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Computer simulation study for the effect of potential energy on the behavior of grain boundary using Molecular dynamics

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Abstract

In this study, MD simulations have been performed to observe the behavior of a grain boundary in an α-Fe plate under 2-dimensional loading. In MD simulation, the acceleration of every molecule can be achieved from the potential energy and the force interacting between each molecule, and the integration of the motion equation by using Verlet method gives the displacement of each molecule. Initially, four α-Fe rectangular plates having different misorientation angles of grain boundary were modeled by using the Johnson potential and Morse potential. We compared the potential energy of the grain boundary system with that of the perfect structure model. Also, we could obtain the width of the grain boundary by investigating the local potential energy distribution. The tensile loading for each grain boundary models was applied and the behavior of grain boundary was studied. From this study it was clarified that in the case using Johnson potential, the obvious fracture mechanism occurs along the grain boundary, in the case of Morse potential, the diffusion of the grain boundary appears instead of the grain boundary fracture.

Keywords : Molecular Dynamics, grain boundary, grain boundary fracture, misorientation angle

1. INTRODUCTION

There are many problems dealing with mechanical and thermal properties of materials which play critical role at the interfaces of materials. Because the region for such processes is often a few atomic layers, micro-scale or molecular level consideration should be introduced in the studies of interfacial systems. The atomic-scale simulation methods of molecular dynamics (MD) and Monte Carlo can satisfy those resent trends, if only the interatomic potential is available and adequate for the used material. However, since it is fundamentally difficult to choose the proper interatomic potential, many studies about potentials have been performed.[1,2,3,4]

MD was first applied to the fracture problem by the crack propagation because the fracture of a material occurs in atomic level and MD is a powertul tool to simulate the microscale behavior of atoms.[5,6] Another principal factor to cause the fracture in a material is a grain boundary(GB) which is considered as a non-homogeneous phase where dislocations or impurities are accumulated. The GB systems in metallic materials have the differences in atomic structure from regular crystal body and show various characteristics. For example, grain boundaries may provide an easy path for atomic diffusion because in grain boundaries the atoms are disturbed and sparsely located. When a grain boundary is influenced by an external vibration, viscous slip occurs and causes the friction between grains. Thus, a grain boundary has great and important effect on properties of metallic polycrystal, so many studies about the structures, physical properties and microscale behavior of GB have been performed. However, most of the studies were concerned with the direct observation and experiment by electronic microscope and SEM. Vitek et al.[7] investigated the symmetric structure of a grain boundary having (001) and (110) axes as its rotation axes in bcc metal, and Broughton et al.[8] examined the stability of grain boundary at high temperatures, and proved that the grain boundary structure of =123 is the most stable around melting point. Nakatani[9] analyzed the influence of the temperature on the slip system of a grain boundary under the shear stress state, and George et al.[10] used the model having two grain boundaries and investigated the extinction of a grain boundary due to slip system and

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interaction of a grain boundary.

In this study, we modeled α-Fe material having misoriented grain boundary and studied its deformation behavior under tensile loading. And, influences of potential energy on the behavior of grain boundary were examined and also the effects of misorientation angles between grains were examined. Moreover, the grain boundary width can be achieved by investigating local potential energy distribution across the grain boundary.

2. THEORETICAL BACKGROUND

2.1 Potential energy

In this simulation, two types of potentials, Morse potential and Johnson potential, are employed to clarify its effect on the behavior of a grain boundary. The Morse potential is as follows.[9]

$$\Phi(r_{ij}) = a[e^{\{-2b(r_{ij}-r_o)\}} - 2e^{\{-b(r_{ij}-r_o)\}}] \quad (1)$$

where, $a = 6.68758E03 g\text{Å}^2/s^2$, $b = 1.3885\text{Å}^{-1}$, and $r_o = 2.845\text{Å}$. r_{ij} is the distance between molecules.

Also, the Johnson potential is represented in what follows.[1,11]

$$\Phi(r_{ij}) = c(r_{ij}+d)^3 + fr_{ij} + g \quad (2)$$

Table 1 shows the variables in eqn. (2) and Fig.1 displays the Morse potential and Johnson potential energy.

