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The Investigation of Mechanical Properties of Polycrystalline Nb Nanowire Under Applied Tensile Deformation by Molecular Dynamics Simulation

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Abstract: In this study, the change in the mechanical properties of Niobium (Nb) nanowire with different grain numbers under applied uniaxial tensile deformation was tried to be investigated by Molecular Dynamics (MD) simulation method. The Embedded Atom Method (EAM), which includes many-body interactions, was used to determine the force interactions between atoms. To determine the effect of grain number on the mechanical properties of Nb nanowire, stress-strain curve, young modulus, yield strain and atomic images obtained from the common neighbor analysis method (CNA) were used. It has been determined that necking and breaking of the model nanowire occur at the grain boundaries, however, the number of grains has important effects on the mechanical properties.

Key words: Nanowire, grain boundary, molecular dynamics, mechanical properties.

Polikristal Nb Nano Telinin Uygulanan Çekme Deformasyonu Altında Mekanik Özelliklerinin Moleküler Dinamik Benzetimi ile İncelenmesi

Öz: Bu çalışmada farklı tane sayılarına sahip Niyobyum (Nb) nano telinin uygulanan tek eksenli çekme deformasyonu altında mekanik özelliklerindeki değişim Moleküler Dinamik (MD) benzetim yöntemi ile incelenmeye çalışıldı. Çok cisim etkileşmelerini içeren Gömülmüş Atom Metodu (GAM), atomlar arasındaki kuvvet etkileşmelerini belirlemek için kullanıldı. Nb nano telinin mekanik özellikleri üzerine tane sayısının etkisini belirlemek için zor-zorlanma eğrisi, elastiklik modülü, akma zorlanması ve genel komşu analiz yönteminden (Common Neighbor Analysis-CNA) elde edilen atomik görüntülerden yararlanıldı. Model nano telde boyun verme ve kopmanın tane sınırlarında meydana geldiği bununla birlikte tane sayısının mekanik özellikler üzerinde önemli etkilerinin olduğu tespit edildi.

Anahtar kelimeler: Nano tel, tane sınırı, moleküler dinamik, mekanik özellikler.

1. Introduction

The rapid technical progress in nanowire fabrication in recent years has greatly supported the development and application of nanoelectromechanical systems. The structural safety and reliability of nanoelectromechanical systems largely depend on the mechanical behavior of these newly developed nanoscale materials. The properties of nanostructured materials depend on the internal microstructure size and the external sample size. Nanostructured materials can be developed by refining the grain size [1] by embedding nanotwined lamellas in sub-micrometer sized grains [2, 3] or nanowires [4, 5] or by adjusting the layer thickness of nanoscale metallic multilayers [6, 7]. They are also used in the development of new products such as nanoelectronic devices [8-10], energy storage and conversion systems [11, 12], biomedical devices and sensors [13].

Research on the mechanical properties of polycrystalline materials is of great importance in terms of both theory and practice [14-16]. It is known that grain boundary plays an important role on the mechanical properties of polycrystalline materials [17-19]. A good understanding of crystallographic deformation in mechanical processes due to nano-dimensional effects [20, 21] is very important for devices to be developed. Atomic force microscopy [22] and high-resolution transmission electron microscopy [23] are used to experimentally examine the properties of nano-sized metallic materials at the atomic level. Nanowires always exhibit a special and unpredictable behavior under applied tensile loading as they are affected by factors such as temperature, crystallographic orientations, strain rate, multiple grain structures, surface and boundary conditions.

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Nb element is used in both experimental and theoretical studies due to its ductility at room temperature, melting at high temperatures, low density and low neutron capture cross section [24, 25]. In addition, Nb and Nb alloys are preferred in the aerospace industry, in the production of reactor pipes, and in implants [26, 27]. Although there are many studies on bulk, clustered and thin film structures of Nb element [28-30], the number of studies on nanowire structure is few.

