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Effect of stiffness contrast on the dislocation equilibrium positions in a multi-layered structure

Jérôme Colin^{1,*}

Abstract

The equilibrium positions of two edge dislocations lying in the same gliding plane have been theoretically determined in a structure composed of a thin layer embedded in an infinite-size matrix of different elastic constants, when the two dislocations are symmetrically distributed with respect to the axis of symmetry of the problem parallel to the interfaces. When the Burgers vectors of the two dislocations are equal and the matrix is stiffer than the layer, the equilibrium positions have been found to be unstable in the central layer and stable in the matrix. No equilibrium position is found when the matrix is softer than the layer. When the Burgers vectors are of opposite sign (same norm and direction) and the layer is stiffer than the matrix, the equilibrium positions are stable in the central layer and unstable in the matrix, no equilibrium position being found when the layer is softer than the matrix.

Keywords: Dislocations, Plasticity, Modeling, Multilayers

1. Introduction

The control of the mechanical stability of composite materials such as thin films on substrates, coatings and multilayers are of paramount importance because of the numerous applications of such multilayered structures in a number of the technological applications among which nanoelectronics and nanophotonics can be cited. More precisely, it is now well-admitted that the plastic flow in metals is controlled by the motion of dislocations. In this framework, the problem of dislocation pile-ups against an interface has been widely investigated since the first seminal work of Eshelby et al. (Eshelby et al., 1951), who determined the dislocation equilibrium positions when the leading dislocation of the pile-up is locked. Using the method of continuous distributions of dislocations, the equilibrium dislocation positions have been for example determined solving a singular integral equation (Kuang and Mura, 1968). In case of discrete pile-ups, the influence of the applied stress, the elastic coefficients of both phases and pile-up length have been also investigated on the dislocation positions and interface stress (Öveçoğlu et al., 1987). Likewise, the equilibrium positions and

*Corresponding author

Email address: jerome.colin@univ-poitiers.fr (Jérôme Colin)

¹Tel.: (0)549496661, Fax: (0)549497415

resulting stress of pile-ups of edge dislocations has been analyzed near bimetallic interface and circular inhomogeneity (Lubarda, 2017a). Later, the interface stress due to the pile-up of screw dislocations submitted to an applied stress has been estimated against a bimetallic interface (Voskoboynikov et al., 2007) and the problem of an inclined interface against which screw and edge dislocations pile-up has been theoretical investigated, the back stress behind the pile-up being again determined (Lubarda, 2017b, 2018). Following various studies dealing with an edge dislocation near a bimetallic interface (Dundurs and Sendekyj, 1965; Lin and Lee, 1992), a number of papers have been devoted to the dislocation-interface interactions, among which one can cite the works on screw dislocations in presence of a bimaterial interface considering surface strain gradient elasticity (Wang and Schiavone, 2015), and in presence of an imperfect interface (Fan and Wang, 2003). Likewise, the case of edge dislocations near nanoscale inhomogeneities with interface effects should be mentioned (Fang and Liu, 2006; Shodja et al., 2012; Gutkin et al., 2013).

The interactions between dislocations and grain boundaries (GBs) have also been the topics of intensive research since the stopping of the dislocation glide in polycrystalline materials is related, through the Hall-Petch effect, to the hardening of materials. In this context, the absorption, emission and transmission of dislocations at GBs have been studied using discrete dislocation dynamics simulations, and the relaxation effect of the stress fields has been discussed (Quek et al., 2014). Likewise, the competition between the activation of dislocation sources and the dislocation transmission has been theoretically studied through a pile-up model for $< 100 >$ tilt GBs (Liu et al., 2020). It has been found that the transmission phenomenon is activated for low angle GBs while the activation of the dislocation source takes place for high angle GBs (Fedorov et al., 2003). More recently, the possibility of crack initiation has been theoretically studied from a dislocation pile-up at a grain boundary in a crystalline metal. It has been found that the crack initiation mechanism is favored rather than the main crack growth when the main crack is small (Li and Jiang, 2019).

The equilibrium positions of dislocations have been already determined in the vicinity of a planar interface for an isolated dislocation and a dislocation array (Gutkin et al., 1989) as well as, in a bilayer plate, for an isolated dislocation (Gutkin and Romanov, 1992, 1994). In this context, the different equilibrium positions of two edge dislocations have been theoretically investigated in this Paper for a composite structure made of thin layer embedded in an infinite-size matrix, when the dislocations are gliding in the same horizontal plane. Depending on the signs of the Burgers vectors, the existence of stable and unstable dislocation positions in the layer and the matrix has been discussed as a function of the ratio of the shear modulus of both layer and matrix phases.

2. Modeling and Discussion

A two-dimensional thin layer of thickness $2h$, shear modulus μ_0 and Poisson's coefficient ν_0 is embedded in an infinite-size matrix of shear modulus μ and Poisson's coefficient ν (see Fig. 1 for axes). The left part of the matrix for $x \in]-\infty, -h[$ is identified by the $-$ sign, the right part for $x \in]+h, +\infty[$ by the $+$ sign. The central layer for $x \in [-h, +h]$ is identified by the index 0. The first step of this work has been to determine the stress field

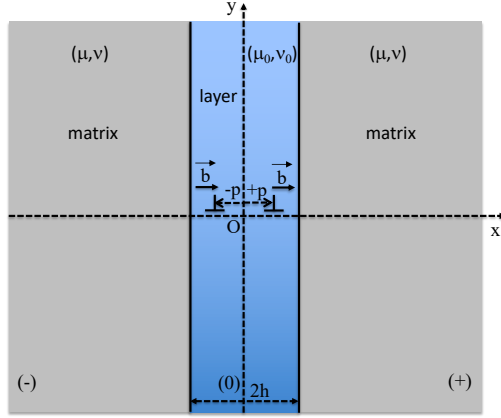


Figure 1: A layer of thickness $2h$ is embedded in a infinite-size matrix. The shear modulus and Poisson's ratio are labelled μ_0 and ν_0 for the layer and μ and ν for the matrix, respectively. Two dislocations of the same Burgers vector $+\vec{b}$ are introduced in the central layer at positions $(p, 0)$ and $(-p, 0)$.

