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Investigation of the Effect of Grain Size and Wire Size on the Mechanical and Structural Properties of Polycrystalline Ni Nano Wire Using Molecular Dynamics Simulation

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Abstract: The effect of grain size and length-to-diameter ratio (LDR) on the mechanical properties of polycrystalline Ni nanowire was examined by molecular dynamics simulation as a result of uniaxial tensile deformation applied at a temperature of 300 K. The Embedded Atom Method (EAM) was used to determine the forces acting on the nanowire atoms. Elastic modulus (E), yield strength and fracture stress values were determined from the stress-strain relationship determined as a result of the deformation process. Microstructural changes resulting from plastic deformation were examined from the atomic positions determined using the common neighbor analysis method (CNA). It was determined that grain size and LDR had a significant effect on the deformation behavior of Ni nanowire, and plastic deformation and breaks resulted from the rearrangement of atomic positions by surface effect and also the nanowires with small grain size and LDR exhibited superplasticity behavior. The grain size in the modeled polycrystalline nanowire system affected the movement mechanisms of the grains, grain boundaries, and the relationship between grain size and flow force was investigated. From this relationship, the Hall-Petch effect and the reverse Hall-Petch effect were observed after a certain critical grain size.

Key words: Polycrystal, nanowire, superplastic, molecular dynamics, Hall-Petch effect.

Tane Büyüklüğü ve Tel Boyutunun Polikristal Ni Nano Telinin Mekanik ve Yapısal Özelliklerine Etkisinin Moleküler Dinamik Benzetimi ile İncelenmesi

Öz: Polikristal Ni nano telinin mekanik özelliklerine tane büyüklüğü ve uzunluk-çap oranının (Length-to-Diameter-Ratio-LDR) etkisi, 300 K sıcaklık değerinde uygulanan tek eksenli çekme deformasyonu sonucu moleküler dinamik benzetimi ile incelendi. Gömülmüş Atom Metodu (GAM) nano tel atomları üzerine etki eden kuvvetlerin belirlenmesinde kullanıldı. Deformasyon işlemi sonucu tespit edilen zor-zorlanma ilişkisinden Elastiklik modülü (E), akma dayanımı, kopma gerilmesi değerleri belirlendi. Ortak komşu analiz yöntemi (Common Neighbor Analysis-CNA) kullanılarak tespit edilen atomik konumlardan plastik deformasyon sonucu meydana gelen mikro yapısal değişimler incelendi. Tane büyüklüğü ve LDR'nin Ni nano telinin deformasyon davranışları üzerinde önemli bir etkiye sahip olduğu ve plastik şekil değişimi ve kopmaların, atomik konumların yüzey etkisi ile yeniden düzenlenmesinden kaynaklandığı belirlendi. Küçük tane boyutuna ve LDR'ye sahip nanotellerin süper plastiklik davranış sergilediği tespit edildi. Modellenen polikristal nano tel sistemde tane boyutunun, tanelerin hareket mekanizmalarını, tane sınırlarını ve tane boyutu ile akma zoru arasındaki ilişkiyi etkilediği tespit edildi. Bu ilişkiden Hall-Petch etkisi ve belirli bir kritik tane büyüklüğünden sonra ters Hall-Petch etkisi gözlemlendi.

Anahtar kelimeler: Polikristal, nano tel, süper plastik, moleküler dinamik, Hall-Petch etkisi.

1. Introduction

The studies on the mechanical properties of nanowires are becoming an increasingly important area of materials science and also nanowires have been extensively studied in recent years for their use as building blocks in nano-electromechanical devices due to their superior thermal, mechanical, electronic and optical properties resulting from their nanoscale scale [1-5]. The use of metallic nanowires as building blocks and connectors in electronic and optical devices as well as chemical and biological sensors requires an understanding of their structure and mechanical properties [6].

The properties of nanostructured materials can vary depending on the intrinsic microstructure size and extrinsic sample size [7]. An important property of metallic nanowires is the surface effects resulting from their large surface/volume ratio. Internal stresses resulting from surface tension in nanowires lead to mechanical properties that are quite different from bulk structures [8]. As a result of experimental studies, it has been determined that the grain boundaries of metallic nanowires significantly affect their mechanical properties [9-11]. Reducing the sample size to nanoscale reduces the formation and probability of defects in the material. The size, shape, number of grains in the sample, crystal orientations and boundary structures in the grains have a significant impact on the thermodynamic, mechanical and electrical properties of materials. Although there are many theories

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explaining how these parameters affect large grains, this number is quite small at the nanoscale [12]. If metal nanowires are used in practice, the most important elements to know are their elastic behavior and durability during tensile deformation [13,14]. Young's modulus, yield stress and fracture stress are determined as a result of tensile deformation tests applied to the sample [15]. Although it is easy to perform these tests at macro scale to determine mechanical properties, they are quite difficult at nano dimensions.

