

Simulation of Deformation of Ni Twinned Nanocrystal Model by Molecular Dynamics

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Molecular dynamics simulation of nickel crystal under uniaxial tensile and compressive deformation was performed for single nanocrystal model and twinned nanocrystal model composed of 1550 atoms using EAM(embedded atom method) potential with the object of investigating deformation induced phase transformation (especially twin deformation). In the case of single nanocrystal model, the evolution and development of twin deformation, $(111)[11\bar{2}]$, is observed under compressive loading in $[001]$ direction, whereas either slip or twin deformation is not recognized under tensile loading. In the case of twinned nanocrystal model, twin, $(111)[11\bar{2}]$, decreases and disappears under tensile loading, and develops under compressive loading. It is suggested from the difference of results between single nanocrystal model and twinned nanocrystal model that it is easy for twin to induce local deformation.

1. INTRODUCTION

It is well known that the local phase transitions (for instance, twinning⁽¹⁾, precipitation of atomic vacancies⁽²⁾ and martensitic transformation of metallic compounds⁽³⁾, inverse transformation of metastable phase such as ω phase⁽⁴⁾) are caused by deformation, and that they lead to local deformation followed by nucleation of crack. Since the deformation induced phase transformation has been often observed in alloys, it may be observed in pure metals during the process of mechanical nanocrystalization. But it seems difficult to investigate experimentally such a phenomenon at present.

Twin deformation, one of the phase transitions, results from shearing of the lattice to a specific direction in a specific plane. For FCC crystals, twin deformation, which is composed of shearing in $[11\bar{2}]$ direction of (111) plane, has been found in Ni and Cu⁽⁵⁾.

In this study, molecular dynamics (MD) simulation of uniaxial tensile and compressive deformation of Ni single nanocrystal and Ni twinned nanocrystal has been performed.

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2. METHOD OF SIMULATION

2.1 Simulation Model

(1) Single Nanocrystal Model

Single nanocrystal model consists of $5a \times 5a \times 16a$ (a : lattice constant) FCC structure of Ni atoms, and is composed of 31 layers, each layer having 50 atoms (Fig.1). The highest two and the lowest two layers were rigid, where the atoms were fixed. Deformation of the model was carried out by moving the position of two rigid blocks. In this study, periodic boundary condition was not applied in order for local deformation like twin to occur.

(2) Twinned Nanocrystal Model

This model was based on the single nanocrystal model above described. A twin, $(111) [\bar{1}1\bar{2}]$, was introduced by displacing three (111) planes, shearing strain being 0.707. Simulation of relaxation and deformation was in the same way as single nanocrystal model. The initial configuration of atoms on the middle (110) plane, depicted in Fig.2(a), of twinned nanocrystal model is shown in Fig.2(b).

