Molecular Dynamics Analysis of Elementary Nucleation Events in Structural Transformation[†]

Takehiko Makino, Kazuki Itoigawa^{††} and Shoichi Matsuda

Department of Mechanical Engineering, Nagoya Institute of Technology, Nagoya 466-8555, Japan

The structural transformation from fcc to bcc was modeled using a potential-change procedure and a constraint method in the molecular dynamics calculation. To model the transformation, inter-atomic potentials were changed before and after the transformation. To obtain a definite image of the elementary event of nucleation, the following was investigated: (a) how individual atoms move and (b) how an orientation relationship forms during the formation of a crystal. The elementary event of the structural change consists of a contraction, an expansion and a rotation. The contraction and the expansion relate to the structural change and are described in terms of a Bain deformation. The rotation relates to the development of an orientation relationship. The structure changes at an early stage of the nucleation process. On the other hand, the orientation relationship develops gradually during the process.

(Received April 30, 1999; In Final Form July 27, 1999)

Keywords: Molecular dynamics calculation, face-centered cubic (fcc)/body-centered cubic (bcc) transformation, nucleation process, Finnis-Sinclair potential, crystal structure, Bain deformation, crystallographic orientation

I. Introduction

Microstructure formation starts from nucleation. Because nucleation is essentially an atomic process, it is difficult to investigate experimentally. The molecular dynamics calculation is effective for the research of a rapid transition such as diffusionless transformation⁽¹⁾. The reason for which the structural transformation occurs is still far from understanding at present, therefore the molecular dynamics method using simple inter-atomic potentials was selected to know how the transformation occurs. Constructing a simple model is important to know the relationship between the conditions and the results and their physical implications. In this calculation, we assume only the inter-atomic potentials and the method of applying the potentials.

We have reported⁽²⁾ that the structural change could be modeled by the method in which applying potentials are changed within a constraint condition. The objective of the study was to obtain a definite image of the atomic nucleation process of structural transformation by clarifying the spatial change with time, and the role of dislocations in the nucleation process in crystals. The following were obtained: (a) formed crystals can grow only around the dislocation, (b) the crystallographic orientation relationship that is observed experimentally in fcc/bcc crystals is satisfied, and (c) the orientation of formed crystals is restricted around the dislocation. These aspects coincide well with experimental facts. Detailed analysis is needed to obtain more essential infor-

mation from the calculated results.

The objective is to obtain a definite image of the atomic movements during structural transformation in crystals by analyzing the calculated results obtained in the previous study⁽²⁾. The purpose of this study is to learn (a) how individual atoms move and (b) how an orientation relationship forms during the formation of a crystal.

II. Procedures

The calculating procedure is the same as reported in a previous paper⁽²⁾. The NPT ensemble is attained by the constraint method proposed by Evans and Morriss⁽³⁾⁽⁴⁾. The pressure and the temperature of the system are set to be 0.0 Pa and 582 K, respectively. To model an fcc/bcc transformation, (a) the relaxation of the initial configuration of fcc crystal is done by using the potential that stabilizes fcc structure, and then (b) the crystal is set to be transformed by changing the potential to a bcc stabilizing potential to all atoms at once. Finnis-Sinclair (F-S) potentials for copper⁽⁵⁾ (lattice constant = 3.615×10^{-10} m) and bcc iron⁽⁶⁾ (lattice constant = 2.866×10^{-10} m) are used for obtaining fcc and bcc structures, respectively. The initial configuration has an fcc structure and the surfaces of the calculating cell are {001} planes. The cubic calculating cell of the perfect crystal contains 2048 atoms. An edge dislocation is introduced in order to work as a nucleation site⁽²⁾. Before the relaxation of the fcc structure, one half plane which is parallel to (001) is removed. As a result of the relaxation, neighboring atoms close the vacant half plane and the dislocation can be introduced.

Voronoi polyhedra analysis⁽⁷⁾ is utilized to distinguish the crystal. Voronoi polyhedra analysis can classify the crystal structure on an atomic scale. The crystallographic orientations of transformed regions are analyzed by the

[†] This Paper was Presented at the Spring Meeting of the Japan Institute of Metals, held in Tokyo, on March 30, 1999.

^{††} Graduate Student, Nagoya Institute of Technology, Present address: Sansei Yusoki Co. Ltd., Suita Japan.

configuration of the atoms confirmed as bcc-constituent. This procedure distinguishes three directions of formed bcc crystals by examining which $\{001\}$ plane of the original fcc crystal is nearly parallel to (001) plane of the formed bcc crystals. The movements of the reference atom and its neighboring atoms are observed and the changes in distances between sampling atoms within a bcc crystal are plotted to know the elementary process of the structural transformation. The changes in the direction of the planes made up by the neighboring three atoms are plotted against time in a stereo diagram.

III. Results

To observe the elementary process of nucleation, we paid attention to the bcc crystal formed around the dislocation in the fcc crystal; we know that the formed bcc crystal is found to grow in the defected crystal⁽²⁾, and the process can be recognized as a nucleation. Shown in Fig. 1 is the movement of a reference atom and its first and second nearest-neighbor atoms that will belong to the bcc crystal, of which $[001]$ direction is nearly parallel to $[100]$ of the fcc crystal. This bcc crystal is one of the first crystals formed in the original fcc crystal. Light toned particles represent (001) fcc and (110) bcc. It can be seen that the atomic distances along $[100]$ fcc direction decrease and that along $[010]$ fcc and $[001]$ fcc directions increase simultaneously. Thus the fcc lattice deforms to be a bcc lattice continuously. It is noted that the process of transformation coincides with the well-known Bain deformation⁽⁸⁾. The group of the atoms starts to rotate around near $[001]$ fcc from the early stage of the nucleation, as shown in Figs. 1(a) and (b).

