A pile-up of edge dislocations to relax Misfit strain

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Abstract

It is shown that very large stresses may be present in the thin films that comprise integrated circuits and magnetic disks and that these stresses can cause deformation and fracture of the material. For a crystalline film on a non deformable substrate, a key problem involves the movement of dislocations in the film. An analysis of this problem provides insight into both the formation of misfit dislocations in epitaxial thin films and the high strengths of thin metal films on substrates.Just as for bulk structural materials, it is important to understand the microscopic processes responsible for deformation and fracture of these thin film materials so that the mechanical properties of these materials can be changed through the control of microstructure.These remarks have motivated much of the work described in this paper. We develop in this paper, theoretical calculations for dislocation nucleation phenomena in nanomaterials obtained by hetero-epitaxial growth of thin films on substrates having lattice mismatch defects $(such\,as\,growth\,3C-SiC\,film\,and\,Si-Ge)$. After experimental observations by electronic atomic force microscopy, which proved the nucleation of dislocations from free lateral surfaces to relax the " misfit " strain and following a limiting resolution, here we explain the principle of nucleating edge dislocations from these surfaces by the theoretical calculation, of the stresses of interaction (dislocation-surface, dislocation -dislocation ...) using the method of image stress and energy study. We begin our study, by treating the case of a single dislocation and then generalize the work at a pile-up of n interface dislocations. We study the nucleation conditions and the possibility to impose on the epitaxial strain and the thickness h of the thin film to relax the instability of the design course material.

Keywords : *epitaxial thin films, misfit dislocations, nucleating edge dislocations, hetero-epitaxial growth*

1 Introduction

As is known the technical of thin-film deposits by various techniques such as the technique heteroepitaxy the nanoscale level have become the method of obtaining the best materials in various application areas as diverse as ferroelectric materials, optics materials with reflective layers and electric field with the metallic conductive layers... Plastic deformation of crystalline materials is often associated to the mobility of dislocations [2, 3, 4, 5, 6, 7, 8],see (figure.1)[1]. In contrast, the ductility is maintained as dislocations have good mobility ; the material is then deformed conserving the unit of its structure. Transmission electron microscopy of heterostructures has enabled the onset and subsequent development of misfit dislocations to be followed for increasing strained-layer thicknesses, from sub- to supercritical.A well-known mechanism is that of Frank-Read [9, 10, 11] by which a dislocation pinned at its two ends gives rise to numerous dislocation loops.In nanostructured materials, the reduced dimensions make the dislocation sources of activation more unlikely, often the number of pre-existing dislocations is also very low,so this is a very challenging problem, because the relaxation mechanism involves nucleation and motion of threading dislocations through the thin film .Their multiplication is not the primary mechanism during the deformation of the material. Plasticity works by the formation of new dislocations from particular sites such as grain boundaries, the crack fronts, precipitates, interfaces, or surface defects (steps, terraces, islands ...).The surfaces have a special role because they are present for any size of the sample studied.In materials having one or more nanoscale, They play a major role ; multiple experimental methods are used to study the formation of dislocations from the free surfaces, but experience encounter major difficulties in studying the earliest stages of plasticity at the atomic scale and with sufficient time resolution, hence the idea to turn to theoretical models.Elastic theory, which describes the dislocations as linear defects moving in a continuous medium, allowed a first approach to solve this ambiguity.The modes of the most observed plasticity are irreversible deformation induced by nucleation, multiplication and dislocation motion.These movements can be glides (conservative shear) or mounted (non-conservative)[2, 3, 4, 5, 6, 7, 8].In bulk materials, one of the known mechanisms of multiplication of dislocations is Frank-Read process [9, 10, 11].In nanostructures materials free of dislocations, no source of Frank-Read can not be created,recent experimental observations using the atomic force microscope showed that the plasticity operates differently : stress relaxation dislocations are nucleated from particular sites such as grain boundaries, cracks fronts, precipitates, interfaces, defects and surface irregularities such as steps [38], terraces, islands etc...see (figure.2)[38].

