Molecular Dynamics Simulation of Temperature Dependence of Dislocation Behavior in fcc Ni Single Crystal under Tensile Condition ^{*1}

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A molecular dynamics (MD) simulation of plastic deformation under a uniaxial tensile strain condition for fcc Ni single crystals is performed in order to clarify the temperature dependence of the edge dislocation behavior. Simulations are performed for the temperature range from 77 to 1200 K using Finnis-Sinclair-type potentials. An edge dislocation first forms at the surface and propagates inside of the crystal on the {111} planes in the <112> direction. The temperature dependence of the simulated Young's modulus is quite similar to the experimental results. The transverse sound velocity is estimated from the simulated elastic constants at each temperature. Below 600 K, the dislocation speed reaches up to 70% of the transverse sound velocity. The dislocation speed decreases with increasing temperature linearly above 600 K. Dislocations at elevated temperature propagate under lower stress than at room temperature. The extrapolated dislocation speed becomes zero at 1200 K. At this temperature, no dislocations are observed in the present simulation system. The temperature dependence of macroscopic deformation behavior and the possibility of the existence of supersonic dislocations are discussed.

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1. Introduction

A dislocation is a carrier of plastic deformation of a crystal.¹⁾ A dislocation is accelerated by a stress field. Phonon (thermal vibration of atoms) and electrons give resistance to the motion of dislocations by scattering and viscous interactions.²⁾ It is important to understand the mobility of dislocations in order to control deformation and brittle fracture of metallic crystals. The speed of edge and screw dislocations in LiF were measured experimentally as a function of the resolved shear stress by Johnston and Gilman.³⁾ Both dislocation speeds vary as the power of the resolved shear stress. In the past, analytical treatments for the speed of dislocations were performed.^{2,4)} Recently, molecular dynamics (MD) simulations have been applied for mesoscopic deformation and fracture phenomena.^{5,6)} Schiotz *et al.* reported the dislocation speed in fcc Cu under tensile condition by MD simulation.⁷⁾ They found that the upper limit of edge dislocation speed is in the order of transverse sound velocity. However, the temperature condition is not apparent in their report. Gumbsch and Gao calculated the edge dislocation speed in bcc W under a forced shear strain condition MD with the boundary condition similar to machining by cutting tool.⁸⁾ Since they use a microcanonical ensemble, temperature changes from 10 to 70 K during deformation. They reported occurrence of supersonic dislocations over 8% shear strain. Aihara *et al.* have performed MD simulation for deformation of Zr-Ni amorphous alloy^{5,9)} and Ni, Ni₃Al and their composites.¹⁰⁻¹³⁾ However,

the relation between dislocation speed and temperature in crystalline materials is still unclear.

In this paper, the authors report the results of MD simulation of plastic deformation of a single crystal Ni under a uniaxial tensile strain condition at various temperatures. The purpose of the present study is to clarify the trend of temperature dependence of the edge dislocation behavior.

2. Simulation Procedure

A single crystal consisting of 4000 Ni atoms with $10 \times 10 \times 10$ fcc unit cells was simulated by MD. The periodic boundary condition is applied in the [010] direction and the {001} free surface condition is done in [100] and [001] directions. The tensile deformation is performed at 77, 298, 600, 800, 1000 and 1200 K. After the system was relaxed at each temperature, the tensile deformation starts at time $t = 0$ ps. The tensile strain in [010] direction is loaded stepwise by 0.1% scaling of initial MD cell length (3.5574 nm at every temperatures) per 0.5 ps. The authors call the ratio of the change in the instant MD cell length in the [010] direction to the initial MD cell length as raw strain. The raw strain rate is $2 \times 10^9 \text{ s}^{-1}$. The authors use the Finnis-Sinclair-type potentials proposed by Cleri and Rosato¹⁴⁾ for the binary Ni-Al system. Geometrical parameters are modified by Aihara and Sho¹¹⁾ to fit for experimentally reported lattice constant¹⁵⁾ at room temperature. The cutoff distance of the potential is 1.0 nm. The authors use a Nosé thermostat to keep the temperature constant.¹⁶⁾ The equations of motion are solved using Gear's fifth-order predictor corrector with a time step of 1 fs. The position of dislocation is numerically detected by the algorithm proposed by Aihara and Sho.¹²⁾ The speed of a propagating dislocation is defined as the slope of a linear plot of the dislocation position versus time during about 1 ps. The