Table 1 Values of c, d, f, and g for α-Fe

Range(Å)	$c(g/s^2\text{Å})$	$d(\text{Å})$	$f(g\text{Å}/s^2)$	$g(g\text{Å}^2/s^2)$
1.9~2.4	-3.52E04	-3.098	4.33E04	-1.19E05
2.4~3.0	-1.02E04	-3.116	7.66E03	-2.53E04
3.0~3.44	-1.79E04	-3.066	7.48E03	-2.48E04

2.2 Local Stress

In the two-body potential such as Johnson potential and Morse potential, the local stress is defined as follows.[11]

$$\sigma_i^{\alpha\beta} = -\frac{1}{\Omega}(m_i v_i^{\alpha} v_i^{\beta} + \sum_{j=1, j\neq i}^{neighbours} q_{ij}^{\alpha} F_{ij}^{\beta}) \quad (3)$$

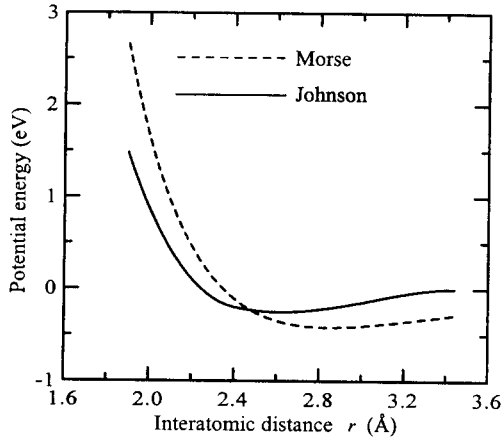


Fig.1 Morse potential and Johnson potential

where q_{ij}^{α} is the α-component of the position vector $\mathbf{q_{ij}}$ between molecules i and j. m_i is the mass of a molecule i and v_i^{α} is the α-component of the velocity vector, $\mathbf{v_i}$. Ω is the volume of a molecule and represented as $\Omega = a^3/2$ where a is the initial lattice constant. $\mathbf{F_{ij}}$ is obviously the force vector between molecules.

3. ANALYSIS CONDITIONS

In this study, four α-Fe models were introduced. In order to simulate the grain boundary having misorientation angle θ in shown in Fig.2, the molecules are bonded together like in Fig.2~Fig.5, which show the geometrically constructed models. They have 5°, 10°,

