Deformation slip and twinning in bulk and nanocrystalline semiconductors

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Abstract. Yielding and twinning in bulk and nanocrystalline semiconductors are considered based on the activation of perfect or partial dislocation loops. Assuming that the yield stress of the crystal is proportional to the critical stress necessary for the activation of a perfect Frank-Read source, it is shown that for a range of crystal orientations with respect to the applied shear stress, the Hall-Petch relationship for a silicon polycrystal fails when the average grain diameter is of the order of 3 nm or less. It is further shown that, assuming the double-cross-slip mechanism of twin formation in silicon, twinning is easier than slip for a range of crystal orientations in nanocrystals.

1. Introduction
The double-cross-slip mechanism of twinning, proposed in 1987 [1], arose out of two experimental observations about semiconductors. The first was that glide dislocations in all semiconductors that had been investigated up to then had been shown to be dissociated [2-4] and, secondly, the experiments of Wessel and Alexander [5] had indicated that the mobility of the leading and trailing partials in Si and in Ge [6] were different. This was quite unexpected because, unlike the case of compound semiconductors, where the core of partial (or perfect) dislocations can be different thus leading to so-called α and β dislocations with different dislocation velocities, the core of partial dislocations in elemental semiconductors is the same atom and one would not expect a mobility difference. It was thus interesting to see what difference the dissociation of dislocations and the difference in mobility of partials would make to the classical mechanism of Frank and Read [7] for dislocation multiplication that was based on the expansion of a pinned segment of perfect dislocation under the action of a shear stress \( \tau \) (figure 1). In particular, it was interesting to consider the case where the mobility of the leading partial was sufficiently larger than that of the trailing partial such that the former expands to the unstable semicircular position while the latter lags behind. This led to the interesting situation that the leading partial forms a faulted loop that surrounds the trailing partial. Clearly, as the leading partial – that is now behind the trailing partial – approaches the latter and the separation distance, \( d \), between them decreases, the repulsive force between the two partials increases rapidly thus preventing a recombination of the two partials into a perfect dislocation. However, even if such a recombination could occur, say under an immensely large stress, a second dissociation could not be envisaged because of the resulting high energy AA-type stacking configuration. In such a case, the applied stress \( \tau \) could not be relieved by the operation of the Frank-Read source and the latter would come to a stop after the formation of only one faulted loop. On the other hand, at the two pinning points X and X' (figure 1), the two partials are naturally recombined into a perfect dislocation.
One could thus envisage that if the perfect dislocation had a screw character, it would be able to relieve the applied stress $\tau_{lz}$ by double cross-gliding on the cross-slip plane (csp) and repeating the formation of a second faulted loop on a glide plane parallel to the original one. In fact this process could be repeated many times and $n$ faulted loops could form on $n$ parallel planes until the cross-slip stress is not enough for further double cross-glide of the screw dislocation. Assuming that these planes are all adjacent to one another, the result would be a twin band with a thickness $nd_{111}$ [1], where $d_{111}$ is the inter-planar spacing for the $\{111\}$ set of slip planes and $n$ is an integer. It was later realized [8] that the cross-slip stage of the twinning, could be described much more naturally and conveniently by the Escaig-Friedel [9-11] model. Also, since it was very likely that the mobility difference of partial dislocations would increase with decreasing temperature, it could be concluded that while nucleation and glide of perfect dislocations is the predominant mode of deformation at moderate to high temperatures in semiconductors, twinning would become more important at low temperatures or higher strain rates [1]. This model was actually more applicable to compound semiconductors because the core of two 30° partials of a screw dislocation are known to have different identities and their velocities can be appreciably different [12]. Further extension of this model could also explain polytypic transformation in SiC [13], and twinning in BCC crystals [14], basal [15-17] and rhombohedral [18] twinning in sapphire and in the Laves phases [19, 20].

2. Dislocation Plasticity of Semiconductors

Recently Estrin et al. [21] considered the role of Frank-Read sources in the plasticity of nanomaterials. Following the suggestion of other investigator [22, 23], these authors attributed the breakdown of the classical Hall–Petch relationship in nanocrystalline materials to a non-monotonic grain-size dependence of the required stress for the operation of Frank-Read sources. The length $\lambda$ of the source dislocation segment acting as the F-R source in figure 1 is assumed to scale with the grain size $d$, and the origin of this non-monotonic dependence is the logarithmic term in the self-energy or elastic energy, $E_{st}$, of a dislocation line of length $\lambda$, see e.g. Ref. [24, 25]:

$$E_{st} = \frac{Gb^2 \lambda}{4\pi(1-\nu)} \left[ \left(1 + \frac{\nu}{2} \cos^2 \theta - \frac{3\nu}{2} \sin^2 \theta \right) \ln \left(\frac{\lambda}{b}\right) + \left(2.0\nu\sin^2 \theta - 0.4\nu\cos^2 \theta\right) - 2.05 \right]$$  (1)