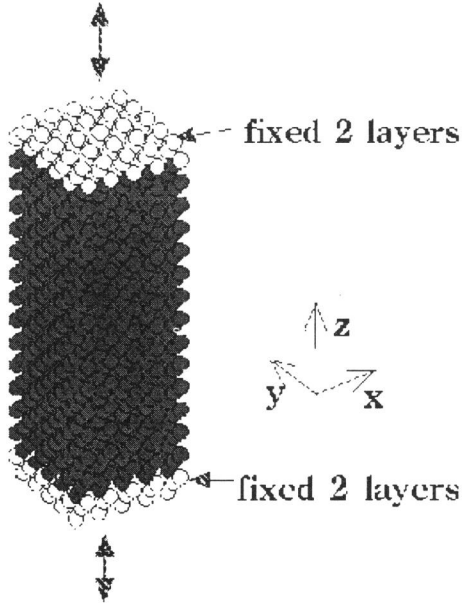


Fig.1 Simulated nanocrystal

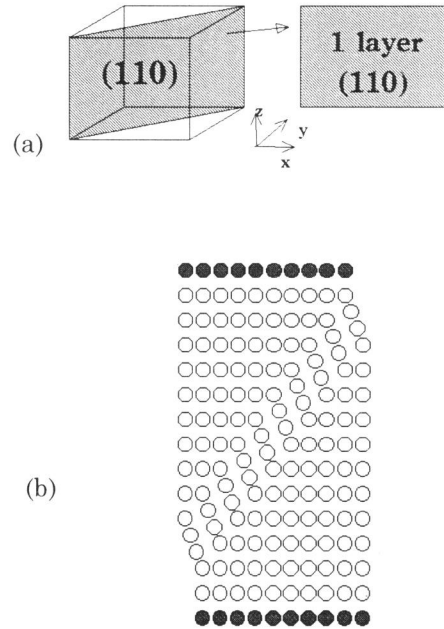


Fig.2 Initial configuration of atoms in (110) plane for twinned nanocrystal model simulation

2.2 Method of Deformation

After relaxation, the cells were deformed in the tensile or the compressive direction. The positions of the highest and the lowest two layers were displaced to make 0.2% strain at a time after relaxation of 200 time steps each. The initial velocity of atoms was set zero. If temperature was higher than 5K during the relaxation, velocity of all the atoms was reduced to zero.

2.3 Atomic Potential

EAM (embedded atom method)^(6,7) potential which was proposed by Daw and Baskes, was used in the present simulation.

Total potential energy function by EAM can be expressed as follows,

$$E_{tot} = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} \phi_{ij}(r_{ij})$$

ϕ_{ij} : Pair potential energy

r_{ij} : Interatomic distance between atoms i and atom j

$F_i(\rho_i)$: Embedded energy of atom i

ρ_i : Electron density

In this total potential energy function, ϕ_{ij} can be expressed as follows

$$\phi_{ij}(r) = \frac{\{Z_0(1 + \beta r^\gamma) \exp(-\alpha r)\}^2}{r}$$

In addition, the total electron density is given by

$$\rho_i = \sum_j \rho_j(r_{ij})$$

$$\rho_j(r) = n_s \rho_s(r) + n_d \rho_d(r)$$

The spherically averaged s - and d -like densities were computed by Clementi⁽⁸⁾ as

$$\rho_r(r) = \frac{\sum_i c_i R_i(r)}{4\pi} \quad (r ; s \text{ または } d)$$

$$R_i(r) = \frac{(2\xi_i)^{(n_i+0.5)}}{\{(2n_i)!\}^{0.5}} r^{n_i-1} \exp(-\xi_i r)$$

Parameters used for the calculation are shown in Table 1 and Table 2.

Table 1 Parameters used for the calculation of potential

α	18.633	n_s	1.5166
β	8.957	n_d	8.4834
γ	1	Z_0	1.266×10^{-19}

Table 2 Parameters used for the calculation of electronic density

	i	n_i	$\xi_i(\text{nm}^{-1})$	c_i
s	1	1	548.8885	-0.00389
	2	1	384.8431	-0.02991
	3	2	274.2703	-0.03189
	4	2	208.8204	0.15289
	5	3	109.5707	-0.20048
	6	3	73.1958	-0.05423
	7	4	39.2650	0.49292
	8	4	21.5289	0.61875
d	1	3	126.7582	0.42120
	2	3	54.3253	0.70658

3. RESULTS AND DISCUSSION

3.1 Deformation of Single Nanocrystal Model

Stress-strain relation of single nanocrystal model under tensile loading is shown in Fig.3. In this figure, elastic deformation is observed until about 18% strain, then stress falls down quickly. The elastic constant is about $1.3 \times 10^{11} \text{Pa}$, in good agreement with the experimental value, $1.198 \times 10^{11} \text{Pa}$. The maximum stress is 22GPa. Configuration of atoms in the (110) plane is shown in Fig.4. Crystal shows a little necking in the elastic range due to the elastic lateral contraction under the constraint of two rigid blocks. A part of the crystal started to lose crystallinity at 20% strain, at last the disorder spread across the crystal at about 30% strain. Either slip or twinning deformation could not be observed in this simulation. Yashiro *et al.*⁽⁹⁾ observed partial dislocation was in the simulation under tensile loading of 1800 atoms of Ni crystal. In their simulation, deformation was given by increasing all the spacings between layers at a time to avoid stress wave, while in this study it was given by displacing the highest and the lowest rigid blocks. The relaxation time was 1000 time steps in their simulation, longer than that in the present study, 200 time steps. These differences may result in the disordering crystallinity in this study.

