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Increase of Grain Boundary Mobility by Radiation Damage under Thermal Gradient Condition using Molecular Dynamics Simulation

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1. Introduction

Most transformations of microstructure, such as recrystallization, grain growth are based on migration of grain boundaries. These transformations greatly influence on thermal, electrical transport and mechanical properties of materials. Material industries always set aim to design and produce decent materials by controlling microstructure evolution under various conditions. Since understanding grain boundary migration is critical for predicting the microstructural evolution in material [1], it has been very widely investigated for several decades. Also simple information from GB migration can give the clue to depict complicated and scale-up microstructural evolution.

Grain boundary (GB) motion is generally described by migration velocity quantitatively. Migration velocity is the product of driving force and grain boundary mobility. (Eq.1.)

$$v = M \times F \qquad (1)$$

v is migration velocity, M and F is mobility and driving force respectively. Driving force is mainly originated from grain curvature, stress, strain and thermal gradients [2]. These driving forces in the unit of pressure are created when free energy stored in grain of material system is released in order to make system stable. And mobility of the grain boundary is also important factor of grain boundary movement. Since it is intrinsic properties of material, it should shows consistent values regardless of types and magnitudes of driving forces. And it follows Arrhenius relation (Eq.2.)

$$M = M_0 \exp(-E_m/k_B T) \qquad (2)$$

M_0 is pre factor of GB mobility, E_m is activation barrier. k_B and T are Boltzmann constant and temperature respectively.

Although GB migration has been actively studied for materials in general conditions such as high temperature, stress and strain. There is no report on GB migration when the material is under irradiation condition. In this work, we investigate the effect on migration when energetic particles are collided with uranium dioxide GB structure using molecular dynamics (MD) simulation and which factor in migration velocity is mainly influenced by irradiation.

2. Methods and Results

2.1 Interatomic Potential

The LAMMPS MD simulation package [3] is introduced to study the GB migration in UO_2. For MD simulation, empirical potential form between atoms is crucial. In this simulation, we selected embedded atom method (EAM) potential form for uranium dioxide, which is the first many-body potential [4]. It introduce many body effect on existing simple pair-wise potential formula. Potential formula of atom i are described via eq.3. Also, ZBL potential was considered to depict collision [6].

$$E_i = \frac{1}{2}\sum_j \phi_{\alpha\beta}(r_{ij}) - G_\alpha \sqrt{\sum_j \sigma_{\alpha\beta}(r_{ij})} \qquad (3)$$

First term is pair-wise term which is the combination of conventional Buckingham and Morse potential with Coulombic potential which treat charged ions. Second term indicate many – body term. By introducing new many body term, verification result is well fitted with experiment rather than existing potential form.

As seen in figure 1, new many body potential can predict bulk modulus of uranium dioxide more accurately, rather than result by simple pairwise Yakub potential.

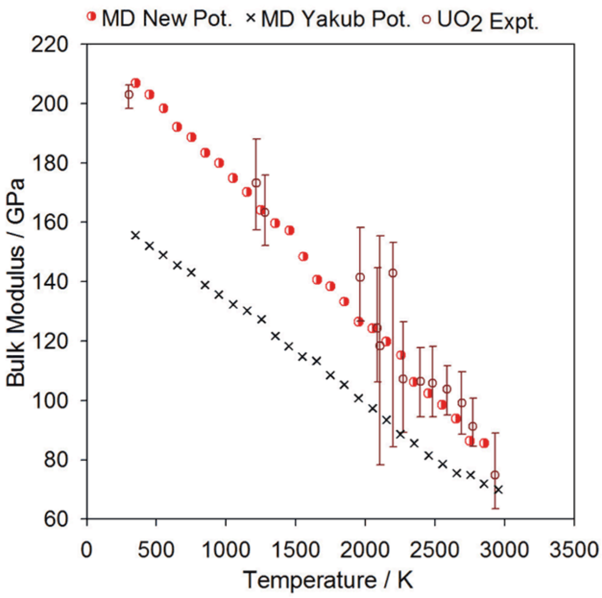

Fig. 1. Bulk modulus using new many body potential and comparison with experiment and existing Yakub potential [4].

Also, in our previous work, thermal conductivity calculation of single crystal result using this potential shows very close with Ab-initio MD calculation result, compared with outcome using simple pair wise potential.

2.2 Construction of GB structure

In order to investigate many phenomena occurred in grain boundary, planar grain structures are introduced. Planar grain structure is made via GB studio [5]. <100>Σ5{031} CSL symmetric tilt grain boundary type is used to simulate grain boundary migration (Fig.2). After construction of original structures of planar grain, it is thermally equilibrated for 100ps at 1500K in NPT ensemble with zero external pressure.

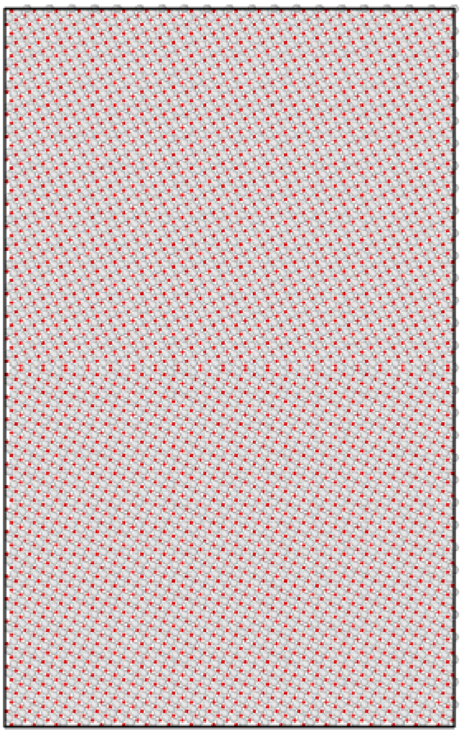

Fig. 2. Cross section of <100>Σ5{031} CSL symmetric tilt grain boundary. Gray and red sphere are uranium and oxygen atoms respectively.