where $b$ is the magnitude of the dislocation Burgers vector and $G$ and $\nu$ are, respectively, the elastic modulus and Poisson’s ratio of the material. The line tension $T$ of the dislocation line is simply the self-energy per unit length of dislocation, i.e.:

$$T = \frac{dE_{st}}{dl} = \frac{Gb^2}{4\pi(1-\nu)} f(\lambda)$$  (2a)

where:

$$f(\lambda) = \left[1 - \frac{\nu}{2} \left(3 - 4\cos^2 \theta \right)\right] \ln \left(\frac{\lambda}{b}\right) - 1 + \frac{\nu}{2}$$  (2b)
Figure 1. Straight dislocation segment AB with line direction ξ and Burgers vector b bows out under the action of the resolved shear stress $\tau_{z\varphi}$ that makes an angle $\varphi$ with respect to the dislocation line direction lying in the plane of the paper, normal to the $z$-axis.

According to the Peach-Kohler equation [26], the glide force $F_g$ per unit length of a dislocation with line direction ξ and Burgers vector b caused by the stress tensor $\sigma$ is [25]:

$$F_g = \frac{[(b \cdot \sigma) \times \xi] \cdot [\xi (b \times \sigma)]}{|b \times \xi|}$$  \hspace{1cm} (3a)

If we denote the shear stress component of the stress tensor acting at an angle $\varphi$ to the dislocation line direction by $\tau_{z\varphi}$ (figure 1), this equation reduces to:

$$F_g = \tau_{z\varphi} b (\sin \theta \sin \varphi + \cos \theta \cos \varphi)$$  \hspace{1cm} (3b)

where $\theta$ is the angle between the Burgers vector b of the source dislocation segment and ξ (figure 1). Note from Eq. (3b) that the glide force on a screw dislocation segment is zero when $\varphi = 90^\circ$.

Under the applied shear stress $\tau_{z\varphi}$, the pinned dislocation segment bows to a radius of curvature $r$ subtending an angle $\vartheta$ at O (figure 1), a process that increases the dislocation length – from AB to ACB - and thus its line tension $T$. The bow out of the dislocation line is also opposed by the lattice resistance, or Peierls stress $\tau^p$, given by [25]:

$$\tau^p = \frac{2G}{K} \exp \left[ - \frac{2\pi d_{111}}{Kb} \right]$$  \hspace{1cm} (4)

where $d_{111}$ is the interplanar spacing of the {111} set of slip planes in semiconductors; in this equation, $K \approx 1$ for a dislocation with a screw character and $K = 1 - \nu$ for one with an edge character [25].

Thus, balancing the bow-out force $F_g$ with the opposing forces due to the line tension $T$ and the Peierls stress $\tau^p$, we get (figure 1):

$$F_g = \frac{T \sin \vartheta}{r} + b \tau^p$$  \hspace{1cm} (5)

Substituting (2a), (3b) and (4) in Eq. 5 gives the radius of curvature of the bowed out segment under the resolved shear stress $\tau_{z\varphi}$:

$$r = \frac{Gb \sin \vartheta}{4\pi (1 - \nu) \tau_{z\varphi} (\sin \theta \sin \varphi + \cos \theta \cos \varphi - \tau^p)} f(\lambda)$$  \hspace{1cm} (6)
Clearly as the stress $\tau_{z\phi}$ increases, the radius of curvature $r$ of the bowed-out segment decreases until the pinned dislocation segment attains a semi-circular shape (ADB in figure 1) at which point it becomes unstable leading to the formation of a loop and re-generation of the original straight dislocation segment [25]. Thus the critical stress $\tau_{z\phi}^*$ required to form an unstable configuration is obtained by the condition $2r = \lambda$ at $\phi = \pi/2$, i.e.

$$\tau_{z\phi}^* = \frac{1}{\sin \theta \sin \phi + \cos \theta \cos \phi} \left[ \frac{Gb}{2\pi(1-\nu)} \lambda f(\lambda) + \tau^p \right]$$

(7)

$\tau_{z\phi}^*$ is plotted for silicon as a function of $\lambda$ and $\phi$ in figure 2; in these calculations, it is assumed that $G = 52$ GPa and $\nu = 0.28$.

As expected, $\tau_{z\phi}^*$ is a minimum along the line where the applied stress is parallel to the Burgers vector $b$, i.e. when $\phi = 0^\circ$. Notice that $\tau_{z\phi}$ increases with decreasing source length (Hall-Petch effect) but reaches a maximum in the small nanometer length scale after which it decreases. This is more clearly shown in figure 3, which is a section of the three-dimensional plot at $\phi = 0^\circ$.

