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# The effect of stress on the cross-slip energy in face-centered cubic metals: a study using dislocation dynamics simulations and line tension models

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## Abstract

Dislocation dynamics simulations were used to calculate the energy barrier of cross-slip via Friedel-Escaig mechanism in face centered-cubic copper. The energy barrier in the unstressed case was found to be 1.9 eV, as reported by B. Ramírez *et al.*<sup>[1]</sup>. The energy barrier was reduced by applying an external stress. The most effective way of reducing it, was by applying a compressive stress on the glide plane. Furthermore, it was confirmed using dislocation dynamics simulations, that both the Schmid and Escaig stress have a comparable effect in reducing the energy barrier, in qualitative agreement with the atomistic simulations performed by K. Kang *et al.*<sup>[2]</sup> in face-centered cubic nickel. Most of the energy barrier values for stressed cross-slip fell within the experimental error of  $1.15 \pm 0.37$  eV measured by J. Bonneville *et al.*<sup>[3]</sup>. Moreover, the activation enthalpy obtained from K. Kang's *et al.*<sup>[2]</sup> line tension model of cross-slip and the general expression for the activation enthalpy proposed by A. Malka-Markovitz *et al.*<sup>[4]</sup> were in good quantitative agreement with the simulation results. Hence, both could be used to calculate the activation enthalpy of screw segments in dislocation dynamics simulations.

### *Keywords:*

activation energy, cross-slip, dislocation dynamics, line tension model, Escaig stress, Schmid stress

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## 1. Introduction

Cross-slip is a thermally-activated process by which screw dislocations change their glide plane, allowing them to overcome obstacles and populate other slip planes<sup>[5]</sup>. It plays an important role in two competing processes during plastic deformation<sup>[6]</sup>. On the one hand, it causes dynamic recovery during stage III by dislocation annihilation<sup>[7]</sup>, and other, it contributes to work hardening by dislocation multiplication<sup>[8,9]</sup>.

Since cross-slip is a thermally activated process, its rate is controlled by an Arrhenius-like equation. Many dislocation dynamics (DD) simulations have successfully model plastic deformation in crystals<sup>[10–14]</sup>. Most of them use the rate equation proposed by L. Kubin *et al.*<sup>[15]</sup>. In their model, the cross-slip probability explicitly depends on the resolved shear stress at the onset of stage-III

plastic deformation, which is a macroscopic parameter obtained from the stress-strain curve of the material.

This probability law has demonstrated to be robust enough to allow the formation of persistent slip bands in the low-cycle fatigue regime<sup>[16]</sup>, or to study the recovery dynamics in copper<sup>[17]</sup>. However, it is not sufficient in many situations. As an example, in the case of irradiated materials, the local level of stress is very high because of the large number of obstacles associated with the defect density. In this case, the cross-slip events are too frequent<sup>[18]</sup>. Contrarily, when the stress level is very low, the probability of inducing cross-slip events will be very low or nonexistent.

Based on the work of L. Kubin *et al.*<sup>[15]</sup>, A. Hussein *et al.*<sup>[19]</sup> recently proposed a more physical rate equation that depends only on microstructure parameters, e.g. the energy barrier required to form a constriction point on a screw dislocation, the Debye frequency of the material, the activation volume and the local stress. This allowed them to implement DD simulations considering the different cross-slip mechanisms identified from molecular dynamics (MD) simulations. Quantifying the effect of stress on the activation barrier is thus of great importance to generate realistic DD simulations.

The two most plausible cross-slip models for Face-Centered Cubic (FCC) crystals are the Fleischer (FL) and Friedel-Escaig (FE) mechanisms.

The FL model was developed by R. Fleischer<sup>[20]</sup>. In his model, the leading partial in a stacking-fault dissociates into two partials; one glides on the cross-slip plane and the other remains sessile at the intersection of the two planes (stair-rod dislocation). The trailing partial then reacts with the stair-rod dislocation to form another Shockley partial in the conjugate plane, which completes the cross-slip process.

The FE model was developed by B. Escaig<sup>[21]</sup> based on J. Friedel's ideas<sup>[22]</sup>. Moreover, he used the line tension (LT) model of cross-slip developed by A. Stroh<sup>[23]</sup> to study the effect of the widening stress (Escaig stress) on the energy barrier. In the FE model, the extended dislocation stops moving in the glide plane due to an obstacle. An already-existing constriction then splits into two halves and then separate in the cross-slip plane. This process proceeds spontaneously due to the stress on the cross-slip plane until the dissociation is completed.

Although there have been some controversy on which cross-slip model prevails<sup>[24]</sup>, recent atomistic simulations confirm that both FL and FE mechanisms can occur. The determination of which process would dominate depends on many factors.

C. Jin *et al.*<sup>[25]</sup> used the nudged-elastic-band method to study FCC Al. They concluded that there is a critical dislocation length below which the screw dislocation cross-slips only via FL mechanism, whereas longer ones would cross-slip either via FL or FE mechanisms, depending on the initial and final positions of the dislocation. The critical length they found was of the order of  $22b$ , where  $b$  is the magnitude of the Burgers vector.

S. Xu *et al.*<sup>[26]</sup> reported similar findings in FCC Ni using dynamic concurrent atomistic-continuum and MD simulations. They found that screw dislocations of length 6.47 nm cross-slip via FL mechanism, whereas longer dislocations (of length 12.94 nm) can cross-slip via either the FE or FL mechanisms. They also suggested that the critical shear stress for both FE and FL mechanisms

depends on the dislocation length.

Recently, W. Kuykendall *et al.*<sup>[27]</sup> used atomistic simulations to examine the effect of stress on the energy barrier of cross-slip via FE and FL mechanisms in FCC Ni. They concluded that the FE mechanism prevails when the Escaig stress on the glide plane is dominant, and that increasing the Schmid and Escaig stress on the cross-slip plane promotes the FL mechanism.

The material of study in this work is FCC Cu due to its broad literature. The mechanism of cross-slip in Cu has been fully examined using atomistic simulations and it was reported that dislocations in this material cross-slip via FE mechanism<sup>[28,29]</sup>. The activation energy of Cu has been calculated using both elasticity theory and atomistic simulations. However, the vast majority of energy barrier calculations employ atomistic simulations<sup>[29–34]</sup>.

Alternatively, B. Ramírez *et al.*<sup>[1]</sup> used a network-based formulation of dislocation dynamics to study the effect of a general stress on the energy barrier of cross-slip via FE mechanism. They found that the stress-free activation energy in Cu is 1.9 eV when the core is represented by two partials, and that it converges to 1.43 eV when the core is distributed by 20 Volterra partial fractional dislocations, the later value being in better agreement with the experimental results. They also found that the cross-slip energy reduces to 0.62 eV in presence of a Lomer-Cottrell junction.

In recent years, K. Kang *et al.*<sup>[2]</sup> extended Escaig’s LT model to include the effect of gliding stress (Schmid stress) on the cross-slip plane. Contrary to Escaig’s claim that the Schmid stress had a negligible effect on the energy barrier, they found that it had a comparable effect to the Escaig stress. They calculated the energy barrier in FCC Ni using atomistic methods at different stress conditions and found good qualitative agreement with their LT model.

More recently, A. Malka-Markovitz *et al.*<sup>[4]</sup> solved Strohs’s LT model of cross-slip<sup>[23]</sup> exactly by linearizing the interaction force between the partials. They obtained a general expression for the activation enthalpy as function of the elastic constants and local stress.

The DD simulations of fatigue mostly rely on the energy barrier, which is often calculated using atomistic simulations. However, the interatomic potential quantitatively affects the simulation results<sup>[30]</sup>. Hence, they may not be reliable. On the other hand, in DD simulations, the core-width used to compute the elastic energy can be determined using the theory developed by G. Schöck<sup>[35]</sup>, as suggested by B. Ramírez *et al.*<sup>[1]</sup>. Moreover, DD simulations naturally enable the possibility to study the effect of complex structures on the energy barrier. In this way, they offer an attractive alternative to large-scale atomic simulations.