With the rapid development of computer technology and computational methods, atomic simulation techniques have become a popular and effective tool widely used to identify new properties of nanomaterials [31] and to detect atomic details of the deformation mechanism [32, 33]. Especially in recent years, the MD simulation method has been used effectively to examine the deformation characteristics of polycrystalline metals [34, 35]. When Wolf et al. [36] examined the deformation behavior of nanocrystalline materials, they revealed that dislocations predominate in the deformation of larger grain size materials, while grain boundaries are effective in smaller grain size materials. A study on the plastic deformation of nanocrystalline Mo showed that a large component of the strain is settling through the formation of cracks at the grain boundaries [37]. However, studies on mechanical properties have mainly focused on single-crystal metallic nanowires with fcc structure. Compared to single crystal nanowires, polycrystalline nanowires are composed of multiple grains. The deformation behavior and breakage of nanowires are highly dependent on grain size [38]. The compatibility of the results obtained in the MD simulation method with the experimental data depends on the potential energy function selected for the system to be modeled [39]. There are many potential energy functions developed for different element and alloy systems [40, 41]. EAM, which includes multi-body interactions, is one of the most preferred functions in MD studies in terms of its simple mathematical structure and effective results.

In this study, it was tried to determine the effects of uniaxial tension deformation applied to polycrystalline Nb nanowires with single and different grain numbers on the mechanical properties of the nanowire. LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) MD simulation program was used for calculations [42]. It was determined that the tension strain applied to the Nb nanowire caused significant changes on the mechanical and structural properties of the wire, such as the stress-strain curve, the young modulus, the yield strain, and the atomic positions, depending on the number of grains.

2. Material and Method

In the classical MD simulation method, the equations of motion of a system composed of N atoms are derived from the Lagrangian function.

$$L_{PR}\left(\mathbf{r}^N, \dot{\mathbf{r}}^N, \mathbf{h}, \dot{\mathbf{h}}\right) = \frac{1}{2}\sum_{i=1}^{N} m_i(\dot{\mathbf{s}}_i^t \mathbf{G} \dot{\mathbf{s}}_i) - \sum_{i=1}^{N}\sum_{j>i}^{N} \phi\left(\left|\mathbf{h}\mathbf{s}_{ij}\right|\right) + \frac{1}{2} M \mathrm{Tr}\left(\dot{\mathbf{h}}^t \dot{\mathbf{h}}\right) - P_{ext} V \quad (1)$$

obtained. Here, the $\boldsymbol{s}_i$, **h, G** and P_{ext} parameters represent the scaled coordinate, the axes of the calculation cell, the metric tensor and the external pressure, respectively. For a system subjected to deformation, the strain is calculated by the microscopic stress tensor as given in equation (2) [43, 44].

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

An object under the influence of external forces is said to be in a strained state. The stress tensor is determined by the nine components of the state of the force at any point in the matter.

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

The normal components of the stress tensor σ_{11}, σ_{22}, σ_{33} (also referred to as σ_x, σ_y, σ_y, respectively) are known as the shear components of the stress. The positive and negative values of the normal components of the stress tensor correspond to the tensile stress and compression stress, respectively. Only the σ_x component changes with uniaxial loading applied along the x-axis. On the other hand, the other components are zero [45]. The expression $\varepsilon_x = (l_x - l_{x0}) / l_{x0}$ determines the strain along the x-axis. l_{x0} and l_x are the length of the wire before and under load in the x direction, respectively [46].

