• *Letters*

Dislocations in the Crystallites of Nanocrystalline α-Fe — A Molecular Dynamics Study

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Molecular dynamics simulations are carried out in order to study the atomic structure of crystalline component of nanocrystalline α-Fe when it is consolidated from small grains. A two-dimensional computational block is used to simulate the consolidation process. All the preset dislocations in the original grains glide out of them in the consolidation process, but new dislocations can generate when the grain size is large enough. It shows that dislocations exist in the consolidated material rather than in the original grains. Whether dislocations exist in the crystalline component of the resultant model nano-material depends upon grain size. The critical value of grain size for dislocation generation appears to be about 9 nm. This result agrees with experiments qualitatively.

1. Introduction

Nanocrystalline materials have abnormal performances, including mechanical properties, which predicts undoubtedly broad prospect for applications in science and technology[1]. The studies on the structure and the deformation mechanism of these materials are paid attention to more and more[2~5]. With respect to the structures of nano-materials, the effect of macroscopic factors, *e.g.*, the size and shape of the crystallites as well as the distribution of grain size, is important, which has been investigated in experimental work widely. From microscopic point of view, two problems are noticeable, that is, whether grain boundary (GB) component is of some kind of ordered structure or not, and whether dislocations as well as other defects exist in the crystalline component.

About the first problem, there are two different opinions on whether the GB structure is gas-like or liquid-like, and it is still an open question[4,5]. In our previous works, we have studied the structure of nanocrystalline α-Fe by using molecular dynamics method (MD), and found that the atomic structure of its grain boundary component has some short range order[6,7].

On the second problem, Trudeau *et al.*[5] found a lot of dislocations in the crystalline component of nanocrystalline alloy NiMo, but it is dislocation free when its grain sizes are below 10 nm[5]. Li *et al.*[8] observed that dislocations as well as other defects can be found in nanocrystalline Pd, whose grain size is about 10 nm. That is to say, whether dislocations and other defects exist in the crystalline component of a nanocrystalline material might depends upon its grain size. It is very important for declaring the mechanism of plastic deformation. In our previous MD simulations, we found that the crystalline component of nanocrystalline α-Fe is dislocation free. However, we could not specify how the existence of dislocations depends upon grain size, because the grain size was only 2.86 nm. In this work, a two-dimensional model is adopted, so that, we can use a relatively small number of atoms with grain size over 10 nm, in order to analyse this phenomenon with MD method.

2. Model and Procedure of Simulation

Generally speaking, dislocations might generate during consolidation process of a nanocrystalline material or simply exist in the original grains. One way is to verify it by simulating the consolidation process with preset dislocations in some of the original grains. A basic computational block with four cylindrical grains is adopted, which is extended with three dimensional periodic border conditions (Fig.1). All the axes of the grains are parallel to Z-axis. Several

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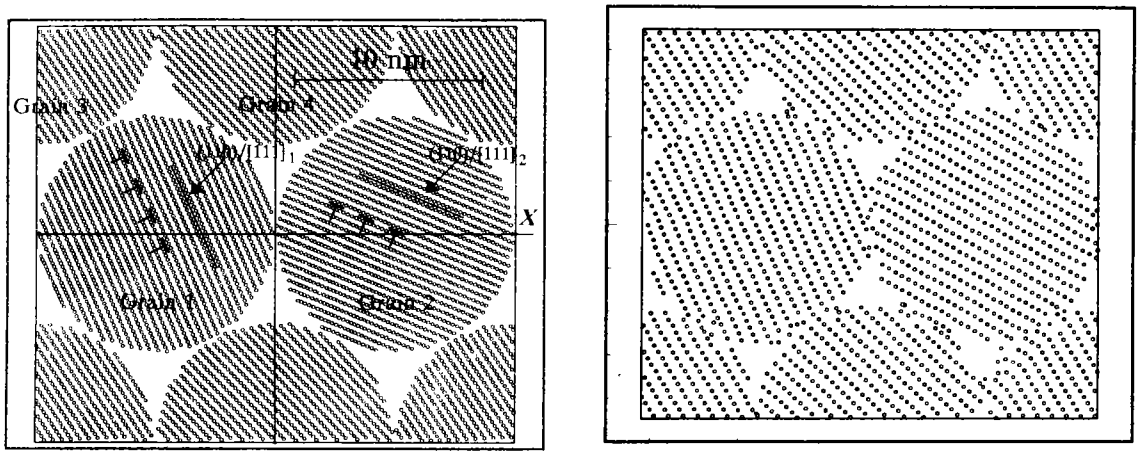

Fig.1 Atomic configurations for the small grain size (7.62 nm, 10562 atoms, 4 preset dislocations (a) initial, (b) final