of an edge dislocation of Burgers vector $+\vec{b}$ located at (x_p, y_p) in the central layer, in the framework of the linear and isotropic elasticity theory (Timoshenko and Goodier, 1952; Hirth and Lothe, 1982). At this point, it is worth noting that the stress field of a screw dislocation in and near a lamellar inclusion, including the case of thin films with straight surfaces, has been derived using the method of image dislocations and the image force on the screw dislocation has been determined (Chou, 1966). The effects of the inclusion thickness and rigidity have been thus discussed. Likewise, the force on an edge dislocation in interaction with a lamellar inhomogeneity has been determined using the complex potential method (Stagni and Lizzio, 1987) and the differences with the bimetallic interface case have been highlighted. Considering interface stress and interface tension, the interaction between an array of edge dislocations and a bimetallic interface has been also investigated (Grekov and Sergeeva, 2020). The stress field at the interface has been then determined as well as the image forces on the dislocations. In this work, the Airy's function formalism has been used in the plane strain hypothesis (Timoshenko and Goodier, 1952; Dundurs and Sendeckyj, 1965). The biharmonic Airy's function of the dislocation, labelled ϕ_i in the region i , satisfies:

$$\Delta^2 \phi_i(x, y; x_p, y_p) = 0, \text{ with } i = -, 0, +, \quad (1)$$

where $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$ is the Laplacian's operator. It allows for determining the stress tensor $\bar{\sigma}^i$ through the formulas (Timoshenko and Goodier, 1952):

$$\sigma_{xx}^i(x, y; x_p, y_p) = \frac{\partial^2 \phi_i}{\partial^2 y}(x, y; x_p, y_p), \quad (2)$$

$$\sigma_{xy}^i(x, y; x_p, y_p) = -\frac{\partial^2 \phi_i}{\partial x \partial y}(x, y; x_p, y_p), \quad (3)$$

$$\sigma_{yy}^i(x, y; x_p, y_p) = \frac{\partial^2 \phi_i}{\partial^2 x}(x, y; x_p, y_p), \quad (4)$$

$$\sigma_{zz}^i(x, y; x_p, y_p) = \nu_i(\sigma_{xx}^i(x, y; x_p, y_p) + \sigma_{yy}^i(x, y; x_p, y_p)), \quad (5)$$

where the elastic displacement fields \vec{u}^i can be derived from the classical laws of linear elasticity (Timoshenko and Goodier, 1952), with $i = -, 0, +$. Considering first an infinite-size solid of shear modulus μ_0 and Poisson's coefficient ν_0 , the well-known Airy's function of an edge dislocation of Burgers vector $+\vec{b}$ located at (x_p, y_p) in this medium has been written as (Hirth and Lothe, 1982):

$$\phi_0^{(0)}(x, y; x_p, y_p) = \frac{\mu_0 b}{2\pi(1-\nu_0)} \int_0^{+\infty} \frac{1+k|x-x_p|}{k^2} e^{-k|x-x_p|} \sin[k(y-y_p)] dk, \quad (6)$$

and the Airy's function modifications due the elastic coefficient heterogeneity between the layer and the matrix have been then determined introducing the total Airy's functions in the three different regions $(-, 0, +)$ as:

$$\phi_-(x, y; x_p, y_p) = \int_0^{+\infty} (C_- + D_- x) e^{+kx} \sin[k(y-y_p)] dk, \quad (7)$$

$$\phi_0(x, y; x_p, y_p) = \phi_0^{(0)}(x, y; x_p, y_p) + \phi_0^{(sup)}(x, y; x_p, y_p), \quad (8)$$

$$\phi_+(x, y; x_p, y_p) = \int_0^{+\infty} (A_+ + B_+ x) e^{-kx} \sin[k(y-y_p)] dk, \quad (9)$$

with:

$$\phi_0^{(sup)}(x, y; x_p, y_p) = \int_0^{+\infty} [(A_0 + B_0 x) e^{-kx} + (C_0 + D_0 x) e^{+kx}] \sin[k(y-y_p)] dk, \quad (10)$$

where $C_-, D_-, A_+, B_+, A_0, B_0, C_0$ and D_0 are constants to be determined using the mechanical equilibrium and total displacement continuity conditions at the interfaces $x = \pm h$. The general expressions of the different stress and displacement fields derived from ϕ_-, ϕ_+ and ϕ_0 being given in the Appendix, it yields:

$$\sigma_{xx}^0(\pm h, y; x_p, y_p) = \sigma_{xx}^\pm(\pm h, y; x_p, y_p), \quad (11)$$

$$\sigma_{xy}^0(\pm h, y; x_p, y_p) = \sigma_{xy}^\pm(\pm h, y; x_p, y_p), \quad (12)$$

$$u_x^0(\pm h, y; x_p, y_p) = u_x^\pm(\pm h, y; x_p, y_p), \quad (13)$$

$$u_y^0(\pm h, y; x_p, y_p) = u_y^\pm(\pm h, y; x_p, y_p). \quad (14)$$

Solving the above set of Eqs. (11), (12), (13) and (14), the different constants have been determined but have not been displayed in this Paper for the sake of compactness. Once the stress field of the dislocation in the central layer is known, the problem of the determination of the equilibrium positions of two edge dislocations of equal Burgers vectors \vec{b} , located at $(x_p = -p, y_p = 0)$ and $(x_p = p, y_p = 0)$ in this layer, with $0 < p < h$, has been then addressed through the Peach-Koehler (PK) force calculation (Peach and Koehler, 1950). Indeed, the

