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Stability of a Screw Dislocation in a $\langle 011 \rangle$ Copper Nanowire

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The stability of a screw dislocation in a free $\langle 011 \rangle$ copper nanowire is investigated using atomistic calculations. This study reveals a strong anisotropy of the Eshelby potential well (EPW) that traps the dislocation. Moreover the depth of the EPW is found to vanish when the radius of the nanowire decreases. It is demonstrated that this behavior is due to the dissociated state of the dislocation.

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Axial screw dislocations may appear in metal nanowires either during growth [1] or under mechanical loading [2]. Understanding the stability of these defects in such small objects is of fundamental interest. The case of a single perfect screw dislocation in an isotropic cylinder was addressed by Eshelby with a well-known solution based on the elasticity theory [3,4]. This solution should, however, be revisited in the case of metal nanowires where additional ingredients are to be considered. First, face-centered-cubic (fcc) crystalline nanowires preferentially grow along a $\langle 011 \rangle$ orientation [5] and therefore require an anisotropic description of the energetic barrier that stabilizes the screw dislocation. Second, in such fcc nanowires, the screw dislocation is made of two parallel Shockley partial dislocations separated by a distance that may be comparable to the diameter of the wire. If the latter has no effect on the energetic barrier in the classical theory, its influence remains unknown at the nanoscale. It is the aim of this work to study both this size effect and the influence of the anisotropy on the energetics of the Eshelby dislocation by performing atomistic simulations of copper nanowires which currently attract lots of attention [6].

In his pioneering article [3], Eshelby shows, using isotropic elasticity, that a screw dislocation can occupy a metastable state along a wire by causing its torsion. This so-called Eshelby twist that was observed afterwards in whiskers [7] reappears today more dramatically in nanowires [8–10], a smaller radius producing a larger twist [11]. To leave its metastable state and reach the lateral surface of the wire, the screw dislocation (parallel to the cylindrical wire axis) must overcome an energy barrier whose maximum is located roughly halfway and whose height does not depend on the radius of the wire in the isotropic theory. This barrier is illustrated in Fig. 1 with the case of a fcc copper wire having the $\langle 100 \rangle$ orientation and a circular cross section of radius $R = 30$ nm. The variation of the elastic strain energy of the wire ΔE (per unit length) is plotted as a function of the relative position $x = \xi/R$ of the screw dislocation. According to Eshelby's original derivation ΔE writes

$$\Delta E = E^d \ln(1 - x^2) - E^t x^2 (x^2 - 2), \quad (1)$$

where $E^d = E^t = C_{44}^0 b^2 / (4\pi)$ for this $\langle 100 \rangle$ orientation that behaves isotropically. b is the magnitude of the Burgers vector equal to the lattice parameter $a = 3.62$ Å for this orientation and $C_{44}^0 = 82$ GPa is the shear elastic constant. In Eq. (1), the first term is due to both the screw dislocation and its image that is located at the position R^2/ξ to cancel the traction on the lateral free surface. The second term in Eq. (1) comes from the Eshelby twist $\alpha_E = b(1 - x^2)/(\pi R^2)$ of the wire that is necessary to cancel the torque induced by the screw dislocation. In terms of forces, the image force tends to drive the dislocation out of the cylinder while the torsion tends to attract the dislocation at the center. In the isotropic case, the energy core of the dislocation is considered as constant with ξ/R and has no role on ΔE . In Fig. 1, ΔE is also recovered by performing atomistic simulations with a tight-binding potential that mimics the interactions between copper atoms. Details on the simulations are given in Ref. [11] and in the Supplemental Material [12]. In the present work, the molecular statics (MS) calculations are

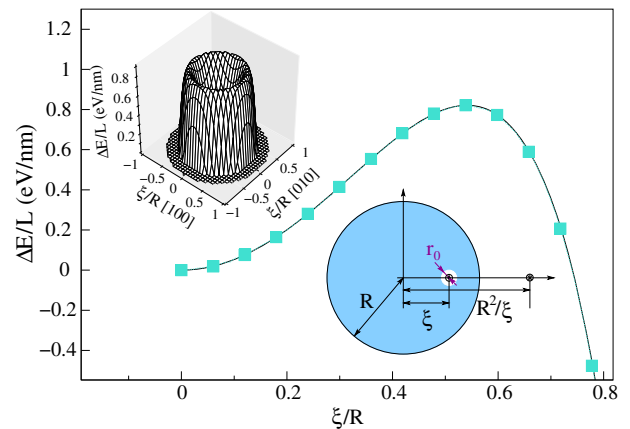


FIG. 1 (color online). Isotropic Eshelby potential well that stabilizes the perfect screw dislocation in a $\langle 100 \rangle$ nanowire of radius $R = 30$ nm. The energy ΔE per unit length is plotted as a function of the position $x = \xi/R$ from either the elasticity theory using (solid line) Eq. (1) or (square) our MS atomistic simulations. In the latter, a small cylinder of radius $r_0 = 1$ nm containing the dislocation core is excluded.