Table 1 Number of dislocations preset in each grain and existed at final state

Run no.	Grain size/nm	Consolidation pressure/GPa		Dislocations situated in grain 1	grain 2	grain 3	grain 4	total
1	7.62	6	preset	2	2	0	0	4
			final	0	0	0	0	0
2	12.78	6	preset	4	3	0	0	7
			final	1	0	1	0	2
3	12.78	4	preset	4	3	0	0	7
			final	0	0	1	0	1
4	12.78	4	preset	0	0	0	0	0
			final	2	0	0	0	2
5	9.40	6	preset	2	2	0	0	4
			final	0	0	1[1)]	0	1[1)]

1) center of this dislocation is not very clear

edge dislocations are preset in two of these grains, whose dislocation lines are parallel to the axes of the crystallites. The easiest gliding directions [111] of the four grains are randomly set in X-Y plane. Therefore, the configuration ensures the dislocations easily to glide. The variation of cross section area of the crystallites gives model nanocrystalline materials with different grain sizes. Based upon the above consideration, simulation of the consolidation process was carried out by using MD method. The simulation of consolidation process was performed as that in the previous paper[6]. The atomic configurations at the end of each step are recorded and gliding behaviour of the dislocations was observed.

3. Results

Five runs are arranged with different conditions in order to examine the effects of grain size, consolidation pressure and preset dislocation. The results are summarized in Table 1.

From Table 1, it is seen that grain size is really a main factor for dislocation generation within the crystallites. When the grain size is 7.62 nm, no dislocation can exist in the crystalline component. When the grain size is 12.78 nm, dislocations can exist in grain 1 and 3 in spite of whether dislocations are preset or not. However, when grain size is 9.4 nm, the condition is somewhat critical for dislocation generation. It this case, although there is one dislocation left in grain 3, its center is not very clear. It appears that the critical grain size for dislocation generation is about 9 nm.

Comparing the results of grain 2 and 3, it is concluded that preset dislocations can not effect the existence of dislocations at final state. In fact, preset dislocations have glided out in all the cases when consolidation finishes. Dislocations existed in final state are all those generated during consolidation. It means that dislocations come from consolidation rather than

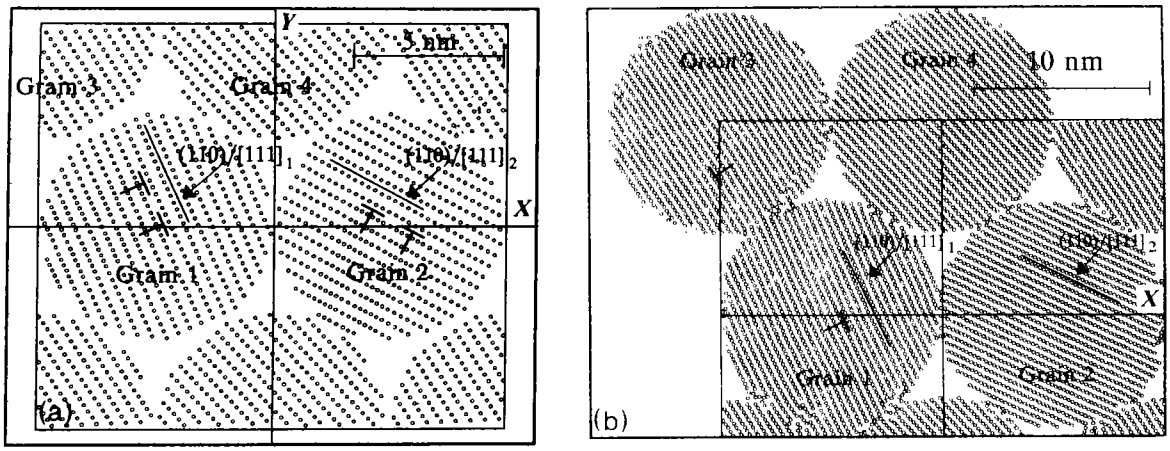

Fig.2 Atomic configurations for the large grain size (12.78 nm, 30360 atoms, 7 preset dislocations (a) initial , (b) final

exist in the original grains. Figure 1 shows atomic configurations of initial and final states in Run 1, and Fig.2 shows those in Run 2.

4. Conclusion

Dislocation can exist in the crystallites so as the grain size is large enough, for example, 12.78 nm. However, when the grain size is 7.62 nm, dislocation can not survive within the crystallites. In the case that the grain size is 9.4 nm, although dislocation appears in the crystallite also, its center is not very clear. Therefore, whether dislocation will exist within the crystalline component depends mainly upon grain sizes of nano-materials. 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. Preset dislocations can not survive during consolidation process and they have no effect on the dislocation generation in any crystallite. It shows that all the dislocations left within crystallites at final state are those generated during consolidation process, but not those come from the orinal grains.

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