Due to the difficulty and time-consuming processes of experimental studies at the nanoscale, the computer simulations were used to establish a connection between theory and experiment. There are effective simulation techniques used in modeling systems at the atomic level. One of these techniques is the Molecular Dynamics (MD) simulation method. MD simulation method is widely used to investigate the physical and thermodynamic properties of alloy systems, glassy structures, polymers, semiconductors and nanomaterials [16-18]. However, MD simulations are a powerful modeling tool used to examine the structure, mechanical properties and deformation behaviors of metallic nanowires under different strain conditions, especially at the atomic level [19-21]. However, studies on the mechanical properties of polycrystalline nanowires are still not sufficient.

In this study, the uniaxial tensile deformation process applied to polycrystalline Ni nanowires with different LDR and grain sizes at a temperature of 300 K and a strain rate of $1x10^{10}$ s^{-1} was examined with the MD simulation software package LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). Calculation of forces between Ni atoms was performed with the EAM potential function. The main advantage of EAM is that the calculation time is short and it provides the opportunity to work with a large number of particles. The effect of grain number and LDR on the mechanical properties of the model polycrystal was tried to be determined from the strain curves and the atomic-sized deformation mechanism of the nanowire during strain from the CNA analysis obtained from the OVITO program. In addition, the development processes of dislocations in the nanowire within the structure during the tensile deformation process were detected by Dislocation Extraction Algorithm (DXA) analysis method.

1. Material and Method

The extent to which the results obtained from MD simulation are in agreement with the experimental results depends on the correct selection of the interatomic potential. EAM, proposed by Daw and Baskes [22] and whose validity has been proven by many studies, produces very effective results in determining the mechanical properties of materials. The general structure of EAM as a semi-empirical potential energy function is defined as Eq.1;

$$E_{top} = \sum_i^N F_i\,(\rho_i) + \frac{1}{2}\sum_{i\neq j} \Phi\left(r_{ij}\right) \tag{1}$$

In this function, which includes many-body interactions, N is the number of atoms in the model system, $F_i(\rho_i)$, corresponds to the embedding energy and $\Phi(r_{ij})$ corresponds to the binary interaction energy [23]. Details of EAM and its potential parameters for the Ni element can be found in the literature [24]. The expression of force in the tensile or compression strain to be applied in MD studies is calculated by the microscopic force tensor given as Eq.2 [25,26].

$$\boldsymbol{\sigma} = V^{-1}\left[\sum_{i=1}^{N} m_i \vartheta_i \vartheta_i - \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{F_{ij}}{r_{ij}} \mathbf{r}_i.\,\mathbf{r}_j\right] \tag{2}$$

The difficult tensor with nine components is expressed as Eq.3;

$$\sigma_{ij} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix} \tag{3}$$

Positive values of the normal components of the force tensor correspond to tensile force, and negative values correspond to compression force [27].

One of the algorithms used to analyze the details of the atomic configurations in the system to be modeled in the MD simulation method is CNA analysis [28]. The basis of this method is to assign 4 characteristic integers (*i, j, k, l*) to a selected reference atom to define a structure and analyze its surrounding neighbors. Details of this method can be found in the literature [29]. In the study, CNA analysis was performed with the OVITO program and atomic positions were determined [30].

The effects of grain size and LDR on the deformation behavior of polycrystalline Ni nanowire were examined by MD simulation under a strain rate of $1x10^{10}s^{-1}$ at 300 K temperature. In this study, grains were created in the

nanowire with the Voronoi tessellation algorithm by the Atomsk program [31]. To determine the average grain size d in the model system, the expression $n = [6V / (\pi d^3)]$ was used, where n is the grain number and V is the MD cell volume [32]. The points where the grains would grow were determined randomly and the grains grew by focusing on these points. The study consists of three parts. In the first part, basic mechanical properties were determined for the model nanowire from the strain curves obtained as a result of the applied tensile deformation for LDR values 1, 1.5, 2, 3 and 4. The base cross-sectional area of all nanowires used in the study is 70.4Åx70.4Å, the number of atoms in the nanowire is N and the average grain size is d, respectively: 32000-3.21 nm for LDR=1, 48000-3.68 nm for LDR=1.5, LDR=2. It was determined as 64000-4.05 nm for LDR=3, 96000-4.64 nm for LDR=3 and 128000-5.1 nm for LDR=4. In the second part, the effect of grain size on the mechanical properties of the nanowire was tried to be determined by creating 10, 12, 15, 20, 30, 50, 70 and 80 grains in the nanowire for LDR = 4 value. Hall-Petch and reverse Hall-Petch effect were determined from the relationship between grain size and flow strain. In the last part, the change in mechanical properties was examined by creating grains of fixed size (d = 5.1 nm) in nanowires for different LDR ratios, as in the first part.