Assuming that $\lambda$ scales with the average grain size diameter $d$ and that the yield stress of polysilicon varies as $\tau_{z\phi}$, figures 2 and 3 show that - similar to polycrystalline metals [21] - its yield stress goes through a maximum. For silicon, this occurs at $\lambda = 2.22$ nm, indicating that for a silicon polycrystal with a grain size smaller than 2.22 nm, the inverse Hall-Petch relationship holds and the crystal softens as the grain size become smaller. According to this figure, the stress required to activate a Frank-Read source in bulk silicon is about 17 MPa. This stress increases to about 2.6 GPa at $\lambda = 2.22$ nm before it starts to decrease. The large stress value is not surprising considering the calculations do not take temperature into account, i.e. they are 0 K calculations.
Figure 3. Variation of the critical resolved shear stress $\tau^*_{op}$ required to activate a perfect screw dislocation loop from a Frank-Read source as a function of $1/\sqrt{\lambda}$ when the stress acts in a direction parallel to the dislocation line direction (i.e., $\theta = \phi = 0^\circ$ in figure 1).

3. Deformation twinning in semiconductors

Let’s use the same methodology as in section 2 to study the effect of the source length in the double cross-slip model of twinning [1]. The source dislocation segment now has a screw character and is dissociated into two $30^\circ$ partials with Burgers vectors $b_l$ and $b_t$ making angles of $\theta_l$ and $\theta_t$ with respect to their line direction $\xi$ (the sub/superscripts $l$ and $t$ denote leading and trailing, respectively). We shall again assume that the applied shear stress makes an angle $\phi$ with respect to $\xi$ (figure 4). As before, both partial dislocations bow out under the action of the applied shear stress, but since the Burgers vectors of the two partials, $b_l$ and $b_t$ are different (even though $b_l = b_t$), they bend to different radii $r_l$ and $r_t$.

We can now write a similar equation to (5) except that we need to incorporate the forces exerted by the stacking fault energy $\gamma$, generated by the leading partial dislocation, and the interaction force $F_{lt}$ between the two partials. The latter is given by [27]:

$$F_{lt} = \frac{G b_l b_t}{2\pi d} \left[ \cos \theta_l \cos \theta_t + \frac{\sin \theta_l \sin \theta_t}{1 - v} \right]$$

(8)
The force balance for the two partials is as follows [27, 28]:

- for the leading partial:

\[ F_g + F_u = \frac{\sin \vartheta}{r_i} T + \gamma + \tau^l_i b_l \]  

(9a)

i.e.,

\[ \tau^l_i b_l \left( \sin \theta_i \sin \phi + \cos \theta_i \cos \phi \right) + \frac{G b_p^2}{2 \pi d} \left( \cos \theta_i \cos \theta_i^l + \frac{\sin \theta_i \sin \theta_i^l}{1 - \nu} \right) = \frac{G b_l^2 \sin \vartheta}{4 \pi (1 - \nu) r_i} f_l \left( \lambda \right) + \gamma + \tau^l_i b_l \]

(9b)

- for the trailing partial:

\[ F_g + \gamma = \frac{\sin \vartheta}{r_i} T + F_u + \tau^r_i b_i \]

(10a)

i.e.,

\[ \tau^r_i b_i \left( \sin \theta_i \sin \phi + \cos \theta_i \cos \phi \right) + \gamma = \]

\[ \frac{G b_l^2 \sin \vartheta}{4 \pi (1 - \nu) r_i} f_l \left( \lambda \right) + \frac{G b_p^2}{2 \pi d} \left( \cos \theta_i \cos \theta_i^l + \frac{\sin \theta_i \sin \theta_i^l}{1 - \nu} \right) + \tau^r_i b_i \]

(10b)

where \( r_i \) and \( r_t \) are the radii of curvature of the leading and trailing partials, \( b_l = b_t = b_p \), and \( f_l(\lambda) \) and \( f_t(\lambda) \) are the same as Eq. (2b) with the Burgers vector of the dislocation replaced by \( b_l \) or \( b_t \).

Solving for \( 2r_t = \lambda \) and \( 2r_t = \lambda \), when \( \vartheta = \pi/2 \), we get the critical resolved shear stresses \( \tau^*_{cp} \) and \( \tau^*_{cp} \) for activating the leading and trailing partials, respectively:

\[ \tau^*_{cp} = \frac{1}{b_t \left( \sin \theta_i \sin \phi + \cos \theta_i \cos \phi \right)} \times \left\{ \frac{G b_t^2}{2 \pi \lambda (1 - \nu) f_l \left( \lambda \right)} + \frac{G b_p^2}{2 \pi d} \left( \cos \theta_i \cos \theta_i^l + \frac{\sin \theta_i \sin \theta_i^l}{1 - \nu} \right) - \gamma + \tau^r_i b_i \right\} \]