2 The first nucleated dislocation

Stresses and forces acting on the dislocation :

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).
Epitaxial stresses are calculated from distributions of dislocations interfaces, characterized by Burgers vectors $\vec{b} = \vec{\delta a}$ ($+\delta a$ in the plane $y = h$ and $-\delta a$ in the plane $y = -h$) with a density $\frac{dx}{a}$,a is the lattice parameter.
One edge dislocation of Burgers vector (b,0) is introduced from the free lateral surface (x = 0, y), concerned interface : $y = h$. The sign of b being opposite the sign of δa.

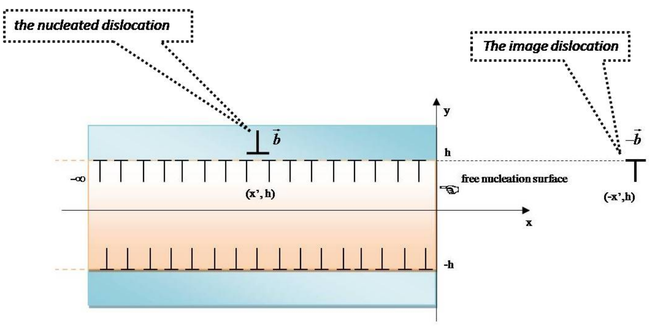

FIGURE 1. The effect of epitaxial shear stress and Image stress illustration

We have determined total stress, total force and the total energy of edge dislocation studied

So for y=h, the total force one dislocation considered, is given by the formula Peach and Koehler [2, 3] :

$$\overrightarrow{f_{tot}} = (\overline{\overline{\sigma_{xy}^{image}}}.\vec{b}) \wedge \vec{\xi} + (\overline{\overline{\sigma_{xy}^{epit}}}.\vec{b}) \wedge \vec{\xi}$$

$$\overrightarrow{f_{tot}} = \frac{-.b^2}{4.\pi(1-\nu).x}\overrightarrow{e_x} + \frac{4..b}{2.\pi(1-\nu)}.\epsilon^{epit}.(1 - \frac{x^2}{x^2+4.h^2})\overrightarrow{e_x}$$

$\vec{\xi}$: *line vector* and $\epsilon^{epit} = \frac{\delta a}{a}$: *epitaxial deformation*

For a very simple study, reduced coordinates are used :

$$\begin{cases} + X = \frac{x}{2.h}; B = \frac{b}{2.h} \\ k \quad = \frac{\epsilon^{epit}}{B} \quad < \quad 0 \\ + F = \frac{f.2.\pi(1-\nu)}{2..h.B^2} \end{cases}$$

Therefore total force and total energy are given by :

- The total force :

$$\begin{cases} F_{im} = \frac{-1}{2.X} > 0 \\ F_{epit} = \frac{4.k}{X^2+1} < 0 \\ F_{tot} = \frac{4.k}{X^2+1} - \frac{1}{2.X} \end{cases}$$

- The total energy :

$$\begin{cases} + W(X) = -\int_{X_0}^{X}(F_{im}(X') + F_{epit}(X')).dX' \\ + W(X) = \frac{1}{2}.Log(\frac{X}{X_0}) - 4.k.Arctg(X) - Arctg(X_0) \end{cases}$$

3 A pile-up of dislocations

We now consider a pair of two, a pile-up of n=3 oder 4 dislocations nucleated one after the other to relax the misfit strain.
Burgers vector (b, 0) at the interface y = h and respectively X_1 , X_2, X_3 and X_4 : see figures 2, 3 ad 3.

- F_i : Force acting on the dislocation number (i)

$$F_i(X_i, X_j) = \frac{-1}{2.X_i} + \frac{4.k}{X_i^2+1} + \sum_{j \neq i}^{n}(\frac{1}{X_i - X_j} - \frac{1}{X_i + X_j} + 2.X_j.\frac{X_j - X_i}{(X_i + X_j)^3})$$

- F_j : Force acting on the dislocation number (j)

$$F_j(X_i, X_j) = \frac{-1}{2.X_j} + \frac{4.k}{X_j^2+1} + \sum_{i \neq j}^{n}(\frac{1}{X_j - X_i} - \frac{1}{X_j + X_i} + 2.X_i.\frac{X_i - X_j}{(X_j + X_i)^3})$$