total Peach-Koehler force per unit length $\vec{F}_{tot}^{p,0}$ exerted on the dislocation located at $(p, 0)$ in the (0) region is expressed as (Peach and Koehler, 1950):

$$\vec{F}_{tot}^{p,0} = \vec{b}\vec{\sigma}^{tot,0} \wedge \vec{u}_z, \quad (15)$$

where \vec{u}_z is the unit vector along the (Oz) axis parallel to the dislocation line and $\vec{\sigma}^{tot,0}$ the stress field composed of the total stress field in the (0) region due to the dislocation located at $(-p, 0)$ and characterized by the Airy's function $\phi_0(x, y; -p, 0)$ defined in Eq. (8) plus the stress tensor modification $\vec{\sigma}_0^{(sup)}$ for the dislocation at $(p, 0)$ due to the elastic constant heterogeneity and characterized by the Airy's function $\phi_0^{(sup)}(x, y; p, 0)$ defined in Eq. (10). Since the two edge dislocations are lying in the same horizontal plane, only the horizontal gliding part of the PK force in Eq. (15) has been considered which is given by:

$$F_g^{p,0} = \vec{F}_{tot}^{p,0} \cdot \vec{u}_x, \quad (16)$$

with \vec{u}_x the unit vector along the (Ox) axis. Assuming in the following that $\nu_0 = \nu = 0.3$, and introducing the shear modulus ratio $\mu_* = \mu/\mu_0$, the dimensionless variable $\tilde{p} = p/h$ and dimensionless force $\tilde{F}_g^{p,0} = F_g^{p,0}h/(\mu_0b^2)$, it yields:

$$\tilde{F}_g^{p,0}(\tilde{p}) = \int_0^{+\infty} \frac{\Psi_1(\tilde{p}, k)}{\Psi_2(\tilde{p}, k)} dk, \quad (17)$$

with

$$\begin{aligned} \Psi_1(\tilde{p}, k) &= (1 - \mu_*)(\mu_* + 3 - 4\nu)\tilde{p}k + (-3 + 4\nu + \mu_*(-2 - 3\mu_* \\ &+ 4(2 + \mu_*)\nu - 8\nu^2))\tilde{p}k \cosh[2k(\tilde{p} - 1)] \\ &- 8\mu_*(1 - \nu)^2\tilde{p}k \cosh[2\tilde{p}k] \sinh[2k] \\ &+ ((\mu_* - 1)((\mu_* + 3 - 4\nu)(1 - \tilde{p})^2k^2 + 2\mu_*(1 - 2\nu)(1 - \nu)) \\ &+ 8\mu_*(1 - \nu)^2\tilde{p}k \cosh[2k]) \sinh[2\tilde{p}k], \end{aligned} \quad (18)$$

$$\begin{aligned} \Psi_2(\tilde{p}, k) &= \pi(-1 + \nu)(2(1 - \mu_*)(\mu_* + 3 - 4\nu)k \\ &+ 8(1 - \nu)^2\mu_* \cosh[2k] + (3 + 2\mu_* + 3\mu_*^2 - 4(1 + \mu_*)^2\nu \\ &+ 8\nu^2\mu_*) \sinh[2k]). \end{aligned} \quad (19)$$

Likewise, when the two dislocations are now positioned in the $(-)$ and $(+)$ regions, an equivalent stress state determination procedure to the one already developed for the dislocations in the (0) region has been conducted, and the gliding component $\tilde{F}_g^{p,+}$ of the PK force applied on the dislocation placed at $(p, 0)$ in the $(+)$ region of positive x has been found to be:

$$\tilde{F}_g^{p,+}(\tilde{p}) = \int_0^{+\infty} \frac{\Phi_1(\tilde{p}, k)}{\Phi_2(\tilde{p}, k)} dk, \quad (20)$$

with

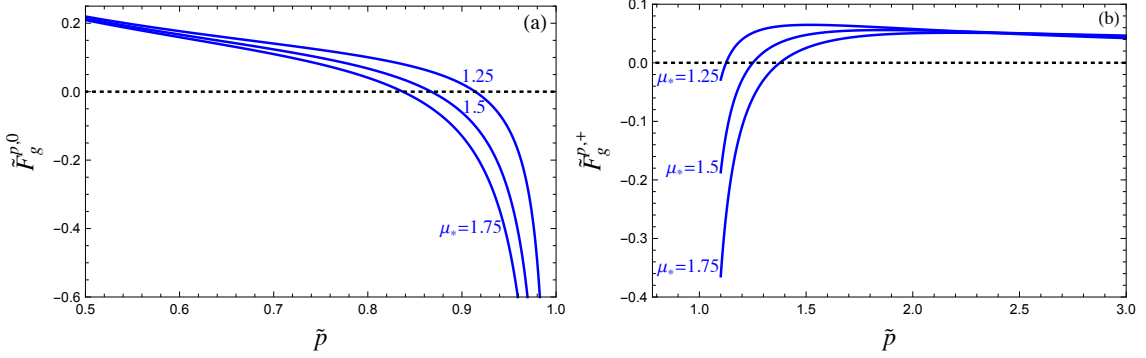


Figure 2: Total forces $\tilde{F}_g^{p,0}$ and $\tilde{F}_g^{p,+}$ versus \tilde{p} in case of two dislocations of the same Burgers vector $+\vec{b}$, when the central layer is softer than the matrix, with $\nu = \nu_0 = 0.3$. (a) The dislocations are in the central layer. (b) The dislocations are in the matrix.