The contribution of this work is twofold. First, the effect of stress on the cross-slip activation enthalpy is carefully calculated using DD simulations, which is an interesting alternative to the common atomistic approach found in the literature. Second, the results are compared with those obtained from two recent LT models of cross-slip in order to verify their consistency. The objective is to determine whether the aforementioned LT models could be reliably used in DD simulations to calculate the activation enthalpy of screw segments.

The rest of this paper is organized as follows. Section 2 introduces the DD simulation methodology, K. Kang’s *et al.*<sup>[2]</sup> LT model of cross-slip and the general expression for the activation enthalpy proposed by A. Malka-Markovitz *et al.*<sup>[4]</sup>. Section 3 describes the effect of stress on the activation

enthalpy obtained using DD simulations and the two LT models. Finally, Section 4 presents the summary and conclusions of this work.

## 2. Methodology

### 2.1. DD simulations

#### 2.1.1. Force computation

Dislocation dynamics is a modeling approach to study crystal plasticity, in which dislocation lines are discretized in linear segments and their motion is determined<sup>[36]</sup>. A segment is defined by two nodes on its ends and a tangent line  $\hat{\xi}$  that connects them. The Burgers vector  $\mathbf{b}$  associated to it indicates the displacement's magnitude and direction as the segment moves.

The force exerted by the local stress at each node is calculated using the Peach-Köhler formula. Similarly to other discrete DD codes<sup>[37]</sup>, NuMoDis<sup>[38]</sup> uses the formalism developed by A. Arsenlis *et al.*<sup>[39]</sup> to compute the nodal forces. This force affects the nodal velocity through a given mobility law. Thus, the dislocation dynamics can be determined by updating the position of all nodes after a simulation step.

In order to study cross-slip in FCC crystals, the dissociated character of dislocations must be considered. The SF produces a force that tends to attract the partials towards each other, compensating the elastic repulsion between them. This results in an equilibrium separation distance in the SF ribbon.

Perfect dislocations dissociate into partials if it decreases its elastic energy. However, discrete DD codes are based on nodal forces and do not consider the systems energetics to determine its evolution. In consequence, E. Martinez *et al.*<sup>[40]</sup> proposed to account for the **intrinsic** SF energy  $\gamma_i$  by introducing a SF force ( $\mathbf{f}_{sf}$ ). They derived that  $\mathbf{f}_{sf}$  should be of magnitude  $\gamma_i$ , and perpendicular to both the tangent line and SF plane  $\hat{\mathbf{n}}$ . The equation satisfying these conditions is given by:

$$\mathbf{f}_{sf} = \gamma_i \hat{\mathbf{n}} \times \hat{\xi} \quad (1)$$

In NuMoDis<sup>[38]</sup>, the SF ribbon is defined by an ordered list of nodes conforming the dislocation partials and the plane that contains them. The SF forces acting on a partial, in order to be physical, must point towards the opposite partial. Thus, given a slip plane orientation, the node order defining the circuit must be such that the SF force given by Eq. 1 satisfy this condition.

#### 2.1.2. Velocity computation

In FCC metals, the relationship between forces and velocities is linear due to the small intrinsic lattice resistance<sup>[41]</sup>. The total force at a node  $\mathbf{f}$  is given by  $\mathbf{f} = \mathbf{f}_{PK} + \mathbf{f}_{sf}$ , where  $\mathbf{f}_{PK}$  is the Peach-Köhler force. The projections of  $\mathbf{f}_{PK}$  and  $\mathbf{f}_{sf}$  on the glide plane act perpendicular to the line segment. Therefore, the mobility law is of the form:

$$\mathbf{f} = \underline{\underline{B}} \cdot \mathbf{v} \quad (2)$$

where  $\mathbf{v}$  is the nodal velocity and  $\underline{\underline{B}}$  the viscosity matrix:

$$\underline{\underline{B}}(\hat{\xi}) = B(\mathbf{I} - \hat{\xi} \otimes \hat{\xi}) \quad (3)$$

where  $B$  is the viscosity coefficient.

Thus, the nodal velocity is obtained by inverting the viscosity matrix from Eq. 2:

$$\mathbf{v} = \underline{\underline{B}}^{-1} \cdot \mathbf{f} \quad (4)$$

At each simulation step, the force at every node due to the influence of all other segments and SF is computed; the nodal velocities are thus calculated and their new positions are updated.

### 2.1.3. Elastic energy

W. Cai *et al.*<sup>[42]</sup> showed that the non-singular interaction energy  $E^{ns}$  between a segment with ends  $\mathbf{x}_1$  and  $\mathbf{x}_2$  and Burgers vector  $\mathbf{b}$  with another segment with ends  $\mathbf{x}_3$  and  $\mathbf{x}_4$  and Burgers vector  $\mathbf{b}'$  is given by:

$$\begin{aligned} E^{ns} = & -\frac{\mu}{8\pi} \int_{\mathbf{x}_3}^{\mathbf{x}_4} \int_{\mathbf{x}_1}^{\mathbf{x}_2} \partial_k \partial_k R_a b_i b'_j dx_i dx'_j \\ & -\frac{\mu}{4\pi(1-\nu)} \int_{\mathbf{x}_3}^{\mathbf{x}_4} \int_{\mathbf{x}_1}^{\mathbf{x}_2} \partial_i \partial_j R_a b_i b'_j dx_k dx'_k \\ & +\frac{\mu}{4\pi(1-\nu)} \int_{\mathbf{x}_3}^{\mathbf{x}_4} \int_{\mathbf{x}_1}^{\mathbf{x}_2} \partial_k \partial_k R_a b_i b'_i dx_j dx'_j \\ & -\frac{\mu\nu}{4\pi(1-\nu)} \int_{\mathbf{x}_3}^{\mathbf{x}_4} \int_{\mathbf{x}_1}^{\mathbf{x}_2} \partial_k \partial_k R_a b_i b'_j dx_j dx'_i \end{aligned} \quad (5)$$

where  $\mu$  is the shear modulus,  $\nu$  the Poisson's ratio,  $R_a = \sqrt{\mathbf{R} \cdot \mathbf{R} + a^2}$ ,  $\mathbf{R} = \mathbf{x} - \mathbf{x}'$ , and  $a$  the core-width parameter.

The analytical expressions resulting from the solution of Eq. 5 for parallel and non-parallel segments were provided by W. Cai *et al.*<sup>[42]</sup>. These formulas were used to calculate the interaction and self-energies of the segments in NuMoDis<sup>[38]</sup>.

The core-width parameter  $a$  affects the elastic energy both qualitatively and quantitatively. G. Schöck<sup>[35]</sup> developed a theory based on the Peierls framework<sup>[43]</sup> to obtain a physical value of  $a$ . He showed that the total energy of a single straight dislocation is given by<sup>[35]</sup>:

$$E^P = E_L(\phi) \left[ \ln \left( \frac{r}{2\bar{w}(\phi)} \right) + 1 \right] \quad (6)$$

where  $\phi$  is the angle between the Burgers vector and the line direction,  $r$  is the outer cut-off radius,  $\bar{w}(\phi)$  is the average width of its edge and screw components, and  $E_L(\phi)$  is the pre-logarithmic elastic line energy factor:

$$E_L(\phi) = \frac{\mu b^2}{4\pi} \left( \cos^2(\phi) + \frac{\sin^2(\phi)}{1-\nu} \right) \quad (7)$$

G. Schöck<sup>[35]</sup> argued that  $\bar{w}(\phi)$  can be approximated as the width of a single dislocation in an isotropic medium passing through two equilibrium positions i.e. with SF energy  $\gamma = \gamma_u$ <sup>[35]</sup>:

$$\frac{\bar{w}(\phi)}{b} = \frac{\cos^2(\phi) + \sin^2(\phi)/(1-\nu)}{b/c + 2\pi^2\gamma_u/(\mu b)} \quad (8)$$

where  $c$  is the interplanar glide plane spacing,  $\gamma_u$  the unstable SF energy and  $b$  is the magnitude of the Burgers vector.