performed to simulate an infinite twisted copper nanowire containing a perfect screw dislocation that is located at different ξ/R positions from the center. MS simulations directly give access to the elastic strain energy and the fully relaxed positions of each atom in such nanowires. Figure 1 shows that for this orientation the MS simulations agree very well with the prediction made by Eshelby. The dislocation is in a metastable equilibrium at the center, being trapped in a potential well of depth $E^t(1 - \ln 2)/2$ and radius $x^{\max} = \sqrt{1 - 1/\sqrt{2}} = 0.54$ for any R as expected in the classical theory.

For a real $\langle 011 \rangle$ fcc metal nanowire, two important properties might change Eshelby's conclusions on the stability of a screw dislocation. First, the two-fold symmetry of a $\langle 011 \rangle$ axis leads to an anisotropy of the shear modulus that controls the depth of the potential well. Second, in metal, the perfect $\langle 011 \rangle$ screw dislocation dissociates into two Schockley partials separated by a distance that can be significant in comparison to the radius of the nanowire [4]. Figure 2 shows a typical snapshot resulting from our simulations. Initially, a perfect screw dislocation parallel to the wire axis, with Burgers vector $\mathbf{b} = 1/2a[011] = 2.56 \text{ \AA}$, is created at a given distance ξ and direction. Then during the quenched molecular dynamics, the screw dislocation first dissociates into two Schockley partials in a $\{111\}$ plane separated by a stacking fault whose width 2δ is around 14 \AA for large radii. Then, a second relaxation regime is observed where the two partials glide together in the $\{111\}$ slip plane. Depending on its initial position and the wire torsion, the pair of partial dislocations either reaches a metastable state near the center or moves out of the nanowire. During this stage, the kinetic energy of the system can be neglected in comparison with the searched well potential. The torsion α is dynamically adjusted according to the instantaneous positions of the partials. For this purpose, the above expression of α_E can be used for each partial dislocation since it remains valid for

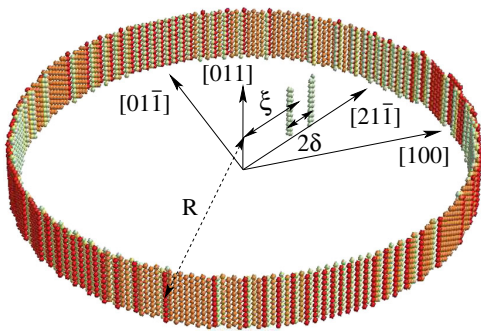


FIG. 2 (color online). Typical nanowire (slice) studied in this work using atomistic simulations. A free $\langle 011 \rangle$ crystalline nanocylinder of copper (here of radius $R = 10 \text{ nm}$) contains a pair of Shockley partial dislocations. Only copper atoms with high energy are shown, revealing a screw dislocation dissociated in a $(1\bar{1}1)$ plane containing the wire axis.

the present anisotropic case of a circular cylinder [17]. Thus, for a mean relative position x , the torsion α now writes

$$\alpha = b[1 - x^2 - (\delta/R)^2]/(\pi R^2), \quad (2)$$

where the separation distance 2δ tends to reduce α . Values of α given by Eq. (2) are confirmed by our MS simulations.

By performing a large set of MS simulations, we obtained the map of the Eshelby potential well for a $\langle 011 \rangle$ copper wire containing the dissociated dislocation. The case of a large radius ($R = 30 \text{ nm}$) is first shown in Fig. 3. Clearly, the potential well exhibits a strong anisotropy with a barrier that is maximum along the $[01\bar{1}]$ direction and roughly 3 times smaller in the perpendicular $[100]$ direction. The position of the maximum x^{\max} also varies with the direction. Along $[100]$, the potential well is significantly closer to the center ($x^{\max} \approx 0.43$) while along $[01\bar{1}]$ it is higher ($x^{\max} \approx 0.58$) than the isotropic value. Interestingly, the ΔE curves obtained for large R in Fig. 3 can be reproduced quite well by using again the expression of Eq. (1) with a term E^d that now varies directionally. The latter is the only parameter which has to be adjusted since in Eq. (1) the coefficient E^t related to the torsion is known $E^t = C_{44}C_{55}b^2/[(C_{44} + C_{55})2\pi]$ and takes the value $E^t = 1.36 \text{ eV/nm}$ [11]. The agreement between Eq. (1) and our simulations shown in Fig. 3 is obtained for $E^d = 1.18 \text{ eV/nm}$ along $[01\bar{1}]$ and $E^d = 1.79 \text{ eV/nm}$ along $[100]$. Furthermore, the 2D potential well resulting from the simulations is fairly well fitted using a $\sin 2\theta$ dependence of E^d , where θ is the azimuth of the dislocation. Within this simple formulation, it is also convenient to express the maximum height in the form