$$\begin{aligned}
\Phi_1(\tilde{p}, k) &= 2\mu_* e^{2(2-\tilde{p})k} (2(1-\mu_*)^2 (1-\tilde{p})^2 k^3 \\
&+ 4(1-\nu)(1-\mu_* + 2\mu_*\tilde{p} - 2(1+\mu_*(\tilde{p}-1))\nu) \\
&+ (1-\mu_*)(2(1-\nu)(1-2\nu) \\
&+ (1-\tilde{p})^2(1+\mu_*(3-4\nu))k^2) \sinh[2k], \tag{21}
\end{aligned}$$

$$\begin{aligned}
\Phi_2(\tilde{p}, k) &= \pi(1-\nu)(4(1-\mu_*)(\mu_* + 3 - 4\nu)ke^{2k} \\
&- (3-4\nu)(1-\mu_*)^2 + (\mu_* + 3 - 4\nu)(1 + (3-4\nu)\mu_*)e^{4k}). \tag{22}
\end{aligned}$$

It is underlined at this point that due to the symmetry of the problem, the forces $\tilde{F}_g^{-p,0}$ and $\tilde{F}_g^{-p,-}$ acting on the dislocation located at $(-p, 0)$ in the (0) and (-) regions can be easily derived from the ones given in Eqs. (17) and (20), respectively. It is also emphasized that both integrals in Eqs. (17) and (20) have been numerically estimated except in a few limit cases that has been now discussed. Indeed, when the layer and the matrix have the same shear modulus, i.e. when $\mu_0 = \mu$, the forces $\tilde{F}_g^{p,0}$ and $\tilde{F}_g^{p,+}$ reduce to the classical expression of the interaction force between two edge dislocations of the same Burgers vector in an infinite-size medium (Hirth and Lothe, 1982):

$$\tilde{F}_g^{p,0}(\tilde{p}) = \tilde{F}_g^{p,+}(\tilde{p}) = \frac{1}{4\pi(1-\nu)} \frac{1}{\tilde{p}}, \tag{23}$$

and the two dislocations should repeal each other, no equilibrium position being reached. When $\mu_0 = 0$, the problem reduces to the study of two isolated dislocations, each one in a semi-infinite medium. The applied force on the dislocation in the (+) region with positive x writes (Hirth and Lothe, 1982):

$$\tilde{F}_g^{p,+}(\tilde{p}) = -\frac{1}{4\pi(1-\nu)} \frac{1}{\tilde{p} - \tilde{h}}. \tag{24}$$

It corresponds to the attracting force of the free-surface, the two dislocations being now disconnected such that no interaction force exists. As a consequence, the dislocations should

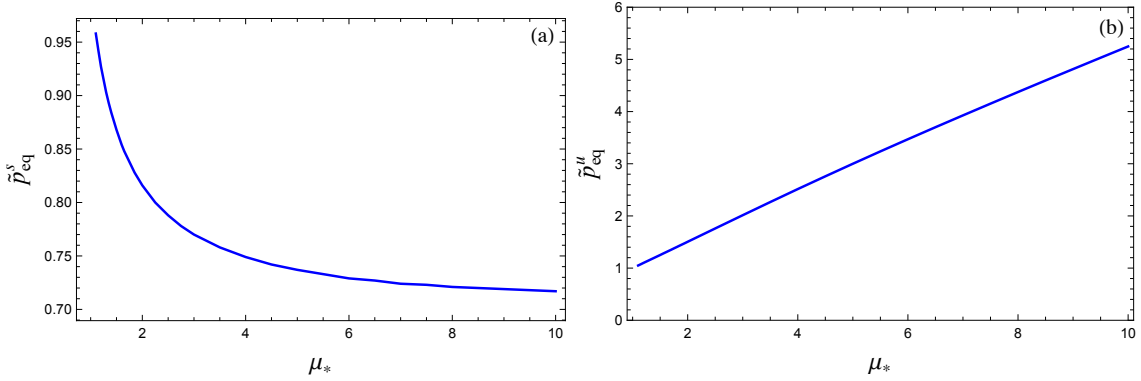


Figure 3: Equilibrium positions of the dislocations of the same Burgers vector $+\vec{b}$ versus the shear modulus ratio. (a) Stable equilibrium position \tilde{p}_{eq}^s in the layer versus μ_* . (b) Unstable equilibrium position \tilde{p}_{eq}^u in the matrix versus μ_* .

be absorbed by the free-surface. When $\mu_0 \rightarrow +\infty$, $\tilde{F}_g^{p,+}$ is found to be:

$$\tilde{F}_g^{p,+}(\tilde{p}) = \frac{1}{4\pi(1-\nu)} \frac{1 + (1-\nu)(1-2\nu)}{(1-\nu)(3-4\nu)} \frac{1}{\tilde{p} - \tilde{h}}, \quad (25)$$