2.3 Introduction of radiation damage under thermal gradient as GB migration driving force

Among several types of driving forces in order to make GB migration simulation, such as curvature, thermal gradient, strain, stress and artificial potential methods, thermal gradient driving forces is chosen despite the fact that thermal gradient driving force is very much low. [1] Because radiation damage simulation on grain boundary is usually conducted on flat grain boundary, not curved boundary, also, there is no external elastic strain or stress condition on grain boundary structure in previous radiation damage simulations.

Thermal gradient is set to 10K/nm. It is very extreme gradient condition compared to typical nuclear fuel temperature gradient environment (~10^-4 K/nm), but its driving force is quite low to trigger the movement of GB. Using above thermally equilibrated structure, Thermostats are installed in upper and lower region of planar grain structure on the temperature range of 1400K to 1600K.

After that, energetic three uranium atoms as irradiation with kinetic energy of 5keV are introduced and designed to make cascade morphology on GB. Thermal gradient condition (Fig.3.) play a role in driving force under NVE and NVT ensemble but not insufficient magnitude. In this simulation, radiation dose was approximately 0.01 dpa (displacements per atom). 1 dpa means that every atom in the irradiated volume has been displaced once from its equilibrium lattice site. Dpa is the most commonly used damage correlation parameter.

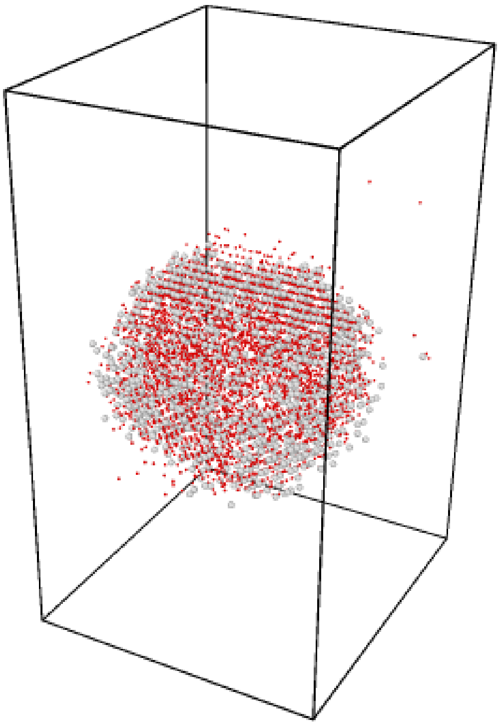

Fig. 3. Right after the introduction of radiation damage, cascade morphology is created. Only interstitial defects are expressed. Gray and red sphere are uranium and oxygen atoms respectively.

2.5 Result

After collision cascade by radiation damage, GB structure is continuously relaxed under thermal gradient condition. GB migration is also simultaneously progressed. In figure 3, left figure indicate arrangement of uranium atoms right after radiated and right one shows grain boundary migration after 1ns. Oxygen atoms and upper and lower part is removed due to comfortable comparison and limited space. Interesting point is that GB migrate despite the fact that thermal gradient driving force is not enough to make the movement of GB.

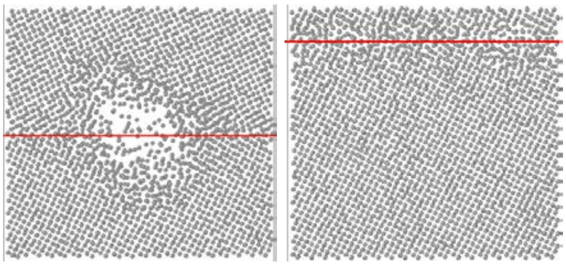

Fig. 4. GB migration under thermal gradient condition after 1ns from collision cascade. Oxygen atoms and upper and lower part is removed due to comfortable comparison and limited space.

3. Conclusions

In this work, we investigated the grain boundary migration after the radiation damage. Without radiation damage, thermal gradient driving force was insufficient to cause the movement of grain boundary. However, with introduction of radiation damage, grain boundary showed the migration behavior while it is restored from damaged state. This is due to the fact that kinetic energy of energetic particles trigger the migration of GB by increasing temperature at GB region enormously. Rapid collision supplies the energy to exceed energy barrier to make the movement of migration As temperature of local regoin goes up due to radiation damage, mobility of GB should rise according to the eq.2. Therefore, radiation damage act as the trigger of local gratin boundary migration.

This implies that mobility of GB can be changed sufficiently by radiation damage. That means, grain growth also can be influenced by radiation damage through enormously sharp increase of temperature in local region which can induce rapid change of GB mobility. it is not considered yet in grain growth modeling of nuclear materials, such as phase field method. Quantitative evaluation about relations among radiation dose, GB mobility and driving force will be investigated.

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