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MOLECULAR DYNAMICS STUDIES ON DISLOCATIONS IN CRYSTALLITES OF NANOCRYSTALLINE α-IRON

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Abstract *— Molecular dynamics simulations have been carried out to study the atomic structure of the crystalline component of nanocrystalline α-iron. A two-dimensional computational block is used to simulate the consolidation process. It is found that dislocations are generated in the crystallites during consolidation when the grain size is large enough. The critical value of the grain size for dislocation generation appears to be about 9 nm. This result agrees with experiment qualitatively. All dislocations that are preset in the original grains glide out during consolidation. It shows that dislocations in the crystallites are generated in consolidation process, but not in the original grains. Higher consolidation pressure results in more dislocations. Furthermore, new interfaces are found within crystallites. These interfaces might result from the special environment of nanomaterial. ©1998 Acta Metallurgica Inc.*

1. INTRODUCTION

It is well known that nanocrystalline materials have superior performance including mechanical properties, which can undoubtedly have a broad prospect for applications in science and technology (1). For this reason, more and more studies have been conducted regarding the structure and the deformation mechanism of these materials(2-5). Many experiments have been done to study the effect of grain size, morphology and distribution on the properties of nanomaterials. Two most critical questions need to be answered: does the grain boundary component have an ordered structure, and do any dislocations and other defects exist in the crystalline component?

Zhu *et al.* concluded that the structure of the interfacial component should be gas-like because the measured X-ray interference function could be matched with the calculated one when a disordered structure of grain boundary (GB) had been assumed (4). However, Trudeau *et al.* argued that whether the interface structure was gas-like or liquid-like depended upon the free volume per atom in the GB (5). We have studied previously the structure of nanocrystalline α-iron using molecular dynamics (MD) method. The simulation showed that the atomic structure of the grain boundary component had a short range order similar to that of amorphous materials (6-7).

Trudeau *et al.* found a large number of dislocations in the crystalline component of nanocrystalline alloy NiMo (via mechanical milling) when the grain size was larger than 10 nm, but no dislocation when the grain size was smaller than 10 nm (5). Dislocations and other defects could also be found in nanocrystalline Al and Pt when the grain size was larger than 10 nm (8). These results indicated that dislocations and other defects could exist in the crystalline component of nanocrystalline materials, depending upon the grain size. The purpose of this work is to analyze this phenomenon using MD method. A two-dimensional model is adopted and various grain sizes are considered.

2. MODEL AND PROCEDURE OF SIMULATION

We are interested in whether dislocations can exist in the crystalline component in nanocrystalline material when its grain size is large enough. Generally speaking, dislocations might either be generated during consolidation process of a nanocrystalline material or they can simply exist in the original grains. For the understanding of this phenomenon, one way is to simulate the consolidation process with dislocations preset in some of the original grains.

For simplicity, the basic computational block consists of four cylindrical grains with equal cross-section. The block is extended using three-dimensional periodic boundary conditions (Figure 1). All the axes of the grains are parallel to the Z-axis. The stacking of the grains is in ABA... sequence. Several edge dislocations are preset in two of these grains. The dislocation lines are parallel to the grain axes and along $[1\bar{1}2]$; therefore, the easy gliding surfaces (110) in different grains are always parallel to Z-axis. Such a configuration ensures that dislocations can glide easily.

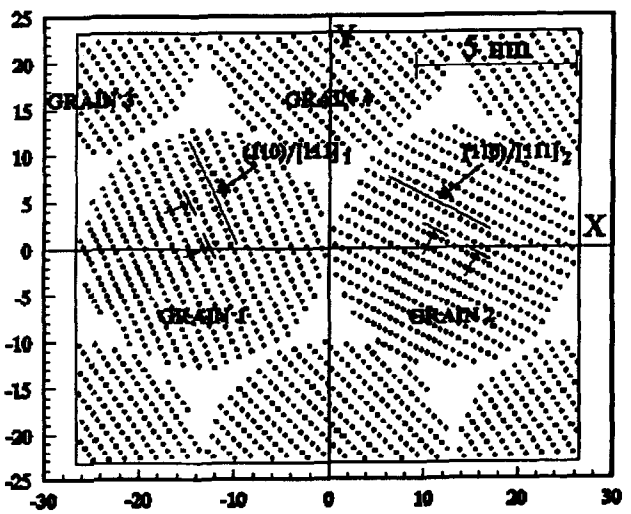


Figure 1. Initial atomic configuration in consolidation of nanocrystalline α-iron (two-dimensional model) (7.62 nm, 10562 atoms, 4 preset dislocations).

