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Edge dislocation near a wedge-shaped solid: elastic force calculation

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Abstract

Using a finite elements procedure, the gliding force acting on an edge dislocation localized near a wedge shaped solid has been numerically calculated as a function of its position coordinates. An analytic function of this force has been then established, considering results obtained for a screw dislocation near two orthogonal free surfaces.

Keywords: Modeling, finite elements, Castem2000, Edge dislocation.

1. Introduction

During the elaboration of multilayers or thin films on substrates, high residual stresses usually appear, which can strongly modifies the mechanical behavior of these nano-structures. Stresses in thin films and in substrates can have different origins like for example the difference of the lattice parameters between the two materials (epitaxy), the thermal expansion differences, the phase transitions or the defects like dislocations or precipitates [1,-3]. During the past few years, many papers have dealt with the determination of the stress field in materials since stresses are fundamental to understand the propagation of cracks and dislocations at the interfaces, the buckling of thin films on substrates, etc [4-10].

The problem of determination of stresses in a semi-infinite solid containing edge or screw dislocations near its free surface has been now solved [11-13] using different technics like Green's functions, distributions of Boussinesq's forces or surface dislocations. The stability of screw and edge dislocations near interfaces in multilayers structures, with different elastic constants and compositions has been also investigated using Muskhelishvili method [15, 16], Fourier series developments [17], etc.

In the case of wedge-shaped bodies, the stress state determination is much more complex. Different methods have been used for an edge dislocation, like for example the Mullin transformation [18] which gave an integral representation of the stress of an edge dislocation or a disclintion. For a screw dislocation, the shear stress has been determined as a function of the angle of the material-filled region [19].

In this paper, the gliding force of an edge dislocation has been first computed near two orthogonal free surfaces, using a finite elements method. An analytic expression of this force has been then established considering the expression of the gliding force obtained for an edge dislocation in a semi-infinite solid and for a screw dislocation in a wedge shaped solid.

2. Method of calculation

An edge dislocation of Burgers vector $\vec{b}\,(b,0)$ is considered at point (x,y) in a wedge shaped 2D solid of shear modulus and Poisson's ratio μ and ν respectively (see figure 1 for axes). The total stress $\sigma_{ij}^{tot}(x,y)$ in the material due to this edge dislocation can be written as:

$$\sigma_{ij}^{tot}(x,y) = \sigma_{ij}^{0}(x,y) + \sigma_{ij}^{rel}(x,y),$$

where $\sigma_{ij}^{0}(x,y)$ is the initial stress of the dislocation in an infinite medium and $\sigma_{ij}^{rel}(x,y)$ is the stress relaxation induced by the two orthogonal free surfaces S_1 and S_2. First to determine numerically this stress relaxation $\sigma_{ij}^{rel}(x,y)$, a finite elements procedure (with CASTEM 2000) has been used. The finite element method is a numerical analysis technique for obtaining approximate solutions to a wide variety of physical problems. This approximation allows to obtain a linear algebraic system $[K]\{u\}=\{F\}$, Or K is a Stiffness matrix, F is a Force vector, u is a displacement vector . The stresses are calculated from the displacements.
On the free surfaces S_1 and S_2, the mechanical equilibrium of forces gives the following conditions:

$$\sigma_{ij}^{tot}\, n_j = 0 \text{ on } S_1 \text{ and } S_2$$

$$\Rightarrow \sigma_{xx}^{tot}(x,0) = \sigma_{xy}^{tot}(x,0) = 0 \text{ on } S_1$$

$$\Rightarrow \sigma_{yy}^{tot}(0,y) = \sigma_{xy}^{tot}(0,y) = 0 \text{ on } S_2$$

where n_j is the component of the unit normal vector to the free surfaces.