The Nb model nanowire system, to be applied uniaxial tensile deformation, was created in 5 different ways: single crystal and multi-grain structure. During the study, the single crystal structure was expressed as Nb1, while the 2, 3, 4 and 5 grain nanowire structures were named Nb2, Nb3, Nb4 and Nb5, respectively. Nb1, Nb2, Nb3, Nb4 and Nb5 nanowires consist of 4672, 4492, 4433, 4417 and 4463 atoms, respectively. Each grain in the model nanowire is defined as gr (grain). In the Nb1 nanowire with a single crystal structure, atoms are arranged in the x, y and z directions with <100>, <010> and <001> crystallographic orientations, while for Nb2 < $6\bar{1}0$>, <$16\bar{4}$>, <169> for Nb3, they are placed in orientations <410>, <$\bar{1}40$>, <001> and <$1\bar{1}1$>, <$1\bar{1}\bar{2}$>, <110> for Nb4, and <$1\bar{1}0$>, <$11\bar{2}$> and <111> for Nb5. While the length of the nanowire in the x direction is 12 nm, its length in the y and z directions varies between 2.59 nm and 2.71 nm due to the different orientations of the atoms.

In MD studies, it is very important to detect microstructures such as fcc, hcp, bcc, which are formed as a result of thermal or mechanical processes applied to the model system, and to determine their development. Many numerical analysing methods have been developed to determine these structures. Assigning a structural type to each particle is the main goal of these methods. In addition, these methods try to determine how close they are by matching a local structure with an idealized structure. For structure analysis in MD simulation studies, centrosymmetry parameter analysis, common neighbor analysis, bond-order analysis, bond-angle analysis, Honeycutt -Andersen, Voronoi analysis is used quite frequently [47, 48].

In this study, atoms were placed at bcc lattice points for the Nb nanowire system as the initial structure. While periodic boundary conditions were applied along the [100] direction of the nanowire, boundary conditions were not applied along the [010] and [001] directions. The initial velocities of the atoms in the model system were randomly determined in accordance with the Maxwell-Boltzman velocity distribution. By using the velocity form of the Verlet algorithm, the numerical integration of the system's equations of motion was performed in 1 fs time steps. Uniaxial drawing processes were applied to the NVT statistical ensemble, where the particle count, volume, and temperature were kept constant at certain values. Before applying tensile loading, $5x10^4$ MD steps were waited for all nanowires to reach stable structure. The strain rate was chosen as $1x10^9$ s^{-1} in the study. In addition, the EAM potential function was used to calculate the interactions between Nb atoms in the model calculation cell. Details on potential can be found in the literature [49]. The cut-off distance of the potential function used was determined as $r_c = 2a_{Nb}$.

3. Results and Discussion

In this study, the effect of uniaxial tensile deformation applied along the [100] direction at 10 K temperature and $1x10^9$ s^{-1} strain rate on the mechanical properties of Nb nanowire system with different grain structures was tried to be investigated using the MD method. Figure 1 shows the stress-strain curve obtained until rupture occurs in a single-grained Nb1 nanowire, which is called gr1 and has the arrangement of atoms along the crystallographic orientations of <100>, <010>, <001>. This graph shows two peaks and a region where the hard value changes within certain limits with the increase in the stress in the middle. The hard-strain curve exhibits an almost linear change until ε (tensile stress), which begins to be applied to the model system, reaches a value of 0.09. This region in the graph is referred to as the elastic region. The highest value reached by the stress before the sudden drop in stress starts is known as the yield strainand has a value of 9.8 GPa. In addition, in Figure 1, the young modulus of the model nanowire system was determined as a result of the regression analysis of the linear region where elastic deformation occurs. High values of the young modulus, which is known as a measure of elastic deformation under the applied force, indicate that the elastic property of that material decreases. The young modulus for the Nb1 nanowire was determined as 104.3 GPa. After a critical strain value is reached, a sudden decrease in strain occurs (point b). This sudden decrease in the graph is an indication of the onset of plastic deformation in the model system. When a stress above the strain corresponding to the yield strain value is applied to the material, plastic deformation begins and the sliding mechanism is activated. This is a wide strain range from point b to point e and there is no significant change in difficulty. At point e, the hard-strain curve starts to change as it did at the beginning of the strain process (e-f interval). As the strain continues, when the strain reaches 0.72 after the second maximum, the strain suddenly drops to zero (g point). This corresponds to the breaking of the nanowire. The deformation phases seen in the stress-strain graph have also been observed in studies for other metallic nanowires [50, 51].