Using W. Cai's *et al.*<sup>[42]</sup> model, the line energy for screw  $E_S$  and edge dislocation  $E_E$  are found to be<sup>[35]</sup>:

$$E_S = \frac{\mu b^2}{4\pi} \ln \left( \frac{r\sqrt{e}}{a_S} \right) \quad (9)$$

$$E_E = \frac{\mu b^2}{4\pi(1-\nu)} \ln \left( \frac{r}{a_E} \right) \quad (10)$$

where  $a_S$  and  $a_E$  are the core spreading parameters of the screw and edge components, respectively, and  $e$  is the base of the natural logarithm.

The continuum description in Eqs. 9 and 10 must be consistent with the Peierl's atomistic treatment in eq. 6. Imposing this condition,  $a_S$  and  $a_E$  are required to be<sup>[35]</sup>:

$$a_S = \frac{2\bar{w}(0)}{\sqrt{e}} \quad \text{and} \quad a_E = \frac{2\bar{w}(\pi/2)}{e} \quad (11)$$

Following the work of B. Ramírez *et al.*<sup>[1]</sup>, the core-width parameter can be considered as an averaged value of  $a_S$  and  $a_E$ :

$$a \approx \frac{2\bar{w}(0)}{e} = \frac{2}{e} \left( \frac{b}{b/c + 2\pi^2\gamma_u/(\mu b)} \right) \quad (12)$$

#### 2.1.4. Effective stacking-fault energy

Dislocations in FCC crystals dissociate into partials. The dislocation moves due to the action of an external stress. The partial at the front respect to the direction of motion is called the "leading" partial, and the other "trailing" partial. Let  $L = \{\vec{P}_1, \vec{P}_2, \dots, \vec{P}_N\}$  and  $\tilde{L} = \{\vec{Q}_1, \vec{Q}_2, \dots, \vec{Q}_N\}$  represent the set of nodes conforming the leading and trailing partials, respectively (see Fig. 1).

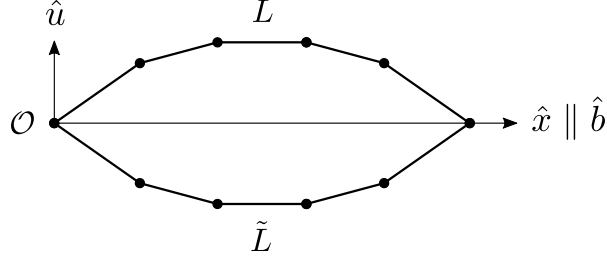


Figure 1: The solid dots denote the nodal positions; the shape of the leading and trailing partials are described by  $L$  and  $\tilde{L}$ , respectively.

The effective SF energy is given by the SF energy  $W_{SF}$  plus the work done by the applied forces  $W_{app}$ , which can be calculated as follows:

$$W_{SF} = \gamma_i \sum_{j=1}^N \left[ \frac{y_{j+1} + y_j}{2} \Delta x_j - \frac{\tilde{y}_{j+1} + \tilde{y}_j}{2} \Delta \tilde{x}_j \right] \quad (13)$$

$$W_{app} = \sum_{j=1}^N F y_j \Delta x_j + \tilde{F} \tilde{y}_j \Delta \tilde{x}_j \quad (14)$$

where:

$$y_j = \vec{P}_j \cdot \hat{u}, \quad \tilde{y}_j = \vec{Q}_j \cdot \hat{u}, \quad \Delta x_j = (\vec{P}_{j+1} - \vec{P}_j) \cdot \hat{b}, \quad \Delta \tilde{x}_j = (\vec{Q}_{j+1} - \vec{Q}_j) \cdot \hat{b} \quad \text{for } j = 1, 2, \dots, N \quad (15)$$

$\hat{u} = \hat{n} \times \hat{b}$  is an unitary vector contained in the slip plane of normal  $\hat{n}$ , perpendicular to the normalized Burgers vector  $\hat{b}$ . In absence of Schmid stress, the partials are indistinguishable from each other due to the spatial symmetry with respect to the  $\hat{x}$  axis. For that reason, the sign of  $\hat{u}$  does not affect the energy. However, the leading and trailing partials are univocally defined in the presence of a Schmid stress. In that case,  $\hat{u}$  must point towards the bowing-out direction because the energy barrier does not depend on the sign of the Schmid stress<sup>[2,4,27]</sup>.

The proportionality factors  $F$  and  $\tilde{F}$  are given by:

$$F = -\frac{b\sigma_E}{2\sqrt{3}} - \frac{b\sigma_S}{2} \quad \text{and} \quad \tilde{F} = \frac{b\sigma_E}{2\sqrt{3}} - \frac{b\sigma_S}{2} \quad (16)$$

where the subscripts  $E$  and  $S$  refer to the Escaig and Schmid stress, respectively.

All the nodes were mobile except those two at the extremes, which simulate the constriction points at the equilibrium configurations. Therefore, the partials always satisfied  $y_1 = \tilde{y}_1 = y_N = \tilde{y}_N = 0$ .



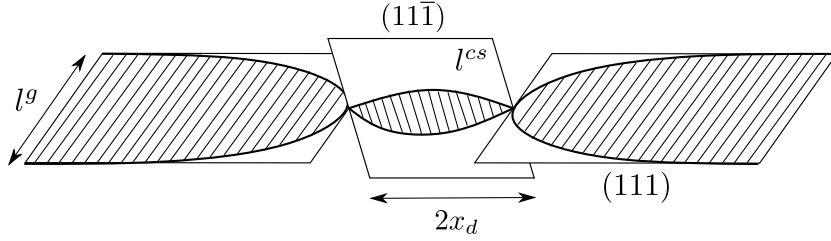


Figure 2: An equilibrium configuration during cross-slip via FE mechanism. The process is completed when the constriction separation tends to infinity. In this limit, the dislocations are completely contained in the conjugate plane with separation between the partials  $l^{cs}$  for all  $x$  (figure adapted from K. Kang *et al.*<sup>[2]</sup>).

### 2.1.5. Cross-slip simulations

Cross-slip via FE mechanism was assumed in all simulations. The DD code was used to find the equilibrium configurations at different cross-slip stages. The total energy of a configuration consisted of its total elastic energy plus the effective stacking-fault energy, which were computed as described in sections 2.1.3 and 2.1.4. The applied stresses were small enough such that the Frank-Read source remained deactivated in all simulations.

According to the FE mechanism, the dislocation must stop moving before cross-slipping. Therefore, the Schmid stress on the glide plane  $\sigma_S^g$  was always assumed to be zero. The dislocation width in the glide plane was affected by the Escaig stress  $\sigma_E^g$ . Soon after stop moving, an already-existing constriction splits into two halves and the dislocation expands in the cross-slip plane until equilibrium is reestablished (see Fig. 2). This occurs in the limit when the distance between the constriction points in the cross-slip plane  $2x_d$  tends to infinity.

In DD codes, an infinite dislocation does not really exist. Thus, the initial configuration consisted of a dislocation with length of 1000 Å lying in the  $(\bar{1}\bar{1}\bar{1})$  plane. **The dislocation was pinned at its ends.** The Burgers vector of the partials pointed away from each other as shown in Fig. 3(a). This was a long-enough dislocation such that most part of it attained equilibrium i.e the distance  $l^g$  between the partials.

An intermediate cross-slip configuration consisted of a semi-infinite dislocation on the glide plane with a constricted cross-slipped segment on the conjugate plane  $(\bar{1}\bar{1}\bar{1})$ . The Burgers vector of the partials pointed towards each other on the cross-slip plane. The total configuration length was fixed to 1000 Å, in agreement with the initial state. The intermediate cross-slip configuration was thus characterized by the distance between its constriction points.