Two arbitrary surfaces S_3 and S_4 have been introduced to block the total displacements of the solid (figure 1). After the numerical computation of the stress tensor of relaxation $\overline{\Sigma}^{rel}$ induced by the two free surfaces S_1 and S_2, the gliding force of the dislocation has been easily derived using the relation:

$$\vec{F}^{num}(x,y) = \vec{b}\,\overline{\Sigma}^{rel} \wedge \vec{l} \Rightarrow F_x(x,y) = b\,\sigma_{xy}^{rel}(x,y)$$

where, $\vec{l}$ is the unit line vector of the dislocation in the (0z) direction.

The numerical force $F_x^{num}(x,y)$ acting on the edge dislocation in the (0x) direction has been determined as a function of x for different values of y, see figure 2. Considering thus the dimensionless function $y\,F_x^{num}(x/y)$, it has been observed figure 3 that, for the different values of y, the curves of $y\,F_x^{num}(x/y)$ were superimposed. This scalling allows one to consider the dimensionless expression of the force acting on the edge dislocation, as a function of x, in only one plane parallel to the free surface S_2, i.e. for one arbitrary constant value of y.

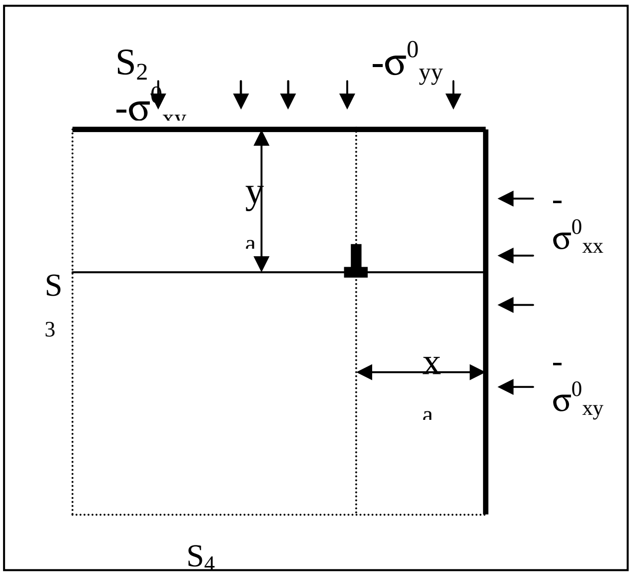

Fig. 1. Position of a dislocation

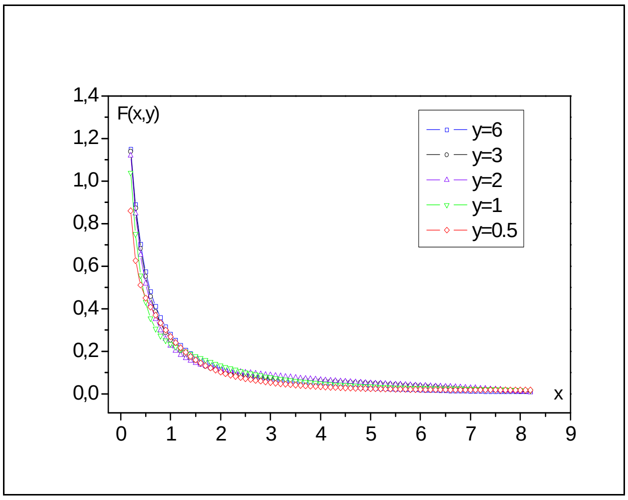

Fig. 2. Numerical force function of x for different value of y

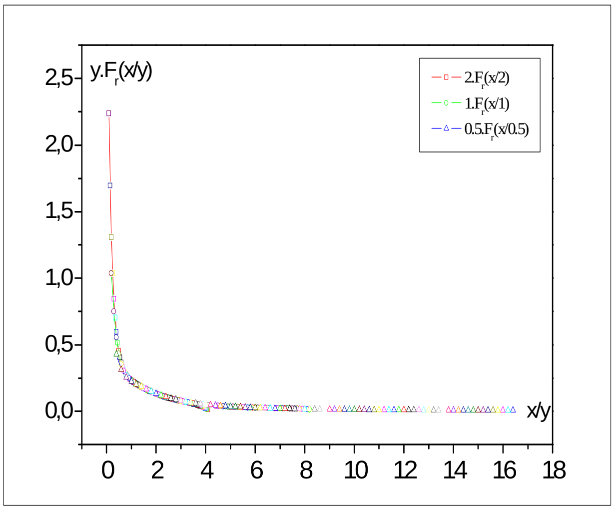

Fig.3. Dimensionless function for different value of y

An analytic expression of the force $y\,F_x^{num}(x/y) = \varphi_x^{num}(\xi)$ can be now established. Since the dimensionless gliding force induced by one free surface S_1, in the case of a semi-infinite solid, is well known [4-8]:

$$\varphi_x^{S_1}(\xi) = \frac{\mu b}{2\pi(1-\nu)}\ \frac{1}{\xi},$$

only the effects of the second free surface S_2 on the dimensionless force $\varphi_x^{num}(\xi)$ calculated in the corner of the solid has to be determined: $\varphi_x^{num} - \varphi_x^{S_1}$.

To quantify the influence of the free surface S_2 on the gliding force acting on the edge dislocation, the expression of the gliding force for a screw dislocation, in the corner of one solid induced by two free surfaces S_1 and S_2, has to be first established. Considering the 3 screw dislocation images of the dislocation in the material filled region (figure 4), the gliding force, in the (0x) direction, has been found to be:

