Possible Slip Systems in Body Centered Cubic Iron

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The slip systems along the (111) direction in bcc iron are investigated by the energy of the generalized stacking fault, or of the stacking fault between two adjacent crystallographic planes of perfect crystals, in order to obtain the knowledge of the slip phenomena in bcc single crystals. For systematic study, the 15 kinds of slip systems along the (111) direction from {110}(111) up to [954](111), [972](111) and [981](111) slip systems are taken into account. The energy of the stacking fault is evaluated by the molecular mechanics method with the embedded atom potential of Finnis-Sinclair type as a function of relative displacement of one side of the two half-crystals across the fault plane in the (111) direction. The maximum values of the fault energies for the slip systems whose slip planes have angles of less than approximately 15 degrees to the (110) plane are nearly as that for the most preferable [110](111) slip system. The maximum value for the [321](111) slip system is the greatest among the currently analyzed 15 slip systems. The maximum value for the [211](111) slip system is in the middle of those for the [110](111) and [321](111) slip systems, and those for the slip systems whose slip planes have angles between approximately 20 degrees and 30 degrees to the [110] plane are close to that for the [211](111) slip system. In general, there is not inverse correlation between the maximum value of the fault energy for the slip system and the interplanar spacing of the considered slip system, although there is inverse correlation between them within the three slip systems which have three lowest index planes, namely, the [110](111), [211](111) and [321](111) slip systems. [doi:10.2320/matertrans.47.1886]

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1. Introduction

It is confirmed that the observed slip lines of bcc metals are often wavy and ill-defined, and that slip occurs in the close-packed (111) direction, where the [110](111) slip system is most preferable. Moreover experimental observations are generally classified into two categories. The first type is that slip occurs in the (111) direction on [110], [211] and sometimes [321] planes,1-4 and the second one is that slip occurs in the (111) direction on maximum resolved shear stress planes or noncrystallographic planes.5-8 A common interpretation of these experimental observations described in the literatures on the theory of dislocations or the plastic deformation is as follows.9-12 The crystallographic slip planes are [110], [211] and [321] planes, and higher index planes could not become slip planes because the theoretical shear stress is inversely proportional to the interplanar spacing of the considered slip system. The wavy slip lines are indicating a result of cross slips of dislocations on different [110] planes or combinations of [110], [211] and [321] planes. However, some of the above literatures slightly refer to the slips on maximum resolved shear stress planes, and it seems to us that the existence of maximum resolved shear stress planes as slip planes cannot always be denied.

Meanwhile, one of semi quantitative indices of evaluation of the easiness of slip against shear stress is the energy of the generalized stacking fault, which corresponds to the potential energy for the theoretical shear stress, proposed by Vitek, who dealt with only {110} and {211} planes in bcc iron.13 Recently, an atomic level calculation of the fault energies for the {431}(111) slip system in bcc iron is reported, however the values do not show the asymmetry same kind of that between twinning and anti-twinning directions.14 Although an ab-initio calculation is performed for the [110](111) and [211](111) slip systems in bcc iron,15 at present, there is not systematic and reliable evaluation for the potential energy for the theoretical shear stress for slip systems.

It is the purpose of this paper to evaluate systematically the energy of the generalized stacking fault or the potential energy for theoretical shear stress for the slip systems along the (111) direction in bcc iron.

2. Method of Simulation

The energy of the generalized stacking fault γ is the energy of the stacking fault between two adjacent crystallographic planes of perfect crystals,15 and corresponds to the potential energy for the theoretical shear stress. In this calculation, the fault energy γ, whose unit is joule per square meter in the SI unit system, appears as a function of x (0 ≤ x ≤ 1) which is the relative displacement of one side of the two half-crystals across the fault plane in the (111) direction and normalized by the magnitude of the Burgers vector 1/2 · (111). Thus the values of x = 0 and x = 1 are equivalent. For systematic study, the 15 kinds of slip systems along the (111) direction, [110](111), [211](111), [321](111), [431](111), [532](111), [541](111), [651](111), [743](111), [752](111), [761](111), [853](111), [871](111), [954](111), [972](111) and [981](111) slip systems, are taken into account. The stereographic projection of their normals is shown in Fig. 1.

The atomic structure of the lattice with the generalized stacking fault is relaxed by the steepest decent molecular mechanics method with the embedded atom potential of bcc iron of Finnis-Sinclair type,16 which has the effects of the electronic charge distribution and is often used in simulations of surfaces and grain boundaries. The relaxation procedure is continued until the convergence of the total energy of the system is attained. The simulation system is composed of two coupled regions, namely, the computation region with the fault plane in the middle is inserted into the surrounding region.
frozen bulk regions. Two-dimensional periodic boundary condition is adopted in the directions parallel to the fault plane. The length of the computation region perpendicular to the fault plane is fixed to that for the perfect crystals in relaxation procedure. The numbers of atoms on each atomic layer in the computation region are taken approximately from 32 to 48, and the lengths of the computation regions perpendicular to the fault plane are taken approximately 2 nm, which means approximately 1 nm in each side across the fault plane. In the case of the \( (981) \{111 \} \) slip system, for example, the simulation system consists of 86 atomic layers with 32 atoms on each atomic layer, which is the largest size among the 15 slip systems evaluated here. The calculation is performed at intervals of 0.005 for the relative displacement \( x \).