In the limiting case when the constrictions points are infinitely apart, the dislocation must be completely contained in the cross-slip plane (see 3(b)). Unlike in the glide plane, the dislocation was allowed to move by bowing-out on the conjugate plane. The sign of the Schmid stress on the cross-slip plane  $\sigma_S^{cs}$  was affected only the bowing-out direction, and not the total energy. As in the glide plane, the width of dislocation in the conjugate plane was affected by the Escaig stress  $\sigma_E^{cs}$ .

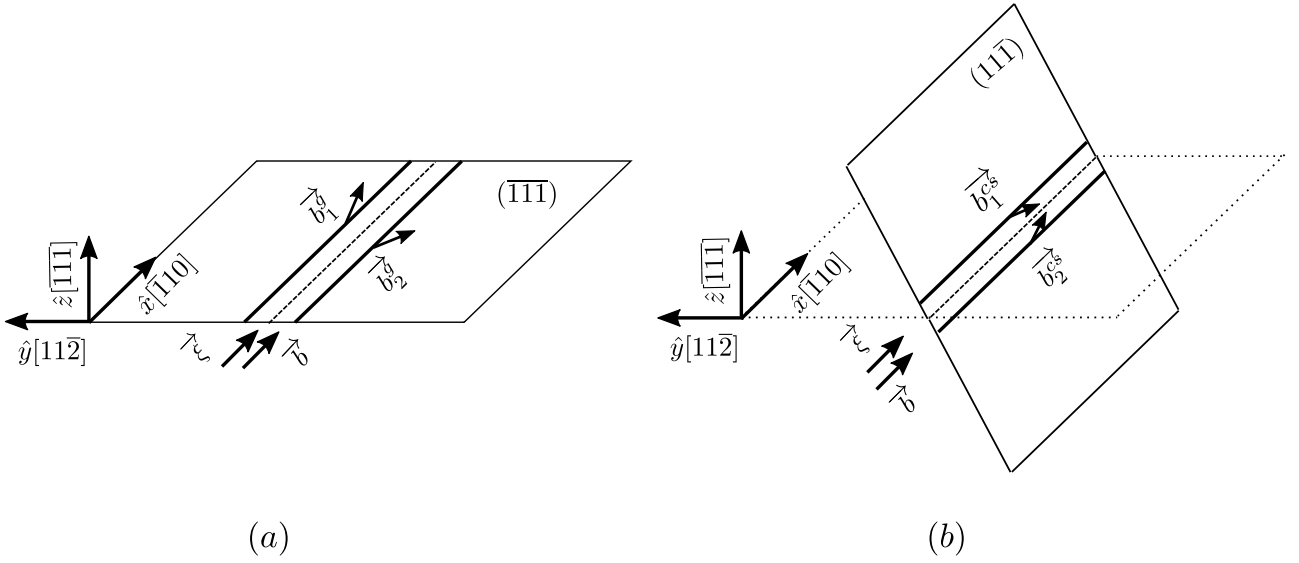


Figure 3: Simulation setup. (a) The reference configuration consists of a dissociated right-handed screw (RHS) dislocation at equilibrium on the glide plane  $(\bar{1}\bar{1}\bar{1})$  with partials' Burgers vector  $\vec{b}_1^g = \frac{a_0}{6}[\bar{1}2\bar{1}]$  and  $\vec{b}_2^g = \frac{a_0}{6}[\bar{2}1\bar{1}]$  pointing away from each other. (b) The final configuration consists of a dissociated RHS dislocation at equilibrium in the cross-slip plane  $(11\bar{1})$  with partials' Burgers vector  $\vec{b}_1^{cs} = \frac{a_0}{6}[\bar{1}21]$  and  $\vec{b}_2^{cs} = \frac{a_0}{6}[\bar{2}1\bar{1}]$  pointing towards each other.

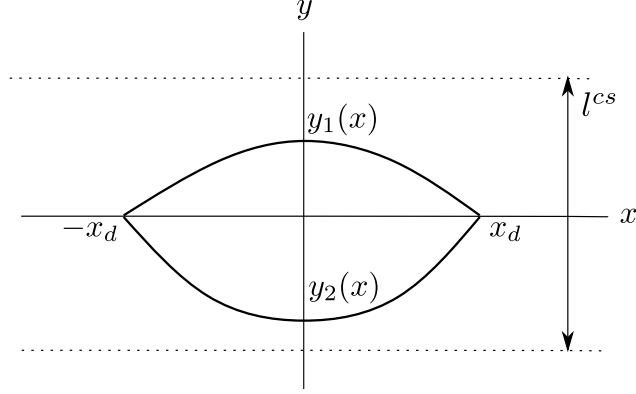


Figure 4: The shape of the partials in the cross-slip plane are described by the  $y_1(x)$  and  $y_2(x)$ , and satisfy the boundary conditions  $y_1(\pm x_d) = y_2(\pm x_d) = 0$  (figure adapted from K. Kang *et al.*<sup>[2]</sup>).

In order to study the effect of  $\sigma_E^g$ ,  $\sigma_S^{cs}$  and  $\sigma_E^{cs}$ , the coordinate system was rotated such that the  $[\bar{1}\bar{1}\bar{1}]$  direction matched with the  $\hat{z}$  axis and the Burgers vector  $[\bar{1}10]$  with the  $\hat{x}$  axis. Thus, the stress on the glide and cross-slip planes as function of the tensor components in the Cartesian coordinate system were given by:

$$\sigma_S^g = \sigma_{xz} \quad (17)$$

$$\sigma_E^g = \sigma_{yz} \quad (18)$$

$$\sigma_S^{cs} = \frac{2\sqrt{2}\sigma_{xy} - \sigma_{xz}}{3} \quad (19)$$

$$\sigma_E^{cs} = \frac{7\sigma_{zy} + 2\sqrt{2}(\sigma_{yy} - \sigma_{zz})}{9} \quad (20)$$

The energy of an intermediate cross-slip configuration was measured with respect to the energy of the initial state i.e. the energy of the dislocation resting at equilibrium in the glide plane under stress  $\sigma_E^g$ . Thus, the energy barrier was defined as the maximum energy among all intermediate cross-slip configurations as function of the distance between the constriction points.

## 2.2. Line tension model

In K. Kang's *et al.*<sup>[2]</sup> LT model of cross-slip, the FE mechanism is assumed. Thus, the dislocation does not move before cross-slipping i.e. the Schmid stress on the glide plane is zero ( $\sigma_S^g = 0$ ). However, the Escaig stress on the glide plane  $\sigma_E^g$  is not necessarily zero. The equilibrium separation between the partials in the glide plane  $l^g$  depends on  $\sigma_E^g$ :

$$l^g = \frac{A}{F^g} \quad (21)$$

where for a screw dislocation dissociated into two 30° partials<sup>[44]</sup>:

$$A = \left( \frac{1}{4} - \frac{1}{12(1-\nu)} \right) \frac{\mu b^2}{2\pi} \quad (22)$$

$$F^g = \gamma_i - b\sigma_E^g / (2\sqrt{3}) \quad (23)$$

The convention used in this framework is that positive  $\sigma_E^g$  increases the distance between the partials and negative decreases it.

Analogously, if the dislocation does not move in the cross-slip plane, its equilibrium distance  $l^{cs}$  is given by:

$$l^{cs} = \frac{A}{F^{cs}} \quad (24)$$

where

$$F^{cs} = \gamma_i - b\sigma_E^{cs} / (2\sqrt{3}) \quad (25)$$

The shape of the partials is described by continuous functions  $y_1(x)$  and  $y_2(x)$  (see Fig. 4). The constriction points are located in the  $x$  axis at  $\pm x_d$  and thus  $y_1(\pm x_d) = y_2(\pm x_d) = 0$  must be satisfied.