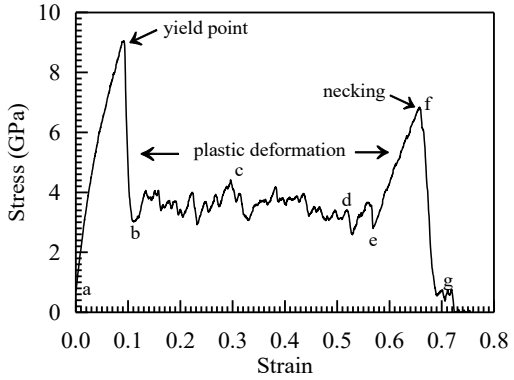

Figure 1. Stress-strain curve of Nb1 nanowire.

In this study, the CNA topological analysis method proposed by Honeycutt and Andersen was used to determine the regional structures with unit cells such as bcc, fcc, hcp that may occur around the atoms in the model system during the drawing process. CNA analysis is a characterization technique used to determine the structural evolution of crystal structures such as agglomeration defects, grain boundaries, deformation and different phases. The CNA algorithm performs a geometric analysis of the nearest neighbors around a reference atom. The minimum value of the radial distribution function between the first two peaks and the arrangement of the selected atoms within a certain distance are analyzed one by one [52]. In this analysis, each atom in the model system is classified according to regional crystal structures determined by the bonds between an atom and its nearest neighbors. Here, atoms are divided into 4 classes called bcc, fcc, hcp and “other”. Atoms in a regional bcc arrangement are considered bcc atoms, and atoms in a regional fcc arrangement are considered fcc atoms. Atoms in a regional hcp arrangement are considered as hcp atoms, which are seen as stacking defect structures formed in the fcc crystal. Atoms in all other local arrangements are called "other" atoms. Generally, blue bcc, green fcc, red hcp and white color represent atoms called “other” [53].

In Figure 2 (a-g), atomic positions taken from the (001) plane section obtained by CNA analysis from the OVITO [54] program at different MD steps for the Nb1 nanowire during the drawing process are given. In Figure 2(a), it was determined that 68% of the structure was bcc and 32% was other structures before applying tensile stress to the nanowire. Since periodic boundary conditions are not applied in the y and z directions of the nanowire, atoms on and near the surface of the wire are not considered as bcc unit cell structure. It is seen in Figure 2(b) that after the strain applied to the nanowire passes the yield point, where plastic deformation begins, regions of atomic rearrangement are formed at the top and bottom ends of the nanowire. These regions, where atoms with different orientations are located, are separated from each other by white colored atoms. Figure 2(c-d) shows the evolution of these differentially oriented regions within the structure with increasing strain. It is seen in Figure 2(e-f) that when the e and f points are reached in the stress-strain curve, the reorientations are completed and the nanowire begins to give neck in the region determined by the dotted circle. In Figure 2(g), the atomic structure of the nanowire when it is broken by thinning and stretching is given.

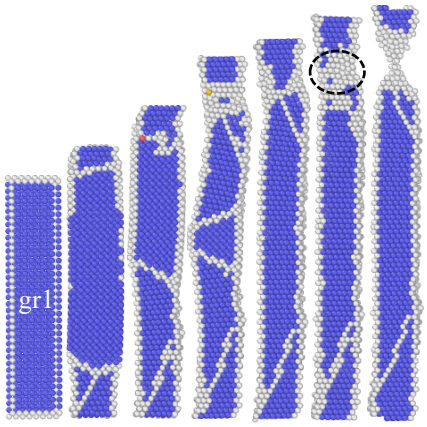

Figure 2. Atomic positions determined for different strain values from CNA analysis for Nb1 nanowire.