(11a)

and:

\[ \tau^*_{cp} = \frac{1}{b_t \left( \sin \theta_i \sin \phi + \cos \theta_i \cos \phi \right)} \times \left\{ \frac{G b_t^2}{2 \pi \lambda (1 - \nu) f_l \left( \lambda \right)} - \frac{G b_p^2}{2 \pi d} \left( \cos \theta_i \cos \theta_i^l + \frac{\sin \theta_i \sin \theta_i^l}{1 - \nu} \right) + \gamma + \tau^l_i b_l \right\} \]

(11b)

A 3D plot of the critical resolved shear stresses \( \tau^l_{cp} \) and \( \tau^r_{cp} \) to activate the leading and trailing partials, respectively, is presented in figure 5.
Figure 4. Bow out of pinned leading and trailing partial dislocation sources under an applied shear stress $\tau_{\phi}$. Under this stress, the leading and trailing partials with Burgers vectors $\mathbf{b}_l$ and $\mathbf{b}_t$ expand to radii $r_l$ and $r_t$, respectively.

Figure 5. Variation of the resolved shear stresses, $\tau_{l\phi}^*$ and $\tau_{t\phi}^*$, required to activate the leading (blue – light - surface) and trailing partial (red – dark - surface) dislocation loops, respectively, from a dissociated dislocation source as a function of $1/\sqrt{\lambda}$ (where $\lambda$ = source length) and $\phi$ (angle between the direction of the applied stress with the dislocation line direction). For clarity, the surface for the perfect dislocation is not shown in this figure.

Note that in different regions of the plot $\tau_{\phi}^*$ may be larger than $\tau_{l\phi}^*$ or vice versa, i.e. whether $\tau_{\phi}^* > \tau_{l\phi}^*$ or, conversely, $\tau_{l\phi}^* > \tau_{t\phi}^*$ depends on the source length $\lambda$ and the direction of the applied shear stress with respect to the source dislocation $\xi$ - this is because as $\phi$ is varied, the angles between the direction of...
the applied stress $\tau_{z\phi}$ and the partial Burgers vectors $b_l$ and $b_t$ vary. In particular, when the applied shear stress is parallel to the Burgers vector of the leading partial, $\tau_{zl\phi}$ is much smaller than both $\tau_{zt\phi}$ and the critical stress required for activation of a perfect F-R loop. Under such conditions, twinning is favoured over slip. This is shown in the 2D plot of figure 6 where $\varphi = \theta_l = 30^\circ$.

![Figure 6](image_url)

**Figure 6.** Variation of the critical resolved shear stresses, $\tau_{zl\phi}$ and $\tau_{zt\phi}$, and $\tau_{pz\phi}$, required to activate the leading partial (continuous dark line - blue), trailing partial (continuous light line - purple), and perfect (dashed line - yellow) dislocation loops, respectively, from a Frank Read source as a function of $1/\sqrt{\lambda}$ (where $\lambda$ = source length) when the shear stress is parallel to $b_l$ ($\varphi = \theta_l = 30^\circ$). Note that under this condition, twinning is favored at all length scales (elasticity equations, upon which the above figures are based, are not valid when $\lambda$ has atomic scale dimensions, say below 1 nm).

A number of approximations have been used in our calculations that can be improved in future work. As an example we have taken the separation distance $d$ between the two partials to stay constant at the equilibrium separation $d_{eq}$. This effectively eliminates the two terms $\gamma$ and $F_{lt}$ from equations (9a) and (10a). In reality, as $d$ increases, the repelling force between the two partials, $F_{lt}$, decreases while the attractive force due to the stacking fault energy $\gamma$ does not change.

4. Conclusions

The critical stress for the activation of a pinned segment of perfect and dissociated dislocation in silicon has been evaluated as a function of the source length $\lambda$ and the angle $\varphi$ between the applied stress and the dislocation line. For different values of $\varphi$ and the source length, initiation of either perfect dislocation or the leading partial dislocation is favored. In the first case, this leads to plastic deformation by slip while in the second case, the first stage of twinning by the mechanism of double cross-glide is satisfied. The variations of the critical stress with the source length indicates that while the crystal strengthens with decreasing grain size for bulk polycrystals of silicon (the Hall-Petch relationship), softening of the crystal can occur when the dimensions of the grain is in the small nanoscale regime. Moreover, for a wide range of stress orientations, the critical resolved shear stress for activation of the leading partial dislocation, $\tau_{zl\phi}$, is much less than that required for the activation of
the trailing partial, $\tau^*_t z^*$, or for the perfect dislocation $\tau^*_P z^*$, indicating that in such orientations, twinning is favored. Moreover, the stress difference $\tau^*_t - \tau^*_P$ increases with decreasing grain size indicating that twinning is generally more likely in nanocrystals than in bulk silicon.

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