In order to give the model a diversified feature, the lattice orientations of different grains are randomly given. Therefore, the dislocation gliding directions $[\bar{1}11]$ of the four grains are not in coincidence with each other. The variation of cross-section area of the crystallites provides model of nanocrystalline materials with different grain sizes so that we are able to study how the dislocation gliding behavior depends upon grain size.

The simulation is carried out by means of MD method. The dynamic equations of N atoms with mass m are solved with the central difference scheme (9). The force exerted on each atom is calculated through Johnson's pair-wise potential (10). The initial velocities of the atoms are given with Maxwellian distribution corresponding to a given temperature. The unit of length takes the value of lattice constant $a_0 = 2.86668 \times 10^{-10}$ m, the unit of energy is leV = 1.60207×10^{-19} Joule and the unit of mass is the atomic mass of Fe, and then the time unit can be obtained in 2.18×10^{-13} seconds.

The simulation of the consolidation process is divided into several stages. First, an initial equilibrium state is obtained through atomic relaxation of the computational block. Second, the compression is done by contracting the block in X,Y and Z directions until the pressure reaches an assigned value, *e.g.*, 6 GPa. Third, the load is removed to normal pressure. Then, an equilibrium state is obtained. In order to make the simulations close to experimental conditions, a quasi-static loading procedure is used. The loading process is divided into many steps. In each step, a small contraction (*e.g.* 0.02-0.1%) is set and then atomic relaxation is performed to obtain a relative equilibrium state. In a typical run, the loading process takes about fifteen steps. The time for obtaining an equilibrium state in each step takes about 40-80 time units. The pressures exerted in X, Y and Z directions are controlled uniformly increasing from zero to the highest pressure and the temperature is kept at 300 K. Similar procedure is also used in the unloading process. The atomic configurations at the end of each step are recorded and the dislocation gliding behavior is observed.

3. RESULTS AND DISCUSSION

3.1 Small Grain Size: (Dislocation Absorption)

The simulation is carried out using a small initial computational block that contains 10562 atoms and has a size of $15.24 \times 13.33 \times 0.70$ nm^3. The diameter of the crystallites is 7.62 nm. Four edge dislocations are preset in grain 1 and grain 2 (Figure 1). Through primary atomic relaxation, the initial equilibrium state is obtained and the density becomes 7.16g/cm^3 at the time t=20. All the four dislocations disappear at this stage. Figure 2a-c shows the dislocation gliding process from bulk to the GB. Then, the quasi-static procedure on consolidation is carried out. The compression and expansion processes are divided into 10 and 17 steps, respectively. After consolidation, the density becomes 7.30g/cm^3, *i.e.* 92.79% of single crystal density. The consolidation pressure, which is the highest pressure during compression, is 6 GPa. Figure 3 gives the relation between pressure and density. It shows that the consolidation process is irreversible. The atomic configurations during the whole consolidation process indicate that the four crystallites remain dislocation free. Figure 2d gives only the final atomic configuration at t=3000. It is seen that dislocations cannot exist in the crystalline component when the grain size is 7.62 nm.