The energy contribution from the cross-slipped segment (measured with respect to the energy of an infinite straight screw dislocation resting at equilibrium in the glide plane) is given by<sup>[2]</sup>:

$$E^{cs} = W_1 + W_2 + W_3 \quad (26)$$

where  $W_1$  is the change in elastic repulsion between the partials,  $W_2$  is the change of the line energy and  $W_3$  the change in SF energy and the work done by the stress.

Specifically,

$$W_1 = A \int_{-x_d}^{x_d} \ln \left( \frac{l^g}{y_1 - y_2} \right) dx \quad (27)$$

$$W_2 = T \int_{-x_d}^{x_d} \left( \sqrt{1 + (y_1')^2} + \sqrt{1 + (y_2')^2} \right) dx - 4T x_d \quad (28)$$

$$W_3 = \int_{-x_d}^{x_d} (F_1^{cs} y_1 + F_2^{cs} y_2) dx - 2F^g l^g x_d \quad (29)$$

where

$$F_1^{cs} = F^{cs} - b\sigma_S^{cs}/2 \quad (30)$$

$$F_2^{cs} = -F^{cs} - b\sigma_S^{cs}/2 \quad (31)$$

The energy functional in Eq. 26 was minimized using the conjugate gradient method as suggested by Kang *et al.*<sup>[2]</sup>.

The line energy per unit length was given by<sup>[2]</sup>:

$$T = \alpha\mu b^2/2 \quad (32)$$

The variable  $\alpha$  was treated as a fitting parameter to match the DD simulations of cross-slip (see section 3).

Formally, the energy barrier is given by:

$$E_b(\sigma_E^g, \sigma_S^{cs}, \sigma_E^{cs}) = \max_{x_d} E(x_d; \sigma_E^g, \sigma_S^{cs}, \sigma_E^{cs}) \quad (33)$$

where

$$E = \min_{y_1, y_2} E^{cs}(y_1, y_2; x_d; \sigma_E^g, \sigma_S^{cs}, \sigma_E^{cs}) + E^g(\sigma_E^g) \quad (34)$$

$E^g$  being the energy of an isolated constriction on a perfect screw dislocation:

$$E^g = 2l^g\sqrt{AT} \int_0^1 [-\ln t + (t-1)]^{1/2} dt \quad (35)$$

The activation energy can be obtained for a given stress condition by solving Eq. 34 numerically.

Another useful formulation of the LT model of cross-slip was proposed by A. Malka-Markovitz *et. al.*<sup>[4]</sup>, who solved Strohs's LT model<sup>[23]</sup> exactly by linearizing the interaction force between the partials. They obtained the following general expression for the activation enthalpy as function of the elastic constants and local-stress components:

$$\begin{aligned} \frac{\Delta H(\sigma)}{\Delta E_0} &= \frac{\beta^g}{2} + \left(\frac{\beta^{cs}}{2}\right) \tanh(l_C) \\ &- \left(\frac{\beta^{cs}}{2}\right) \left[ \frac{2\alpha_L}{1.55} l_C E^* + \frac{\alpha_{Ls}^3}{1.55} \frac{\delta}{\beta^{cs}} l_C^3 \right] \end{aligned} \quad (36)$$

where  $\Delta E_0 = 1.9$  eV is the energy barrier of copper obtained in this work using DD simulations and  $\alpha_L \approx 0.6$  is a scale factor.

$\beta^g$  and  $\beta^{cs}$  are functions of the Escaig stress:

Property	Value
$a_0$	<sup>[46]</sup> 3.61 Å
$b$	<sup>[47]</sup> $a_0/\sqrt{2}$
$\gamma_i$	<sup>[48]</sup> 42 mJ/m <sup>2</sup>
$\gamma_u$	<sup>[1]</sup> 182 mJ/m <sup>2</sup>
$\nu$	<sup>[49]</sup> 0.324
$\mu$	<sup>[50]</sup> 54.6 GPa
$B$	<sup>[51]</sup> $1.5 \times 10^{-5}$ Pa-s

Table 1: Parameters used for FCC Cu;  $a_0$  is the lattice parameter,  $b$  the magnitude of the Burgers vector,  $\gamma_i$  the intrinsic SF energy,  $\gamma_u$  the unstable SF energy,  $\nu$  the Poisson's ratio,  $\mu$  the shear modulus and  $B$  the viscosity coefficient at room temperature.

$$\beta^g = \frac{1}{1 + \frac{\sqrt{3}b}{6\gamma_i}\sigma_E^g} \quad \text{and} \quad \beta^{cs} = \frac{1}{1 + \frac{\sqrt{3}b}{6\gamma_i}\sigma_E^{cs}} \quad (37)$$

whereas  $\delta$  is a quadratic function of the Schmid stress on the cross-slip plane:

$$\delta = \frac{1}{6} \left( \frac{b\sigma_S^{cs}}{\gamma_i} \right)^2 \quad (38)$$

The  $E^*$  function is a dimensionless off-set in the interaction energy between the glide and cross-slip planes<sup>[45]</sup>:

$$E^* = \ln \left( \frac{\beta^{cs}}{\beta^g} \right) \quad (39)$$

The critical length  $l_C$  in Eq. 36 can be found by solving the following equation numerically<sup>[45]</sup>:

$$\frac{1.55}{\cosh^2(l_C)} - \frac{3\delta}{\beta^{cs}} l_C^2 = 2E^* \quad (40)$$

In contrast with the convention used in K. Kang's *et al.*<sup>[2]</sup> LT model of cross-slip, positive  $\sigma_E^g$  decreases the distance between the partials and negative increases it.

In this work, the sign convention of K. Kang's *et al.*<sup>[2]</sup> was used in the plots.

The elastic constants of Cu used in both the DD simulations and LT model are shown in Table 1.

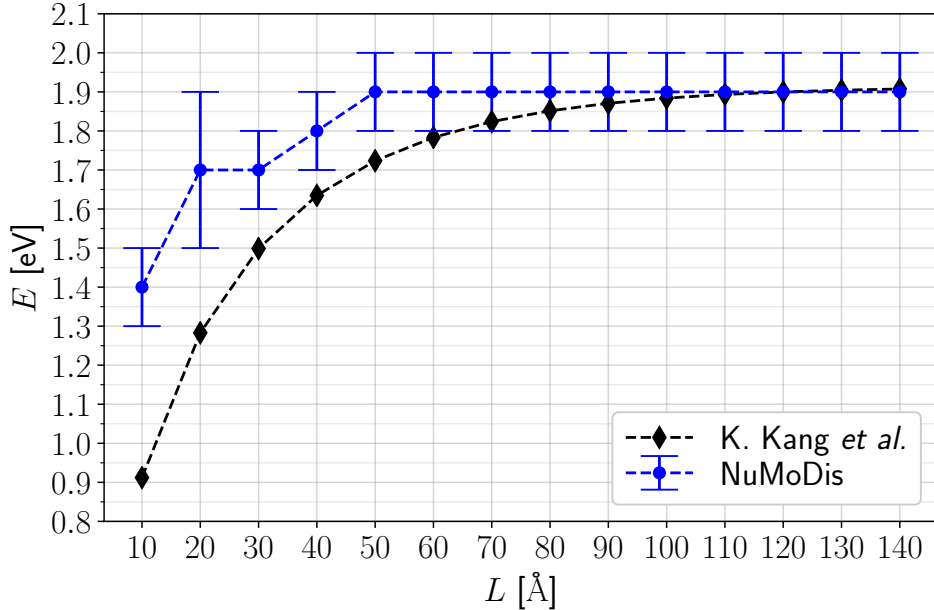


Figure 5: The energy barrier as function of the constriction separation at zero stress.