In the polycrystalline Ni nanowire system modeled in this study, atoms were placed at fcc lattice points with a lattice parameter of 3.52 Å. Periodic boundary conditions were applied only along the x direction of the nanowire. However, the y and z directions of the nanowire are freed. The initial velocities were assigned to the atoms randomly, taking into account the Maxwell-Boltzman velocity distribution. The velocity form of the Verlet algorithm was used for the numerical solution of the equations of motion at 1 fs time intervals. The NVT statistical ensemble was used to ensure that all model polycrystalline nanowires reached equilibrium at target temperature and pressure values before applying the drawing process.

2. Results and Discussion

In this study, the changes in mechanical properties and the plastic deformation mechanism that occurred as a result of $1x10^{10}$ s^{-1} tensile strain applied along the x-axis under a constant temperature of 300 K and a pressure of 0 GPa on polycrystalline Ni nanowires with different initial structures and grain sizes were tried to be examined by MD simulation method.

2.1. Effect of LDR variation on mechanical properties of constant grain number polycrystalline Ni nanowire

Figure 1 shows the different initial structure obtained from the (001) plane section of the 12-grain Ni nanowire from the OVITO program. In the atomic configuration obtained from CNA analysis, green atoms indicate fcc unit cell structures. However, the white atoms represent the irregularly structured atoms at the grain boundary, which are not defined as any unit cell structure by CNA, and the surface atoms of the nanowire, where periodic boundary conditions are not applied.

In this study, first of all, the changes in the mechanical properties of nanowires with different LDR values as a result of uniaxial tensile stress was tried to determine. To reduce the effect of the random nature of sample generation throughout the entire study, the number of grains in the nanowires was fixed and set at 20. The fixed number of grains caused the formation of grains of different sizes in the nanowire system, depending on the LDR ratio. The strain curve obtained as a result of the tensile deformation applied to the polycrystalline Ni nanowire with LDR change is given in Fig. 2. In all nanowires, it is clearly seen that the stress-strain curve, where the elastic properties of the sample are determined, changes almost linearly up to a certain value of the applied strain. The elastic modulus of Ni polycrystalline nanowires was determined by linearly fitting the elastic region of the stress curve up to 2 strain value. The first maximum point on the stress-strain curve where plastic deformation begins is expressed as the yield force. It is thought that the zig-zag changes seen in Fig. 2 arise from the atomic arrangements within the structure [33]. Parameters expressing the mechanical properties of the polycrystalline Ni nanowire such as elastic modulus, yield strain, and fracture stress depending on the LDR values are given in Table 1. It has been determined that as the grain size decreases, the elastic modulus and yield force value decrease. Experimental results show that the elastic modulus of nanowires increases with decreasing wire diameter [34,35].

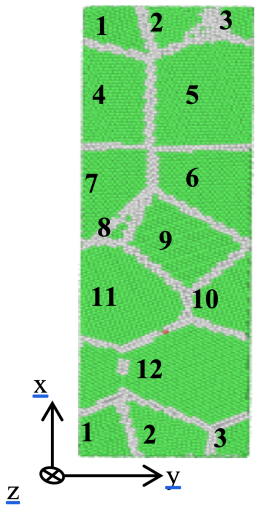

Figure 1. Initial structure of the polycrystalline Ni nanowire system containing 12 grains for LDR = 4.

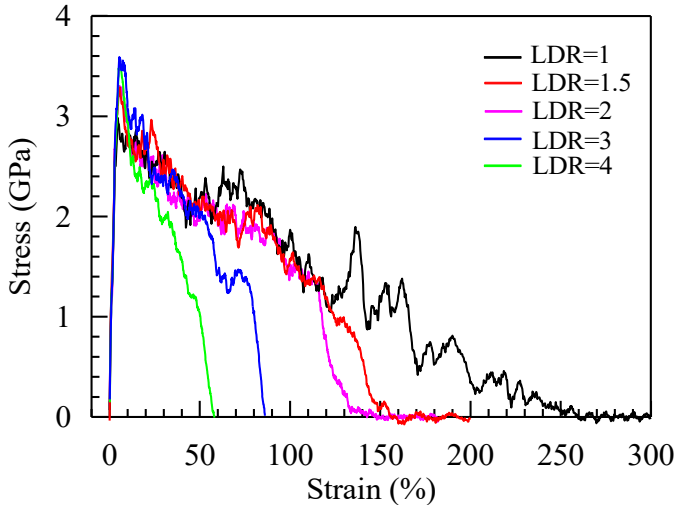

Figure 2. Stress-strain curves of polycrystalline Ni nanowire for different LDR values.