and the dislocation is repelled by the "wall" layer. Equivalent results can be drawn for the expression of the force applied on the dislocation located in $(-\tilde{p}, 0)$. In Figs. (2), the dimensionless forces $\tilde{F}_g^{p,0}$ and $\tilde{F}_g^{p,+}$ applied on the dislocation located at $(p, 0)$ in the (0) and (+) regions have been numerically calculated from Eqs. (17) and (20) and have been plotted versus the dimensionless dislocation position \tilde{p} for different values of the shear modulus ratio μ_* , with $\nu_0 = \nu = 0.3$. In Fig. (2)a, it is observed that when the matrix is harder than the central layer ($\mu_* > 1$), the two edge dislocations of the same Burgers vector can occupy stable equilibrium positions such that $F_g^{p,0}(p_{eq}, 0) = 0$ (and $F_g^{-p,0}(-p_{eq}, 0) = 0$), with $\partial^2 F_g^{p,0}/\partial p^2(p_{eq}, 0) > 0$ (and $\partial^2 F_g^{-p,0}/\partial p^2(-p_{eq}, 0) > 0$). It is also observed that as the stiffness of the matrix increases, the resulting repulsive forces on the dislocations increase, and the equilibrium positions move away from the layer/matrix interfaces. Likewise, in Fig. (2), two equilibrium positions can be identified in the matrix for the dislocations when the matrix is still harder than the layer, but in this case, the equilibrium positions are found to be unstable ($\partial^2 F_g^{p,0}/\partial p^2(p_{eq}, 0) < 0$ and $\partial^2 F_g^{-p,0}/\partial p^2(-p_{eq}, 0) < 0$). As the shear modulus ratio increases, these equilibrium positions move away from the interfaces. No equilibrium position has been found in case of a hard layer embedded in a soft matrix, i.e. when $\mu_* < 1$. In Figs. (3), the equilibrium positions of the dislocations have been displayed versus the shear modulus ratio μ_* , with $\nu_0 = \nu = 0.3$. It is confirmed in Fig. (3)a that the stable equilibrium position \tilde{p}_{eq}^s decreases as μ_* increases, due to the matrix repulsion. As the shear modulus of the matrix tends to infinity, it is found that \tilde{p}_{eq}^s goes to the minimum value of the order of 0.712 at which the repulsive force between the two dislocations of the same Burgers vector prevents the dislocation to get closer to each other. In Fig. (3)b, the unstable equilibrium position \tilde{p}_{eq}^u increases with μ_* , the dislocations also moving away from the interface, the variation being almost linear in this case. The problem of the determination

of the equilibrium positions of two edge dislocations of opposite Burgers vectors has been also addressed taking advantage of the results previously obtained. Considering an edge dislocation of Burgers vector $-\vec{b}$ at $(-\tilde{p}, 0)$ and another one of Burgers vector $+\vec{b}$ at $(\tilde{p}, 0)$, the gliding components of the two PK forces exerted on these dislocations can be easily derived from the ones already calculated for the two dislocations of the same Burgers vector. Indeed, the force exerted by one dislocation on the other changes sign while that resulting from the elastic coefficient heterogeneity keeps the same sign as that of the previous case. As a consequence, the dimensionless force $\tilde{F}_g^{p,0}$ in the central layer has been found to be:

$$\tilde{F}_g^{p,0}(\tilde{p}) = \int_0^{+\infty} \frac{\Psi_3(\tilde{p}, k)}{\Psi_4(\tilde{p}, k)} dk, \quad (26)$$

with

$$\begin{aligned} \Psi_3(\tilde{p}, k) &= (\mu_* - 1)(\mu_* + 3 - 4\nu)\tilde{p}k \\ &+ (3 + 2\mu_* + 3\mu_*^2 - 4(1 + \mu_*)^2\nu + 8\mu_*\nu^2)\tilde{p}k \cosh[2(\tilde{p} - 1)k] \\ &+ 8\mu_*(1 - \nu)^2\tilde{p}k \cosh[2\tilde{p}k] \sinh[2k] + ((\mu_* - 1)((1 - \tilde{p})^2(\mu_* \\ &+ 3 - 4\nu)k^2 + 2\mu_*(1 - \nu)(1 - 2\nu)) \\ &- 8\mu_*(1 - \nu)^2\tilde{p}k \cosh[2k]) \sinh[2\tilde{p}k], \end{aligned} \quad (27)$$

$$\begin{aligned} \Psi_4(\tilde{p}, k) &= -\pi(1 - \nu)(2(\mu_* - 1)(\mu_* + 3 - 4\nu)k + 8\mu_*(1 - \nu)^2 \cosh[2k] \\ &+ (3 + 2\mu_* + 3\mu_*^2 - 4(1 + \mu_*)^2 + 8\mu_*\nu^2) \sinh[2k]), \end{aligned} \quad (28)$$

and the force $\tilde{F}_g^{p,+}$ in the matrix part of positive x is given by:

$$\tilde{F}_g^{p,+}(\tilde{p}) = \int_0^{+\infty} \frac{\Phi_3(\tilde{p}, k)}{\Phi_4(\tilde{p}, k)} dk, \quad (29)$$

with

$$\begin{aligned} \Phi_3(\tilde{p}, k) &= \mu_*e^{2(1-\tilde{p})k}((1 - \mu_*)(e^{4k} - 1)(-2 + 6\nu - 4\nu^2 \\ &+ (1 + \mu_*(3 - 4\nu))(2 - \tilde{p})\tilde{p}k^2) + 2e^{2k}k(2(1 - \mu_*)^2(1 - \tilde{p})^2k^2 \\ &- 4(1 - \nu)(\mu_* - 1 - 2\mu_*\tilde{p} + 2(1 - \mu_*(1 - \tilde{p}))\nu) \\ &- (1 - \mu_*)(1 + \mu_*(3 - 4\nu))k \sinh[2k]), \end{aligned} \quad (30)$$

$$\begin{aligned} \Phi_4(\tilde{p}, k) &= \pi(1 - \nu)(4e^{2k}(1 - \mu_*)(\mu_* + 3 - 4\nu)k + (3 - 4\nu)(1 - \mu)^2 \\ &- e^{4k}(\mu_* + 3 - 4\nu)(1 + \mu_*(3 - 4\nu))). \end{aligned} \quad (31)$$

