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A Short Review on the Stress Field of a Screw Dislocation in a Thin Film – Substrate

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Abstract An analytical Fourier series analysis of the elastic field of a misfit dislocations along a thin film-substrate interface is proposed in the context of a plane strain. When the period is sufficiently large, this solution tends assymptotically towards that of an isolated dislocation in the thin film substrate system. Numerical applications are illustrated to evaluate the effect of elastic properties of the materials used as well as the effect of the film thickness and the position of the dislocation in the substrate.

Keywords Screw dislocation, Film–substrate interface, Free surface

1. Introduction

For about a four decades, experimental studies of epitaxial layers on monocrystalline substrate have developed considerably since the first moments of nucleation until reaching the desired thickness, which exceeds general 10 nm in silicon substrate applications (e. g) [1-2]. In parallel with these experimental studies, different theoretical models were developed to evaluate the field of dislocation stresses present in the thin-film substrate system. Since the works of Liebfried and Dietz [3] and Head [4], several other investigations have been developed Bai and Wang [5], Ogbonna [6] and Wang et al. [7]. Bonnet et al [8] have proposed a analytical solution for the stress field of a familly of misfit dislocations at the interface of a thin film – semi infinite substrate. Recently, Gharahi et al [9] have studied the interaction of a screw dislocation with a thin film–substrate interface in the anti-plane deformations of a couple stress elastic solid. They have discussed the contribution of couple stresses to the interaction force acting on the dislocation.

In this paper, we develop an analytical solution of the problem of a screw dislocation interacting with a thin-film–substrate structure based on Fourrier series. The elastic field of such a dislocation is that of a periodic family of misfit dislocations periodically distributed along the semi-coherent interface. In the case of a large period, this field tends towards that of an isolated dislocation. Numerical applications are developed to show the effect of the elasticity of the medium, the thin film thickness as well as the position of the dislocation in the substrate.

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2. Stress Field in a Semi – Infinite Bicristal

The geometry of the problem and the conventions used are illustrated in Figure 1, the system of Cartesian axes $Ox_1x_2x_3$ and some symbols used in the analysis. A series of misfit dislocations are periodically distributed (of period T) along the planar hetero-interface denoted (+)/(-), the thickness of the media (+) is h^+, the media (-) is supposed infinite. A thin film of thickness h^* is placed above the media (+).

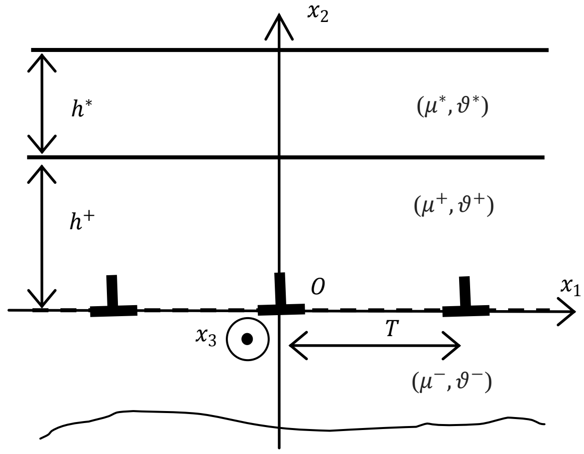

Figure 1. Thin film of thickness h^* on a semi-infinite substrate. A periodic distribution of a screw dislocation of a period T along the plane $x_2 = 0$. The elastic constants of Lamé and Poisson relative to the media (*), (+) and (-) are noted respectively (μ^*, ϑ^*), (μ^+, ϑ^+) and (μ^-, ϑ^-)

The stress field of such distribution of dislocations was given by Bonnet [8,10], the displacement field is written under a Fourier series:

$$u_i = \sum_{n=-\infty}^{\infty} U_i^n e^{in\omega x} \quad i = 1, 2, 3 \tag{1}$$