A softening of the material is observed with decreasing grain size. It is thought that this softening occurs because the grain boundaries occupy a larger part of the total volume in samples with smaller grain sizes and grain boundary sliding becomes easier [36]. The elastic weakness of grain boundaries and triple junctions at small grain size significantly affects the elastic properties of polycrystalline nanowires. Looking at the fracture percentage values given in Table 1, it can be seen that two deformation behaviors occur in the model nanowire sample: plastic and superplastic. At LDR values of 1, 1.5 and 2, the fracture strain value for nanowires was over 100% and superplastic deformation was observed. Especially for LDR=1, the percentage of fracture strain is quite high. Super plasticity is known as the ability of the sample to change shape greatly without bending at certain temperatures and strain rates. In superplastic materials, the deformation area can increase from 100% to 1000% without giving way. It is accepted that superplastic deformation will occur mostly with grain boundary sliding. The idea that grain boundary shifting will be effective in superplastic deformation arises from the fact that these materials have a small-grained structure [37]. Fig. 3 shows the atomic positions obtained from CNA analysis for different strain percentages, from the initial state ε=0%, where no strain is applied, for LDR value 1, to the value ε=259%, where fracture occurs in the sample. Plastic deformation is observed without any neck formation up to ε=100% of the tensile stress applied to the sample. At ε=20% value and beyond, hcp unit cell structures, indicated by red atoms, are formed in almost all grains. These structures are known as stacking defects that occur as a result of the nucleation of Shockley partial dislocations in the model nanowire [38,39].

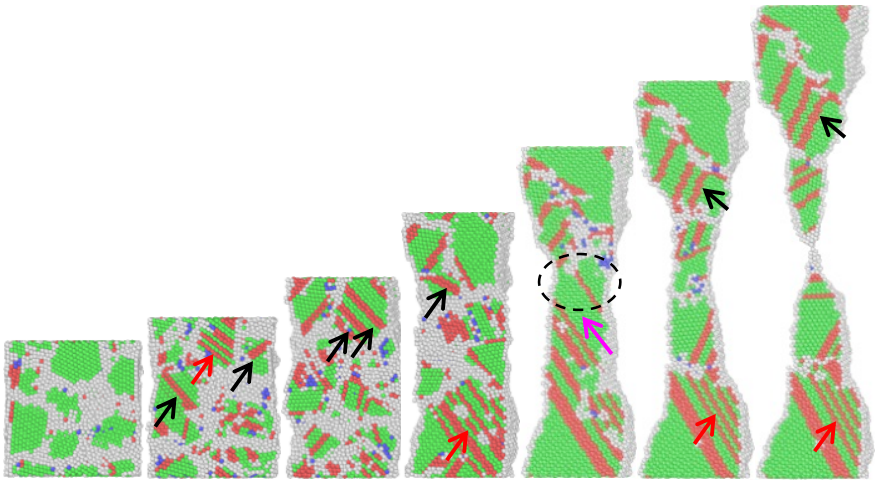

Figure 3. Atomic images obtained at different strain percentages of the polycrystalline Ni nanowire system with d = 3.21nm grain size for LDR = 1 at a strain rate of $1x10^{10}$ s^{-1}.

Table 1. Parameters of some elastic and plastic properties of polycrystalline Ni nanowires with different LDR and grain sizes containing 20 grains.

LDR	1	1.5	2	3	4
Grain size (nm)	3.21	3.68	4.05	4.64	5.10
E (GPa)	68.2	71.1	78.6	78.9	79.2
Yield strength (GPa)	2.96	3.28	3.29	3.58	3.58
Fracture strain (%)	259	155	148	86.0	59.0