In Figure 3, the stress-strain curve obtained until rupture occurs in the Nb2 nanowire, which consists of two grained structures called gr1 and gr2, is given. It is seen that the yield strength is 6.02 GPa and the hard-strain curve exhibits an almost linear change until ε=0.08 is reached. The elastic constant for Nb2 nanowire was determined as 99.07 GPa. The change in the stress-strain curve with increasing strain is almost similar to the Nb1 nanowire structure. It was determined that the rupture occurred at a value of 0.58 of the strain.

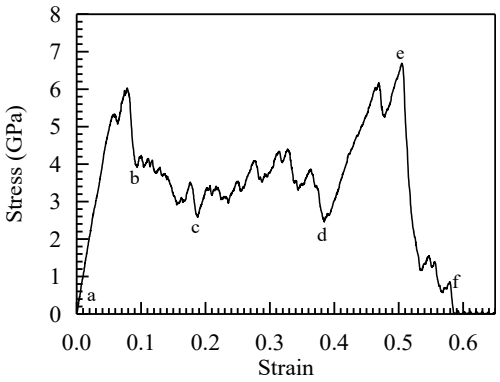

Figure 3. Stress-strain curve of Nb2 nanowire.

In Figure 4, atomic images of the nanowire obtained from CNA analysis are given for the different points (a-f) determined in the stress-strain curve. Figure 4(a) shows the initial structure composed of bcc unit cells of the Nb2 before nanowire is strain applied. Grains of gr1 and gr2, which have different atomic orientations, are separated from each other by the grain boundary indicated by white colored atoms. When the point b on the hard-strain curve, where plastic deformation occurs by increasing the strain applied on the nanowire, is reached, a region begins to form as indicated by the arrow with different crystallographic orientation by rearranging the atoms at the grain boundary, as seen in Figure 4(b), and as the strain continues to increase, this change occurs. The development of the region within the structure (Figure 4(c)) is seen. It is determined from Figure 4(d) that this reorientation and diffusion within the structure ends when the d point is reached in the strain curve. It can be seen from Figure 4(e-f) that the applied strain from this moment on creates a neck in the region marked with a dotted circle in the grain boundary region instead of creating plastic deformation in the structure, and the deformation of the nanowire ends with rupture.

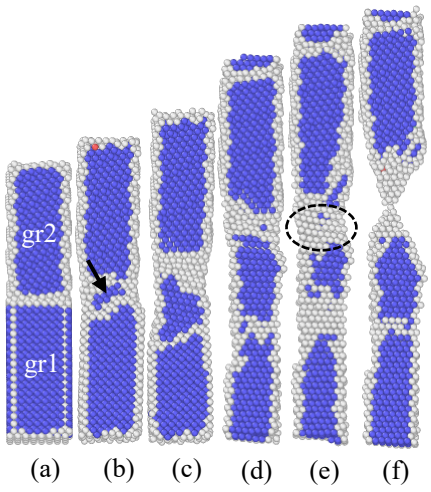

Figure 4. Atomic positions determined for different strain values from CNA analysis for Nb2 nanowire.

In Figure 5, the stress-strain curve obtained as a result of uniaxial tensile deformation applied to the Nb3 nanowire, which consists of three grained structures called gr1, gr2 and gr3, is given. The change in the stress-strain curve with increasing strain is almost similar to that of other granular nanowire structures. From the stress-

strain curve, yield strain was determined as 5.42 GPa, ε=0,068 and elastic constant 87.2 GPa for Nb3 nanowire. It was observed that when ε=0,56 reached the value, rupture occurred.

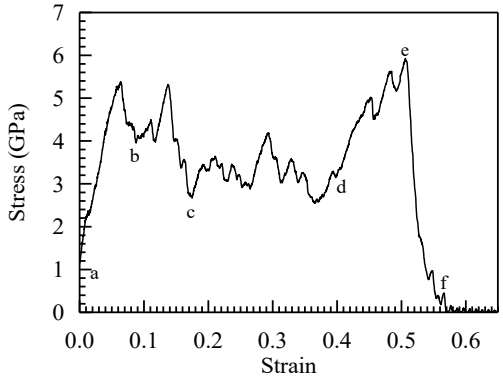

Figure 5. Stress-strain curve of Nb3 nanowire.

