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INTERACTION BETWEEN LATTICE DISLOCATIONS AND GRAIN BOUNDARIES
IN F.C.C. MATERIALS

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Introduction

The interaction between dislocations and grain boundaries is generally believed to be of great importance to the mechanisms of mechanical failure in metals. Especially the difference between ductile and brittle fracture might be explained by variations in the way of interaction between dislocations and grain boundaries. In this paper we concentrate on the detailed phenomena, at the atomic level, which occur when extrinsic lattice dislocations impinge on the grain boundary. One of the topics of interest is the meaning of the well known structural unit model [1] for the interaction between dislocations and grain boundaries. The mechanisms for the interaction between dislocations and grain boundaries have to do with the DSC lattice [2]. A grain boundary dislocation has a Burgers vector which is a vector of the DSC lattice associated with the grain boundary. Its core may be associated with a step in the boundary plane. In general two mechanisms for the interaction between a lattice dislocation and a grain boundary can be discriminated. The first mechanism is referred to as dislocation absorption, which can be explained by the dissociation in the grain boundary plane of the lattice dislocation into DSC dislocations. As the Burgers vectors of the DSC dislocations are relatively small, the dislocation can reduce its energy in this way. The second mechanism for the interaction is referred to as dislocation transmission. A lattice dislocation in one grain can create another lattice dislocation in the other grain, usually leaving a residue at the boundary. The residue is always a DSC dislocation. A number of experimental studies of dislocation-grain boundary interactions has been carried out in the past. See e.g. ref. [3,4].

The description of the interaction between the long range stressfield of a dislocation and the short range field of a grain boundary with the help of elasticity theory is limited to larger separations. Atomistic simulation can help the study of details of absorption or transmission of dislocations by a grain boundary. The present research is a computer simulation study of the interaction between $1/2 [110]$ screw dislocations and $[110]$ symmetric tilt grain boundaries in f.c.c. materials. In this special case, transmission of the dislocation through the boundary can occur easily, as no residue is left in the boundary plane. In the simulations, no external stress is applied to the bicrystal, so that in this case low energy configurations of the combined system are found. In this setup, the tilt axis of the grain boundary is parallel to the dislocation line, preserving the periodicity along this direction of the combined system, which facilitates the computational procedure. Also, the displacement of the dislocation is not impeded by fixed boundary conditions.

Although from an elastic point of view no interaction between a pure tilt boundary and a pure screw dislocation can be expected, it is clear that there will be core interactions. In addition, the pure screw may split and then there will be elastic interaction with the edge components of the Shockley partial dislocations.

Method of Calculation

For the description of interatomic forces, a Finnis-Sinclair many-body potential representing copper [5] was used. First, the grain boundary was relaxed; the relaxation procedure was carried out at constant volume, using a standard gradient method; details are described elsewhere [1,6].

Secondly, a computational block for the relaxation of a dislocation near the grain boundary had to be constructed. The computational block of the relaxed grain boundary (which had translational symmetry in two directions) was extended, according to the periodicity of the CSL, in the direction perpendicular to the tilt axis, parallel to the boundary plane. A computational block of $40b \times 40b$ perpendicular to the tilt axis (where b is the size of the Burgers vector of the $1/2[110]$ screw dislocation), containing the relaxed grain boundary, was formed.

Next, the displacement field of the dislocation was imposed. Along the dislocation line, periodic boundary conditions were applied. The anisotropic elastic solution (as if there was only one grain present) was used for the boundary conditions perpendicular to the dislocation line. The dislocation-grain boundary relaxation procedure was carried out in the way which is normally used for dislocation relaxation and it utilized the same gradient method that was used for the grain boundary relaxation.

Results

All low-energy configurations that have been found for a boundary are given schematically in a figure showing the relaxed boundary structure (the symbols indicating the atom positions are drawn as if there was no dislocation present). Some examples of dislocation structures are depicted using the differential displacement method, see e.g. [7]. The method indicates the relative displacement of each atom with respect to its neighbours in a certain crystallographic direction. In our case, the direction along the dislocation line is chosen. If the absolute value of the relative displacement exceeds half of the periodicity of the lattice in that direction, an integer number times the period is added or subtracted. In these figures, the relative displacements are indicated by arrows and the symbols indicate the atom positions of the relaxed configuration. In the schematic figures, the regions where the differential displacements have a size between $0.30 a_0$ and $0.354 a_0$ (half the periodicity along the tilt axis) are indicated by lines; the regions where the differential displacements are between $0.15 a_0$ and $0.30 a_0$ are indicated by lobes (two lines parallel).