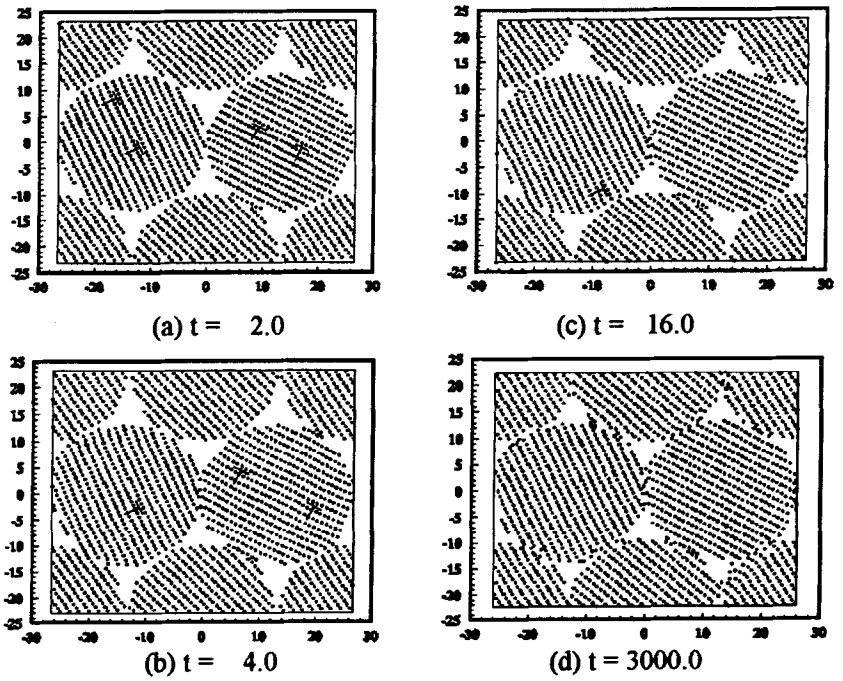


Figure 2. Atomic configurations at different times (7.62nm, 10562 atoms, 4 preset dislocations).

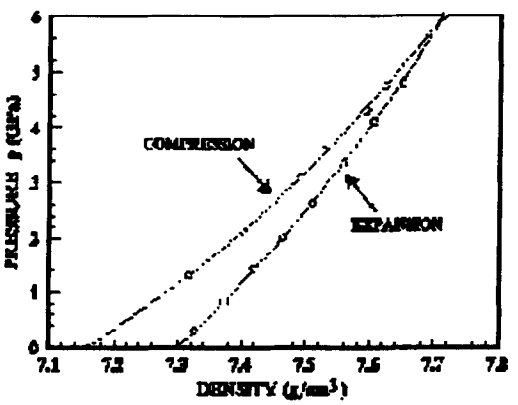


Figure 3. Pressure-Density relation during consolidation (7.62nm, 10562 atoms, 4 preset dislocations).

3.2 Large Grain Size: (Dislocation Generation)

In order to see if dislocations will exist in the crystalline component of nanocrystalline materials with grain sizes larger than 10 nm, a quite large initial computational block is considered

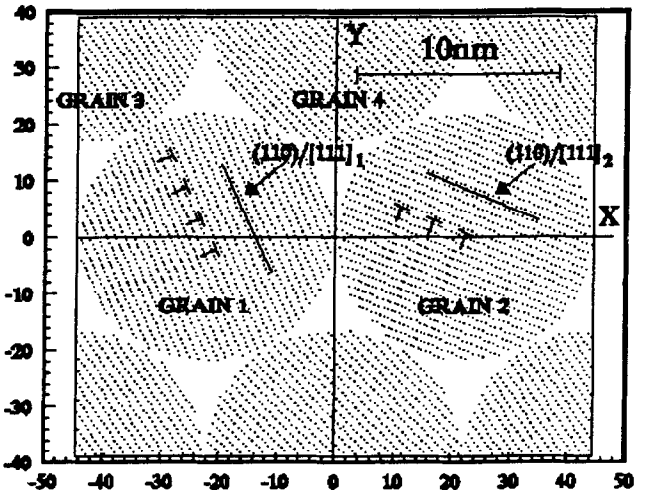


Figure 4. Initial atomic configuration in consolidation of nanocrystalline α-iron (12.78 nm, 30360 atoms, 7 preset dislocations).

in the following simulations. It contains 30360 atoms and has a size of 25.56 x 22.27 x 0.70 nm^3. The diameter of the crystallites is 12.78 nm. The initial density is 7.17 g/cm^3. To observe the effect of consolidation pressure p and the effect of preset dislocations, three different cases have been examined.

