In Eq. (4) E_i is the energy per atom and v_i^α is the velocity component in the *j* direction of atom *α*.
The atomic positions, velocities, and intermolecular forces for each time step are obtained by solving Newton equations of motion in molecular dynamics code [9]. The atomic velocities are scaled during the simulation using the temperature thermostat, thus the temperature of system is kept constant. The formalism of this thermostat can be written as follows,

$$v_i^{new} = v_i^{old} \times \sqrt{\left(\frac{T}{T_0}\right)^{Cstep}} \tag{5}$$

Where T, T_0 and Cstep are temperature of simulation, desired temperature and constant of thermostat, respectively.

In this research, a solid FCC nickel single crystal with a square cross-section is considered. The single crystal is constructed as a regular FCC lattice with

initial surface orientations of [1 0 0], [0 1 0] and [0 0 1] in the X, Y and Z directions, respectively. An infinitely long nickel single crystal is modeled by applying periodic boundary conditions in the [1 0 0] direction. The other two Cartesian directions are simulated considering free boundary condition.

The size of Ni single crystal is $40\times8.5\times8.5$ in terms of lattice parameter (the lattice parameter of the bulk nickel is 3.524 A° at 300 K).

In order to start the simulation, it is needed the system to be relaxed at a known temperature using constant pressure algorithm [10] for duration of 420 ps. This procedure causes the pre-stress to be set to zero in the lattice. Actually when a bulk material is divided into some portions, a new surface is created. Atoms neighborhood to the surface lose their electrons and obtain a force field different from those of bulk atoms. Therefore it is needed to carry out the relaxation process and let the atoms readjust themselves in order to minimize their kinetic energy. Figure 2 shows the variation of stress in the relaxation process.

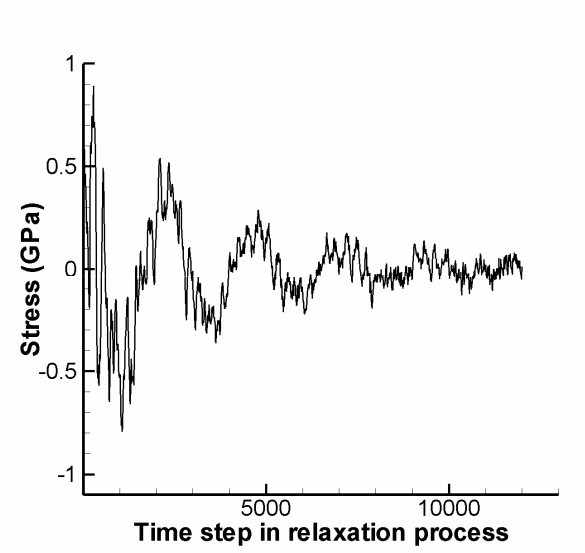

Figure 2. Stress during relaxation process

After relaxation process, the displacement boundary condition is applied to the system. The right zone is moved about 3×10^{-4} lattice parameter while the left zone is fixed and then the system is relaxed for about 35 fs, so the strain rate reads 0.86 $\%ps^{-1}$. The initial configuration of fixed and moveable zones is presented in Figure 3.

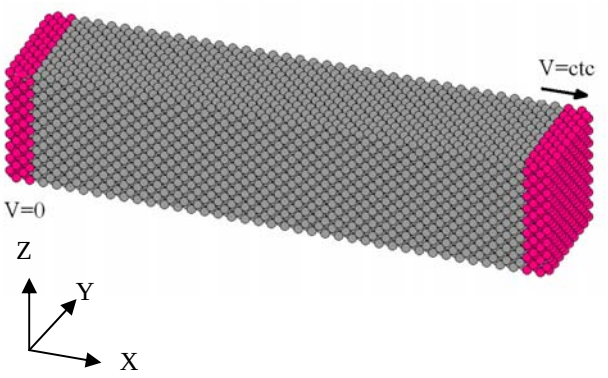

Figure 3. Initial configuration of Ni single crystal and different boundary zones in simulation

IV. RESULT AND DISCUSSION

The stress-strain curve for nickel defect-free single crystal under uniaxial loading (tension and compression) at 300K is shown in Figure 4. According to this figure, the tensile stress increases up to a maximum value of 8.56 GPa corresponding to strain of 0.095, then the stress suddenly decreases to 2.2 GPa where the plastic zone is developed. In this situation the curve is saw-shape. The saw-shape portion of the curve is due to nucleation, transformation and junction of dislocations in single crystal.

