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Research Paper Physics

Dislocation Nucleation at the Lateral Free Surface of A Strained Multilayer.

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ABSTRACT

The nucleation of an edge dislocation from the free surface of a multilayer composed of a buried layer embedded in an infinite-size matrix has been investigated from a theoretical point of view when a misfit stress is present in the layer. From an energy variation calculation, the metastable and stable equilibrium positions of the dislocation have been determined as a function of the misfit stress.

Keywords :

Introduction

Multilayers and coatings have been the topic of intensive researches over the past few years because of the numerous applications of such structures in different engineering fields ranging from micro-electronics and optics to metallurgy. Indeed, the control of the mechanical properties of the multilayered structures is of paramout importance to prevent them from dislcation and crack propagation at the interfaces which may lead to their ageing and final deterioration [1,2]. Following the work of Mattews [1], the nucleation of dislocations from the free surfaces to release the misfit stress has been widely investigated. In the case of an epitaxially strained thin film on a substrate for example, the Mattews' critical thickness has been determined below which the nucleation of a misfit dislocation is favourable.

In this paper, the problem of the nucleation of a misfit dislocation in a buried layer embbeded in a matrix has been investigated from a static energy variation calculation. The different equilibrium positions of the dislocation have been determined as a function of the misift stress.

Consider a semi-infinite solid bounded by a free surface x = 0 and located on the side of negative x. This solid contains a buried epitaxial layer between y = h and y =-h (see Figure.1).

The stresses of epitaxy can be deduced from distributions of dislocations at the interfaces of Burgers vectors

$\pm\delta a$ ($+\delta a$ in the plane y = h and $-\delta a$ in the plane y =-h) of density $\frac{dx}{a}$.

We introduce from the free surface, an edge dislocation Burgers vector $(\vec{b},0)$ in the interface y = h, the sign of b is opposite to the sign of δa. The energy variation associated with the introduction of the dislocation is calculated to characterize its equilibrium position.

1. forces on the dislocation

Image force

The edge dislocation with Burgers vector $\vec{b}$ at the point (x,h)
The image force exerted by the dislocation image is given by:

$$(1) \qquad f_{im} = \frac{-\mu.b^2}{4.\pi(1-\nu)}.\frac{1}{x}$$

Epitaxial force

This force has been calculated by Professor J. Colin [3] :

$$(2) \qquad f_{\acute{e}pit} = \frac{4.\mu.b}{2.\pi.(1-\nu)}.\varepsilon^{\acute{e}pit}.\left(1-\frac{x^2}{x^2+4.h^2}\right)$$

$\varepsilon^{\acute{e}pit}$: the epitaxial deformation

$$(3) \qquad \varepsilon^{\acute{e}pit} = \frac{\delta a}{a} \langle 0$$

a: is the lattice parameter
We set:

$$X = \frac{x}{2.h};B = \frac{b}{2.h};$$

$$(4) \qquad k = \frac{\varepsilon^{\acute{e}pit}}{B}\langle 0; F = f.\frac{2.\pi.(1-\nu)}{2.\mu.h.B^2}$$

Using this notation we obtain:

$$(5) \qquad \begin{cases} F_{im} = -\dfrac{1}{2.X} \\ F_{\acute{e}pit} = \dfrac{4.k}{X^2+1} \end{cases}$$

The total force on the dislocation:

$$(6) \qquad F_{tot} = -\frac{1}{2.X} + \frac{4.k}{X^2+1}$$

We note:

Far from the free surface, the effect of the image force prevails over the effect of epitaxial force:

and $F_{im} = -\frac{1}{2.X}$

$$(7) \quad F_{épit} = \frac{4.k}{X^2+1} \approx \frac{4.k}{X^2} \langle\langle |F_{im}|$$

The energy of the dislocation:

$$-\int_{\varepsilon}^{X} F_{tot}(X')dX'$$

increases with distance from the free surface.