$$\varphi_x^{screw}(\xi) = \frac{\mu b}{2\pi}\left(\frac{1}{\xi} - \frac{\xi^2}{1+\xi^2}\right) = \frac{\mu b}{2\pi}\ f(\xi).$$

Since this function $f(\xi)$ has the good behaviour even for an edge dislocation: $f(\xi) \to 1/\xi$ as $\xi \to 0$ near the free surface S_1 and $f(\xi) \to 0$ as $\xi \to +\infty$ near S_2, this expression of the force φ_x^{screw} has been used in our determination of the expression of the gliding force on the edge dislocation.

Finally, after approximation of the remaining numerical force:

$$\varphi_x^{num}(\xi) - \frac{\mu b}{4\pi(1-\nu)}\left(\frac{1}{\xi} - \frac{\xi}{1+\xi^2}\right),$$

with the help of fractional functions, $\frac{\chi(\xi-a)^{\alpha}}{\left(1+\beta\,(\xi-b)^2\right)^{\delta}}$ where a, b, α, β, χ, δ are numerical constants, the dimensionless force acting on the edge dislocation has been found to be :

$$\varphi_x(\xi) = \frac{\mu b}{4\pi(1-\nu)}\left[\left(\frac{1}{\xi} - \frac{\xi}{1+\xi^2}\right) + \left(\frac{\xi}{1+\xi^2}\right)^2 \left(1 + \frac{1.5(\xi-1)}{\left(1+0.1(\xi-1)^2\right)^2}\right)\right].$$

Finally, the gliding force $F_x(x,y)$ can be written as:

$$F_x(x,y) = \frac{\mu b}{4\pi(1-\nu)}\left[\left(\frac{1}{x} - \frac{x}{x^2+y^2}\right) + \frac{x^2 y}{(x^2+y^2)^2}\left(1 + \frac{1.5(x-y)y^3}{\left(y^2+0.1(x-y)^2\right)^2}\right)\right]$$

This expression of the gliding force can now be used to investigate the mechanical behaviour of thin films on substrates and in particular the delamination of the films calculating for example the activation energy to introduce an edge dislocation on the interface from one free surface.

Conclusion

In this paper, the stress relaxation in a wedge shaped solid containing an edge dislocation has been determined using a finite elements method. An analytic expression of the force acting on the edge dislocation has been then determined which now can be used to investigate the stability of these dislocations in nano-structures like thin films on substrates.

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