In the tensile loading, the Young's modulus is estimated as 81.6 GPa in the elastic region according to the present model, which is lower than the value of 90 GPa reported by Rino and Branico [11] and is close to the value of 80.6 GPa determined by Hen et la. [12].

Also, the stress-strain curve of Ni single crystal in the compression loading (the compressive strain and stress are shown with positive sign) is shown in Figure 4 In the compression loading, the stress increases up to maximum value of 2.75 GPa at strain of 0.05, then a sharp drop in stress follows the nonlinear elastic behavior of the stress–strain curves.

By linear fitting in elastic zone the Young's modulus is obtained as 51.24 GPa. This value is lower than the modulus of elasticity for tension process. The same trend is observed for the yield stress. Uniaxial tensile and compression loadings exhibit asymmetry in the mechanical properties which is associated with free surface effect in material.

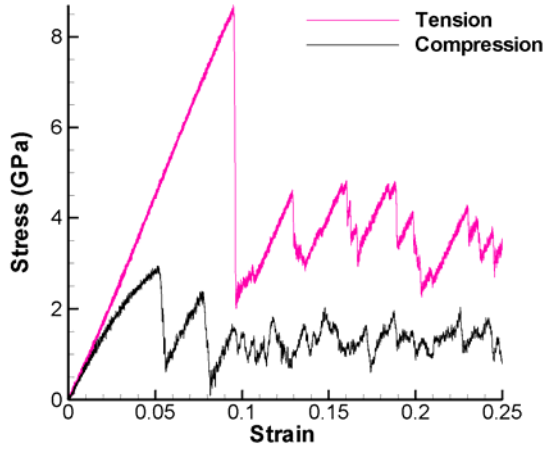

Figure 4. The stress-strain curve under tensile and compressive loading

As mentioned before, Bauschinger effect is intimately tied to the history of loading. Therefore, the system was tested to five different prestrain levels under tension-followed-by-compression process.
First the reversal loading is applied at strain of 0.07 in the elastic zone. The stress-strain curve for this case is shown in Figure 5 In this figure, the reverse yield stress is 2.75 GPa, which is equal to the original compressive yield stress. Thus Bauschinger effect is not observed in this case. This phenomenon is compatible with macro scale.

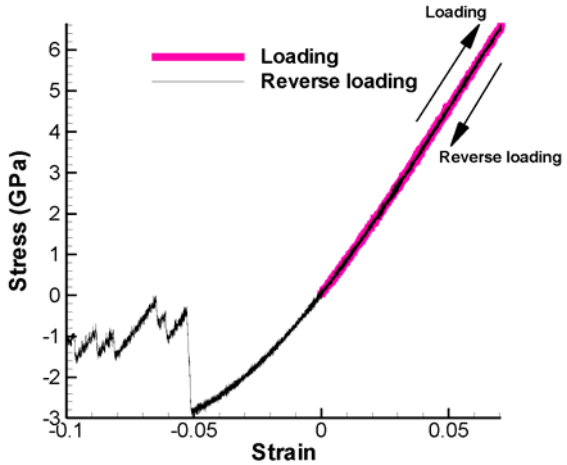

Figure 5. The stress-strain curve of reversed loading in the elastic zone

In the next stage, the specimen is loaded to prestrain of 0.12 and then reversed loading is applied to the material. In this case a reduction in the reverse yield stress is seen. This process is repeated under four different prestrain levels (0.12, 0.15, 0.3 and 0.37). The corresponding stress-strain curves are shown in Figure 6 through Figure 9.

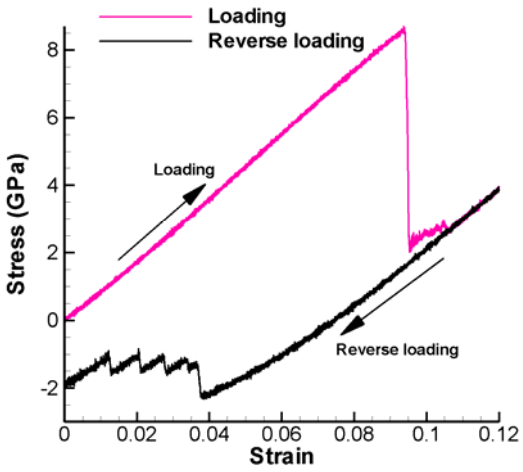

Figure 6. The stress-strain curve of tension-followed-compression loading under prestrain of 0.12