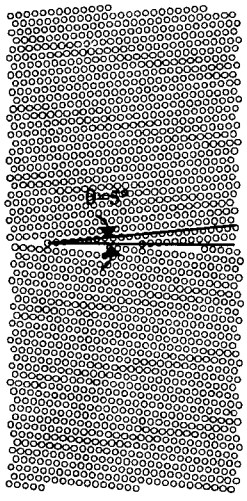


Fig.2 Geometric atomic arrangement for the misorientation angle of θ=5°

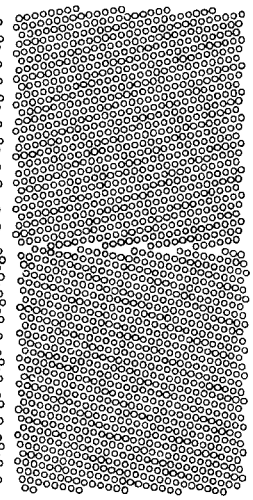


Fig.3 Geometric atomic arrangement for the misorientation angle of θ=10°

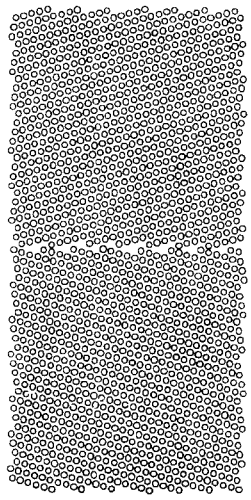


Fig.4 Geometric atomic arrangement for the misorientation angle of θ=15°

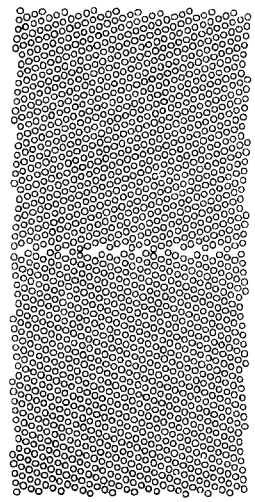


Fig.5 Geometric atomic arrangement for the misorientation angle of θ=20°

15°, and 20° of misorientation angle, respectively. Each model consists of 1600 molecules and has the size of 80Å width and 160Å height. First, four models were thermally relaxed at 300K by using the Morse potential and Johnson potential, respectively. Potential energy during thermal relaxation and the effects of potential function type are investigated. The tensile loading of 3m/s was applied to the upper and lower two layers of these thermally relaxed models vertically and at the same time, the deformation behaviors of grain boundaries of each model were investigated. Time step to update the position of each molecules is 1.5×10^{-15}sec.

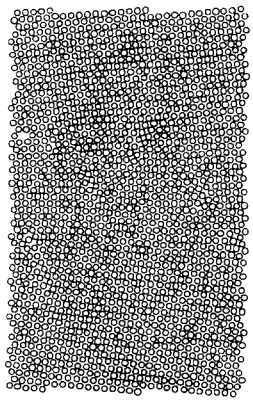


Fig.6 Atomic arrangement for the misorientation angle of θ=5° after thermal relaxation

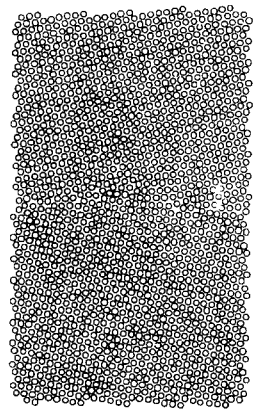


Fig.7 Atomic arrangement for the misorientation angle of θ=10° after thermal relaxation

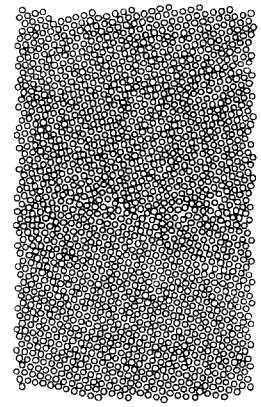


Fig.8 Atomic arrangement for the misorientation angle of θ=15° after thermal relaxation

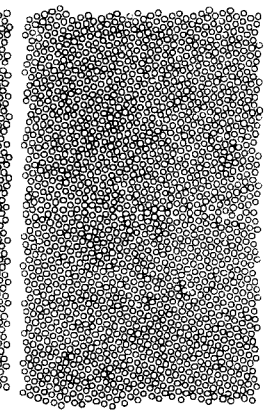


Fig.9 Atomic arrangement for the misorientation angle of θ=20° after thermal relaxation

4. RESULTS AND DISCUSSIONS

Fig.6~Fig.9 represent the thermally relaxed models with Morse potential corresponding to each misoriented angle. The models are relaxed for 8000, 30000, 12000 and 30000 steps, respectively. From the figures, it is noted that as the angle of misorientation increases, more disturbances and more dislocations appear in grain boundaries. The shapes of the thermally relaxed models with Johnson potential are similar to those of Morse potential and are not shown here. However, it took much longer time to be thermally relaxed with Johnson potential. For Johnson potential, the time steps needed to be fully relaxed are 170000, 150000, 60000, and 200000 steps for 5°, 10°, 15°, and 20° misoriented specimens, respectively.