For a distribution of screw dislocations with a Burgers vector $(0,\ 0, b_3)$ only the component u_3 is not zero. This field sastisfy the equilibrium equation of elasticity, then the pre-exponential coefficients of expression (1) are written in the following way, leaving, for simplicity, the upper index (n) on U_i^n.

$$U_3^* = T^* e^{-n\,\omega\,x_2} + U^* e^{n\,\omega\,x_2} \tag{2a}$$

$$U_3^+ = T^+ e^{-n\,\omega\,x_2} + U^+ e^{n\,\omega\,x_2} \tag{2b}$$

$$U_3^- = U^- e^{n\,\omega\,x_2} \tag{2c}$$

In total for the three mediums and each harmonic of order n, it is necessary to determine five unknown complex coefficients: T^*, U^*, T^+, U^+ and U^-. These coefficients are the unknowns of a system of five equations with five unknowns. This system is obtained by writing the boundary conditions, linear discontinuity of the displacement field at $x_2 = 0$ [10], continuity of the normal stresses at $x_2 = 0$ and $x_2 = h^+$ and nullity of the stresses at the level of the free surface $x_2 = h^+ + h^*$. The solutions are purely complex, they are written:

$$T^* = \frac{i\,b_3\,e^{2\,n\,\omega\,h^*}}{2\,n\,\pi\,(1-k+(1+k)\,e^{2\,n\,\omega\,h^*})} \tag{3}$$

$$U^* = \frac{i\,b_3\,e^{-2\,n\,\omega\,h^+}}{2\,n\,\pi\,((1+e^{2\,n\,\omega\,h^*})+(-1+e^{2\,n\,\omega\,h^*})k)} \tag{4}$$

$$T^+ = \frac{i\,b_3}{4\,n\,\pi} \tag{5}$$

$$U^+ = \frac{i\,b_3\,e^{-2\,n\,\omega\,h^+}(1+e^{2\,n\,\omega\,h^*}+k\,(1-e^{2\,n\,\omega\,h^*}))}{4\,n\,\pi\,(1+e^{2\,n\,\omega\,h^*}+k\,(-1+e^{2\,n\,\omega\,h^*}))} \tag{6}$$

$$U^- = -\frac{i\,b_3\,e^{-2\,n\,\omega\,h^+}((-1+e^{2\,n\,\omega\,h^+})(1+e^{2\,n\,\omega\,h^*})+k(1+e^{2\,n\,\omega\,h^+})(-1+e^{2\,n\,\omega\,h^*}))}{4\,n\,\pi\,(1+e^{2\,n\,\omega\,h^*}+k\,(-1+e^{2\,n\,\omega\,h^*}))} \tag{7}$$

Where $k = \frac{\mu^*}{\mu^+}$ the ratio of Lamé coefficient of media (*) and (+) and $\omega = \frac{2\pi}{T}$. These expressions are given when $(\mu^+, \vartheta^+) \equiv (\mu^-, \vartheta^-)$ that means two elastically identical media. When the period T increases, the results around a misfit screw dislocation converge to those of an isolated translation screw dislocation in a substrate near a thin film.