3. Results

The graphs of the energy of the generalized stacking fault for the slip systems as a function of relative displacement of one side of the two half-crystals across the fault plane in the \( (111) \) direction are shown in Figs. 2(a) and (b). The order of the maximum values of the fault energies for the slip systems with the three lowest index planes is \( (110) \{111 \} < (211) \{111 \} < (321) \{111 \} \), as shown in Fig. 2(a). The maximum value for the \( (431) \{111 \} \) slip system is nearly same as that for the \( (110) \{111 \} \) slip system, the latter is the smallest among the 15 slip systems evaluated here, and besides the shape of the graph for the \( (431) \{111 \} \) slip system is similar to that for the \( (110) \{111 \} \) slip system. The graph for the \( (211) \{111 \} \) slip system shows the asymmetry of slip between twinning and anti-twinning directions. Similar asymmetries are observed in the cases of the \( (321) \{111 \} \) and \( (431) \{111 \} \) slip systems. The difference between the fault energies with and without optimization of the length of the computation region perpendicular to the fault plane, for example, for the \( (321) \{111 \} \) slip system at \( x = 0.4 \) is approximately 0.6%.

As an example for the slip systems with higher index slip planes, the graphs of the fault energy for several slip systems are shown in Fig. 2(b). The shapes of the graphs for the \( (752) \{111 \} \) and \( (981) \{111 \} \) slip systems are similar to that for the \( (110) \{111 \} \) slip system, and those for the \( (853) \{111 \} \) and \( (954) \{111 \} \) slip systems are similar to that for the \( (211) \{111 \} \) slip system. With respect to the slip systems not appeared in Figs. 2(a) and (b), the shapes of the graphs for the \( (541) \{111 \} \), \( (651) \{111 \} \), \( (761) \{111 \} \), \( (871) \{111 \} \) and \( (972) \{111 \} \) slip systems, whose slip planes have angles of less than 15° to the \( (110) \) plane, are similar to that for the \( (110) \{111 \} \) slip system. Those for the \( (532) \{111 \} \) and \( (743) \{111 \} \) slip systems, whose slip planes have angles between 20° and 30° to the \( (110) \) plane, are similar to that for the \( (211) \{111 \} \) slip system.

The maximum value of the fault energies for the slip system \( \gamma_{\text{max}} \) as a function of \( \theta \), the angle of the slip plane to the \( (110) \) plane, is shown in Fig. 3. The maximum fault energies for the slip systems whose slip planes have angles of less than approximately 15° to the \( (110) \) plane are nearly same as that for the most preferable \( (110) \{111 \} \) slip system, and those for the slip systems whose slip planes have angles between approximately 20° and 30° to the \( (110) \) plane are close to that for the \( (211) \{111 \} \) slip system. The maximum fault energy for the \( (321) \{111 \} \) slip system with angle of
19.1° to the \{110\} plane is the greatest among the currently analyzed 15 slip systems.

The maximum value of the fault energies for the slip system $\gamma_{\text{max}}$, as a function of $1/d$, where $d$ is the interplanar spacing of the considered slip system, is shown in Fig. 4. The maximum fault energies for the slip systems do not indicate inverse correlation with the corresponding interplanar spacing, although there is inverse correlation between them within the three slip systems which have three lowest index planes, namely, the \{110\}{111}, \{211\}{111} and \{321\}{111} slip systems.

4. Discussion

There are steep steps in the fault energies for the \{211\}{111}, \{321\}{111}, \{853\}{111} and \{954\}{111} slip systems in Figs. 2(a) and (b). At the foot part of the graphs, the interplanar spacing across the fault plane of relaxed structure is almost same as that of the perfect crystal and the strain parallel to the fault plane is shared with several layers across the fault plane. On the other hand, at the plateau part of the graphs, the interplanar spacing across the fault plane is expanded several percent compared to that of the perfect crystal and the strain parallel to the fault plane is concentrated on the fault plane only. This kind of expansion of interplanar spacing at interfaces is usually appeared in grain boundary structures. Here, we think that the steps in the fault energy is intrinsic, although there may be some effects by the shortness of the potential range and the transition of the initial configuration of neighboring atoms accompanied by the change of relative displacement.

The dislocations during the slip deformation may be subject to the energy field similar to the generalized stacking fault energy field, and a similar assumption is taken into the model of the Peierls-Nabarro stress. If we assume the maximum value of the fault energies to be an index for estimation of the easiness of slip, our results that the maximum fault energy for slip systems and the interplanar spacing have never been made. So we think that it is an open question whether the above expression for the theoretical shear stress in perfect crystals is inversely proportional to the interplanar spacing, can be applicable for metallic crystals with positive charged ions in the electron gas.

The calculation of the fault energy for two dimensional relative displacement parallel to the slip plane is now in progress. There may not be preferable slip systems around the \{111\}{110} slip system in fcc metals, for which similar calculation is under consideration.

5. Conclusion

The energy of the generalized stacking fault for the slip systems along the \{111\} direction in bcc iron is evaluated by the molecular mechanics method with the embedded atom potential of Finnis-Sinclair type as a function of relative displacement of one side of the two half-crystals across the fault plane. The 15 kinds of slip systems along the \{111\} direction from \{110\}{111} up to \{954\}{111}, \{972\}{111} and \{981\}{111} slip systems are taken into account.

The maximum value of the fault energies for the \{110\}{111} slip system is the smallest among the currently analyzed 15 slip systems, and that for the \{321\}{111} slip system is the greatest. Those for the slip systems whose slip planes have angles of less than approximately 15° to the \{110\} plane are nearly same as that for the most preferable \{110\}{111} slip system, whose maximum fault energy is in the middle of those for \{110\}{111} and \{321\}{111} slip systems. There is no inverse correlation between the maximum value of the fault energies for the slip system and the interplanar spacing of the considered slip system.

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