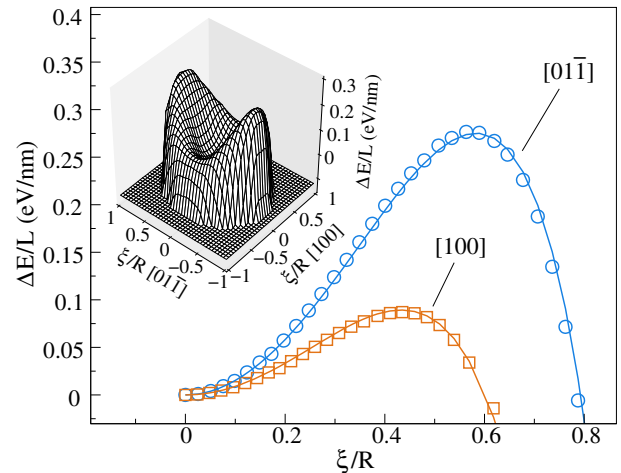


FIG. 3 (color online). Molecular statics calculation of the full 2D (inset) Eshelby potential well of a screw dislocation in a free $\langle 011 \rangle$ crystalline cylinder of copper with large radius $R = 30 \text{ nm}$. Profiles along the two main $[100]$ and $[01\bar{1}]$ directions are plotted according to our MS simulations (symbols) and modeled using Eq. (1) (solid lines).

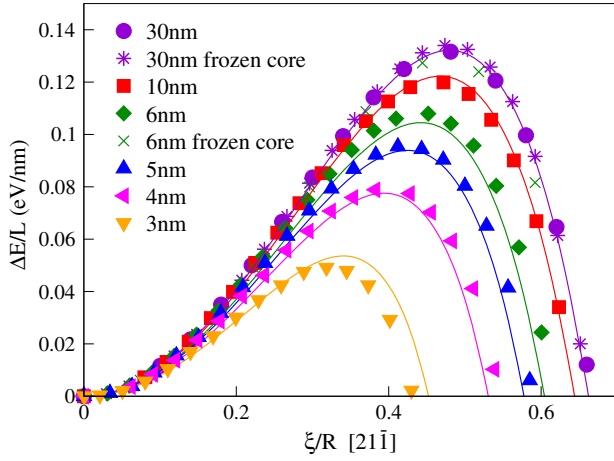


FIG. 4 (color online). Eshelby potential wells along the $[21\bar{1}]$ direction obtained from our MS simulations (symbols) in free $\langle 011 \rangle$ copper nanowires of different radii $R = 3, 4, 5, 6, 10$, and 30 nm containing a $b = 1/2a[011]$ screw dislocation. The decrease of the Eshelby barrier happens only when the dislocation is dissociated into two Shockley partials and for $R < 30$ nm. This is shown by considering frozen dislocation cores for $R = 6$ and 30 nm. The solid lines are given by our model expressed in Eq. (7).

$$\Delta E^{\max} = E' [2\beta^2 \ln \beta + (1 - \beta^2)] \quad (3)$$

and the radius $x^{\max} = \sqrt{1 - \beta}$ with $\beta = \sqrt{E^d / (2E')}$. Thus, for a given E' and $E^d < 2E'$, the barrier decreases and moves to the center when E^d increases.

In order to quantify a possible size effect on the stability of the pair of partial dislocations we focus our analysis along the $[21\bar{1}]$ direction imposed by one of the two $\{111\}$ gliding planes containing the nanowire axis. Different radii are considered in Fig. 4 with R ranging from 3 to 30 nm. Clearly the pair of dislocations is less stable in small nanowires. Both the depth of the potential well and the position of its maximum x^{\max} decrease markedly when R decreases. Moreover, our simulations show that this nano-size effect is directly due to the dissociated state of the screw dislocation. Indeed in Fig. 4, if one prevents the dissociation by freezing the dislocation core as in the previous isotropic case, the energetic barrier becomes invariant with R . This effect vanishes for $R = 30$ nm where allowing (or not allowing) the dissociation gives similar results.

