ORAL/POSTER REFERENCE: ICF100721OR

THE INFLUENCE OF LATTICE DISTORTION REGION NEAR THE GRAIN BOUNDARY ON MECHANICAL PROPERTIES IN NANO-CRYSTALLINE MATERIALS

Xiaowei Wang[1,2], J.Y. Wang[1,2], J. Rifkin[3], D.X. Li[2]

[1]International Centre for Materials Physics, Institute of Metal Research,
Chinese Academy of Sciences, Shenyang 110016, China
[2] Shenyang National Laboratory for Materials Science, Institute of Metal Research,
Chinese Academy of Sciences, Shenyang 110016, China
[3] Institute of Materials Science, University of Connecticut, USA

ABSTRACT

In this paper, the distortion structure in nano-crystalline NiAl is studied using molecular dynamics simulation. In these simulations the lattice structures within these small grains show a distortion relative to the large grained lattice structure. They are mainly located near grain boundary. Our results show that rounded grain boundaries in these nano-grains (as opposed to the planar faceted grain boundaries found in conventional-sized grains) are a direct factor in the production of the observed lattice distortion. The grain size directly affects the volume fraction of the distorted lattice in the nano-grain. The smaller the grain sizes, the larger the distortion region contributes to improved mechanical properties.

KEYWORDS: Molecular dynamic simulation, Nano-crystalline, Distortion

INTRODUCTION

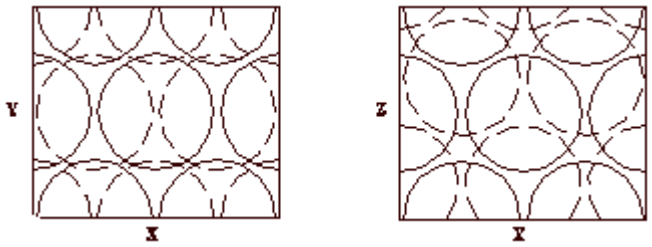
Research on the structure of nano-crystalline materials is motivated by their advanced properties. The influence of grain size on mechanical properties is first considered as the most important influential factors. Except for a number of experimental observation, previous computer simulation studies have focused on the relation between grain size and properties of nano-crystalline. For example, Schiøtz *et al.* [1] studied the softening of nano-cystalline metals at small grain size. In their work, the conventional faceted grain boundary is studied. In fact, the types of the interface structure between

nano-grains is also an very important factor. Li *et al.* [2] reported results from high-resolution electron microscopic (HREM) observation in nano-crystalline materials. Their results indicate that there are three types of interface structures. The first is similar to the planar, faceted interfaces in conventional coarse grains. The second type of interface structure exhibits an imperfect or disordered grain boundary region. The third type is a rounded grain boundary (as opposed to a planar, faceted grain). HREM observation clearly shows a lattice distortion near grain boundary for the last two types of grain boundaries, the disordered grain boundary and the rounded grain boundary, but not for the conventional faceted grain boundary. Otherwise, the existence of this distortion region is also supported by X-Ray diffraction observations (Sui *et al*. [3]). These observations show lattice distortions in individual grains as an average result, but cannot determine where in the grain the distortions are located, nor even if the distortions are localized. The influence of distortion structure on properties of materials and how these lattice distortion region form have not been studied specially in previous works.

The present work concentrates on the character of the lattice distortion region near the grain boundary and the formation of this region. This paper aims to show the influence of the lattice distortion region on the mechanical behavior of nano-crystalline grain and its forming mechanism.

SIMULATION METHOD

The atomic configuration is designed to model nano-crystalline grains with rounded grain boundaries, it consists of a number of small spherical nano-grains embedded in an amorphous matrix. Each simulation contains eight equal-sized nano-grains arranged in a closed packed structure. The initial configuration is shown in Figure 1. Periodic boundaries condition are used in all three directions.



(a) (b)

Figure 1: Initial simulated nano-crystalline configuration.The system contains 8 equal-sized grains arranged in 3-layer close packed structure. The solid line corresponds to the first and third layer of grains. The dashed line corresponds to the second layer of grains. Two projective directions, (a) and (b), is selected.

Simulations are done for varying sizes of nano-grains, but with a fixed separation between grain boundaries. In other words, the width of the amorphous region between grains remains fixed. This was done to judge the effect of grain size and by extension, the grain boundary curvature on the intergranular region.