As the strain increases, accumulation defects increase as a result of the nucleation and propagation of new dislocations. Two side by side atomic layers consisting of hcp unit cells are defined as internal stacking defects, the structure with an fcc atom layer between two hcp atomic layers is defined as external stacking defect, and the structure consisting of many fcc unit cells between two hcp layers is defined as deformation twins [40,41]. Accordingly, internal stacking defect formation was detected in the places marked with black arrows in Fig. 3, and external stacking defects were detected in the places marked with red arrows. However, deformation twins were detected in the area indicated by the pink arrow. It can be seen that at ε=150%, the nanowire begins to neck in the region indicated by the dotted circle, at ε=200%, the neck area gradually becomes thinner with increasing strain, and at ε=259%, fracture occurs. In an experimental study conducted by Lu, it was observed that excessive elongation (ε=5000%) occurred in the Cu nanowire synthesized in high purity under tensile deformation [42]. For the strain percentages from ε=0% to ε=259% given in Fig. 3, the percentage changes obtained from the CNA analysis of the atoms called "other" were determined as 50, 50.6, 46.3, 36.8, 28.4, 27.8 and 27.3, respectively. Accordingly, it is thought that the decrease in the percentage of surface atoms and "other" atoms representing grain boundaries due to periodic boundary conditions with increasing strain occurs as a result of the grains in the nanowire coalescing with increasing strain and the grain boundaries disappear.

2.2. Effect of grain size on mechanical properties of polycrystalline Ni nanowire

In Figure 4, for the fixed initial structure of the MD calculation cell (LDR = 4), polycrystalline Ni nanowires containing 10, 12, 15, 20, 30, 50, 70 and 80 grains are applied with a strain rate of $1x10^{10}$ s^{-1} along the x-axis direction. The stress-strain curves obtained as a result of tensile deformation are seen. The grain numbers used in the study were chosen randomly to determine the effects of grain size on the mechanical properties of the nanowire. The elastic modulus, yield strength and fracture strain percentages obtained from the stress-strain curves determined as a result of the uniaxial drawing process applied to nanowires with different grain sizes are given in Table 2. From Figure 4, it is clearly seen that the strain-strain curve changes almost linearly up to a certain value of the applied strain in all nanowires with different grain numbers. The elastic modulus values obtained from the

regression analysis of this change, known as the elastic deformation region, are given in Table 2. It is clearly seen that the elastic modulus is affected by grain size. As the number of grains increases, in other words, as the grain size decreases, the elastic modulus decreases. When the strain applied to the nanowires reaches the value corresponding to the yield strength, which is the maximum point of the stress-strain curve, the mechanisms required for plastic deformation begin to take effect and permanent deformations begin. When Table 2 is examined, increasing the number of grains in nanowires with 10, 12 and 15 grain numbers caused an increase in the yield strength values. Polycrystals are stronger than single crystals, and the increase in flow force as the number of grains increases, in other words as the grain size decreases, causes an increase in the strength of the material due to the "smaller is stronger" effect [7].

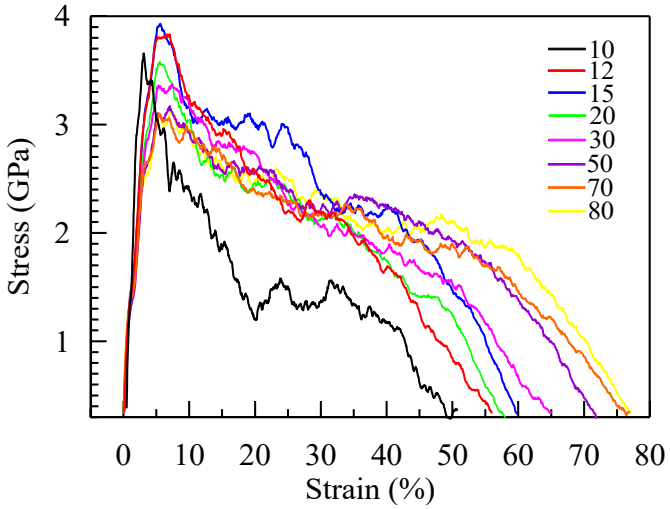

Figure 4. Strain curves of polycrystalline Ni nanowire containing different numbers of grains for a constant value of LDR = 4.

Table 2. Parameters of some elastic and plastic properties of polycrystalline Ni nanowires with different grain numbers for the constant value of LDR = 4.