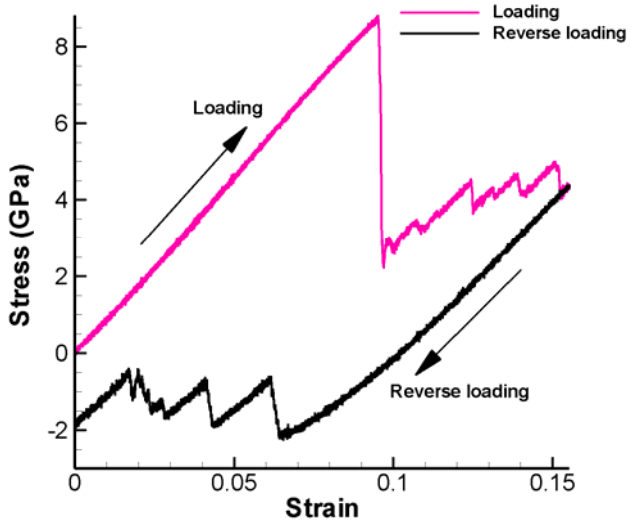

Figure 7. The stress-strain curve of tension-followed-by-compression loading under prestrain of 0.15

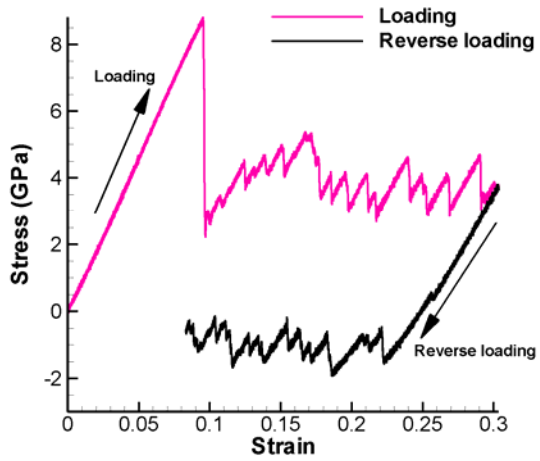

Figure 8. The stress-strain curve of tension-followed-by-compression loading under prestrain of 0.3

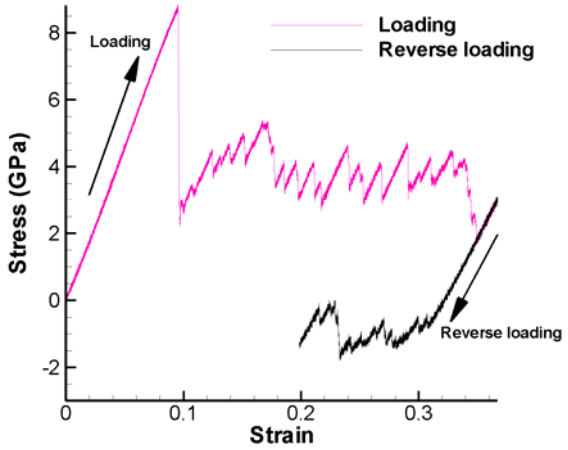

Figure 9. The stress-strain curve of tension-followed-by-compression loading under prestrain of 0.37

In order to quantitatively describe the Bauschinger effects for nanoscale simulations, the introduced BP parameter is employed here. The value of this parameter and reverse yield stress according to Figures (6-9) for four different strains is calculated and shown in Table 1.

Table 1: The BP parameter for different strain

Strain	σ_y^r (GPa)	BP
0.07	-2.75	0
0.12	-2.15	0.21
0.15	-2.1	0.24
0.3	-1.5	0.45
0.37	-0.7	0.75

It is seen that the larger BP value reveals the stronger Bauschinger effect. According to Table 1, with increasing the prestrain level, BP is increased and the stronger Bauschinger effect is seen.

In another words, it can be interpreted that the larger prestrain level causes higher dislocation density in material. Thus the lower reverse yield is occurred in reversal direction**.**

V. CONCLUSION

A MD simulation was employed to investigate the Bauschinger effect of Ni defect-free single crystal in nanoscale using embedded-atom model potential. For this reason the tension-followed-by-compression process was applied to the specimen and the effects of prestrain on reversal yield stress was studied.

It was seen that by increasing the prestrain, the Bauschinger effect increases and more reduction is observed in the reversal yield stress.

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