3. Numerical Application

Figs. 2(a,b,c,d) display, for a thin film – substrate foil (thickness of the film h^* =3 nm), equistress contours related to an screw dislocation oriented along $Ox_3 // U$ according the ratio k. The Burgers vector $\boldsymbol{b}$= (0, 0, b_3). Its line position is at h^+ = 4 nm below the thin film. The Cartesian frame is $Ox_1x_2x_3$, with Ox_2 oriented towards the upper normal **N** to the foil. In Figs. 2(a,b,c,d), the stress fields are derived from the **u** field (1) and the application of Hooke's law from isotropic elasticity theory. For a quicker convergence of the Fourier series the harmonic terms beyond 50 were reduced to their principal values so that they can be summed exactly via simple analytical functions [10]. The equistress contours correspond to σ_{x2x2}= 0 et ±50 MPa. These contours are represented in the region around the screw translation dislocation as $-\frac{T}{3} \leq x_1 \leq \frac{T}{3}$ and $-2h^+ \leq x_2 \leq h^+ + h^*$. The value of the period should reash the value $T = 10h^+$ to obtain visually stable curves for a single screw translation dislocation. The test is useful to examine the validity of the proposed approach relatively to some works reported in the literature for an infinite medium [11]. The dashed line marks the position of the inteface between the film and the substrate. The internal zero stress contours meet of course the free surface of the film. Close to the core, the traction or compression regions are the same than for a dislocation in an infinite medium [11]. These contours are continuous at level $x_2 = 0$ and the interface $x_2 = h^+$. It is interesting to note when k increases from 0.5 to 2, then the film becomes harder, the lobes of stress contours become wider and become more pronounced in the film.

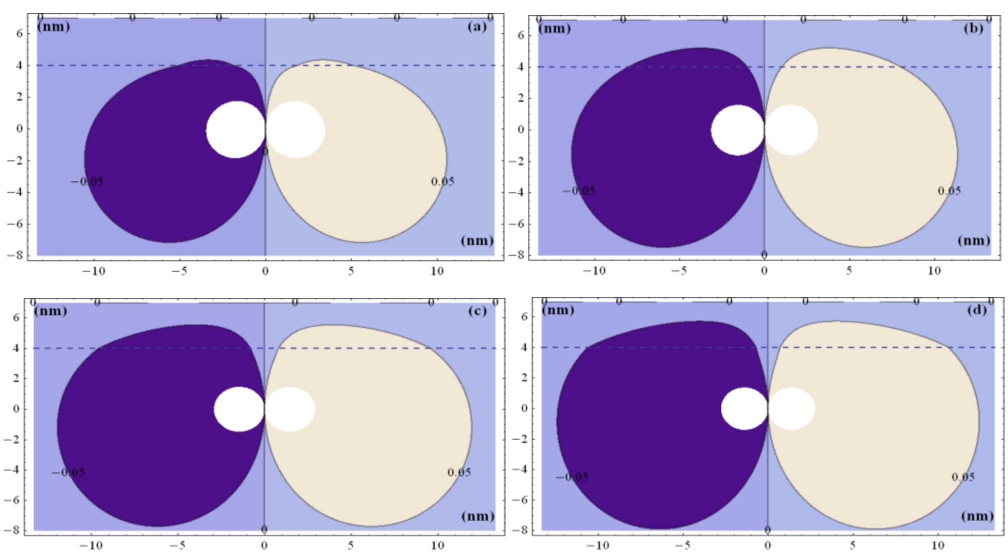

Figure 2(a,b,c,d). Equistress contours σ_{x2x2}= 0 and ±0.05 GPa around a screw dislocation. The ration of Lamé coefficient k are respectively from 0.5, 1, 1.5 and 2. The zero stress contours meet the free surfaces of the thin film. $b_3 = 0.32$ nm, $h^+ = 4$ nm, $h^* = 4$ nm and $T = 10h^+$

Figure 3 superimpose curves of variation of the stress σ_{x1x2} versus x_2 along the plane $x_1 = 4\,nm$ when k increases from 0.5 to 2. In the region $x_2 < 0$, this stress and for all the values of k is the same than for a screw translation dislocation in an infinite medium.

We notice a slight variation with k. This is not the case in the region $0 < x_2 < h^+$, which shows a variation versus k more important when x_2 increases. The discontinuity at $x_2 = 0$ is intensive, it reaches 0.16 GPa, while at the level $x_2 = h^+$ it is more lower and depends on the value of k, it is close to 0.048 GPa for $k = 0.5$. For $k = 1$ and the same level $x_2 = h^+$, the curve is continuous since the elastic properties for the film and the substrate are identical. Finally we propose to calculate the elastic energy E as a function of the depth of the dislocation in the substrate. A cut is first made along the interface $x_2 = 0$. To restore the atomic bonds, it is necessary to exert surface stress. The work of the forces of surface is calculated for the linear relative displacement [8].