As previously mentioned in the case of two dislocations of the same Burgers vector, the following situations where analytical expressions can be obtained for the applied forces on the dislocations of opposite sign Burgers vectors can be briefly discussed. When $\mu_0 = \mu$, the attractive forces $\tilde{F}_g^{p,0}$ and $\tilde{F}_g^{p,+}$ have been found to be from Eqs. (26) and (29):

$$\tilde{F}_g^{p,0}(\tilde{p}) = \tilde{F}_g^{p,+}(\tilde{p}) = -\frac{1}{4\pi(1 - \nu)}\frac{1}{\tilde{p}}, \quad (32)$$

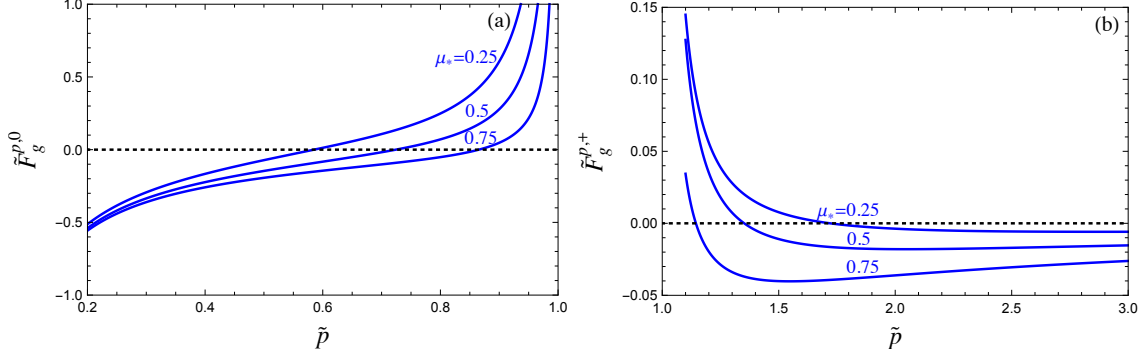


Figure 4: Total forces $\tilde{F}_g^{p,0}$ and $\tilde{F}_g^{p,+}$ versus \tilde{p} in case of two dislocations of opposite sign Burgers vectors, when the central layer is harder than the matrix, with $\nu = \nu_0 = 0.3$. (a) the dislocations are in the central layer. (b) the dislocation are in the matrix.

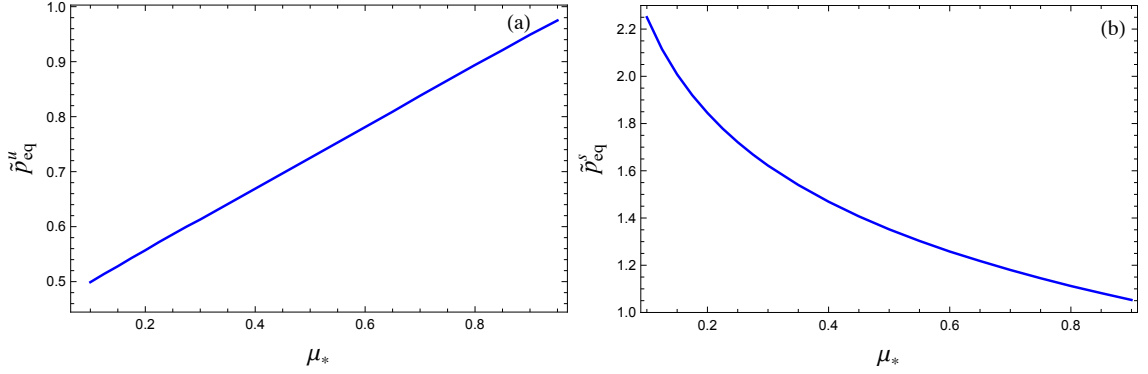


Figure 5: Equilibrium positions of the dislocations of opposite sign Burgers vectors versus the shear modulus ratio μ_* . (a) Unstable equilibrium position \tilde{p}_{eq}^u in the layer versus μ_* . (b) Stable equilibrium position \tilde{p}_{eq}^s in the matrix versus μ_* .

such that the two dislocations should attract each other, and no equilibrium position can be neither reached (Hirth and Lothe, 1982). When $\mu_0 = 0$, the applied force on the dislocation in the semi-infinite (+) region with positive x is:

$$\tilde{F}_g^{p,+}(\tilde{p}) = -\frac{1}{4\pi(1-\nu)} \frac{1}{\tilde{p} - \tilde{h}}, \quad (33)$$

and the dislocation should be again absorbed by the free-surface (Hirth and Lothe, 1982). When $\mu_0 \rightarrow +\infty$, $\tilde{F}_g^{p,+}$ is found to be:

$$\tilde{F}_g^{p,+}(\tilde{p}) = \frac{1}{4\pi(1-\nu)} \frac{1 + (1-\nu)(1-2\nu)}{(1-\nu)(3-4\nu)} \frac{1}{\tilde{p} - \tilde{h}}, \quad (34)$$

and the dislocation is still repelled by the layer of infinite stiffness.

In Figs (4), the forces $\tilde{F}_g^{p,0}$ and $\tilde{F}_g^{p,+}$ applying on the dislocations in the (0) and (+) regions, respectively, have been numerically determined from Eqs. (26) and (29) and have plotted versus \tilde{p} for different values of μ_* , with $\nu_0 = \nu = 0.3$. When the layer is harder

than the matrix ($\mu_* < 1$), it is found in Fig. (4)a that the dislocations can occupy unstable equilibrium positions in the layer, these positions getting closer to the interface as μ_* increases. In the matrix, the equilibrium positions are found in Fig. (4)b to be stable and also move closer to the interface as μ_* increases. When the layer is softer than the matrix, no equilibrium position is found for the dislocations of opposite sign Burgers vectors. Finally, the equilibrium positions \tilde{p}_{eq}^u and \tilde{p}_{eq}^s for the dislocation in the layer and in the matrix (with positive x) have been plotted versus μ_* in Figs. (5). It is confirmed that the unstable equilibrium position \tilde{p}_{eq}^u in the layer increases almost linearly until the interface in Fig. (5)a, while the stable one in the matrix decreases until the dislocation reaches the interface in Fig. (5)b.