### 3. Results and discussion

#### 3.1. The calibration of the line tension model

The relative energy of the intermediate cross-slip configurations at zero stress is shown in Fig. 5. The energy uncertainty of the order of  $\pm 0.1$  eV in all the simulations results can be attributed to the line discretization used in the DD simulations, as well as to the finite core-width size of the non-singular theory of dislocations. The parameter  $\alpha$  in K. Kang’s *et al.*<sup>[2]</sup> LT model was calibrated such that the equilibration energy matched with the DD simulations at zero stress. The value was found to be  $\alpha = 0.22$ . Together with the core-width parameter in the elastic energy, the choice of  $\alpha$  was a key parameter for the good agreement between K. Kang’s *et al.*<sup>[2]</sup> LT model and DD simulations. The effect of compressive Escaig stress was to decrease the SF width. The stressed equilibrium separation obtained from the DD simulations was in great agreement with the LT model, as shown in Fig. 6.

The energy predicted by the K. Kang’s *et al.*<sup>[2]</sup> LT model and that obtained with the simulations does not match for short cross-slipped segments as seen in Fig. 5. This is expected because the LT model approximates the energy of a differential segment as that of a straight dislocation<sup>[52]</sup>. In fact, the LT model breaks down in the limiting case where  $2x_d = 0$  because the elastic repulsion diverges (see Eq. 27). However, this is not relevant since the objective of this work is to quantify the stress effect on the energy barrier, which occurs for longer dislocation lines where the LT model is more physical.

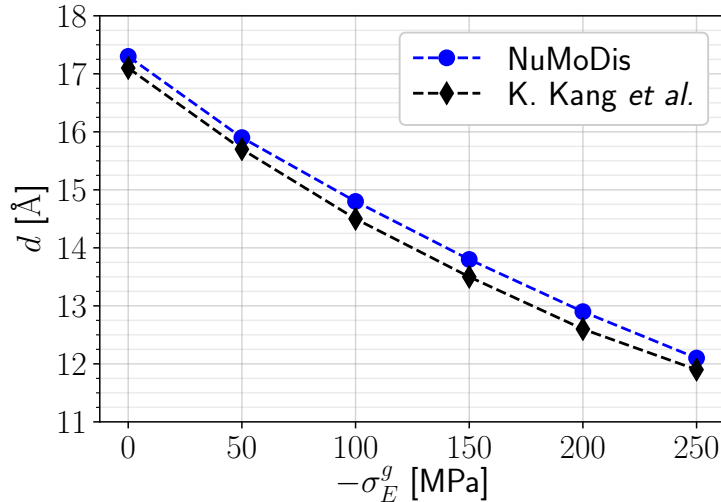


Figure 6: The effect of stress on the equilibrium separation between the partials. The segmented line corresponds to equation 21.

In the unstressed case, the energy monotonically augments as the constriction separation increases, but quickly reaches a maximum value of 1.9 eV. This means that once the cross-slip segment reaches a critical length (around 60 Å), no further energy is required to be invested and the cross-slip process continues spontaneously. **Therefore, the unstressed energy barrier of copper is equal to 1.9 eV, as reported by B. Ramírez *et al.*<sup>[4]</sup>.**

The equilibration energy encountered in the unstressed cross-slip is roughly equal to twice the energy required to form an isolated constriction. It can be argued that at the beginning of cross-slip, when the two constrictions are close to each other, the elastic repulsion between them adds up to the energy required to form them in isolation. However, as the distance between them increases, their interaction further decreases. Thus, if they are sufficiently far apart, the total energy with respect to the relaxed dislocation is roughly equal to that of the two independent constrictions. The planar constriction energy at zero stress is 0.7 eV, according to the DD simulations (see Fig. 7).

A. Stroh *et al.*<sup>[23]</sup> found the energy of a constriction using elasticity theory. Assuming a shear modulus of  $G = 45$  GPa and an equilibration distance between the partials at zero stress of  $d_0 = 18$  Å, one finds that in his model the energy of a single constriction is roughly 2 eV, which is almost three times higher than that found in this work (0.7 eV).

W. Püschl<sup>[53]</sup> estimated a constriction energy of 1.1 eV for FCC Cu using elasticity theory; G. Saada<sup>[54]</sup> generalized A. Strohs’s LT model for arbitrary constricting distance. He obtained different constriction energy values in the range of 0.33 - 0.7 eV, depending on the choice  $r_0/b$ , where  $r_0$  is a cut-off radius. Although these values are in better agreement with the experimental energy barrier, the (arbitrary) choice of  $r_0$  was not clearly determined.

T. Rasmussen *et al.*<sup>[34]</sup> found a constriction energy of 1.6 eV using atomistic simulations, in



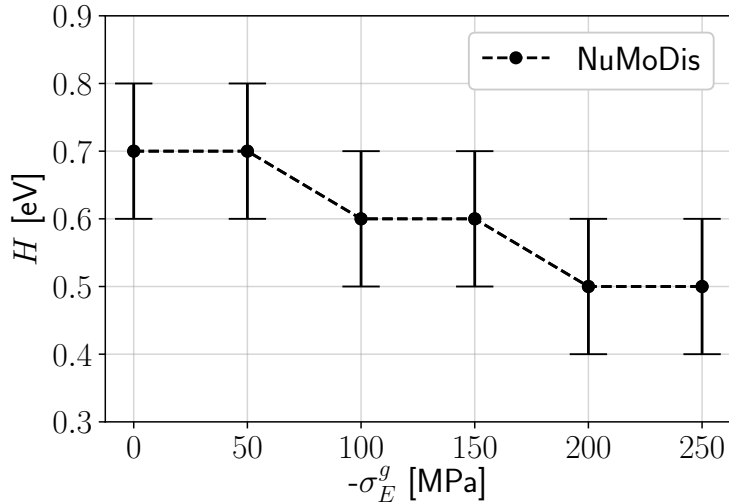


Figure 7: The effect of compressive stress on the constriction energy according to DD simulations.

reasonable agreement with A. Stroh *et al.*<sup>[23]</sup>, but too high according to the experimental energy barrier.

More recently, B. Ramírez *et al.*<sup>[1]</sup> found a constriction energy of 0.7 eV using dislocation dynamics, in excellent agreement with this work.

The effect of pure compressing stress on the constriction energy was found to be negligible. The slight decrease on the constriction energy observed in Fig. 7 is not conclusive. Nevertheless, one can assert that the average constriction energy did not vary much in the given range of stress.

The small effect of stress on the constriction energy can be explained by using the model developed by W. Püschl<sup>[53]</sup>. It predicts a marginal decrease in constriction energy (of less than 0.2 eV) when the splitting width between the partials decreases from  $8b \approx 20.4 \text{ \AA}$  to  $6b \approx 15.3 \text{ \AA}$ . These are roughly the equilibration distances simulated by NuMoDis<sup>[38]</sup> at zero (17.4  $\text{\AA}$ ) and -250 MPa (12.1  $\text{\AA}$ ), respectively. Thus, according to this model, one should not expect the constriction energy to vary much by applying a pure compressing stress for the given range of values.

The asymptotic convergence of the cross-slip energy barrier at zero stress observed in Fig. 5 has been thoroughly reported before.

M. S. Duesbery *et al.*<sup>[55]</sup> calculated the constriction pair energy as function of the stacking-fault energy using a linear-elastic framework, and found that for constriction separation larger than  $\sim 50b$ , the total energy becomes that of two independent constrictions. In particular, for FCC Cu, they found that the asymptotic value of the cross-slipped configuration was 3.7 eV. They also identified the asymmetric nature of the two constrictions in the cross-slip plane, as they asserted that one had lower energy being screw-like, and the other higher energy being edge-like. These are different from the Stroh-type constriction, which are edge-like on the one side, and screw-like on the other.