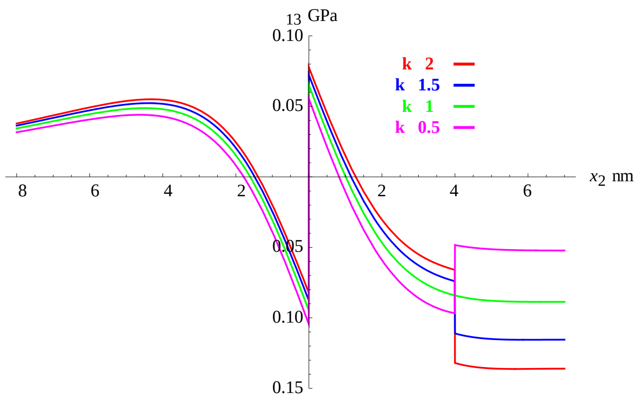

Figure 3. Variation of stress σ_{x1x2} versus x_2 along the plane $x_2 = 4$ nm when k increases from 0.5 to 2

The integration surface extends over a length unit along Ox_3 and along Ox_1 on the interval $(r_0,\ T - r_0)$, where r_0 is the cutoff radius [11]. The elastic energy stored by unit of surface, noted E is therefore:

$$E = \frac{1}{2T}\int_{r_0}^{T-r_0} b_3(-2\bar{\sigma}_{x2x3})_{x2=0}\left(\frac{x_1}{T} - \frac{1}{2}\right)dx_1 \qquad (8)$$

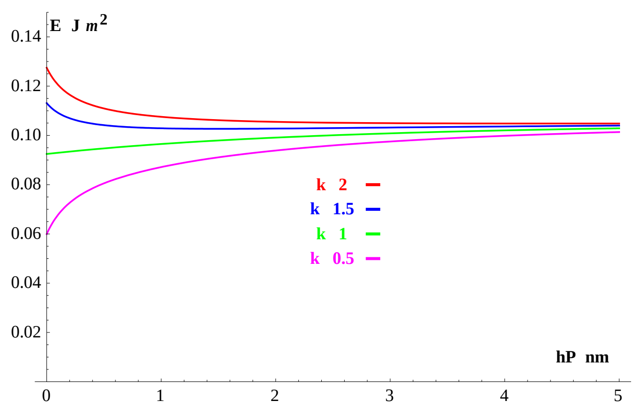

Figure 4. Variation of elastic energy with the depth of the dislocation in the substrate. $r_0 = \frac{b_3}{2}$ and $T = 40$ nm

Figure 4 illustrates the variation of elastic energy by unit of surface versus the depth of the dislocation in the substrate when the ration k increases from 0.5 to 2. It is interesting to note that the value of energy increases as k increases. This increase is due to the crowding of the substrate by the film which becomes more harder. The elastic energy tends towards an asymptotic value when the depth h^+ reaches 3 nm.

Many authors use molecular dynamics method and atomic simulation to analyzed the size-dependent interaction of dislocations in layer–substrate configurations [12,13]. The present method offers an opportunity to prepare an atom block of a heterogeneous bicrystal including one or several relaxed screw misfit dislocation.

4. Conclusions

In this work we present analytical solutions for the displacement and stress fields corresponding to a screw dislocation located inside a substrate near a thin-film interface. The presented solution is in the form of a Fourier series with large period. We discussed the effect of the elastic properties of two mediums on the stress field and the effect of the depth of the dislocation in the substrate on the elastic energy at nanoscale. Since the displacement field has an analytic form its nine derivatives can be easily derived analytically and therefore be useful to refine the contrast simulations of conventional TEM images of such dislocations lines.

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