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zero point of the nominal strain ε is defined by an extrapolation of the stress-strain (raw strain) curve to the zero stress in the [010] direction. Young's modulus is calculated from the slope of the simulated stress-strain curve in linear elastic region from the time 2 to 12 ps. Thermal expansion effect is compensated by a consideration of the experimental thermal expansion data¹⁷⁾ for Young's modulus E and density ρ . Other simulation details are described in the previous reports by Aihara *et al.*^{5,9-13)}

3. Results

Figure 1 shows a stress-strain curve at 800 K. The Ni crystal is elastically deformed at first. At the final stage of elastic elongation (the nominal strain $\varepsilon = 7.4\%$), some point defects appears near the surface. When the nominal strain reaches 8.8%, a partial edge dislocation nucleates at a corner of the free surface. This is the yield point. The first dislocation propagates with changing its length. During the propagation of the first dislocation on the {111} plane the area of stacking fault increases, since the second dislocation does not appear on the same plane. Figure 2 shows a position of the first propagating dislocation on the {111} plane in the $\langle 112 \rangle$ direction as a function of relative time at 800 K. The first dislocation propagates in the crystal at almost constant speed. This means

that effect of the increasing dislocation length and stacking fault area is smaller than the driving force of very high elastic stress energy for the dislocation speed. Present dynamical behavior is different from the solution in static continuous model. These factors should affect the dislocation speed at the conventional stress condition. After the first dislocation propagates on the {111} plane in the $\langle 112 \rangle$ direction of the crystal, other several dislocations are formed and propagate. Motion of these dislocations causes plastic deformation and reduces the true tensile stress from 7.6 to 2.6 GPa. The more detail, for example partial dislocation, is described in a previous report by using snapshot and trajectory of atom.¹²⁾ Owing to the high strain rate and the lack of dislocation sources, the strain and stress reaches to a very high level before any plastic deformation occurs in the MD simulation.⁷⁾ Similar deformation behavior is observed from 77 to 1000 K. At 1200 K, although the stress-strain curve is similar to that at lower temperature, no dislocation is observed. The stress is released by allotropic transformation with cooperative motion of atoms. The speed of the first edge dislocation in the $\langle 112 \rangle$ direction and the nominal strain at the yield point are listed for each temperature in Table 1. The dislocation speed decreases with increasing temperature. The nominal strain at yield point does not much depend on temperature. Its average for all temperatures is $8.42 \pm 0.57\%$. It is suggested that the nucleation of the dislocation at the surface is affected by the minimum interatomic distance of the thermally vibrating atoms.

The temperature dependence of the true yield stress is shown in Fig. 3. Dislocations at elevated temperatures prop-

Fig. 1 Simulated stress-strain curve for fcc Ni single crystal at 800 K. The simulation starts from pre-tensiled state.

Fig. 2 Propagation of first dislocation on the {111} plane in the $\langle 112 \rangle$ direction as a function of relative time at 800 K.

Table 1 Simulated first edge dislocation speed on the {111} plane in the $\langle 112 \rangle$ direction. Edge dislocation nucleates at an edge on the {100} free surfaces of fcc Ni single crystal after stress reaches yield point. Thermal expansion effect is compensated for the nominal strain at the yield point.

Temperature (K)	Dislocation speed ($\text{km}\cdot\text{s}^{-1}$)	Nominal strain at yield point (%)
77	1.76	7.4
298	1.31	8.2
600	1.32	8.9
800	0.88	8.8
1000	0.44	8.2
1200	0	9.1

Fig. 3 Temperature dependence of the true yield stress of fcc Ni single crystal.