The changes in distances between the reference atom and its neighboring atoms with MD steps are shown in

Fig. 2. At zero steps, the group of the atoms has an fcc structure, and the first nearest-neighbor atoms locate at around 2.6×10^{-10} m and second nearest-neighbor atoms locate at around 3.6×10^{-10} m. As the steps advance, the two second nearest-neighbor atoms of the fcc structure rapidly approach the reference atom to be the second nearest-neighbor atoms of the bcc structure. The four first nearest-neighbor atoms of the fcc structure slightly separate to be the second nearest-neighbor atoms of the bcc structure. Similarly, the four second nearest-neighbor atoms of the fcc structure separate to be the third nearest-neighbor atoms of the bcc structure. In the early stages, the atoms move to new positions. It can be seen that each atom oscillates. The amplitude of the first nearest-neighbor atoms is small and that of the second nearest-neighbor atoms is large. At about 5000 MD steps, structural change is completed among these atoms. The changes in atomic distances along $[100]$ fcc and $[011]$ fcc directions at 5000 MD steps are -16.5% and 7.8% , respectively.

The changes with time in the direction of planes formed by the neighboring three atoms sampled are shown in Fig. 3. Six $\langle 110 \rangle$ bcc and three $\langle 100 \rangle$ bcc directions are plotted in a (001) fcc stereo diagram. The lines that have varying tones show the tracks of the plane directions. As MD steps progress, the tone changes from black (0 steps) to white (30000 steps) continuously. It can be seen that each $\langle 110 \rangle$ bcc direction fluctuates about 10 degrees. Some directions oscillate at original directions and some move to new positions. It can be seen that the direction that was originally $[\bar{1}\bar{1}1]$ fcc settles down to $[\bar{2}21]$ fcc. Consequently, the orientation relationship between fcc and bcc crystals is an N-W relation ($(1\bar{1}1)$ fcc $\parallel$ (011) bcc, $[011]$ fcc $\parallel$ $[100]$ bcc, $[\bar{2}21]$ fcc $\parallel$ $[01\bar{1}]$ bcc).

Fig. 1 Movement of atoms that will belong to the bcc crystal of which $[001]$ direction is nearly parallel to $[100]$ of the fcc crystal.

Fig. 2 Changes in distances between the reference atom and its neighboring atoms, against time.

Fig. 3 Changes with time in the direction of the planes formed by the atoms sampled.

IV. Discussion

The elementary event of the structural change from fcc to bcc is analyzed from the movement of atoms. Geometrically, the event is recognized from Fig. 1 as a contraction, an expansion and a rotation of lattices. The contraction and the expansion can be described well in terms of a Bain deformation⁽⁶⁾. The rotation relates to the development of an orientation relationship. However, the combination of the former two changes and the rotation cannot be treated until the molecular dynamics analysis is applied. It is clarified from Fig. 2 and Fig. 3 that the structure changes at an early stage of the nucleation process and the orientation relationship

develops gradually during the process. Comparing the tracks of the directions of the planes nearly parallel to $\langle 100 \rangle_{\text{fcc}}$ directions, the rotation of the lattice is around $[001]_{\text{fcc}}$. However, such a geometrical interpretation is not always significant in the molecular dynamics analysis because an individual atom is conscious of not a part of the planes in a crystal but the relation between neighboring atoms.

It has to be emphasized that the observed elementary event is a result of a calculating condition employed. The combination of the initial and the final states determine even the beginning of the structural change. The validity of the aspects shown in the previous study⁽²⁾ is caused by the elementary event shown in this study. The potential-change method used changes the interaction between atoms all at once. The assumption is thought to be not far from the reality. However, this simple condition is only a first step toward an understanding of the mechanism of the structural transformation. Further analysis on the relationship between the selection of potentials and the results will provide useful information on the significant factors of the transformation.

V. Conclusions

Using the molecular dynamics method, which employs a pressure-temperature-constant condition and potential-change procedure, the elementary event during structural transformation in a modeled crystal was investigated and the results are as follows:

- (1) The elementary event of the structural change from fcc to bcc consists of a contraction, an expansion and a rotation. The contraction and the expansion relate to the structural change and are described well in terms of a Bain deformation. The rotation relates to the achievement of an orientation relationship.
- (2) The orientation relationship between fcc and bcc

crystals is found to be an N-W relation in the modeled crystal.

(3) The crystal structure changes at an early stage of the nucleation process. The orientation relationship is achieved gradually during the process.

REFERENCES

- (1) T. Tonokawa, T. Fukushima and T. Suzuki: *Mater. Trans., JIM*, **37** (1996), 1298–1303.
- (2) T. Makino, K. Okouchi and S. Matsuda: *Mater. Trans., JIM*, **40** (1999), 435–438.
- (3) D. J. Evans and G. P. Morriss: *Chem. Phys.*, **77** (1983), 63–66.
- (4) D. J. Evans and G. P. Morriss: *Phys. Lett.*, **98A** (1983), 433–436.
- (5) G. J. Ackland, G. Tichy, V. Vitek and M. W. Finnis: *Phil. Mag., A*, **56** (1987), 735–756.
- (6) M. W. Finnis and J. E. Sinclair: *Phil. Mag. A*, **50** (1984), 45–55.
- (7) M. Tanemura, Y. Hiwatari, H. Matsuda, T. Ogawa, N. Ogita and A. Ueda: *Prog. Theor. Phys.*, **58** (1977), 1079–1095.
- (8) E. C. Bain: *Trans. AIME*, **70** (1924), 25–46.