On the dissociation of dislocations in semiconductor crystals

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Abstract. An analysis of moving dissociated dislocations subjected to both a quasi-static viscous friction force and a periodic lattice resistance is performed: Metastable configurations are expected, the range of the dissociation distances being asymmetrically distributed with respect to the equilibrium dissociation distance. The data of earlier investigations on the influence of high external stress on the dissociation of dislocations in silicon and germanium, as determined by transmission electron microscopy, are re-examined. It is shown that in most cases the range of observed dissociation widths is consistent with the predictions of the model.

1. Introduction

From a theoretical analysis of the energy of dislocations that are not freely mobile in their dissociation plane, it was recently shown that metastable dissociations are expected [1]. The mean value of the measured partial separation may be higher than the equilibrium distance, as a consequence, the surface energy of the fault connecting the two partials may be underestimated.

In covalent materials such as semiconductors, dislocations are moving through a periodic Peierls-type potential. At low temperature dislocations in semiconductors align themselves along the low energy <110> Peierls valleys. Then perfect dislocations have either 60° or screw character and partial dislocations have either 90° or 30° characters, each with a specific atomic core structure.

In earlier studies [2, 3] the influence of high external stress on the dissociation of dislocations in Si and Ge was investigated by considering that, in addition to the applied forces, moving dislocations are subjected to a quasi-viscous friction force (proportional to their velocity). Then, measuring the dissociation widths under stress can give useful information on the mobilities of dislocations in these materials: it was concluded that partial dislocations have different mobilities, depending not only of their character (90° or 30°), but also on their position (leading or trailing) with respect to the dislocation motion. If the former point is readily explained by considering that 90° and 30° partials have different atomic core structure, the latter result is rather unexpected, because the core structure of a given partial does not depend on its position with respect to the stacking fault ribbon.

In this paper, we investigate the influence of the periodic Peierls-type lattice friction force. It is shown that metastable dissociation configurations are possible, the range of which is asymmetrically distributed with respect to the equilibrium dynamic dissociation distance. In most cases the range of observed dissociation widths is consistent with the predictions of the model. A main conclusion is that the mobility of a partial dislocation (which is defined as the ratio velocity/mean friction force) depends only of its character (30° or 90°) and not of its position (leading or trailing) with respect to dislocation motion.
2. Dynamic dissociation of dislocations

In a strained crystal each partial dislocation \( P \) and \( P_l \) (\( l \) and \( t \) means leading and trailing, respectively) experiences four forces (per unit length): (i) the attractive force exerted by the stacking fault ribbon (equal to the stacking fault energy \( \gamma \)), (ii) the repulsive elastic interaction \( kb^2/d \), with \( b \) the Burgers vector of the perfect dislocation, \( d \) the partial separation and \( k \) the interaction constant which depends on the elastic constants of the crystal and on the dislocation character, (iii) the glide component \( F_i \) (\( i = l \) or \( t \)) of the applied force, which causes the dislocation movement and (iv) a friction force \( R_i \) which opposes to the dislocation movement. According to Wessel and Alexander [2] \( R_i \) is proportional to the mean partial velocity \( v_i \), which defines the mobility \( M_i \) of the partial (\( v_i = M_i R_i \)). The dynamical dissociation width \( d_e \) is obtained by considering that in the stationary regime of velocity, the net force acting of each partial is 0. According to the present authors [4, 5] these results can be analysed by introducing an “effective” stacking fault energy \( \Gamma \), so that the elastic energy \( E \) (per unit length) of a dislocation dissociated in two partials separated by a distance \( d \) writes as:

\[
E = \Gamma d - kb^2 \ln d + \text{(self energy terms)}
\]

(1)

with \( \tau \) the stress component acting in the glide plane on the total dislocation, \( f = (F_l F_t)/tb \) a geometrical factor given by the orientation of the stress axis and \( \mu = M_l/M_t \) the mobility ratio. Then:

\[
d_e = kb^2 / \Gamma
\]

(3)

to be compared to the equilibrium dissociation width in the absence of applied forces \( d_0 \):

\[
d_0 = kb^2 / \gamma
\]

(4)

Then, according to [2, 3] the equilibrium dissociation width in stressed semiconductor crystals is determined not only by the orientation of the stress axis, but also by the ratio \( \mu \) of the mobilities of partial dislocations.