However, the potential energies of the fully relaxed models using Johnson potential are much higher than those of Morse potential for all cases. As a result, it took much more time to be fully relaxed with Johnson potential than Morse potential. Fig.10 shows the variation in the potential energy of 5° misoriented model during thermal relaxation with Morse potential. The potential energy of the initial model of ① in Fig.10 has a very high value due to the forced molecular arrangement and the irregular structure of a grain boundary. As the relaxation continues, however, the molecules in the grain boundary begin to adhere one another and the potential energy shows the steady decrease. Around 8000 relaxation steps, the upper and lower plate fully adhere and the natural grain boundary is made as in ③ in Fi.10. As a result, the model becomes a stable state of an equilibrium and the potential energy

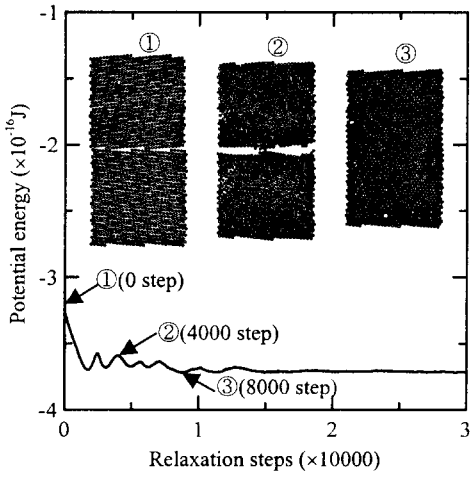


Fig.10 Variation of total potential energy for the misorientation angle of θ=5° during thermal relaxation with Morse potential

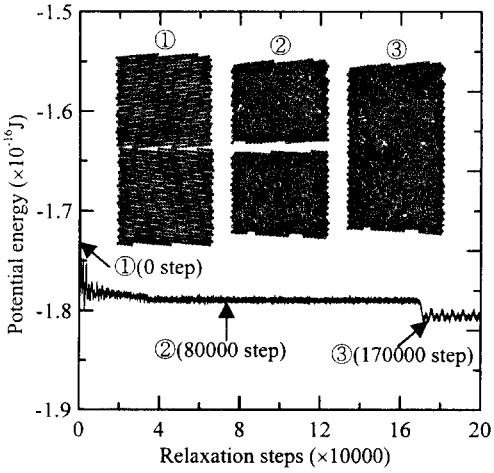


Fig.11 Variation of total potential energy for the misorientation angle of θ=5° during thermal relaxation with Johnson potential

is settled in the least value. Fig.11 represents the potential energy of the model using Johnson potential. In Fig.11, a sudden drop in potential energy around 170000 relaxation steps indicates that the grain boundary in this model is fully made and thus this model becomes the stable state of an equilibrium.

To clarify the effect of the existence of a grain boundary on the potential energy of the system, we investigated the potential energy of a system having the perfect atomic structure of the same number of molecules. The differences of potential energy, ΔρE, between the grain boundary model and perfect structure model during the thermal relaxation are displayed in

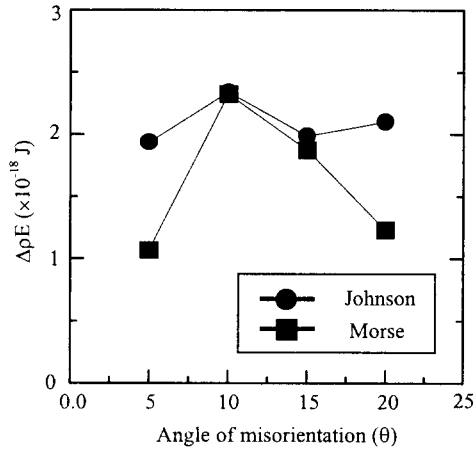


Fig.12 Relation between ΔρE and misorientation angle θ

Fig.12. From Fig.12, we can see that the potential energy of the grain boundary model increases as the misorientation angle of a grain boundary θ increases until θ=10°. After that point, on the contrary, the potential energy suddenly decreases. This decrease in potential energy seems to be caused by the fact that as θ increases the formation of the dislocations increases, and more local disturbances due to the dislocations interrupt molecule's behavior.