3.2.1 p=6.0 GPa, 7 preset dislocations

In the first case, seven edge dislocations are preset in grain 1 and grain 2 (Figure 4). The consolidation pressure is 6 GPa. After consolidation, the density is 7.25g/cm^3, *i.e.* 92.12% of single crystal density. Curve (1) and (2) in Figure 5 give the relation between pressure and density during consolidation process. From the atomic relaxed structure at final state (Figure 6), it is seen that two dislocations are in green 1 and grain 3. It shows that dislocation can exist in the crystalline component of nanocrystalline material when the grain size is 12.78 nm.

It is interesting that the dislocations in grain 1 and grain 3 at final state are not the ones that have been preset in the original grains but those that generated during consolidation. For example, Figure 7 shows the dislocation generation and gliding processes in grain 1. The dislocation 1 and 4 that are preset in grain 1 glide out of the grain at the very beginning of consolidation and, therefore, they cannot be displayed in this Figure. Dislocation 3 also glides out of the grain rapidly (before t=50) as shown by curve (2). (In Figure 7, the unit of time is 21.8 x 10^{-12} s that has been hundred-times magnified to the time unit 0.218 x 10^{-12} s in calculations.) Curve (1) shows that dislocation 2 remains in the central part of the grain until compression process is finished. However, when relaxation starts from 6 GPa, dislocation 2 glides immediately to the right GB (t=1070). At the same time, a new dislocation generates from the left GB and glides to the central part of grain 1, where it survives stably. This result indicates that dislocation can generate during consolidation in the case of large grain size but not exist in the original grains.

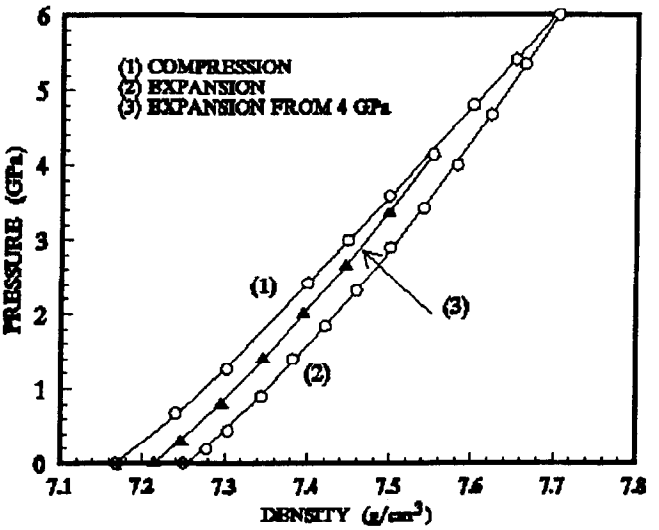


Figure 5. Pressure-density relation during consolidation (12.78nm, 30360 atoms, 7 preset dislocations).

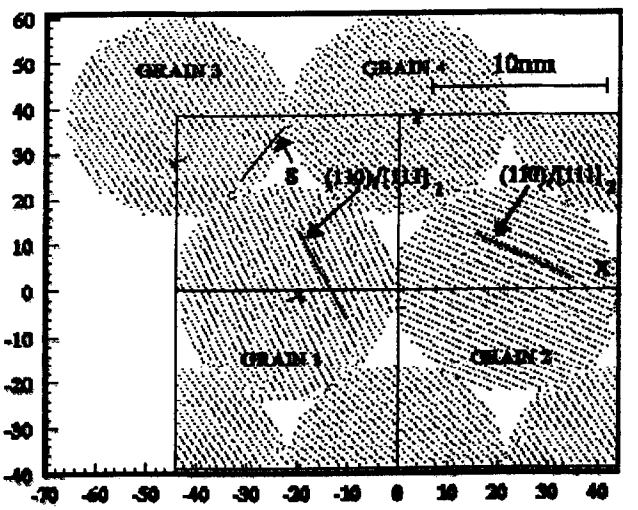


Figure 6. Relaxed atomic structure after consolidation of nanocrystalline α-iron (12.78 nm, 30360 atoms, 7 preset dislocations). [Atoms outside left and upper borders are those extended with periodic boundary condition. Similarly done in Figures 8-10.]