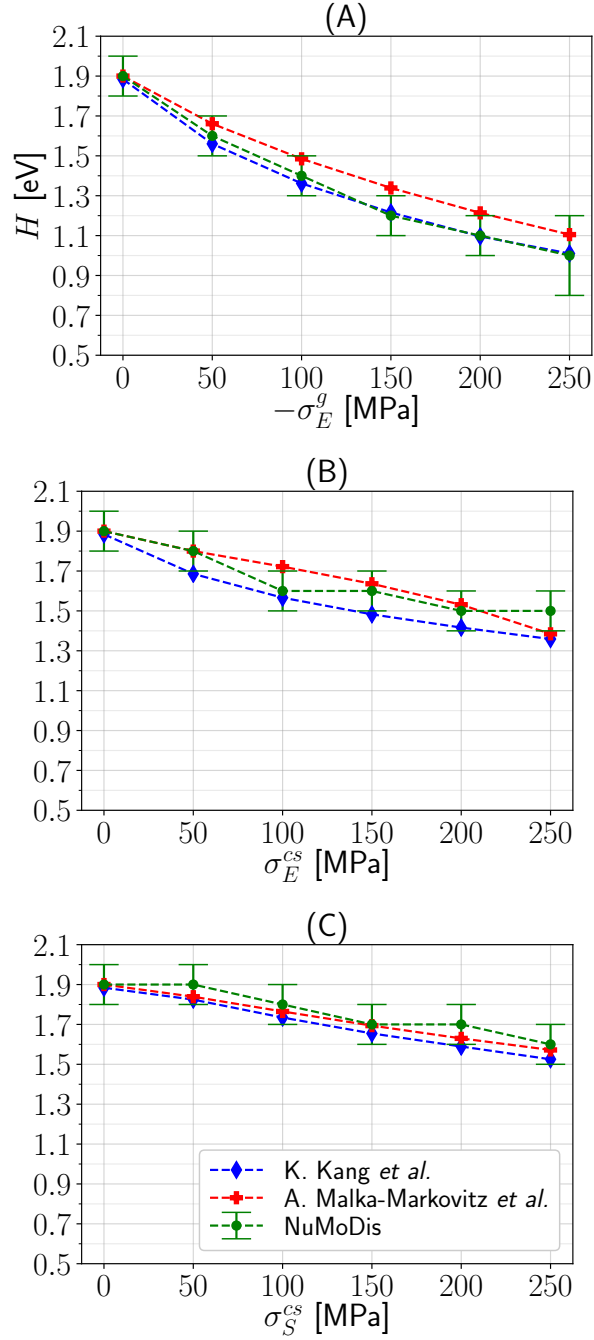


Figure 8: The effect of stress on the energy barrier: (A)  $\sigma_S^g = \sigma_E^{cs} = \sigma_S^{cs} = 0$ , (B)  $\sigma_S^g = \sigma_E^g = \sigma_S^{cs} = 0$  and (C)  $\sigma_S^g = \sigma_E^g = \sigma_E^{cs} = 0$ . The green circles represent the DD simulation results, the blue diamonds correspond to the numerical solution of K. Kang's *et al.*<sup>[2]</sup> LT model of cross-slip (see Eq. 34) and the red crosses were obtained from the general expression for the activation enthalpy proposed by A. Malka-Markovitz *et al.*<sup>[4]</sup> (see Eq. 36).

Later on, T. Rasmussen *et al.*<sup>[34]</sup> corroborated several results of M. S. Duesbery *et al.*<sup>[55]</sup> using atomistic simulations, as they obtained that indeed the total energy converged to the value of two independent constrictions for separations larger than  $\sim 50b$ . They measured a screw-like constriction energy of -3.8 eV, and an edge-like constriction energy of 1.1 eV, which added up to the total energy barrier in FCC Cu (2.7 eV). Although this value is lower than that obtained by M. S. Duesbery *et al.*<sup>[55]</sup>, it is roughly the double of the experimental value obtained by J. Bonneville *et al.*<sup>[3]</sup>.

S. I. Rao *et al.*<sup>[30]</sup> obtained an energy barrier for cross-slip at zero stress in the range of 1.07 - 1.28 eV using molecular statics. This energy is significantly smaller than that predicted by T. Rasmussen *et al.*<sup>[34]</sup>. They argued that it could be due to the difference in interatomic potentials used, as well as the Green's function technique used to relax the boundary forces in the simulations developed by S. I. Rao *et al.*

B. Ramírez *et al.*<sup>[1]</sup> found an unstressed energy barrier of 1.9 eV using DD simulations for dislocations dissociated into two partials. They obtained that the energy plateau was reached for a constriction separation of about 60 Å. Both results are in excellent agreement with the simulations in this work. Furthermore, notice that the critical length is about the half of the value found by previous methods.

The total energy of a solid crystal is all potential energy (assuming of course that the crystal does not move). The potential energy of an elastic system is the difference between the internal energy  $\Pi^{\text{int}}$  and the energy due to external forces  $\Pi^{\text{ext}}$ <sup>[56]</sup>. The  $\Pi^{\text{int}}$  consists of the stress-strain energy due to the stress field introduced by the dislocations (and their interactions) respect to the initial geometry i.e. the perfect crystal. The  $\Pi^{\text{ext}}$  consists of the work done by the applied forces, which is obtained by multiplying the displacement generated by the dislocations as they move with the applied forces. Therefore, the energy barrier can be decreased in presence of an external stress.

In many DD fatigue simulations<sup>[10–14]</sup>, following the pioneering work of L. Kubin *et al.*<sup>[15]</sup>, the driving force for cross-slip is the Schmid stress. However, the screw dislocation does not really move because an obstacle is assumed to stop its motion in the glide plane. Thus, the effect of  $\sigma_S^g$  is to compress the dislocation against the obstacle, reducing the equilibration distance between the partials<sup>[2]</sup>. In this way, the  $\sigma_S^g$  stress plays a similar role to  $\sigma_E^g$ , if the dislocations is assumed to stop completely by being compressed against an obstacle. For this reason,  $\sigma_S^g$  is assumed to be zero in all simulations, following the model developed by B. Escaig<sup>[21]</sup>.

### 3.2. Uncoupled stress

In order to study the independent influence of the stress components on the energy barrier, three cross-slip possibilities were considered: (A) pure compression on the glide plane, (B) pure expansion on the conjugate plane and (C) pure bowing-out on the conjugate plane. The stress was increased up to 250 MPa, because the equilibrium configuration breaks down around 260 MPa<sup>[57]</sup>.

The activation enthalpy obtained from DD simulations, the numerical solution of K. Kang's *et al.*<sup>[2]</sup> LT model of cross-slip and the general expression for the activation enthalpy proposed by A. Malka-Markovitz *et al.*<sup>[4]</sup> are in good quantitative agreement with each other, as shown in Fig. 8.

The largest influence on the energy barrier was obtained by pure compression on the glide plane, which reduced it up to 45% (see Fig. 8 (A)). The minimum energy barrier of 1 eV was obtained by applying a compressive stress of 250 MPa on the glide plane. This is in contrast with the lower energy value of 0.95 eV obtained by B. Ramírez *et al.*<sup>[1]</sup> under a pure  $\sigma_E^{cs}$  of 220 MPa. On the other hand, K. Kang *et al.*<sup>[2]</sup> also concluded that the compressive stress applied on the glide was the most effective way of reducing the energy barrier in FCC nickel. The pure widening stress on the cross-slip reduced it up to 20% (see Fig. 8 (B)) and the pure bowing-out stress on the cross-slip produced a decrease in the energy barrier of about 15% (see Fig. 8 (C)).

The effect of stress was not only to decrease the energy barrier but also the activation length of cross-slip. The maximum of energy at 200 MPa occurred for a constriction separation of about 25 Å. This value is comparable to the activation length of  $12b \approx 30.6$  Å at 220 MPa obtained by B. Ramírez *et al.*<sup>[1]</sup>.