A number of boundaries in the misorientation range 31.59° to 50.48° were relaxed: the $\Sigma=27$ ($\bar{1}15$) ($\Theta=31.59^\circ$), the $\Sigma=9$ ($\bar{1}14$) ($\Theta=38.94^\circ$), the $\Sigma=57$ ($\bar{2}27$) ($\Theta=44.0^\circ$) and the $\Sigma=11$ ($\bar{1}13$) ($\Theta=50.48^\circ$). The results of the grain boundary relaxations compared well to the results of Sutton et al. [1] for Al. The same repetition of structural units along the boundary plane was found: respectively A.A($\Sigma=27$), AB($\Sigma=9$), ABBB($\Sigma=57$), B.B($\Sigma=11$), where the . indicates that the same unit is repeated with a translation of $1/4[110]$ along the tilt axis. See figs. 1, 3, and 5.

The DSC unit vectors of the $\Sigma=11$ and the $\Sigma=27$ boundaries are given in the columns of the two matrices shown below:

$$\begin{array}{cc}
 \Sigma=11 & \Sigma=27 \\
 1/22 \begin{pmatrix} \bar{3} & \bar{2} & 7 \\ 3 & 2 & 4 \\ \bar{2} & 6 & 1 \end{pmatrix} & 1/54 \begin{pmatrix} \bar{5} & \bar{2} & 16 \\ 5 & 2 & 11 \\ \bar{2} & 10 & 1 \end{pmatrix}
 \end{array}$$

For the two favoured boundaries, the $\Sigma=11$ and the $\Sigma=27$ and for the long period boundary, the $\Sigma=57$, an extensive investigation of the grain boundary-dislocation interaction was carried out, together with a study of the $\Sigma=9$ boundary. For the dislocation-grain boundary relaxation, it has to be emphasized that a large number of different initial configurations has to be discriminated, according to the periodicity of the boundary. Therefore, numerous relaxations were carried out with the elastic center of the dislocation at different positions

along the boundary period, a few lattice parameters away from the boundary plane. As the displacement field of an undissociated $1/2[110]$ screw dislocation was imposed, there were two different $\{111\}$ slip planes along which there could be interaction.

For the $\Sigma=27$ boundary four different configurations were found, that were all very similar in energy. All configurations showed splitting into two Shockley partials. One partial dislocation (the one further away from the boundary) had a core structure, similar to the core structure found for a lattice Shockley partial dislocation. The other had its core at the boundary plane with some spreading of the core into the other grain. The splitting occurred on the $(1\bar{1}1)$ plane as well as the $(\bar{1}11)$ plane. The configurations are shown in fig. 1. In addition, it was found that the strainfield caused by the dislocations was not distributed as homogeneously as is the case in perfect lattice. The differential displacements (which give an indication for the local strain) between the atoms at one specific site in the structural unit always were relatively large for each of the four configurations found. (See figure 2).

The $\Sigma=11$ boundary showed only one low energy configuration: (see fig. 3 and 4) the screw dislocation moved completely into the boundary and split into two DSC-dislocations; the $1/22[47\bar{1}]$ and the $1/22[741]$. The Burgers vectors of each of these two dislocations can be decomposed vectorially into two components; one component along the tilt axis and one component perpendicular to the tilt axis, in the boundary plane: $1/4[110] + 1/44[\bar{3}3\bar{2}]$ and $1/4[110] - 1/44[\bar{3}3\bar{2}]$, respectively. The two DSC dislocations cause a step in the boundary plane of $+0.30 a_0$ and $-0.30 a_0$ (+ and - one interplanar spacing) respectively, so that the condition of conservation of step height [8] is fulfilled. The two DSC dislocations moved about $3.5 a_0$ apart. This observation can be compared well with experimental observations of Mori and Tangri [9].

The configurations for the $\Sigma=57$ boundary are very similar to the configurations in the relaxations of the $\Sigma=11$ and $\Sigma=27$ boundaries. In the part of the boundary that can be described by $\Sigma=11$ units, the mechanism of absorption into the boundary and splitting into the two DSC dislocations mentioned above is observed again. The splitting was always limited to the $\Sigma=11$ region. If the core of one of the DSC's was at the separation between a $\Sigma=11$ and a $\Sigma=27$ unit, some spreading of the core into the $\Sigma=27$ unit could be observed. For the $\Sigma=27$ unit three of the four configurations for the $\Sigma=27$ boundary are found here again. The configurations are depicted in fig. 5 and one example in fig. 6. Also in this case some inhomogeneities in the strainfield could be observed: the values of the differential displacements were again relatively large at the same specific site in the $\Sigma=27$ units in the boundary plane as mentioned in the results for the $\Sigma=27$ boundary.