We now wonder how to rationalize this decrease of the Eshelby barrier for small nanowires. How can the depth of the potential well for a pair of partial dislocations be smaller than the one obtained for a single perfect screw dislocation having an equivalent Burgers vector? To study this influence of the dissociation mechanism one needs to estimate the different forces acting on each partial dislocation. Only dislocation Volterra fields are considered [12] and surface stress effects are neglected [11]. To simplify further we assume that the only effect of anisotropy is contained in E^d and we use the isotropic elasticity theory of dislocations.

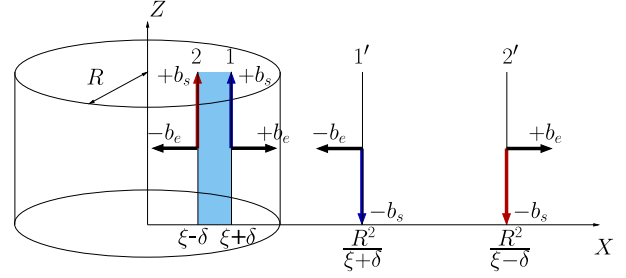


FIG. 5 (color online). The two partial dislocations have equal and opposite edge Burgers vector components ($+b_e$ for the dislocation 1 at $\xi_1 = \xi + \delta$ and $-b_e$ for the dislocation 2 at $\xi_2 = \xi - \delta$) and equal screw components, $b_s = b/2$. To model the Eshelby barrier, we simplify the problem to the case of an isotropic circular cylinder where two image dislocations $1'$ and $2'$ are needed at $\xi_{1'} = R^2/\xi_1$ and $\xi_{2'} = R^2/\xi_2$ to cancel the traction on the lateral surfaces.

In this framework the considered configuration is shown schematically in Fig. 5 to define all the quantities of interest. The two partial dislocations have equal and opposite edge Burgers vector components ($+b_e$ for the dislocation 1 at $\xi_1 = \xi + \delta$ and $-b_e$ for the dislocation 2 at $\xi_2 = \xi - \delta$) and equal screw components, $b_s = b/2$. In the isotropic case, image dislocations and image forces are well described in the literature [18]. The Burgers vectors and the expected positions $\xi_{1'}$ and $\xi_{2'}$ along the X axis for the image $1'$ of the dislocation 1 and the image $2'$ of the dislocation 2 are reported in Fig. 5 accordingly. Using Eshelby's image forces [18] and following the line of thought of Weinberger and Cai [2] who envisaged the same configuration, we obtain the following expression for f_1 , the X component of the force (per unit length) exerted on the dislocation 1:

$$\begin{aligned} f_1 &= \frac{\kappa_{11'}}{\xi_{1'} - \xi_1} + \frac{\kappa_{12'}}{\xi_{2'} - \xi_1} + \frac{\kappa_{12}}{\xi_1 - \xi_2} + f_1^t + f_1^s, \\ \kappa_{11'} &= \frac{\mu}{2\pi} [b_e^2 / (1 - \nu) + b_s^2], \\ \kappa_{12} &= \frac{\mu}{2\pi} [-b_e^2 / (1 - \nu) + b_s^2], \\ \kappa_{12'} &= \kappa_{12} + \frac{\mu}{2\pi} \frac{b_e^2}{1 - \nu} \frac{\xi_{2'} (\xi_{2'} - \xi_2) (\xi_1 - \xi_2)}{\xi_2 (\xi_{2'} - \xi_1)^2}, \end{aligned} \quad (4)$$

where for an isotropic wire having a shear modulus μ and a Poisson ratio ν , the coefficient $\kappa_{11'} > 0$ leads to an attraction with image $1'$, $\kappa_{12} > 0$ induces a repulsion with dislocation 2 while the role of the image $2'$ is captured through the more complicated term $\kappa_{12'} > 0$ that also tends to attract the dislocation 1 out of the nanowire. On the contrary in Eq. (4), the force induced by the torsion

$$f_1^t = -\frac{\mu b_s^2}{\pi R^2} \xi_1 \left[2 - \left(\frac{\xi_1}{R} \right)^2 - \left(\frac{\xi_2}{R} \right)^2 \right] \quad (5)$$

and the force (per unit length) due to the extension of the stacking fault (of energy γ per unit surface) $f_1^s = -\gamma$ are