Stress-strain relation under compressive loading is shown in Fig.5 and configuration of atoms is shown in Fig.6. Deformation is elastic until -7% strain. And stress suddenly changes at about -8.5% strain. In this stage, the evolution of two twin deformations, A and B in Fig.6 (b), is obtained. Both of these twin deformations are (111) $[\bar{1}1\bar{2}]$ and are composed of one layer each. Stress changes abruptly at about -11% strain. The configuration of atoms in this stage is shown in Fig.6.(c). The development of Twin B, becoming two layers, can be observed. This is induced by the movement to $[\bar{1}1\bar{2}]$ direction of the matrix layers over Twin B. Then stress changes abruptly at -12% strain. The configuration of atoms at that time is shown in Fig.6 (d). The development of Twin A, becoming two layers, can be observed. This is induced by the movement to $[\bar{1}1\bar{2}]$ direction of the matrix layers under Twin A. Stress changes abruptly at -15% strain. The configuration of atoms at that time is shown in Fig.6(e). Both Twin A and Twin B has become three layers, increasing one layer each.

In order to investigate the effect of periodic boundary condition, Ni crystal under uniaxial compressive deformation was performed for NVE ensembles applying periodic boundary condition using EAM potential. In this case, a twin, (010)[101], was observed, different from the result of single nanocrystal model. It is considered

that periodic boundary condition resulted in this difference. The result of single nanocrystal is in good agreement with the experimental result⁽⁵⁾, while the result of the model applying periodic boundary condition isn't. It is found that nanocrystal model is better for simulation to investigate deformation induced phase transformation than the model applying periodic boundary condition.

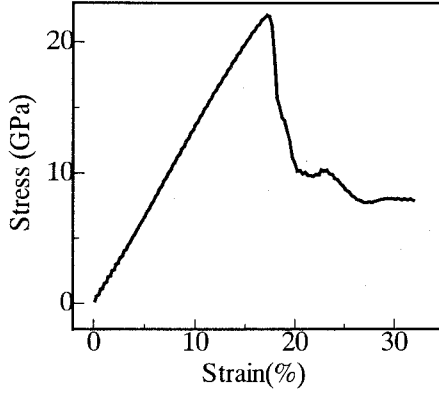


Fig.3 Stress-strain relation under tensile loading of single nanocrystal model

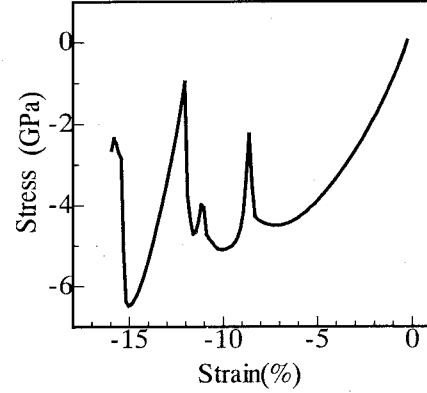


Fig.4 Stress-strain relation model under compressive loading of single nanocrystal

3.2 Deformation of Twinned Nanocrystal Model

Stress-strain relation of twinned nanocrystal model under uniaxial tensile loading is shown in Fig.7. In this figure, elastic deformation is observed until about 7% strain. At that time, stress falls down quickly. Stress starts to increase again from 9% strain and this deformation is still elastic. The change of configuration of atoms at this point is shown in Fig.8.

The twin, initially composed of three layers, decreases to one layer at 9% strain, and finally disappears at 25% strain.

Stress-strain relation under compressive loading is shown in Fig.9 and configuration of atoms is shown in Fig.10. From this figure, twin increases to become four layers at -6% strain. This result agrees with that of single nanocrystal. The yield stress of twinned nanocrystal, however, is about half as high as that of single nanocrystal. It is considered from this fact that local deformation is induced more easily in crystals containing twins than in perfect crystals.