Fig. 4 Temperature dependence of the normalized Young's moduli by that at 298 K for MD simulation and experiment.¹⁸⁾

Fig. 5 Temperature dependence of the normalized edge dislocation velocity by the transverse sound velocity in the $\langle 112 \rangle$ direction on the $\{111\}$ plane at each temperature. Both velocities are results of MD simulation.

agate under lower stress than that at room temperature. The difference of the stress at 77 and 1200 K is 60%. Figure 4 shows the temperature dependence of the Young's modulus. It is normalized by its value at 298 K. The trend of the temperature dependence of the Young's modulus of the simulated results is quite similar to the experimental results of electrolytic nickel (purity 99.98%)¹⁸⁾ at the temperature range from 298 to 800 K. The Young's modulus drastically decreases with increasing temperature. At 298 K, the simulated Young's modulus is 96.7 GPa, and the experimental value is 202.7 GPa.¹⁸⁾ This difference would be caused by imperfectness of fitted potential. Then, sound velocity should be calculated from simulated elastic constant.

The transverse sound velocity v_s^T is estimated from the rigidity G and density ρ by

$$v_s^T = \sqrt{\frac{G}{\rho}}. \quad (1)$$

The rigidity is calculated from Young's modulus and Poisson's ratio ν by

$$G = \frac{E}{2(1 + \nu)}. \quad (2)$$

Since experimental data of the Poisson's ratio of Ni base alloys is almost independent of temperature,¹⁸⁾ the experimen-

tal Poisson's ratio at room temperature, 0.312,¹⁹⁾ is used in eq. (2). Simulated Young's moduli are used for estimation of the transverse sound velocity. The dislocation velocities normalized by the transverse sound velocity at each temperature are shown in Fig. 5. Below 600 K, the dislocation speed saturates to 70% of the transverse sound velocity. The normalized dislocation speed decreases linearly with increasing temperature above 600 K.

4. Discussion

The temperature dependence of the dislocation dynamics is divided into three categories. At low temperature, an edge dislocation propagates with a speed in an order of transverse sound velocity. At intermediate temperature, the dislocation reduces its speed with increasing temperature. Two reasons are suggested. The former is the reduction of the yield stress caused by the softening of Ni with increasing temperature, since the dislocation speeds vary as the power of the stress.³⁾ The latter is the scattering and viscous interactions with phonon,²⁾ *i.e.* thermal vibration. At elevated temperature (1200 K), dislocation can not move under high tensile strain condition. From a macroscopic viewpoint, the first denotes the brittle fracture behavior of a crystalline metal at low temperature. The second denotes the plastically deformable ductile behavior of a crystalline metal at intermediate temperature. The third denotes viscoelastic behavior of a crystalline metal at elevated temperature.

Supersonic dislocations, which propagate in the crystal with a speed greater than the sound velocity, radiate energy as acoustic emission, just as Cherenkov radiation. A steady supersonic motion of dislocation is possible if driving energy is continuously provided by an applied stress or by atomic readjustment in the glide plane.²⁾ From the viewpoint of experiment, such a supersonic deformation can be performed by a Hopkinson pressure bar and a torsional pressure bar methods²⁰⁾ with ultra high strain rate. The former is a compressive deformation and the latter is a shear deformation. An Instron type tensile testing machine with a supersonic crosshead can not give deformation but will fracture materials. A tensile stress can not accelerate a dislocation beyond the transverse sound velocity.

5. Conclusions

A molecular dynamics (MD) simulation of plastic deformation under a uniaxial tensile strain condition for an fcc Ni single crystal is performed at various temperatures. The edge dislocation first nucleates at the surface and propagates inside the crystal on the $\{111\}$ planes in the $\langle 112 \rangle$ direction. The trend of the temperature dependence of simulated Young's modulus is quite similar to the experimental results. The nominal strain at yield point does not much depend on temperature. Its average for temperature is $8.42 \pm 0.57\%$. Below 600 K, the dislocation speed reaches up to 70% of the transverse sound velocity. The dislocation speed decreases linearly with increasing temperature above 600 K and becomes zero at 1200 K. Dislocation at elevated temperatures propagates under lower stress than that at room temperature. At 1200 K, stress is not released by dislocation but by allotropic

transformation with cooperative motion of atoms. The temperature dependence of the dislocation dynamics affects the macroscopic deformation and fracture behavior of the metallic crystal. It is suggested that the supersonic dislocations can not exist in tensile deformation mode.

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