Although the width of a grain boundary is generally known to be a magnitude of several atomic layers, it is not easy to determine the width of a grain boundary with experiments or direct inspection. In this study, we considered the grain boundary as higher local potential energy than other area. Thus we measured the potential

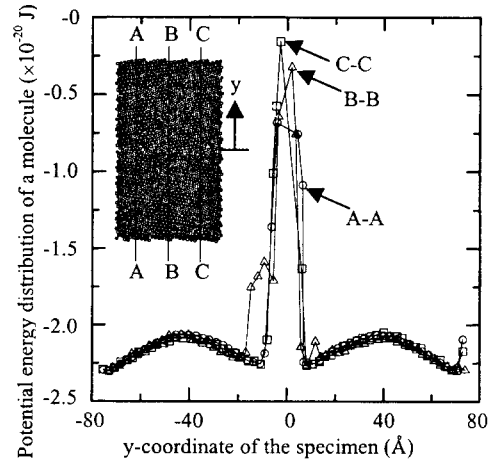
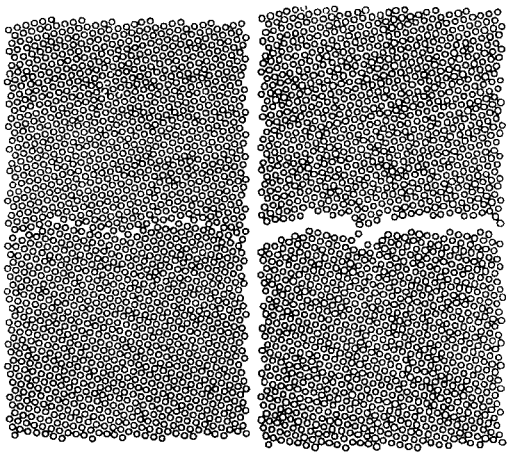
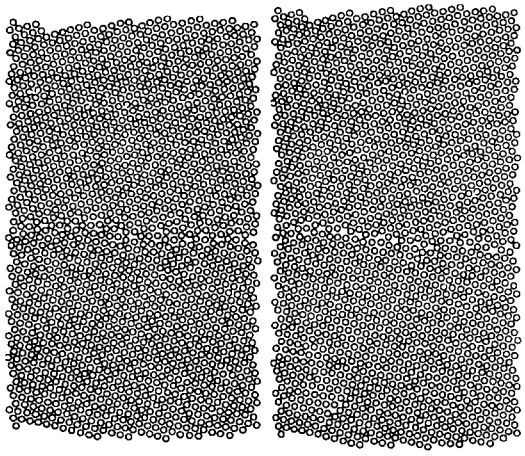


Fig.13 Distribution of atomic potential energy measured along y-direction for the misorientation angle θ=15°



a) ε=0.01 b) ε=0.03

Fig.14 Atomic arrangement for the misorientation angle of θ=15° under 3m/s tensile loading using Johnson potential



a) ε=0.01 b) ε=0.03

Fig.15 Atomic arrangement for the misorientation angle of θ=15° under 3m/s tensile loading using Morse potential

energy distributions across the grain boundary along three vertical lines of thermally relaxed specimen. This clarified the width of a grain boundary of the specimen. Fig.13 represents the distribution of potential energy measured along the y-direction across the grain boundary for 10° misoriented model in the case of Morse potential. From Fig.13, we can say that the width of grain boundary in this case is about 27Å. Other models are omitted here due to their similarities.

For these fully relaxed models, we applied the constraint displacements to two atomic layers in both end sides of each specimen in order to investigate the deformation behaviors of grain boundaries. Fig.14 and Fig.15 show the geometrical arrangement of molecules after the tensile test using Johnson potential and Morse potential, respectively. In case of Johnson potential, the micro fracture along the grain boundary occurs at the strain of about 3%. In models using Morse potential, however, the fracture does not appear until the strain of 4% and the diffusion of grain boundary is noted instead. From these results, we can conclude that the Johnson potential function is more suitable to analyze the behavior of the brittle materials than Morse potential.