Figure 6 shows the atomic positions of different points on the stress-strain curve given in Figure 5 for the Nb3 nanowire. The initial structure of the Nb3 nanowire, which consists of layers with three different atomic orientations, is given in Figure 6(a). It is clearly seen in Figure 6(b-c) that when the yield point is passed and plastic deformation begins, a region in which the atoms take different orientations is formed at the grain boundary of the gr1 and gr2 grains and as a result of the increase in the strain, the atoms in this region move in the shear planes and spread into the gr1 grain structure in a way to form a twin structure. However, no change was observed in the atomic configurations of the gr2 and gr3 grains forming the nanowire, with increasing strain. With increasing strain value, the twin boundary moved until it reached the lower end of the nanowire (Figure 6(d)) and then the rearrangement of the atoms was completed. It is clearly seen from Figure 6(e-f) that the nano wire starts to give neck at the gr1 and gr2 grain boundary and that rupture occurs in this region as the strain continues to increase.

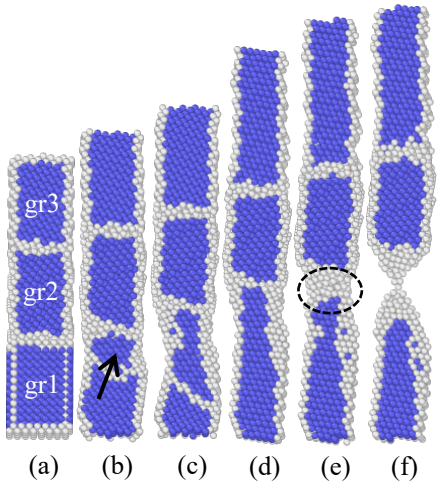

Figure 6. Atomic positions determined for different strain values from CNA analysis for Nb3 nanowire.

In Figure 7, a stress-strain curve is given for Nb4 nanowire, which contains four grained structures called gr1, gr2, gr3 and gr4. The stress-strain curve exhibits a linear change, as in other nanowire structures, until ε=0,069, where the yield strain is 5.98 GPa. The elastic constant of the Nb4 nanowire was determined as 84.7 GPa from the regression analysis. It has been determined that the nanowire rupture occurs when it reaches the value of ε=0,45.

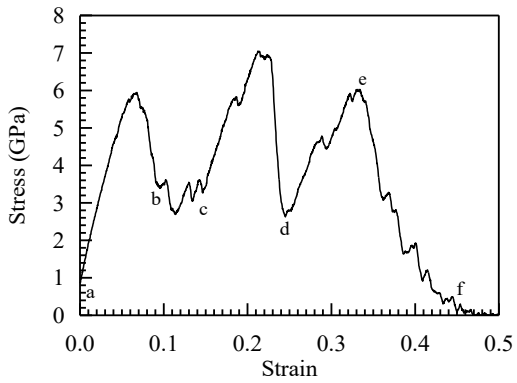

Figure 7. Stress-strain curve of Nb4 nanowire.

Figure 8 shows the atomic positions obtained at different stress values for the Nb4 nanowire. The initial structure of the Nb4 nanowire formed with 4 different crystallographic orientations of atoms is given in Figure 8(a). It is clearly seen in Figure 8(b) that a twinning occurs within the gr1 grain and the atoms take a different orientation when the yield point is passed and the plastic deformation begins. This atomic arrangement formed in the gr1 grain is completed when the strain value reaches the c point in the stress-strain curve (Figure 8c). However, the atomic orientations of the gr2, gr3 and gr4 grains that make up the nanowire did not show any change with the increase in strain. It is clearly seen from Figure 8(e-f) that the neck region begins to form at the gr2 and gr3 grain boundaries at progressive strain values, and then the atoms in this region become thinner and elongate like a chain and rupture occurs, respectively.