The number of grain	Grain size (nm)	E (GPa)	Yield strength (GPa)	Fracture strain (%)
10	6.43	88.87	3.68	49
12	6.05	88.84	3.82	56
15	5.62	86.49	3.91	60
20	5.10	79.20	3.58	59
30	4.46	65.61	3.38	66
50	3.76	66.55	3.18	72
70	3.36	61.03	3.10	77
80	3.21	54.95	3.08	78

However, the flow forces of nanowires containing 20, 30, 50, 70 and 80 grains decrease as the number of grains increases. Hall [43] and Petch [44] determined the Hall-Petch expression, which gives the relationship between flow force and grain size, from the data they obtained as a result of their experimental studies. This relationship states that a small grain size corresponds to a high material strength. Thus, reducing the grain size has become an effective method to change the strength of materials [45-47]. The difficulty of dislocation movement along grain boundaries and the concentration of force resulting from dislocation accumulation are expressed as the physical basis of this behavior. Reducing the grain size to the nanoscale level results in a significant increase in the volume fraction of grain boundaries. As a result, grain boundary-mediated processes such as grain boundary sliding and grain boundary transformation become more important [48, 49]. However, reducing the grain size has a limited effect on the strength of the material [A5 and else]. When the grain size decreases below a certain critical value, the strength of the material decreases and a situation called the reverse Hall-Petch effect occurs. Yip suggested that the highest plastic resistance occurs in polycrystalline materials at grain sizes of approximately 20

nm [36]. Schiotz et al. They determined a softening process at small grain sizes with their simulation studies for nanocrystal Cu [51]. This grain softening phenomenon has also been reported in studies on various nanowires such as Ni and Pt [52-54].

The relationship between flow force and grain size for Ni nanowire is given in Fig.5. It is seen that when the average grain size is larger than d = 5.62 nm, that is, smaller than $d^{-1/2}$ = 0.422 nm, the flow force of the model polycrystalline nanowires increases with the decrease in d. This result is compatible with the Hall-Petch relationship (Eq. 4).

$$\sigma_S = \sigma_0 + k.d^{-1/2} \quad (4)$$

In this equation, σ_0 is the lattice friction force required to move individual dislocations, σ_S is the flow force, k is a constant that varies depending on the material and is known as the Hall-Petch slope, and d is the average grain size [50]. Hall-Petch equation from the fit process using points with $d^{-1/2}$ value less than 0.422 nm, is obtained by the Eq.5;

$$\sigma_S = 0.33 + 8.49.d^{-1/2} \quad (5)$$

It has been determined that when the grain size is smaller than 5.62 nm, that is, the $d^{-1/2}$ value is greater than 0.422 nm, the flow force of the model nanowire system decreases with the decrease of d. This result was first reported by Chokshi et al. It is compatible with the inverse Hall-Petch effect determined by . The inverse Hall-Petch equation for the Ni nanowire system was obtained by fitting the points with $d^{-1/2}$ values greater than 0.422 nm as follows (Eq. 6).

$$\sigma_S = 6.13 - 5.61.d^{-1/2} \quad (6)$$

Nanowire structures with grain sizes larger than 6.43 nm and fewer than 10 grains were not included in the study because no size effect was observed.

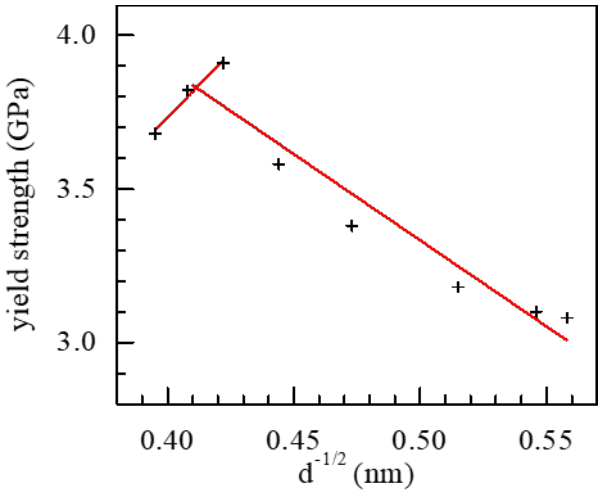

Figure 5. Relationship between grain size and yield-strenght of polycrystalline Ni nanowire.

In crystal structures, grain boundaries act as a barrier against dislocations moving on slip planes. Increasing the orientation angles of the atoms in the grains also increases the strength of this barrier. In Figure 6, in the images of the atomic positions of the nanowire containing 15 grains taken from the elastic deformation region before the plastic deformation started, it is clearly seen that dislocations accumulate at the grain boundaries and the transition of other grains to the slip planes is prevented by these boundaries. In DXA analysis, green color shows 1/6<112> Shockley dislocations, blue color shows 1/2<110> perfect dislocations, and red color shows dislocations that are not defined in DXA analysis and are called “other”.

From Table 2, it can be seen that as the grain size decreases, the strain values at which fracture occurs in the nanowire increase. Li et al. reported that there was an increase in the fracture stress value with decreasing grain size for Mo nanowire [37] determined in their study. In addition to having high strength, small-grained structures also break more slowly due to their high elongation.