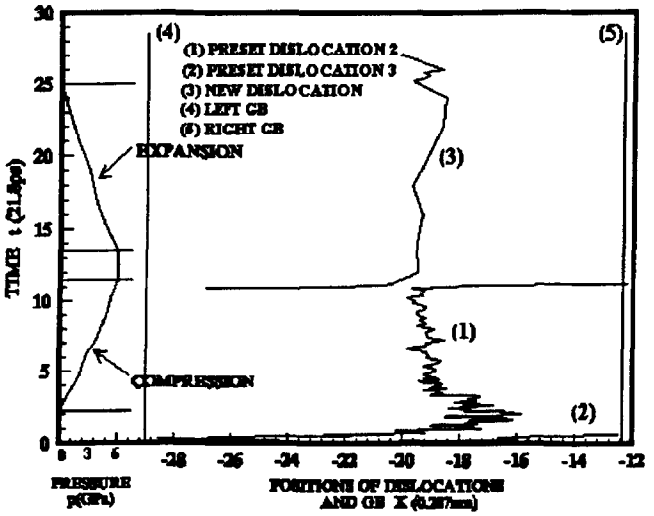


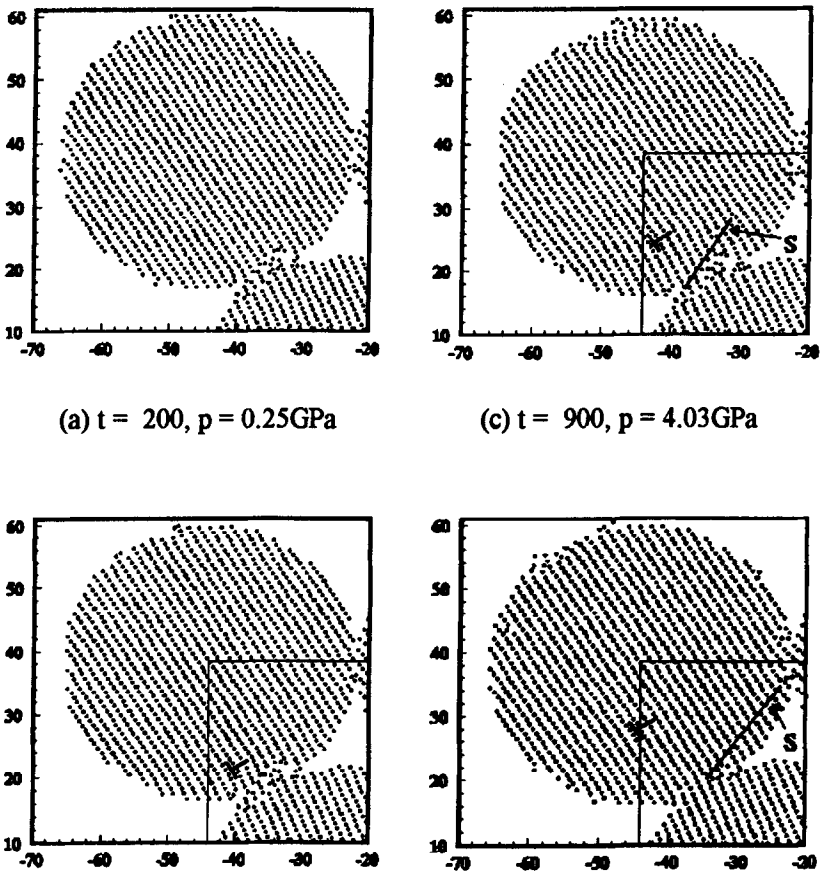
Figure 7. Time evolution of preset and new dislocation centers in grain 1 (12.78 nm, 30360 atoms, 7 preset dislocations).