### 3.3. Coupled stress

In order to study the combined effect of stress on the energy barrier, three cross-slip possibilities were considered: (A) compression on the glide plane and expansion on the conjugate plane, (B) compression on the glide plane and bowing-out on the conjugate plane and (C) expansion and bowing-out on the conjugate plane.

As in the previous case, the activation enthalpy obtained from DD simulations and the two formulations of the LT model of cross-slip analyzed in this work<sup>[2,4]</sup> are in good agreement (see Fig. 9).

The effect of applying a coupling compressive stress on the glide plane lead to the largest decrease in the energy barrier (see Figs. 9 (A) and (B)). These results resemble the effect applying an uncoupled compressive stress on the glide plane (see Fig. 8 (A)), which also lead to an energy barrier reduction of roughly 50%.

The effect of applying coupled stresses on the conjugate plane only (see Fig. 9 (C)) was comparable of applying an uncoupled Schmid stress on the conjugate plane (see Fig. 8 (C)). In both cases, the energy barrier decreased up to 20%.

These observations are validated by the atomistic simulations of G. Esteban-Manzanares *et al.*<sup>[58]</sup>, who studied the effect of stress in aluminum using molecular dynamics and obtained the same qualitative results.

## 4. Summary and Conclusions

In this work, the unstressed constriction energy was equal to 0.7 eV, as reported by B. Ramírez *et al.*<sup>[1]</sup>. The effect of pure compressive stress in the range of -50 to -250 MPa on the constriction energy was negligible, in agreement with W. Püschl<sup>[53]</sup>.

The unstressed energy barrier was found to be 1.9 eV, as obtained by B. Ramírez *et al.*<sup>[1]</sup>. However, it does not lie within the experimental range of  $1.15 \pm 0.37$  eV measured by J. Bonneville *et al.*<sup>[3]</sup>. On the other hand, the energy barrier could be reduced by applying an external stress,

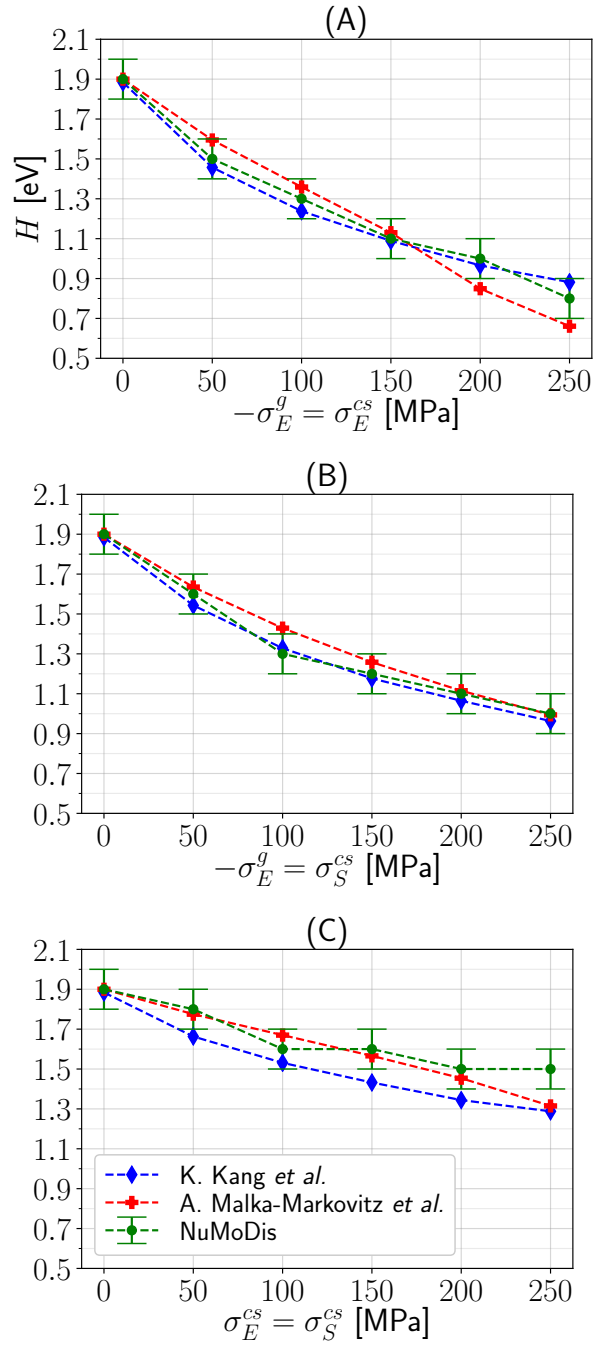


Figure 9: The effect of stress on the energy barrier: (A)  $\sigma_S^g = \sigma_S^{cs} = 0$ , (B)  $\sigma_S^g = \sigma_E^{cs} = 0$  and (C)  $\sigma_S^g = \sigma_E^g = 0$ .

leading to an energy barrier in better agreement with the experimental results. The most effective way of reducing it, was by pure compression on the glide plane. Furthermore, it was found using DD simulations, that both the Schmid and Escaig stress on the conjugate plane have a comparable effect in reducing the energy barrier, in qualitative agreement with the atomistic simulations performed by K. Kang *et al.*<sup>[2]</sup> in FCC nickel.

The energy barrier of FCC Cu at zero stress has been obtained using the line LT model and atomistic simulations before. Some of them reported an energy barrier in better agreement with experiments<sup>[30,54]</sup>. However, the LT model suffers from arbitrariness in the cut-off radius determination<sup>[54]</sup> and the atomistic simulations are highly sensitive to the interatomic potential used<sup>[30]</sup>. In DD simulations, these problems do not exist and the core-width used to compute the elastic energy can be calculated using the theory developed by G. Schöck<sup>[35]</sup> as suggested by B. Ramírez *et al.*<sup>[1]</sup>. Moreover, the effect of non-homogeneous stress on the energy barrier, like those generated by pile-ups and forest dislocations, can be more naturally studied using DD simulations, in comparison with other simulation techniques.

The activation enthalpy obtained from DD simulations was in excellent agreement with both the numerical solution of K. Kang's *et al.*<sup>[2]</sup> LT model of cross-slip and the general expression for the activation enthalpy proposed by A. Malka-Markovitz *et al.*<sup>[4]</sup>. Since the later is an analytical model, it can be easily implemented in a DD code to calculate the activation enthalpy of screw segments.

Acknowledging a limitation of this work, a perfect screw dislocation in FCC crystals can be dissociated in a set of fractional partial dislocations (FPD) pairs, instead of two Shockley partials with Burgers vectors  $\mathbf{b}_1$  and  $\mathbf{b}_2$ . Based on the work of S. Banerjee *et al.*<sup>[59]</sup>, B. R. Ramírez *et al.*<sup>[1]</sup> generalized the dissociation of perfect screw dislocations into  $n$  pairs of fractional partial dislocations (FPD) with Burgers vectors  $\mathbf{b}_1/n$  and  $\mathbf{b}_2/n$ . By using 20 FPDs, they obtained an energy barrier reduction from 1.9 to 1.43 eV at zero stress, which lies within the experimental error of the energy barrier measured by J. Bonneville *et al.*<sup>[3]</sup>.

Regarding the LT model, the constant line energy per unit length  $T$  makes it impossible to distinguish between edge-like and screw-like constrictions. Thus, a more physical description of cross-slip can be made by letting the total energy depend on the angle between the Burgers vector and the local tangent vector<sup>[2,45,52]</sup>. In spite of it, the energy barrier calculated using the LT model was found to be in good quantitative agreement with the DD simulations, at least for the case of dissociation into two partials. Hence, the orientation-dependent LT model might be in better agreement with DD simulations that describe the dislocation core using more than a pair of FPDs.

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**Declaration of interests**

- The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.
- The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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**Margarita Longworth:** Conceptualization, Methodology, Software, Writing - original draft. **Marc Fivel:** Conceptualization, Supervision, Writing - review & editing.