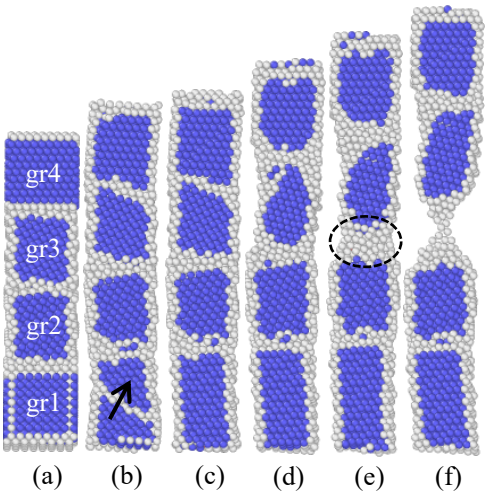

Figure 8. Atomic positions determined for different strain values from CNA analysis for Nb4 nanowire.

The stress-strain curve for five grained Nb5 nanowires called gr1, gr2, gr3, gr4 and gr5 is given in Figure 9. It is clearly seen that the stress-strain graph exhibits an almost linear change until ε=0,085, where the yield strain is 6.2 GPa. The elastic constant of the Nb5 nanowire was found to be 82.4 GPa by using this linear region. It was determined that the nanowire rupture occurred as the strain increased and reached the value of ε=0,3.

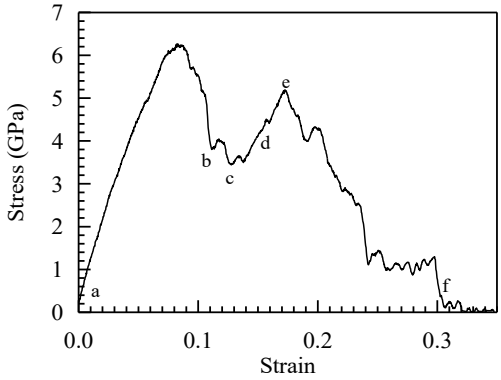

Figure 9. Stress-strain curve of Nb5 nanowire.

In Figure 10, atomic images corresponding to different values of strain are given for the Nb5 nanowire. While the initial structure of the Nb5 nanowire is given in Figure 10(a), it is clearly seen in Figure 10(b) that the atoms in the gr3 grain enter an irregular structural arrangement that does not have a specific unit cell, once the yield point is passed and the plastic deformation begins. It has been determined from Figure 10(c-d) that the irregular structure has been replaced by relatively regular bcc unit cell structures with the increase of the strain and reaching the c and d points in the stress-strain graph, respectively. However, it is seen that the atomic arrangement of the gr1, gr2, gr4 and gr5 grains that make up the nanowire do not show any change with increasing strain. It is clearly seen from Figure 10(e-f) that the neck region starts to form at the gr2 and gr3 grain boundaries and the rupture also occurs at this grain boundary with the increase of the strain.

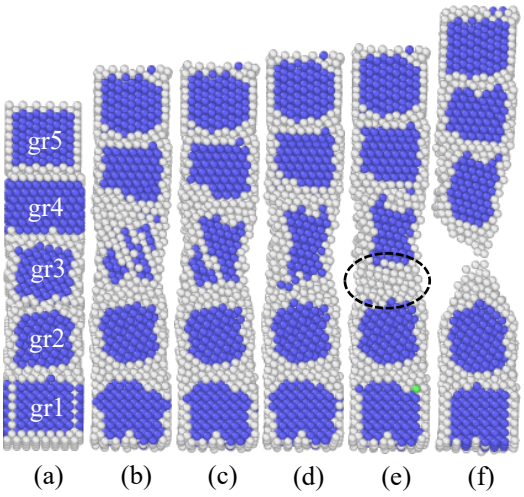

Figure 10. Atomic positions determined for different strain values from CNA analysis for Nb5 nanowire.