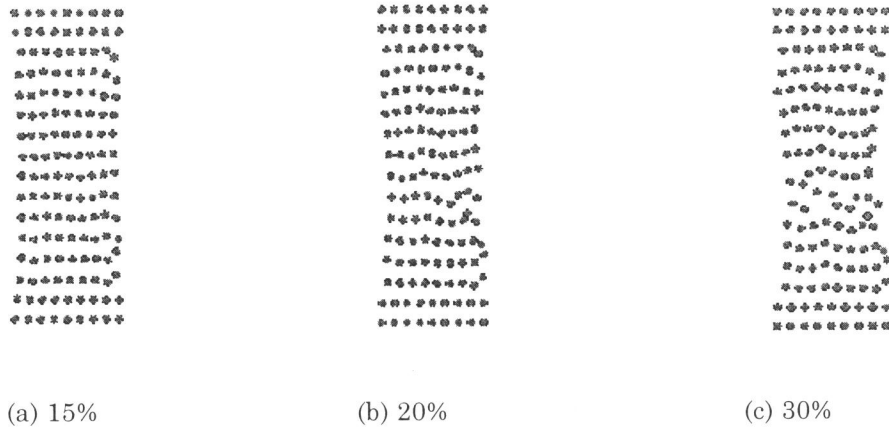


Fig.5 Configuration of atoms in the (110) plane of single nanocrystal model during tensile deformation