The stress and strain curves for each potential during the tensile test are represented in Fig.16 and Fig.17. In Fig.16, the major drops in stress for each misorientation angle mostly appear at about 3% strain except the case of 20° misorientation angle. These drops means that each misoriented model begins to fail there. The stress of 15° misoriented model is the highest and that of 20° misoriented model is the lowest. A sudden drop in stress of 20° misoriented model around 1% strain is due to the generation of a small and local void in the model, not an index of an obvious failure. Because of this local void, the stress value of 20° misoriented model is lower than the others and not uniform. In Fig.17 for the cases using Morse potential, however, any drop in stress does not appear, because the models using Morse potential do not fail during the tensile tests. The stress value of 15° misoriented model is the highest and that of 20° misoriented model is the lowest, but differences in stress between misorientation angles are not prominent. Also it is noted that the diffusion of a grain boundary has little effect on the stress value.

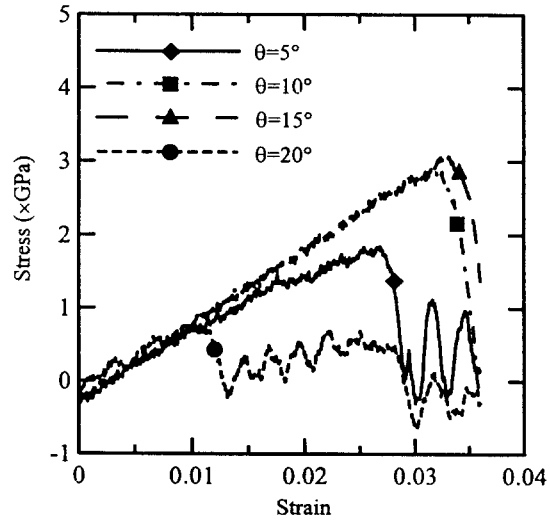


Fig.16 Stress and strain curve under tensile loading Using Johnson potential

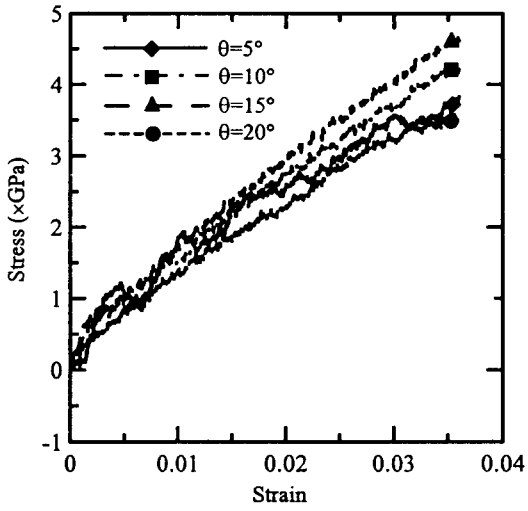


Fig.17 Stress and strain curve under tensile loading Using Morse potential

5. CONCLUSIONS

In this study, a molecular dynamics simulation to analyze the behavior of α-Fe having a grain boundary has been performed. First, the rectangular atomic models having four misoriented grain boundaries were arranged and thermally relaxed at 300K by using Johnson and Morse potential. We could know that it took much shorter time for a atomic system to be thermally relaxed using Morse potential than Johnson potential function due to the relatively lower potential energy of the case using Morse potential. We compared the potential energy of the grain boundary system with that of the perfect structure model. It is then noted that the potential energy of the model increases as the angle of misorientation increases up to 10° of the misorientation angle and at the higher misorientation angles than 10° the potential energy decreases. Also we could obtain the width of a grain boundary by comparing the local potential energy distribution of each molecule and know that the width is about ten times the lattice constant. The tensile loading of 3m/s were vertically applied to the thermally relaxed models. In the case using Johnson potential, the fracture process along the grain boundary occurs clearly in every misoriented angle during the tensile test. In the case of Morse potential, however, the fracture of a grain boundary did not appear and the diffusion of grain boundary is observed. Also, we could see those phenomena in the stress and strain curves. Therefore, we can say that the Johnson potential is suitable to the brittle materials and the Morse potential is suitable to more ductile materials. And it is also noted that the fracture along the grain boundary of each model makes the stress decrease suddenly but the diffusion of grain boundary has little effect on the stress.

6. ACKNOWLEDGEMENTS

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