The simulation was done using the XMD molecular dynamics program. NiAl alloy was selected as the material simulation. The Embedded Atom Method potential due to Voter and Chen [4] was used. The grain diameters used in the simulations are 3.8nm, 6.2nm and 8.7nm, corresponding to 30 327, 131

227 and 344 534 atoms per simulation. The initial percentage of atoms residing in the interface are 34.7%, 35.8% and 36.8%. Four different lattice orientations are used to orient the grains, they are

$$(1\ 1\ 1) \quad (1\ 1\ \bar{2}) \quad (1\ \bar{1}\ 0)$$
$$(1\ 1\ 1) \quad (4\ 1\ \bar{5}) \quad (2\ \bar{3}\ 1)$$
$$(3\ 1\ 2) \quad (1\ 1\ \bar{2}) \quad (\bar{2}\ 4\ 1)$$
$$(2\ 2\ \bar{3}) \quad (3\ 3\ 4) \quad (1\ \bar{1}\ 0)$$

These orientations ensure that there is a common lattice plane between two adjacent grains, this makes it easier to analyze the change of lattice structure between grains.

These nano-grains of defect free lattice are constructed. It is assumed that grains under this small size could not maintain internal defects because any such defects would easily migrate to the nearby grain boundary and reduce the lattice energy.

RESULTS

For the three different initial grain sizes described above we performed a static relaxation of the initial system. This was done using XMD's QUENCH command with a time step of 2E-15 and for 1500 time steps. For each grain size the relaxation shows a reduction in the lattice volume with the corresponding growth of the amorphous region. In addition, within the lattice closest to the amorphous region there formed a distorted region. For future reference we called these three regions as follows: the ‘grain’ is the undistorted lattice, the ‘distortion region’ is the distorted lattice, and the ‘interface region’ is the amorphous region. The ‘grain’ is a roughly spherical region surrounded by a spherical shell of ‘distortion region’, which in turn is embedded in the ‘interface region’. The volume fraction respectively occupied by three region is shown in Figure2 as a histogram.

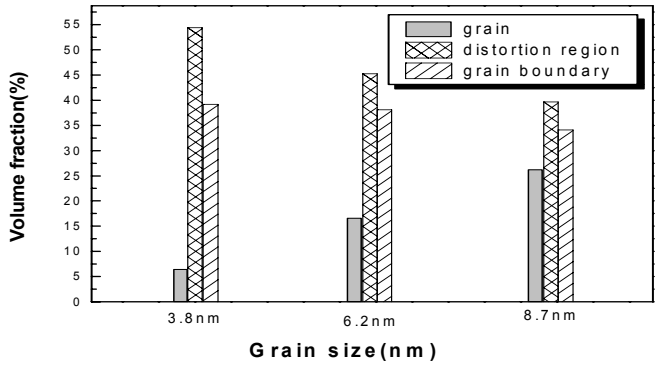


Figure 2: The volume fraction respectively occupied by distortion region, interface region and grain.

Figure 3 gives another indication of the distortion region. It shows the average nearest neighbor distance (nnd) as a function of the distance from the center of interface region to the center of grain. The nearest neighbor distance is expressed in units of the nearest neighbor distance in the bulk d_0. The sharp upturn in the graphs as one travels from the grain to the interface region gives a clear indication of the presence of the distortion region.

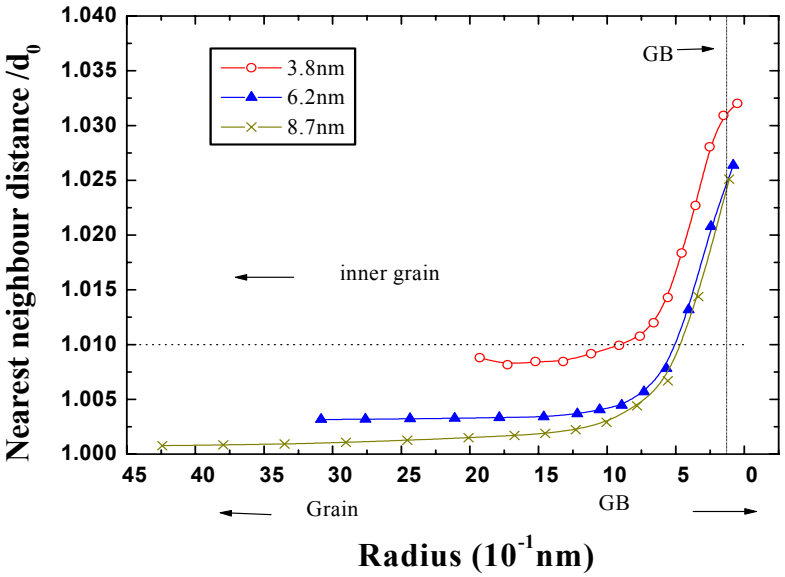


Figure 3: The relationship between the distance from the center of the interface region and the average atomic nearest neighbor distance

Figure 4 shows the deformation behavior of the nano-grains in the amorphous matrix. The horizontal axis displays the amount of uniaxial strain of the system, the vertical axis shows the resulting internal tensile stress. For each data point the atomic system is stretched in one direction while being compressed in the other two directions. Repeating boundary conditions are imposed with these new dimensions and the system is quenched. The resulting internal stress is plotted. This was done for each grain size, and the difference in elastic behavior and yield stress is plainly shown.