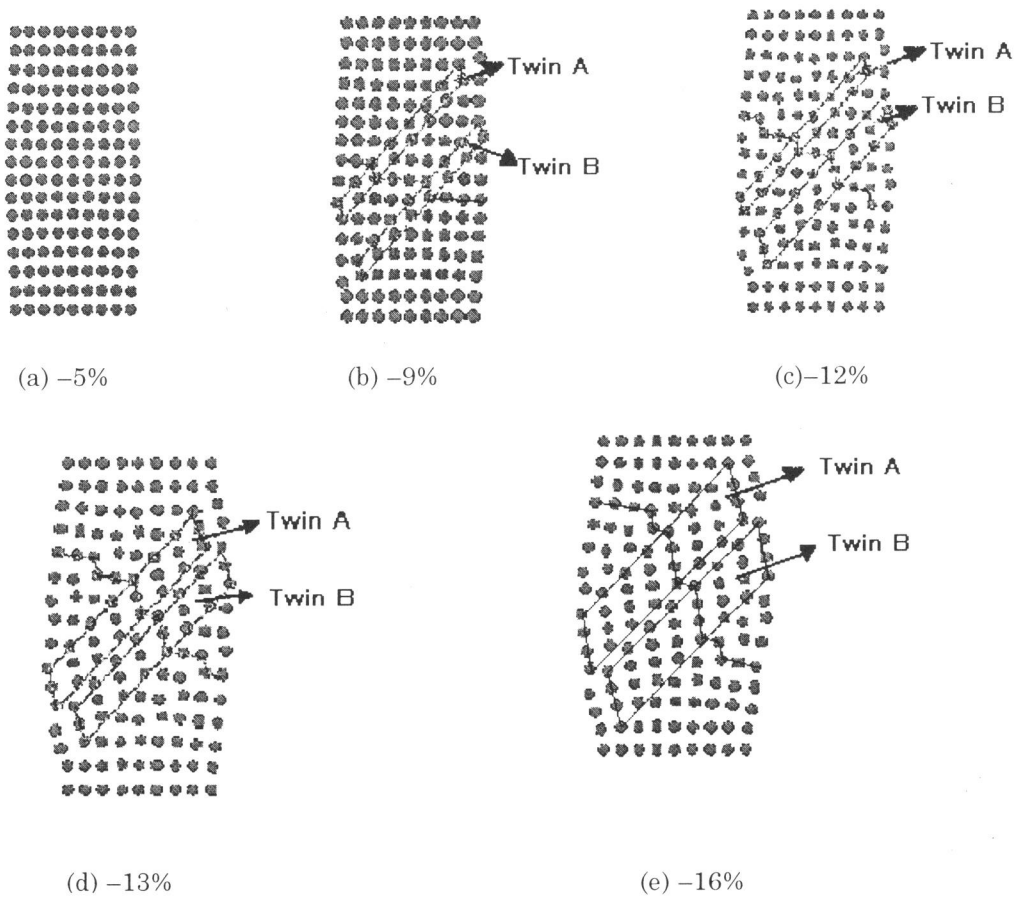


Fig.6 Configuration of atoms in (110) plane of single nanocrystal model during compressive deformation

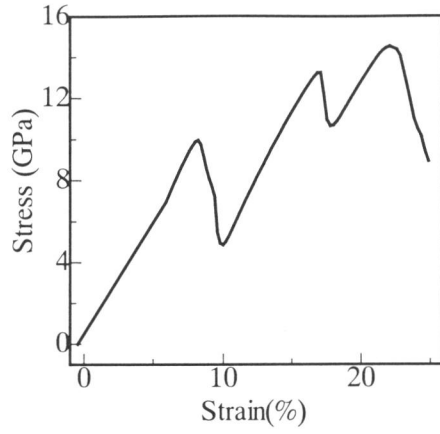


Fig.7 Stress-strain relation under tensile loading of twinned nanocrystal model

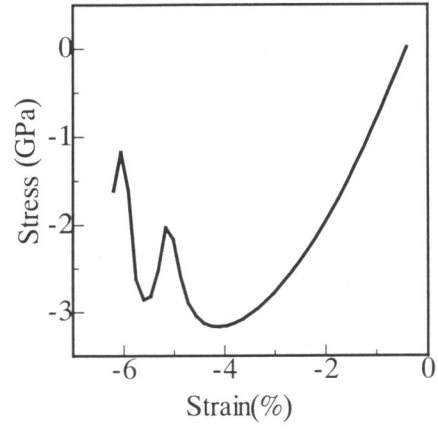
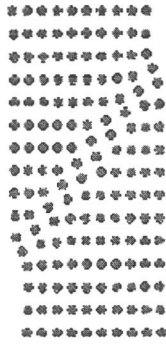
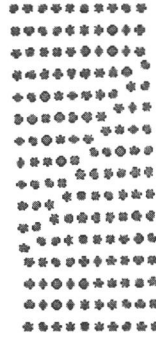


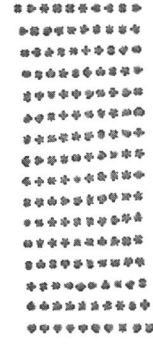
Fig.8 Stress-strain relation under compressive loading of twinned nanocrystal model



(a) 8%

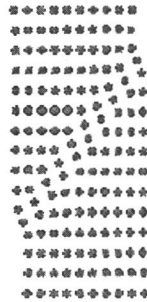


(b) 10%

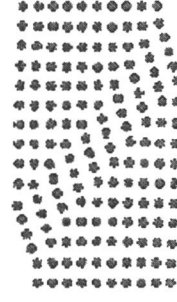


(c) 25%

Fig.9 Configuration of atoms in (110) plane of twinned nanocrystal model during tensile deformation



(a) -5%



(b) -7%

Fig.10 Configuration of atoms in (110) plane of twinned nanocrystal model during compressive deformation

4. CONCLUSION

Simulation was performed for uniaxial tensile and compressive deformation of Ni single nanocrystal and Ni twinned nanocrystal composed of 1550 atoms using EAM(embedded atom method) potential. The conclusion of the present study is as follows.

- (1) Twin, (111) $[11\bar{2}]$, developed under compressive loading, and decreased and disappeared under tensile loading.
- (2) Nanocrystal model is better for simulation to investigate deformation induced phase transformation than the model applying periodic boundary condition.
- (3) Local deformations induced more easily for crystals containing twins than for perfect crystals.

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