3. Conclusion

The different equilibrium positions of two edge dislocations lying in the same horizontal gliding plane of a structure composed of thin layer embedded in an infinite-size matrix has been theoretically investigated from the Peach-Koehler force calculation. When the two dislocations have the same Burgers vector and when the layer is harder than the matrix, the equilibrium positions have been found to be stable in the layer and unstable in the matrix. When the dislocations have opposite sign Burgers vectors and the matrix is harder than the layer, the equilibrium positions are unstable in the layer and stable in the matrix. One possible next step of inquiry of the present work would be to consider in addition to the crystallography of the layer and matrix materials, the nucleation mechanism of the dislocations, their interface crossing and eventual cross-slip. Likewise, the possibility of existence of non-symmetric configurations should be considered, where the two dislocations would not be symmetrically distributed with respect to the axis of symmetry parallel to the interfaces.

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5. Appendix

A dislocation of Burgers vector $+\vec{b}$ is located at (x_p, y_p) in a central layer embedded in an infinite size matrix of different elastic coefficients (see Fig. 1). To determine the resulting stress field in the structure, the Airy's function formalism has been used (Timoshenko and Goodier, 1952; Hirth and Lothe, 1982) such that the biharmonic Airy's function ϕ_i satisfying:

$$\Delta^2 \phi_i(x, y; x_p, y_p) = 0, \quad (35)$$

in the region i allows for determining the dislocation stress tensor $\bar{\sigma}^i$ through the formulas (Timoshenko and Goodier, 1952):

$$\sigma_{xx}^i(x, y; x_p, y_p) = \frac{\partial^2 \phi_i}{\partial^2 y}(x, y; x_p, y_p), \quad (36)$$

$$\sigma_{xy}^i(x, y; x_p, y_p) = -\frac{\partial^2 \phi_i}{\partial x \partial y}(x, y; x_p, y_p), \quad (37)$$

$$\sigma_{yy}^i(x, y; x_p, y_p) = \frac{\partial^2 \phi_i}{\partial^2 x}(x, y; x_p, y_p), \quad (38)$$

$$\sigma_{zz}^i(x, y; x_p, y_p) = \nu_i(\sigma_{xx}^i(x, y; x_p, y_p) + \sigma_{yy}^i(x, y; x_p, y_p)), \quad (39)$$

$i = -, 0, +$. Assuming the Airy's function of the dislocation when the central region is of infinite size is given by:

$$\phi_0^{(0)}(x, y; x_p, y_p) = \frac{\mu_0 b}{2\pi(1-\nu_0)} \int_0^\infty \frac{1+k|x-x_p|}{k^2} e^{-k|x-x_p|} \sin[k(y-y_p)] dk, \quad (40)$$

and using Eqs. (36), (37), (38) and (39), the corresponding stress field has been found to be:

$$\sigma_{xx}^{0,(0)}(x, y; x_p, y_p) = -\frac{\mu_0 b}{2\pi(1-\nu_0)} \int_0^{+\infty} (1+k|x-x_p|) e^{-k|x-x_p|} \sin[k(y-y_p)] dk, \quad (41)$$

$$\sigma_{xy}^{0,(0)}(x, y; x_p, y_p) = \frac{\mu_0 b}{2\pi(1-\nu_0)} \int_0^{+\infty} k(x-x_p) e^{-k|x-x_p|} \cos[k(y-y_p)] dk, \quad (42)$$

$$\sigma_{yy}^{0,(0)}(x, y; x_p, y_p) = \frac{\mu_0 b}{2\pi(1-\nu_0)} \int_0^{+\infty} (-1+k|x-x_p|) e^{-k|x-x_p|} \sin[k(y-y_p)] dk. \quad (43)$$

Likewise, using the classical laws of linear and isotropic elasticity (Timoshenko and Goodier, 1952), the displacement field is found to be:

$$u_x^{0,(0)}(x, y; x_p, y_p) = -\frac{b}{4\pi(1-\nu_0)} \int_0^{+\infty} \left(2(1-\nu_0) \frac{|x-x_p|}{x-x_p} + k(x-x_p)\right) \frac{e^{-k|x-x_p|}}{k} \times \sin[k(y-y_p)] dk, \quad (44)$$

$$u_y^{0,(0)}(x, y; x_p, y_p) = \frac{b}{4\pi(1-\nu_0)} \int_0^{+\infty} (1-2\nu_0 - k|x-x_p|) \frac{e^{-k|x-x_p|}}{k} \cos[k(y-y_p)] dk. \quad (45)$$

Since the central layer in the present problem is of finite thickness, the Airy's function labelled now ϕ_0 is modified as follows:

$$\phi_0(x, y; x_p, y_p) = \phi_0^{(0)}(x, y; x_p, y_p) + \phi_0^{(sup)}(x, y; x_p, y_p), \quad (46)$$

$$(47)$$

with

$$\phi_0^{(sup)}(x, y; x_p, y_p) = \int_0^{+\infty} [(A_0 + B_0 x) e^{-kx} + (C_0 + D_0 x) e^{+kx}] \sin[k(y-y_p)] dk. \quad (48)$$

In the regions $-$ and $+$, the following Airy's function's ϕ_- and ϕ_+ have also been introduced:

$$\phi_-(x, y; x_p, y_p) = \int_0^{+\infty} (C_- + D_- x) e^{+kx} \sin[k(y-y_p)] dk, \quad (49)$$

$$\phi_+(x, y; x_p, y_p) = \int_0^{+\infty} (A_+ + B_+ x) e^{-kx} \sin[k(y-y_p)] dk. \quad (50)$$