In the study, it is seen that single crystal and polycrystalline Nb nanowires exhibit distinctly different tensile deformation behaviors. Microstructure control plays a critical role in nanoscale wires to provide the desired mechanical properties. Grain boundaries are the most basic defects in polycrystalline materials. Material properties are greatly affected by the presence of such defects. Grain boundaries play an important role in plastic deformation since grain sizes are reduced to nanometers [55, 56]. In all model nanowires, necking started at the grain boundary and then fracture occurred with decreasing tensile ductility. High stresses in the grain boundary region clearly play a dominant role in controlling both plastic deformation and fracture processes in nanoscale materials [57]. In the study, yield strain, strain values (ε) and breaking strain values of Nb polycrystalline nanowires are lower than single crystal nanowires. However, yield strain and ε value increase for Nb4 and Nb5 nanowires.

Deformation and rupture behaviors of polycrystalline nanowires show dependence on grain size and length-diameter ratio (LDR). It shows that the polycrystalline nanowires exhibit a ductile characteristic under tensile loading and elongation before breaking. When the tensile stress reaches a certain value, the change of atomic configuration in the grains can be seen. At the elastic limit, the young modulus increases with grain size. It was found that LDR had little effect on the elastic properties, but had a significant effect on the fractures of

polycrystalline nanowires due to the surface effect. [38]. In conventional polycrystalline metals, the volumetric stresses due to interfacial tensions are negligible. However, grain boundary interfacial tensions are important for metallic nanowires with nanometer grains [38]. Because they induce bulk stresses in the order of t/d, where t is wire thickness and d is grain size. Studies have shown that as the t/d ratio increases from 1 to 4, the tensile strength of Ni, Cu and Al films [58] increases, while it decreases in Ag microwires [59]. Obviously, there is controversy regarding the size effect of nanoscale polycrystalline films/nanowires and therefore it is essential to examine this effect and deduce the underlying mechanism. It is thought that the size effect caused by the t/d ratio of 4 and above in Nb4 and Nb5 nanowires is the reason for the increase in yield strain and ε.

The stresses near the grain boundary are quite different from the stresses occurring within the grain. The highest internal stresses and high energy atoms are located at the grain boundary interface due to its heterogeneous structure. The flow mechanism is via nucleation and propagation of partial dislocations at grain boundary interfaces rather than at free surfaces. This causes the yield strain to be much lower than that of single crystal nanowires. In addition, despite the large surface-to-volume ratio, a significantly lower yield strain may also occur as a result of dislocations propagating from the free surfaces [38]. Researchers have determined from experimental and simulation studies that the cause of plastic deformation in many fcc and bcc metallic nanowires is due to partial/full dislocation shifts. However, metallic nanowires with both fcc and bcc structures with suitable orientations can also be plastically deformed by the twinning mechanism [60]. During the tensile deformation process applied to our model nanowire systems, it was determined that the plastic deformation did not occur as a result of any dislocation as a result of the dislocation defect analysis DXA (Dislocation Extraction Algorithm). However, it can be said that plastic deformation in model nanowires occurs due to nucleation, propagation and atomic rearrangements of twinning.

4. Conclusion

The effects of uniaxial tensile deformation applied to single-crystal and polycrystalline nanowires with different grain numbers, where the interactions between Nb atoms are determined by EAM, on the properties of nanowires such as yield strain, young modulus, yield strain were investigated using MD simulation method. It was determined that the number of grains significantly affects the plastic deformation of the nanowire. All nanowires used in the study are plastically deformed by twinning and their propagation. It was determined that grain boundary interfacial tensions are important for metallic nanowires with nanometer grains and necking and breaking of the nanowire occur at these grain boundaries. The size effect resulting from the increase in the number of grains shows its effect on the yield strain and strain of the nanowire. However, it can be said that the atomic orientations that make up the grains may have important structural effects on the nanowire.

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