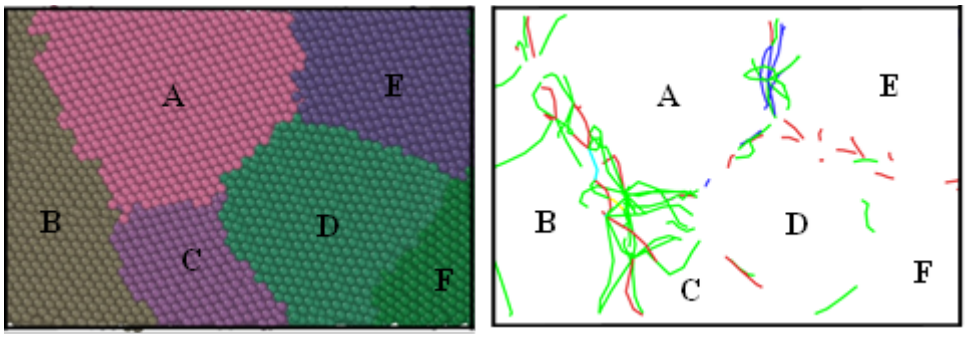

Figure 6. Grain structures in atomic configuration and dislocation distributions at grain boundaries taken from a specific cross-section of the polycrystalline Ni nanowire.

2.3. Effect of LDR change on mechanical properties in polycrystalline Ni nanowire with constant grain size

In this section, the effect of LDR variation of the MD calculation cell with fixed grain size (d = 5.1 nm) on the mechanical properties of polycrystalline Ni nanowire was tried to be examined. The stress-strain curves obtained as a result of the tension deformation applied to the model nanowire system with a strain rate of $1x10^{10}$ s^{-1} along the x-axis direction for different LDR values are shown in Fig. 7. The parameters of the mechanical properties obtained from the figure are given in Table 3. Although the grain size is larger than 4.05 nm, superplastic deformation behavior is still observed in the nanowire at LDR values of 1 and 1.5. LDR affects the deformation behavior and fracture stress percentage, and with increasing LDR, the fracture stress of the sample tends to be small due to the surface effect. It can be seen that the elasticity modulus is almost unaffected by the LDR change. In addition, it has been determined that the yield strength values at which plastic deformation begins are almost unaffected by the LDR change, except for LDR = 3.

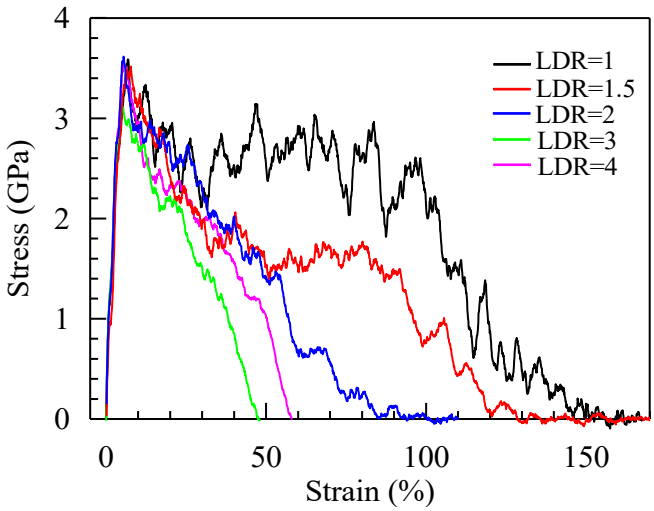

Figure 7. Stress-Strain curves of polycrystalline Ni nanowire for fixed grain size and different LDR values.

Table 3. Parameters of some elastic and plastic properties of polycrystalline Ni nanowires with different LDR for fixed grain size (d = 5.1 nm).

LDR	1	1.5	2	3	4
The number of grain	5	8	10	16	20
E (GPa)	73.2	72.9	74.1	73.9	79.2
Yield strength (GPa)	3.60	3.52	3.61	3.17	3.58
Fracture strain (%)	151	120	85	48	59