The different stress and displacement fields corresponding to ϕ_- , ϕ_+ and $\phi_0^{(sup)}$ have been then determined with the help of the set of Eqs. (36), (37), (38) and (39). It yields:

$$\sigma_{xx}^-(x, y; x_p, y_p) = - \int_0^{+\infty} k^2(C_- + D_-x)e^{+kx} \sin[k(y - y_p)] dk, \quad (51)$$

$$\sigma_{xy}^-(x, y; x_p, y_p) = - \int_0^{+\infty} k(C_-k + D_- + D_-kx)e^{+kx} \cos[k(y - y_p)] dk, \quad (52)$$

$$\sigma_{yy}^-(x, y; x_p, y_p) = \int_0^{+\infty} k(C_-k + 2D_- + D_-kx)e^{+kx} \sin[k(y - y_p)] dk, \quad (53)$$

$$u_x^-(x, y; x_p, y_p) = -\frac{1}{2\mu} \int_0^{+\infty} (C_-k - (1 - 2\nu)D_- + D_-kx)e^{+kx} \sin[k(y - y_p)] dk, \quad (54)$$

$$u_y^-(x, y; x_p, y_p) = -\frac{1}{2\mu} \int_0^{+\infty} (C_-k + 2(1 - \nu)D_- + D_-kx)e^{+kx} \cos[k(y - y_p)] dk. \quad (55)$$

$$\sigma_{xx}^+(x, y; x_p, y_p) = - \int_0^{+\infty} k^2(A_+ + B_+x)e^{-kx} \sin[k(y - y_p)] dk, \quad (56)$$

$$\sigma_{xy}^+(x, y; x_p, y_p) = - \int_0^{+\infty} k(-A_+k + B_+ - B_+kx)e^{-kx} \cos[k(y - y_p)] dk, \quad (57)$$

$$\sigma_{yy}^+(x, y; x_p, y_p) = \int_0^{+\infty} k(A_+k - 2B_+ + B_+kx)e^{-kx} \sin[k(y - y_p)] dk, \quad (58)$$

$$u_x^+(x, y; x_p, y_p) = \frac{1}{2\mu} \int_0^{+\infty} (A_+k + (1 - 2\nu)B_+ + B_+kx)e^{-kx} \sin[k(y - y_p)] dk, \quad (59)$$

$$u_y^+(x, y; x_p, y_p) = -\frac{1}{2\mu} \int_0^{+\infty} (A_+k - 2(1 - \nu)B_+ + B_+kx)e^{-kx} \cos[k(y - y_p)] dk. \quad (60)$$

$$\begin{aligned} \sigma_{xx}^{0,(sup)}(x, y; x_p, y_p) &= - \int_0^{+\infty} k^2((A_0 + B_0x)e^{-kx} + (C_0 + D_0x)e^{+kx}) \\ &\quad \times \sin[k(y - y_p)] dk, \end{aligned} \quad (61)$$

$$\begin{aligned} \sigma_{xy}^{0,(sup)}(x, y; x_p, y_p) &= - \int_0^{+\infty} k((-A_0k + B_0 - B_0kx)e^{-kx} \\ &\quad + (C_0k + D_0 + D_0kx)e^{+kx}) \cos[k(y - y_p)] dk, \end{aligned} \quad (62)$$

$$\begin{aligned} \sigma_{yy}^{0,(sup)}(x, y; x_p, y_p) &= \int_0^{+\infty} k((A_0k - 2B_0 + B_0kx)e^{-kx} \\ &\quad + (C_0k + 2D_0 + D_0kx)e^{+kx}) \sin[k(y - y_p)] dk, \end{aligned} \quad (63)$$

$$\begin{aligned} u_x^{0,(sup)}(x, y; x_p, y_p) &= \frac{1}{2\mu_0} \int_0^{+\infty} ((A_0k + (1 - 2\nu_0)B_0 + B_0kx)e^{-kx} \\ &\quad - (C_0k - (1 - 2\nu_0)D_0 + D_0kx)e^{+kx}) \sin[k(y - y_p)] dk, \end{aligned} \quad (64)$$

$$u_y^{0,(sup)}(x, y; x_p, y_p) = -\frac{1}{2\mu_0} \int_0^{+\infty} ((A_0k - 2(1 - \nu_0)B_0 + B_0kx)e^{-kx}$$

$$+ (C_0k + 2(1 - \nu_0)D_0 + D_0kx)e^{+kx} \cos[k(y - y_p)] dk, \quad (65)$$

where $C_-, D_-, A_+, B_+, A_0, B_0, C_0$ and D_0 are constants to be determined. Considering the mechanical equilibrium and total displacement continuity conditions at the interfaces $x = \pm h$:

$$\sigma_{xx}^0(\pm h, y; x_p, y_p) = \sigma_{xx}^\pm(\pm h, y; x_p, y_p), \quad (66)$$

$$\sigma_{xy}^0(\pm h, y; x_p, y_p) = \sigma_{xy}^\pm(\pm h, y; x_p, y_p), \quad (67)$$

$$u_x^0(\pm h, y; x_p, y_p) = u_x^\pm(\pm h, y; x_p, y_p), \quad (68)$$

$$u_y^0(\pm h, y; x_p, y_p) = u_y^\pm(\pm h, y; x_p, y_p), \quad (69)$$

these constants have been determined but not explicitly displayed in this Paper for the sake of compactness. An equivalent procedure to the one described in this Appendix has been carried out when the dislocation is embedded in the $-$ or $+$ regions, the initial stress field of dislocation in the infinite-size medium \pm being obtained from Eqs. (41), (42), (43), (44), and (45), changing μ_0 and ν_0 in μ and ν , respectively.

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