2. Energy of the dislocation

The energy of the dislocation is obtained by calculating the work of the total force on the dislocation, when it moves from the position x_0 to the position x.

x_0 is of the order of magnitude of the radius of the heart of the dislocation.

In reduced coordinates we obtain:

$$(8) \quad W(X) = -\int_{X_0}^{X} F_{tot}(X').dX'$$

After integration:

$$(9) \quad W(X) = \frac{1}{2}.\ln\frac{X}{X_0} - 4.k.\left[Arctg(X) - Arctg(X_0)\right]$$

3. Equilibrium positions of the dislocation

The equilibrium positions of the dislocation are given by:

$$\overrightarrow{F_{tot}}(X) = \vec{0}$$

or

$$(10) \quad -\overrightarrow{grad}W(X) = \vec{0}$$

Either :

$$F_{tot}(X) = -\frac{1}{2.X} + \frac{4.}{X^2 \quad 1} =$$

$$\Leftrightarrow \quad X^2 - 8.k.X + 1 = 0 \quad (11)$$

3.1 Equilibrium position: discussion

The equilibrium is gievn by:

$$X^2 - 8.k.X + 1 = 0$$

$$\Delta = 64.k^2 - 4 = 4.(16.k^2 - 1) \quad (12)$$

* If $\Delta \langle 0$: ie $(13) \quad |k| \langle |k_{c1}| = \frac{1}{4}$

the dislocation does not have any equilibrium position.

This property is verified when k is small, i.e. when h the thickness of the epitaxial layer is small:

$$k = \frac{\varepsilon^{épit}}{B} = \frac{\delta a}{a}.\frac{2.h}{b}$$

$$(14) \quad 2.h \langle -\frac{b}{4}.\frac{a}{\delta a} \Leftrightarrow |k| \langle |k_{c1}| = \frac{1}{4}$$

* If : ie $(15) \quad |k| \rangle |k_{c1}| = \frac{1}{4} \qquad \Delta \rangle 0$

Position of stable equilibrium:

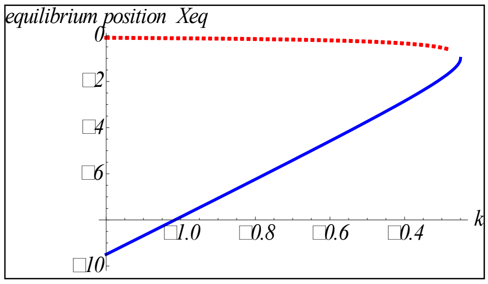
$$X_{st} = 4.k - \sqrt{16.k^2 - 1} \quad (16)$$

Position of unstable equilibrium:

$$X_{ist} = 4.k + \sqrt{16.k^2 - 1} \quad (17)$$

At this point, it can be undelined that the layer thickness h determined in this work is equivalent to the Mattews' thickness obtained for a thin film on a substrate [1].

The dislocation has two positions of equilibrium.



In Figure 2, the variations of the stable and unstable equilibrium positions of the dislocation have been displayed as a function of the parameter k.

Red curve: represents the position of unstable equilibrium.
Blue curve: represents the stable equilibrium position.

3.2 Study of the curves representing the energy

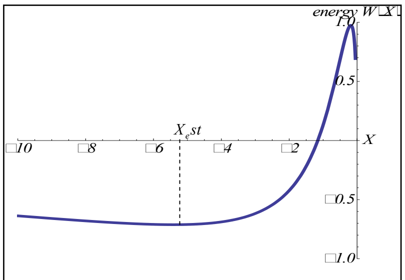


Fig.3: the energy variation as function of X is presented for: k = -0.7

The energy variation as a function of X is presented in Figure 3 for .

$$\left(|k| \rangle \frac{1}{4}\right) \quad k = -0.7$$

The two equilibrium positions stable and unstable are labelled on the graph.