The previous analysis does not take into account the periodic character of the Peierls potential. Let us assume that each partial experiences, in addition to the previous forces, a periodic lattice friction which derives from a Peierls type potential. The corresponding energy can be simply described by a cosine function:

\[
-A_i \cos(2\pi x_i/h)
\]

(5)

where \( x_i \) are the coordinates of the partials \( P_i \) in the slip plane (\( h \) being the distance between the Peierls valleys) and \( A_i \) is temperature dependent (\( A_i \) is the depth of the Peierls potential at 0K, and \( A_i \) decreases as \( T \) increases). That means that the force which opposes to the dislocation movement is the sum of two terms: a mean friction force \( (R_i) \) and a periodically varying force.

The total energy \( E(x_i, x_t) \) of the dissociated dislocation is then (omitting the partials self energy terms which do not depend on the partial separation):

\[
E = \Gamma(x_l - x_t) - kb^2 \ln(x_l - x_t) - \Sigma A_i \cos(2\pi x_i/h)
\]

(6)

Minimising the energy function with respect to \( x_l \) and \( x_t \) and taking account of the balance of forces in the stationary state of steady motion, yields to the dissociation width \( d = (x_l - x_t) \).

When \( A_i = 0 \) (i.e. the Peierls friction is negligible), the partial separation is \( d_e = kb^2 / \Gamma \) (cf Eq. (3)); however when \( A_i \neq 0 \) there are several solutions and metastable dissociation configurations (each with a different energy \( E_m \)) are possible. It turns out that \( E_m \) is minimum for \( d = d_e \); i.e. the most probable dissociation distance (for which the total energy is minimum) is the one given by equation (3).

The range of metastable dissociation widths is controlled by the weakest Peierls valley\(^1\) so that, labelling \( A_m \) which of the two quantities \( A_i \) is the lowest one, one should have:

\[
-2\pi A_m / h \leq kb^2 / d - \Gamma \leq 2\pi A_m / h
\]

(7)

\(^1\) This point was dismissed in previous papers by the present authors [4, 5], where Equation (7) was wrongly written as:

\[
-\pi(A_i + A_j) / h \leq kb^2 / d - \Gamma \leq \pi(A_i + A_j) / h
\]
It is noteworthy that the range of possible dissociation widths is asymmetrically distributed with respect to $d_e$: it is shorter for $d < d_e$ than for $d > d_e$. Therefore the mean value of the measured partial separations may be higher than the equilibrium distance. Indeed, from equation (7):

$$d_{\text{min}} = d_e \frac{1}{1 + \frac{2\pi A_\text{m}}{\Gamma h}} \leq d \leq d_{\text{max}} = d_e \frac{1}{1 - \frac{2\pi A_\text{m}}{\Gamma h}}$$

(8)

Note that we have:

$$\frac{2\pi A_\text{m}}{\Gamma h} \frac{d_{\text{max}} - d_e}{d_{\text{max}}} = \frac{d_e - d_{\text{min}}}{d_{\text{min}}} = \frac{d_{\text{max}} - d_{\text{min}}}{d_{\text{max}} + d_{\text{min}}}$$

(9)

Equation (9) makes it possible to check the consistency of experimental data with the model: $d_{\text{min}}$ and $d_{\text{max}}$ are the limits of the metastable dissociation range (assuming that the whole dissociation range is detected experimentally); $d_e$ is identified as the most frequently measured dissociation distance $d_F$. Note that, although the range of metastable dissociation distances $d$ is asymmetrically distributed with respect to $d_e$, their inverse $1/d$ is symmetrically distributed with respect to $1/d_e$.

3. Are the experimental data consistent with the model?
The dislocation microstructure resulting from a two-step deformation process, the second step being a low temperature-high stress deformation regime, was investigated in [2, 3]:

- (a): Si, T = 420 °C; $\tau$ = 256 MPa;
- (b) Si P-doped Si (labelled Si(P)), $T = 360$ °C; $\tau$ = 296 MPa;
- (c) Ge, $T = 220$ °C ; $\tau$ = 294 MPa ;
- (d) Ge, $T = 220$ °C ; $\tau$ = 343 MPa

The histograms of experimental data present a rather wide scatter: Qualitatively consistent with the model, the asymmetry predicted by the previous analysis is noticed in more than half of the studied configurations (see Table 1): the range of observed dissociation widths ($d$) is larger for $d > d_F$ than for $d < d_F$, where $d_F$ is the most frequent dissociation distance. Consequently, the mean dissociation distance $<d>$ is higher than $d_F$. It should be pointed out that for each configuration, the number of dissociation distance measurements is relatively low (10-20), which could be insufficient to get a correct statistics. (For comparison, in the study on dissociation of superdislocations in the intermetallic alloy Ti$_3$Al, about 100 measurements were performed on a given configuration [6]).