Another phenomenon is the unsymmetrical behavior of dislocation generation in the four grains. Originally, four and three dislocations have been preset in grain 1 and grain 2, respectively, and at final state only one remains in grain 1 and none in grain 2. While no dislocation has been preset in grain 3 and grain 4, one generates in grain 3 and none in grain 4. Although the four grains have completely the same geometrical conditions, the shape and size as well as the stacking of the grains, they are under different microscopic environment, which results from the random lattice orientations of the grains. It is expected that the result will change to a different manner if another random distribution of the lattice orientations is given.

3.2.2 p=4GPa, 7 preset dislocations

In order to examine the effect of consolidation pressure on the dislocation generation, we choose a lower consolidation pressure this time. In fact, we simply use the last result except that the expansion starts from 4 GPa. In Figure 5, curve (3) shows the pressure-density relation. After consolidation, the density becomes 7.21 g/cm^3, which is lower than that in the former case by 0.6%. In this case, all the seven preset dislocations in grains 1 and 2 glide out of the grains, but a new dislocation generates in grain 3. The result is similar to that of the first case but grain 1 is dislocation free. Therefore, higher consolidation pressure results in more dislocations in the crystalline component.

Figure 8 shows different stages of dislocation generation process in grain 3 corresponding to different pressures. From Figure 8b, it is seen that grain 3 is intruded by grain 1 at their boundary and an edge dislocation starts to formulate near the boundary at t=540 when the pressure is 2.25 GPa. When the pressure increases to 4.03 GPa, the dislocation approaches to the bulk of the grain. Finally, this dislocation is situated in the bulk stably (Figure 8d). From this process, it can be seen that dislocation is generated due to compression when the grain size is large enough.



(a) t = 200, p = 0.25GPa (c) t = 900, p = 4.03GPa

(b) t = 540, p = 2.25GPa (d) t = 3000, p = 0.0GPa

Figure 8. Process of dislocation generation in grain 3 with pressure increasing during consolidation of nanocrystalline α-iron. (12.78 nm, 30360 atoms, without preset dislocation in grain 3).

3.2.3 p=3GPa, without preset dislocations

In the above cases, it appears that dislocation can exist in some grains even though no dislocation is preset. In order to observe the effect of preset dislocations directly, an initial atomic configuration without preset dislocations is considered. In this case, the result shows that a dislocation generates in grain 1 as shown in Figure 9, while the consolidation pressure is only 3.6 GPa. It confirms that the generation of dislocation does not depend upon preset dislocations.

3.3 Moderate Grain Size: (Dislocation Generation)

In this simulation, we consider a moderate computational block that contains 17923 atoms and has a size of 19.83 x 17.30 x 0.70 nm^3. The diameter of crystallites is 9.4 nm. Four edge

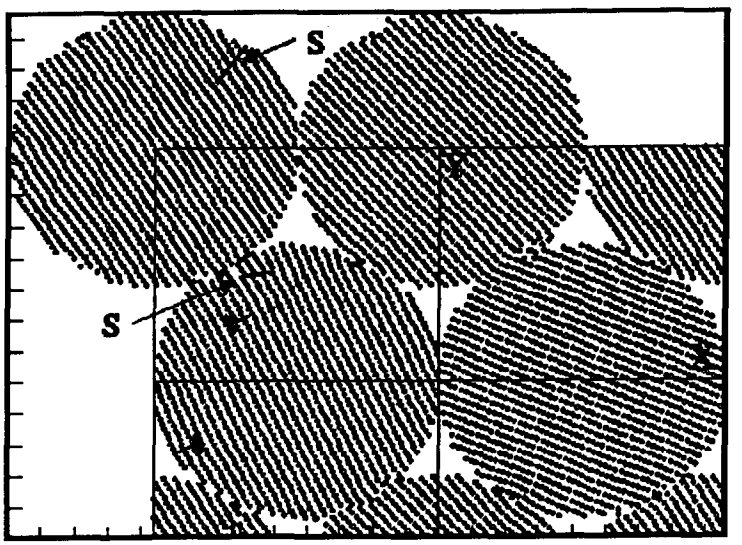


Figure 9. Relaxed atomic structure after consolidation of nanocrystalline α-iron (12.78 nm, 29756 atoms, 3.6 GPa, without preset dislocations).

