Large-scale Molecular Dynamics on Screw Dislocation in Alumina

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Alumina (Al_2O_3) is one of the most common materials used in various industrials sectors. Despite such importance, atomistic-level details of the dislocations, which are responsible for plastic deformation of the material, have not been identified until recently, mainly because of its complex crystal structure. Recent progresses of high-resolution electron microscopes have enabled one to obtain the atomic-level information of alumina dislocations. Shibata *et al*. [1] have reported recently their experimental analysis, based on the scanning transmission electron microscopy (STEM), on the structures and migration properties of a basal edge dislocation with the Burger's vector in $\mathbf{b} = 1/3\langle 11\bar{2}0\rangle$ α-alumina. Tochigi *et al*. [2] have reported also the high-resolution TEM (HRTEM) measurements on atomic-level structure of dissociated $\langle 1\bar{1}00\rangle$ dislocations and their associated stacking fault on $\{1\bar{1}00\}$ planes. On the other hand, screw dislocations in α-alumina have not been studied as extensively as the basal edge dislocations. This is mainly due to difficulty in finding the screw dislocations generated intrinsically in experiment. Primary purpose of the present study is thus to perform a large-scale molecular dynamics computer simulation in order to elucidate the above mentioned discrimination between the edge and the screw dislocations by examining the structures and energetics of screw dislocations in alumina.

We employ a classical Molecular-Dynamics (MD) method for investigating the stability of dislocations in alumina. An empirical potential model for alumina, proposed by Vashishta *et al.*[3], is adopted for descriptions of interatomic forces. We have recently performed [4] a hybrid density-functional-theory/classical MD analysis on local atomistic and electronic structure of perfect dislocation core in alumina. The result showed that the structure predicted by the pure classical MD is qualitatively the same as that examined by the hybrid simulations, indicating the transferability of the empirical model. To reduce the computational cost spent for the present "over-million-atoms" simulation, we adopted a parallel algorithm based on the spatial domain-decomposition technique for calculating interatomic forces.

We examine perfect and partial dislocation energies and stable structure

involving four screw dislocations. The system size is 0.958 nm x 49.4 nm x 51.9nm involving 288,000 atoms. We compare energies between perfect and partial dislocation at 0 K. Figure 1 depicts potential energy (relative to the value for the perfect dislocation) in the system as a function of the partial-core distance. This indicates that the partial dislocation is an unstable structure, which is consistent with the experimental fact that has observed only perfect dislocation. As temperature is increased to 1000 K, the gradient of the slope in Fig. 1 is decreased. Preliminary results on the MD runs at higher temperatures indicate that the energies of the system with partial dislocations dissociated with 2.4 nm distance differ little from that of the perfect dislocation at 1300 K and 1600 K. Also, we employ variable-charge MD method (Es+model) proposed by Streitz and Mintmire [5] for investigating the stability of dislocations in alumina. In the presentation, effects of charge neutrality in the dislocation cores and of temperature on the stability of the dislocations in alumina will also be reported.

References

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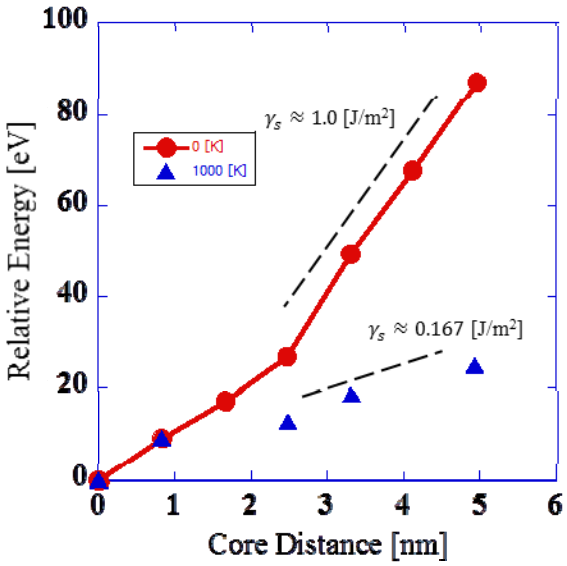

FIG. 1. Relative energy of the system as a function of distance between partial screw dislocations.