Figure 8 shows the atomic positions obtained from CNA analysis for different strain percentages, from ε=%0 initial state, where no strain is applied, to ε=151%, where fracture occurs in the sample, for LDR=1, which contains 5 grains and has a grain size of 5.1 nm. It is seen that no neck formation occurs up to the tension strain value applied to the model system, ε = 100%. However, at ε = 7%, which is the yield strenght at which plastic deformation begins, it has been determined that the atoms in grains 4 and 5 are rearranged and have the same orientation, as a result of which the boundary between them disappears, these grains come together, and hcp unit cell structures shown with red atoms begin to form. These stacking defects occurring in hcp unit cells, known as alignment errors of fcc structures, are thought to occur as a result of the nucleation of Shockley partial dislocations [38,39]. It is clearly seen that as the strain increases, many accumulation defects occur as a result of new dislocations nucleating and spreading within the structure. The black, red and pink arrows in Fig. 8 point to the places where deformation twins with internal and external stacking defects are formed within the nanostructure, respectively. However, it has been determined that as the strain applied to the nanowire increases, the grain boundaries disappear and the grains coalesce. It is seen that at ε=110%, the nanowire begins to yield in the region indicated by the dotted circle, and at ε=151%, fracture occurs in this region. The fact that the percentages of atoms representing free surfaces and grain boundaries atoms, called "other", obtained from CNA analysis, decreased from 36.5% before the strain was applied to 22.3% when the fracture occurred, which is evidence that the different atomic orientations in different grains disappear and the coalescence of the grains occurs.

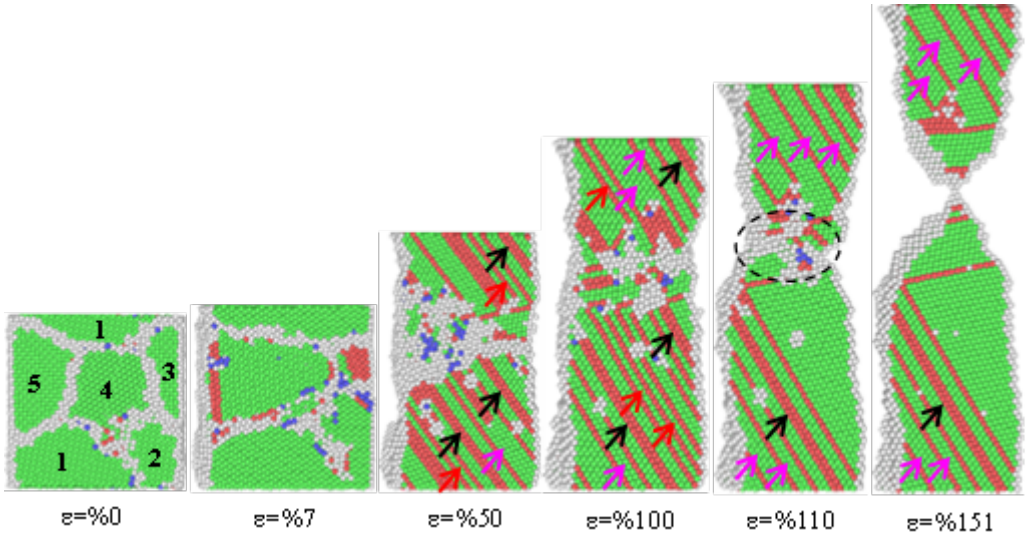

Figure 8. Atomic images obtained at different strain percentages of the polycrystalline Ni nanowire system with d = 5.1 nm grain size for LDR = 1 at a strain rate of $1x10^{10}$ s^{-1}.

4. Conclusion

This study, in which the interactions between Ni atoms are modeled with the EAM potential function, consists of three parts. In the first part, the changes in mechanical and microstructural properties as a result of tension deformation applied to nanowires containing 20 grains and with different LDR values were examined. At LDR values of 1, 1.5 and 2, the nanowire exhibits superplastic deformation behavior. At LDR=1, the fracture percentage of the nanowire reaches its highest value. It has been determined that increasing LDR values cause a decrease in the elastic modulus, which gives the elastic properties of the nanowire, and the flow strain value at which plastic deformation begins. During the superplastic deformation of the nanowire, the formation of deformation twins as well as internal and external stacking defects was observed in the structure. In the second part, nanowires with different grain numbers were subjected to tension deformation for a constant value of LDR = 4. When the average grain size was larger than 5.62 nm, it was determined that the nanowire showed a Hall-Petch relationship from the change in flow force with grain size. However, when the grain size was smaller than 5.62 nm, an inverse Hall-Petch relationship was observed. When the critical grain size of 5.62 nm is reached, the ability of interfacial atoms to resist dislocation transfer and grain rotation is strongest. In the last part, tension deformation was applied to nanowires with different LDR starting structures with a fixed grain size of 5.1 nm. Although the number of grains is large, the structure undergoes superplastic deformation at LDR values of 1 and 1.5. In addition, the elastic

modulus is almost close to each other at all LDR values. It was determined that the grains coalesced during superplastic deformation and many stacking defects formed in the nanostructure.

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