Direct calculation of equilibrium positions X_{eq} becomes impossible. So we used the iterative conjugate gradient method

Using the reduced variables, and the Mathématica code for the calculation we translate the results graphically (see below)

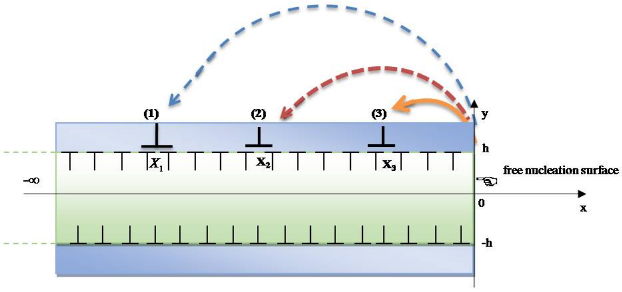

FIGURE 2. introduction of 3 edge dislocations

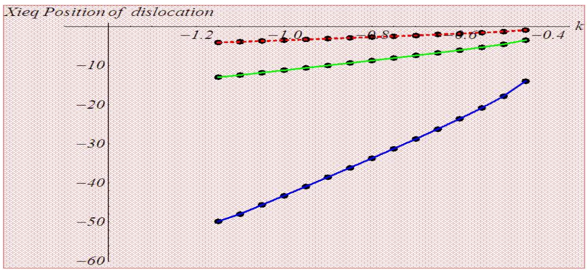

FIGURE 3. stable equilibrium positions of the three dislocations, discontinuous style

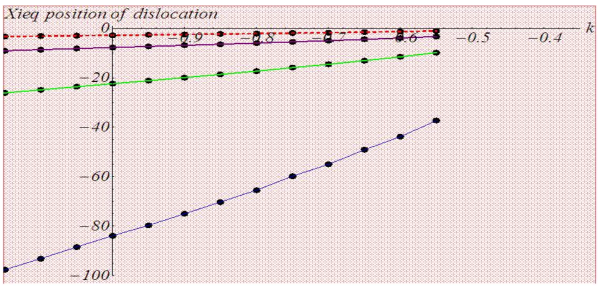

FIGURE 4. Stable equilibrium positions for 4 dislocations, discontinuous style

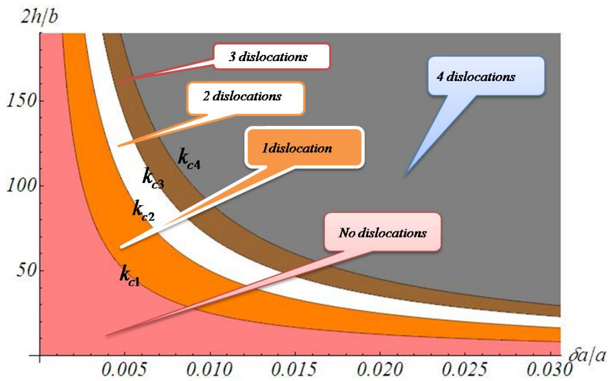

FIGURE 5. graph illustrating the curves $|k| = f(\frac{\delta a}{a}, h) = constant$, stability area, metastability and field of instability

4 General Conclusion

Following this work, we studied how to introduce a pile-up of n dislocations $(n = 2, 3, 4...)$ nucleated from a free lateral surface, experimentally observed at the nanometer level. The method used here, is that of the energy model and theoretical analytic calculations.The introduction of misfit dislocations is Very important and major operation, because it provides a basis for understanding the dislocation processes responsible for plastic deformation of thin films on non deformable substrates. We have shown by calculation and through the curves $k = f(\frac{\delta a}{a}, h)$ that we can control and prevent the emergence of this pile-up of dislocations taking into consideration the misfit strain $\epsilon = \frac{\delta a}{a}$ and the effect of the thickness h of the layer, which are two parameters very significant for controlling constantly during development materials operations by deposits from thin films.There's even better and we can always do better, with a more advanced calculation again, in order to find other conditions much better about this technique of production of high-performance materials. Note that, once again the results of the curves $k = f(\frac{\delta a}{a}, h)$ showing the areas of stability and metastability permits us to reaffirm the validity of the findings of Van der Merwe and Matthews and Blakeslee.

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