dislocations are preset in grain 1 and 2. The initial density is 7.05 g/cm^3. The compression (up to 6 GPa) and the expansion processes are divided into 11 and 25 steps, respectively. After consolidation, the density becomes 7.33g/cm^3, *i.e.*, 93.18% of the single crystal density. Figure 10 gives the final atomic configuration. Although a dislocation exists in grain 3 (near "A"), the center is not very clear. It seems that the condition is somewhat critical for dislocation generation when the grain size is 9.4 nm. Therefore, whether dislocation will exist within the crystalline component or not depends mainly upon grain size of nanomaterial. It appears that the critical grain size for dislocation generation is about 9 nm. It agrees with the experimental results by Trudeau and Li qualitatively.

3.4 Other Defect: (New Interfaces Appear)

Sometimes, new interfaces appear in grain 1 and grain 3 (as marked by S in Figure 6, Figure 8c-d, Figure 9 and Figure 10). They are not in the easiest sliding surfaces (111). These new interfaces represent some kinds of solid defects and result from compression and stress relaxation. This phenomenon is found in the cases of large and moderate grain sizes.

In an extreme case, the crystallite is separated by the interface (grain 1 in Figure 10) into two single crystal structured parts. In fact, the interface is formulated by a shift of both parts. This kind of interface is generally unstable in crystals, but it might exist in nanocrystalline materials. However, this phenomenon has not been seen in real experiment; therefore, it should be examined in further studies.

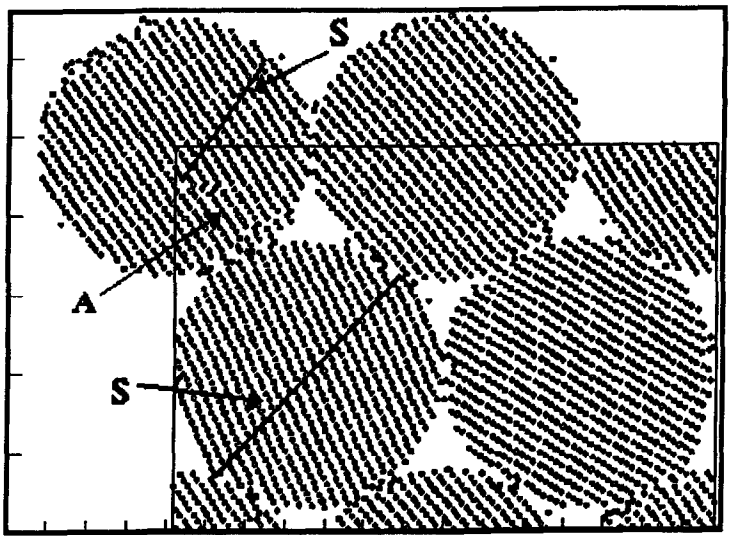


Figure 10. Relaxed atomic structure after consolidation of nanocrystalline α-iron (9.4 nm, 17923 atoms, 4 preset dislocations).

4. CONCLUSIONS

Molecular dynamics simulations have been carried out for nanocrystalline α-iron with grain sizes ranging from 7.62 to 12.78 nm. The result shows that:

(i) Dislocations can exist in the crystallites so long as the grain size is large enough. Whether dislocation will exist within the crystalline component or not depends mainly upon the grain size of nanomaterials. It appears that the critical grain size for dislocation generation is about 9 nm, which agrees with the experimental results by Trudeau and Li qualitatively.

(ii) Preset dislocations cannot survive during the consolidation process and they have no effect on the dislocation generation in the crystallites. All the dislocations that exist within crystallites at final state are generated during consolidation process.

(iii) The consolidation pressure can affect the number of dislocations generated. Higher pressure results in more dislocations.

(iv) Sometimes, a new interface appears in crystallite, although it does not coincide with the easiest sliding surface (111). It is generally unstable in a crystal and might result from the special environment of nanomaterial. This phenomenon has not been seen in real experiment; therefore, it should be examined in further studies.

5. ACKNOWLEDGMENT

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