The $\Sigma=9$ boundary again showed configurations that were similar to the $\Sigma=11$ and $\Sigma=27$ boundaries. Although the boundary shows a repeating sequence of only one $\Sigma=11$ and one $\Sigma=27$ unit, the mechanism of absorption into the $\Sigma=11$ unit was observed here again; the splitting in the boundary plane was limited to the very narrow region of one $\Sigma=11$ unit. The occurrence of one extra configuration showed that there was some interference between the $\Sigma=11$ and the $\Sigma=27$ units.

Discussion and Conclusions

It can be concluded that there is an attractive force between boundary and dislocation core. For the $\Sigma=11$ boundary the tendency towards splitting into two DSC dislocations is evident: the dislocation can lower its energy by splitting, according to the b_2 criterion, and no fault is created between the partials. As the Burgers vector of both DSC's lies in the boundary plane, they should both be able to glide. From an elastic point of view the two DSC's would be expected to separate as far as possible. A possible explanation of the limited splitting in our simulations can be found in the occurrence of an equivalent of what is called the Peierls force for a dislocation moving through perfect lattice.

For the $\Sigma=27$ boundary an analogous mechanism could be envisaged: splitting into b_3 and $(b_3 + b_1)$. Although there is conservation of step height for this mechanism, the associated step in the boundary plane would be $0.7 a_0$ (4 interplanar spacings). As the Burgers vectors of both dislocations lie in the grain boundary plane, glide of both DSC dislocations should be possible. The gliding of the DSC's would require shuffling of atoms, which might impede dissociation. Instead, splitting into two Shockley partials is favoured, and one Shockley is attracted to the boundary. The attraction shows that the partial dislocation core can lower its energy by merging into the boundary core.

The structural unit model may help us to predict the interaction between the screw dislocation and the $\Sigma=57$ long period boundary if we know the interaction between the dislocation and the two delimiting favoured boundaries. Of course, the degree of splitting of the dislocation into two DSC dislocations (as occurred in the $\Sigma=11$ favoured boundary) would be limited, because the $\Sigma=11$ DSC's are not DSC's of the $\Sigma=27$ boundary and therefore cannot glide past the $\Sigma=27$ structural units without causing a fault in the $\Sigma=27$ units in the boundary plane. As the Burgers vectors of the two extrinsic DSC dislocations lie in the boundary plane and the Burgers vector of the intrinsic DSC dislocations describing the misorientation from $\Sigma=11$ ($\mathbf{b}=2/22[\bar{2}26]$) are almost perpendicular to the boundary plane, almost no interaction between these dislocations can be expected from an elastic point of view.

The interaction between a dislocation and the $\Sigma=27$ minority units in the $\Sigma=57$ boundary can be expected to show some differences with respect to the $\Sigma=27$ boundary, because the $\Sigma=27$ minority units in the $\Sigma=57$ boundary can be thought to contain the core of a secondary (intrinsic) DSC dislocation of this boundary; or, equivalently, the misorientation of the long period boundary matches the $\Sigma=11$ majority structural unit better than the $\Sigma=27$ minority structural unit.

The consequences of these results for the grain boundary-dislocation interactions during deformation are now discussed. For the $\Sigma=27$ boundary in this setup, transmission of dislocations can be expected. In this special case, the impinging dislocation can create a dislocation with equal Burgers vector in the other grain and absorption in the grain boundary is less favoured because of the step in the boundary plane that has to be created. Although transmission is also possible for the $\Sigma=11$ boundary, absorption by splitting into two DSC dislocations seems to be favoured because of the smaller associated step and because both DSC dislocations are able to glide in the boundary plane. Because both dislocations can glide, they can very easily reduce their strain field by moving apart and, in the case of extended slip, they can move away freely as the next dislocation is absorbed.