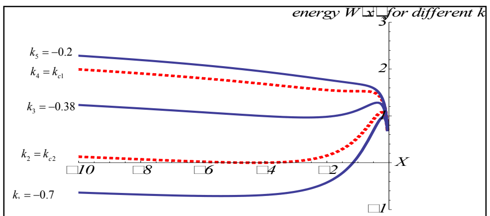


Fig.4: the energy variation as function of X is presented for different values of k

In Figure 4 we represent the energy variation as function of X for different values of k:

$$(k=-)0.7; k_{c2} = -0.569; -0.38; k_{c1} = -0.25; -0.2$$

The red and dashes blue curves represent the energy for two critical values of k:

(the red curve) $k_{c1} = -0.25 = -\frac{1}{4}$

(red discontinuous curve tangent to the k_{c2} x-axis, 0.50)

For $k \rangle k_{c2}$, $W(X_{st})\rangle 0$ and the equilibrium position is metastable.

For $k \langle k_{c2}$,$W(X_{st})\langle 0$ and the equilibrium position is stable.

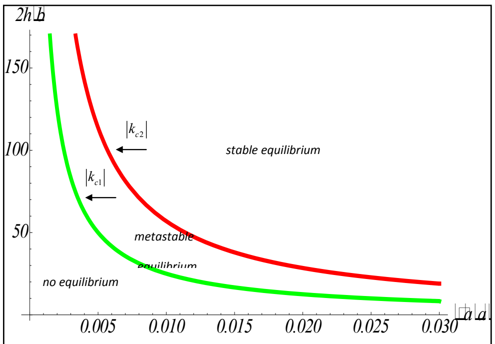


Fig.5: Stability diagram for the dislocation

in the plane ($\frac{2.h}{b}$, $\frac{\delta a}{a}$).

All results are summarized in the graph below Fig.5

According to the relations (12) and (13) , the existence of equilibrium depends on

the values of k: $k = \frac{\delta a}{a} . \frac{2.h}{b}$

k is a function of $\frac{\delta a}{a}$ and $\frac{h}{b}$.

Following the graph above Fig.5, we conclude that:

- For very small $\left|\frac{\delta a}{a}\right|$ such that $|k|\langle|k_{c1}|$: dislocation has no equilibrium position. In absence of other forces the dislocation is attracted by the lateral free surface and exits the solid.

- For $|k_{c1}|\langle|k|\langle|k_{c2}|$ the dislocation has a metastable equilibrium position ($X_{st}\rangle 0$)

- For $|k|\rangle|k_{c2}|$ the dislocation has a stable equilibrium position ($X_{st}\langle 0$)

Conclusion

According to the results of calculations and graphs presented in this work, one can conclude that:

•For $|k|\langle|k_{c1}|$: there is no equilibrium, so in absence of other forces and under the effect of its image force the dislocation is attracted by the free surface and exits the solid (highest blue curve in Figure. 4).

•For $|k_{c1}|\langle|k|\langle|k_{c2}|$: there is a metastable equilibrium position, ($X_{st}\rangle 0$) and $W(X_{st})\rangle 0$ (blue curve in the middle Figure .4).

•For $|k|\rangle|k_{c2}|$ there is a stable equilibrium position (blue curve below in Fig.4), ($X_{st}\langle 0$) and $W(X_{st})\langle 0$.

According to the relations (16) , for h and b constants, if we calculate X_{st} for $\frac{\delta a}{a}=-0.7$, $\frac{\delta a}{a}=-$ and we find respectively:

$X_{st}(-0.7)=-5.415$ and $X_{st}(-1.0)=-7.873$

Therefore to protect the free lateral surface, we can remove the dislocation by increasing the misfit strain $\left|\frac{\delta a}{a}\right|$ caused by a mismatch of lattice parameter between the buried layer and the substrate.

Perspectives

Study of the behavior of several dislocations (b, xi), (number n) in the same interface and determination of the activation energy.

Study of several dipoles of dislocations (one dislocation in each interface), determination of the activation energy.

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