More quantitative agreement could be obtained by checking if the experimental results are consistent with Equation (9). According to the predictions of the model, $d_F$ is put equal to $d_e$. Moreover we assume that the measured minimum and maximum dissociation distances, $d_{\text{min}}$ and $d_{\text{max}}$, respectively, are those corresponding to the limits of the dissociation range.

Table 1 shows the corresponding ratio for 60° dislocations: When the asymmetry with respect to $d_F$ is observed, the equalities (9) are reasonably well satisfied. (It should be keep in mind that the error bar on the dissociation distances measured by the TEM weak beam technique is at least of 0.5 nm, which leads to rather high relative error bars on $d_{\text{min}}$ ($d_{\text{min}} \approx 1-1.5$ nm); of course the incidence of this experimental uncertainty on $d_F$ and $d_{\text{max}}$ is less important). Similar agreement is noticed for screw dislocations.

So, most of the experimental data on dislocation dissociation in low-temperature highly stressed Si and Ge crystals are consistent with the occurrence of metastable configurations originating from the influence of the periodic Peierls potential. As a consequence, to determine the mobility ratio $\mu$ using equations (2, 3), one should use the most frequent dissociation width $d_F$ and not the mean experimental dissociation width $<d>$. This will be done in the next section.

4. The mobility of partial dislocations
Let us first consider the data on screw dislocations (dissociated into two identical 30° partials). It turns out that they can be interpreted in a consistent way without the assumption of different mobilities for leading and trailing 30° partials. Indeed putting $M_l = M_t$ (i.e. $\mu = 1$) in Eq. (2), leads to $d_F = d_e$ within the experimental errors [4, 5].
Table1. 60° dislocations: Comparison between the experimental data and the prediction of the model

| crystal (dislocation) | asymmetry/d_F | d_F - d'^min | d'_max - d_F | d'_max - d'^min |
|-----------------------|---------------|--------------|--------------|-----------------|
| Si^{30°/90°}          | yes           | (0 - 0.80)   | (0 - 0.57)   | (0.13 - 0.37)   |
| Si^{90°/30°}          | no            | /            | /            | /               |
| Si(P)^{(30°/90°)}     | no            | /            | /            | /               |
| Si(P)^{(90°/30°)}     | no            | /            | /            | /               |
| Ge^{30°/90°}          | yes           | (0 - 0.50)   | (0.40 - 0.67) | (0.25 - 0.50)   |
| Ge^{90°/30°}          | yes           | (0.33 - 1.5) | (0.44 - 0.60) | (0.50 - 0.67)   |
| Ge^{30°}(90°/30°)     | yes           | (0 - 1)      | (0.33 - 0.57) | (0.33 - 0.56)   |
| Ge^{90°}(30°/30°)     | yes           | (0.25 - 1)   | (0.50 - 0.62) | (0.50 - 0.63)   |

(a) (b) (c) (d): see text.

For 60° dislocations, let us assume again that the mobility of a given partial depends only of its character (30° or 90°) and not of its leading/trailing position. That means that the ratio (Equation (9) which depend only of A_m, should be the same for both kinds of 60° dislocations, (30°/90°) and (90°/30°), respectively. This is exactly what is observed in Ge (Table 1) for both sets of strained samples. This is a strong indication that the partial mobility depends only of its character and not on its leading/trailing position. (The comparison could not be made for Si since the data for (90°/30°) dislocations are not consistent with the model).

The mobility ratio μ can be estimated either by comparing d_0 (the dissociation distance in the absence of applied forces) and d_F (the most frequent dissociation distance in strained crystals). Unfortunately, stacking fault energies in elemental semiconductors are rather scattered amongst the available reports [7]. This, combined with the relative error bar on dissociation widths measurements leads to a rather rough estimate. One finds:

- Si: 3 ≤ M_{90}/M_{30} ≤ 6
- Ge: 1.5 ≤ M_{90}/M_{30} ≤ 5

5. Conclusion
Taking into account the periodic nature of the lattice friction in covalent materials leads to a possible range of metastable dissociated dislocation configurations. In the frame of this model, we have re-examined the literature data on the dissociation of dislocations in highly stressed elemental semiconductors. The main conclusion is that it is not necessary to postulate that the mobility of a Shockley partial depends on its leading/trailing position, to account for the experimental results.

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