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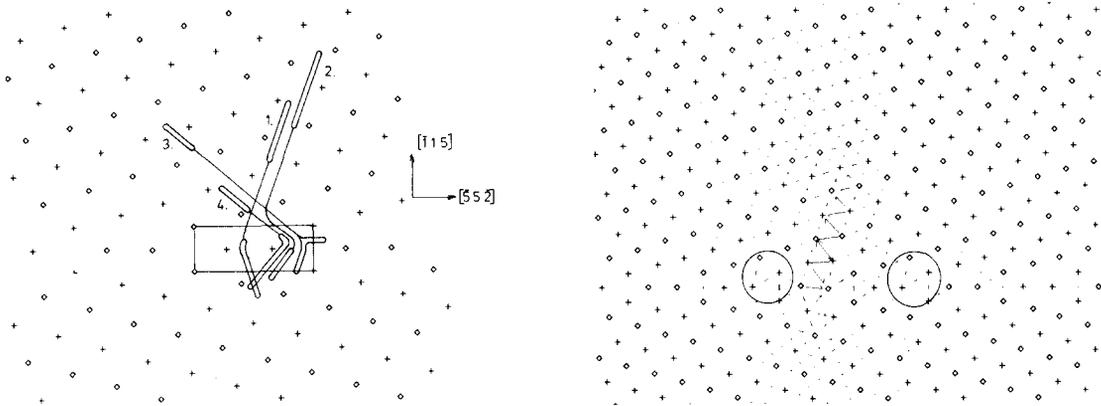


Fig. 1 (Left) The configurations found for the $\Sigma=27$ boundary. The symbols indicate atoms at different heights.

Fig. 2 (Right) Configuration nr. 1 from fig. 1. The symbols again indicate atoms at different heights. These are the heights of the atoms in the grain boundary, before the dislocation was imposed. The inhomogeneous strain distributions are indicated by circles.

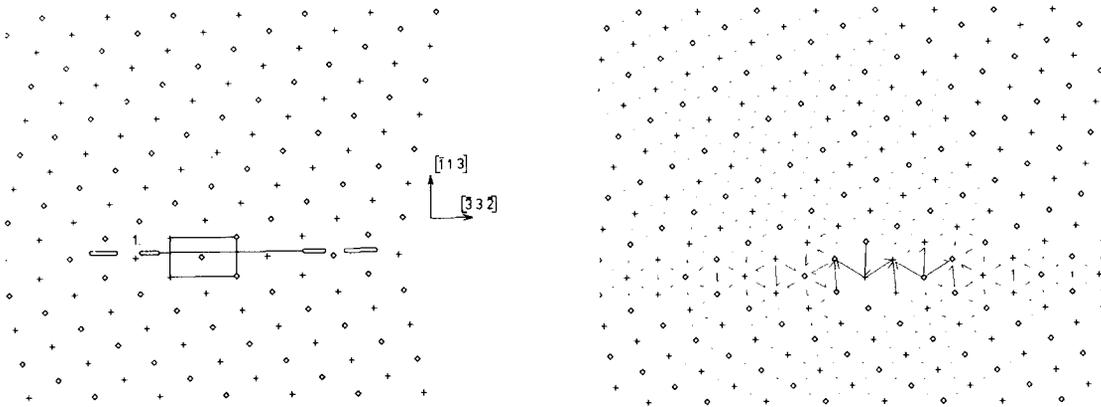


Fig. 3 (Left) The configurations found for the $\Sigma=11$ boundary.

Fig. 4 (Right) Configuration nr. 1 from fig. 3.

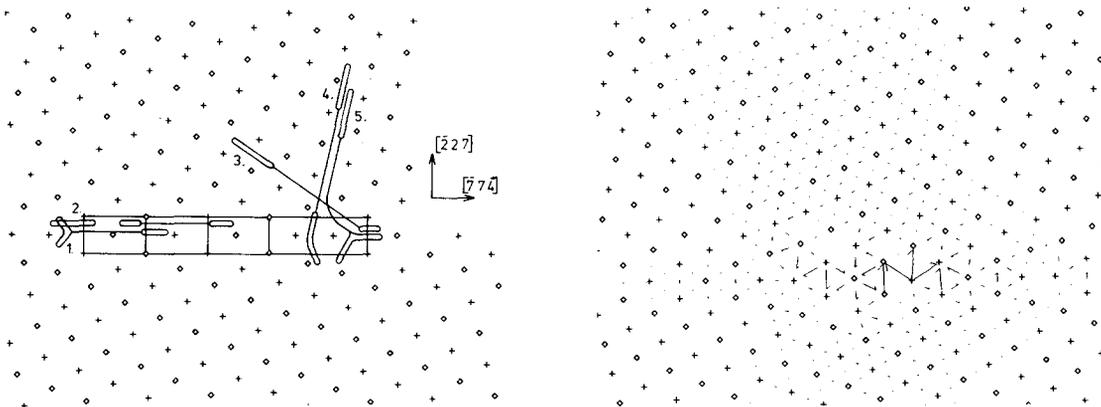


Fig. 5 (Left) The configurations found for the $\Sigma=57$ boundary.

Fig. 6 (Right) Configuration nr. 2 from fig. 5.