both negative and drive the dislocation 1 towards the center. Permuting indexes [19], one gets from Eq. (4) the force component f_2 exerted on dislocation 2 along X and by integration one obtains the energy $E(\xi_1, \xi_2) = E(\xi, \delta)$ of the cylinder containing the two partial dislocations. This simple model will enable us to capture the variation of the potential well ΔE with R observed in Fig. 4 providing that we know how the dissociation distance 2δ varies with ξ for a given R . This latter point is solved in the Supplemental Material [12] where using Eq. (4) and applying the condition $-\partial E/\partial \delta|_{\xi} = f_1 - f_2 = 0$, we derive the following expression of δ that minimizes E [12]:

$$\delta \approx a_1 + \frac{1}{R^2} [a_2 + a_3 f(x)], \quad (6)$$

with $x = \xi/R$, and $f(x)$ is a polynomial function $f(x) = \frac{3}{4}(1-x^2)^{-2} - \frac{1}{4}(1-x^2)^{-1} - (1-x^2) + \frac{1}{2}$ derived for $b_e = b/\sqrt{12}$ and $\nu = 1/3$. By adjusting the parameters a_1 , a_2 , and a_3 , Eq. (6) reproduces remarkably well the dependency of δ with x for R ranging from 3 nm to 30 nm in our simulations [12]. At the center for $\xi = 0$, the distance between partials is found to be smaller in thinner wires and it increases linearly with $1/R^2$. Equation (6) also tells that δ increases with ξ for any radius R .

Using again forces f_1 and f_2 from Eq. (4) and integrating we finally get ΔE for a dissociated screw dislocation:

$$\begin{aligned} \Delta E = E^d & \left\{ \frac{3}{4} \ln \left[\frac{\sqrt{(1-x^2-y^2)^2 - 4x^2y^2}}{1-y_R^2} \right] \right. \\ & + \frac{1}{4} \ln \left[\frac{(1-x^2+y^2)}{(1+y_R^2)} \right] \\ & - \frac{1}{2} \left[\frac{y^2}{(1-x^2+y^2)^2} - \frac{y_R^2}{(1+y_R^2)^2} \right] \\ & \left. - \frac{1}{4} \ln \left[\frac{y}{y_R} \right] + \frac{R}{4\delta_\infty} (y - y_R) \right\} \\ & - E^t [x^2(x^2 - 2 + 2y^2) - y^2(2 - y^2) + y_R^2(2 - y_R^2)], \end{aligned} \quad (7)$$

with $x = \xi/R$, $y = \delta/R$ and $y_R = \delta_R/R$ where δ_R denotes the half dissociation distance for $\xi = 0$ in Eq. (6). In Eq. (7), one can still recognize each interaction that contributes to building the full potential well. The first logarithmic term originates from the interactions between the dislocations and their own images (1 with 1' and 2 with 2'). The second and the third lines in Eq. (7) contain the terms that come from the crossed interactions between dislocation and image (1 with 2' and 2 with 1'). Then in the fourth line, the two terms account for the direct interaction between dislocations 1 and 2 and depend only on the increase of the relative dissociation distance y with respect to its value y_R at the center. Finally, in Eq. (7), the term with

the prefactor E^t is due to the torsion. Only this latter term and the term proportional to $y - y_R$ in Eq. (7) are positive. They increase with x in contrary to the other negative terms that decrease with x .

For large R , Eq. (7) tends to Eq. (1) since $y_R^2 \ll 1$ and $y \approx y_R$ from Eq. (6). This situation is found for $R = 30$ nm in Fig. 4 with $E^d = 1.60$ eV/nm. Below 30 nm for copper, the role of the relative dissociation distance y_R increases. A constant value of y equal to y_R does induce a decrease of the Eshelby barrier when y_R increases. However, it is only by taking into account the way y varies with x and R from Eq. (6) that we obtain a good agreement with the results of our simulations in Fig. 4. In this latter case where all terms count in Eq. (7), the R dependence of both ΔE^{\max} and x^{\max} of the potential well are quantitatively reproduced. The model also predicts the existence of a critical radius below which the dissociated dislocation becomes unstable. This radius is estimated to be around 1.5 nm from the atomistic simulations.

To conclude, we have examined the stability of a screw dislocation in a $\langle 011 \rangle$ copper nanowire. We find that the crystallographic anisotropy of the wire leads to a marked anisotropic Eshelby potential well (EPW) with a two-fold symmetry. In addition, we show that the dissociated state of the screw dislocation into two partials induces a dependence of the EPW with the radius R of the nanowire. By diminishing R from 30 to 3 nm for copper, both our molecular statics simulations and our model based on elasticity theory of dislocations predict a decrease of the EPW barrier ΔE^{\max} by almost a factor 3 and a reduction of the EPW radius x^{\max} from roughly 0.5 to 0.3 in the $\langle 211 \rangle$ directions. The pair of partials is found to be unstable for $R < 1.5$ nm.

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