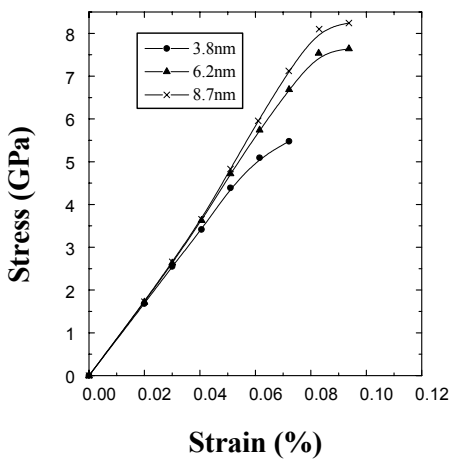


Figure 4: Grain size dependence of tensile Deformation.

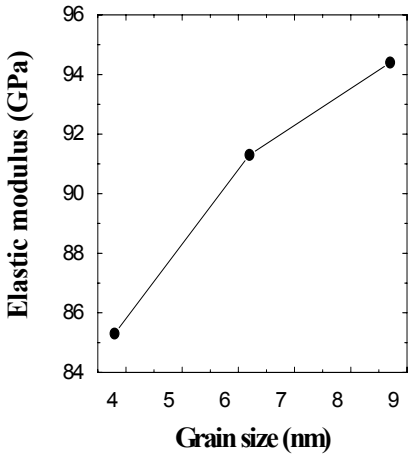


Figure 5: Grain size dependence of elastic modulus.

The results of elastic modulus are given in Figure 5. This is mainly calculated by the slope change of stress-strain curves.

DISCUSSION

Based on the observations of HREM, it is obvious that the structure of nano-crystalline materials (NC) differ from those of coarse grain materials. The distortion region is a transition structure between the perfect NC and the amorphous-like interface. It is also a metastable region in terms of the energy distribution. Therefore, it should be sensitive to a change in external conditions. The presence of the distortion region should have an important influence on the strength of NC. The results of Figure 2 shows clearly the effect of the distortion region and grain size when other conditions are fixed - the smaller the grain size, the higher the proportion of distortion.

Past works have focused on the influence of the grain boundary structure, the distortion structure of NC has received much less attention. But research into the excess enthalpy of NC has exposed a feature of that is different from coarse grain materials. Tschöpe *et al.* [5] showed the unrelaxed strain and non-equilibrium boundary structure in nano-grain are thought to be an important factor that produces the excess enthalpy. Lu *et al.*'s [6] study indicated further two things, (1) that the effective grain boundary energy in NC is smaller than in coarse grain materials despite the fact that the total enthalpy is greater and (2) that the grain boundary energy decreases with decreasing grain size. The excess enthalpy arises mainly from the distortion of the lattice structure. The present work demonstrates that the distortion region near the grain boundary is where the micro-strain is located. This distortion structure is a factor - in addition to the high percentage of grain boundary - that affects the mechanical properties of NC.

The results showed in Figure 4 and Figure 5, the change of deformation behavior with grain size, arise from two factors: the grain size and the size of the distortion region. These two factors have different influence on mechanical behavior. The decrease of grain size causes the increase of distortion region. The change of grain size and distortion region are a correlative factors to affect the yield stress and the elastic modulus of nano-crystalline. When the grain size is smaller, the kind of grain which have the rounded grain boundary will have produced larger distortion region and increased the energy of grain. When we consider the mechanism of deformation in nano-crystalline, the change of distribution of distortion energy is also an important factor except for the change of grain size.

ACKNOWLEDGEMENTS

The authors are grateful to the Nature Science foundation of China (NSFC) (Grants No. 59871056 and 59831020) and The Special Founds for the Major State Baisc Research Projects of China (G2000067104) for financial support.

REFERENCES

1. Schiøtz, J., Di Tolla F. D. and Jacobsen, K. W., (1998) *Nature*, **391**, 561.
2. Li, D.X., Ping, D.H., Ye, H.Q., Qin, X.Y.,and Wu, X.J., (1993) *Mater. letter*, **18**, 29.
3. Sui, M.L. and Lu, K., (1994) *Mater. Sci. Eng.* A, **179/180**, 541.
4. Voter, A. and Chen, S.F., (1987) *MRS Symposia Proceedings*, **82**, 175.
5. Tschöpe, A., Birringer, R. and Gleiter, H., (1992) *J. Appl. Phys.* **71**, 5391.
6. Lu, K. and Sun, N. X., (1997) *Phil. Mag. Lett.*, **75**, 389.