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Dislocations and elastic anisotropy in heteroepitaxial metallic thin films

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ABSTRACT

The influence of elastic anisotropy on the critical thickness for the plastic relaxation of epitaxial layers is examined with the help of a coupled discrete–continuum simulation. The latter incorporates a rigorous treatment of the boundary conditions and of mismatch stresses, as well as the elastic properties of a single threading dislocation. Numerical experiments conducted on model Cu/Cu, Cu/Au and Cu/Ni systems with a (001) interface show that, through several distinct effects, elastic anisotropy induces a significant increase in the critical thickness with respect to the values predicted by Matthews *et al.* The isotropic model of a comparison of the anisotropic critical thicknesses for (001) and (111) interfaces shows that Cu-(111) films on Ni substrates are about 50% 'harder' than (001) films. This feature is discussed in relation to the strength of thin metallic films.

§ 1. INTRODUCTION

The growth of a thin epitaxial film on a substrate with a different chemical nature induces stresses in the film. These stresses are uniform and depend on the mismatch strain ε_0 between the two lattices. Beyond a critical film thickness h_c, the elastic energy of the film is relaxed by misfit dislocations that appear at the film–substrate interface. These dislocations are formed by the glide of pre-existing segments, the so-called threading dislocations. The present work is concerned with the critical stress for the motion of threading dislocations, which governs plastic relaxation in metallic systems (Arzt *et al.* 2001). Processes involving the heterogeneous nucleation of dislocations in dislocation-free films or the possible influence of a passivating layer are not considered here.

When the film thickness h is larger than the critical value h_c, a threading dislocation with suitable Burgers vector magnitude b bows out critically and glides, depositing a misfit dislocation at the interface. The first prediction of the critical thickness value was proposed by Matthews *et al.* (1970), within the framework of isotropic

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linear elasticity. The Matthews *et al.* criterion expresses a minimum-energy condition for an epitaxial layer containing a single threading dislocation. It is written

$$\frac{\varepsilon_0 h_c}{b} = FK\left[\ln\left(\frac{h_c}{r_0}\right) + 1\right]. \tag{1}$$

The term on the right-hand side arises from the dislocation line tension; it contains an outer cut-off radius taken as the film thickness and an inner core radius r_0 of the order of b. The factor K accounts for the dependence of the line tension on dislocation character and the factor F for the orientation of the dislocation glide plane. In semiconductor/semiconductor systems with small misfit strains (typically below 2%), the prediction of the Matthews *et al.* criterion is relatively well verified by experiment (Matthews and Blakeslee 1974). However, with larger misfit values, such as those found in metal/metal systems, the observed critical thicknesses can be substantially larger than predicted by equation (1).

For this reason, Freund (1990) and Nix (1998) extended the Matthews *et al.* model to account for the elastic interactions between dislocations with different Burgers vectors. Indeed, the larger the misfit, the larger is the amount of plastic relaxation in the film and, therefore, the higher is the density of misfit dislocations deposited at the interface. The interactions between these dislocations may cause strain hardening and increase the effective value of the critical strain (see figure 2). These models and several variants have been reviewed by Fitzgerald (1991). A similar problem is encountered with the strength of thin polycrystalline metallic films on substrates, which is significantly higher than that of the corresponding bulk material. This strengthening cannot be rationalized by combining Hall–Petch hardening with a critical thickness model (Arzt *et al.* 2001).

Some aspects of the mutual interactions of dislocations have been analysed with the help of dislocation dynamics (DD) simulations (Schwarz and Tersoff 1996, Gomez-Garcia *et al.* 1999, Pant *et al.* 2001, von Blanckenhagen *et al.* 2001). In the present work, we show that the critical thickness depends sensitively on elastic anisotropy, a feature that is not considered in the currently available models. To estimate the influence of anisotropy, use is made of a hybrid simulation method, the discrete-continuum model (DCM). In the DCM, a DD simulation is coupled to a finite-element (FE) code, which solves boundary value problems. This allows one to obtain the state of stress in the film and in the substrate, in the presence of a threading dislocation and within the framework of isotropic or anisotropic linear elasticity. A few basic features of the DCM and the conditions in which the computations were carried out are described in § 2. In § 3, a validation test for equation (1) is performed on a model Cu/Cu system. Then, the influence of elastic anisotropy on the critical thickness is examined and discussed by considering a Cu film on several substrates with different elastic properties, namely Cu, Ni and Au. Finally, the influence of the interface orientation, (111) or (100), is examined in the case of the Cu/Ni system. The concluding § 4 emphasizes that a rigorous description of the stress fields may account for a large part of the differences observed between predicted and observed values of the critical thickness in epitaxial layers. The same conclusion is thought to apply as well to thin polycrystalline metallic films on substrates.

§ 2. Simulation method

Coupled simulations combining a DD code and an FE code allow the discrete and continuum aspects of plasticity to be treated simultaneously. Their use is for the moment restricted to relatively simple configurations (van der Giessen and Needleman 1995, Fivel and Canova 1999, Lemarchand *et al.* 2001). In essence, the numerical model used here, the DCM, is made up of an FE code, in which the constitutive law is replaced by a DD simulation. The main advantage of this method resides in the fact that the elastic and plastic fields can be determined numerically in a rigorous manner, taking into account the presence of dislocations in a small volume element and with a variety of possible boundary conditions (Lemarchand *et al.* 1999).

2.1. *The threading dislocation: dislocation dynamics simulations*

DD simulations are performed using the 'edge–screw' model, in which the continuous shape of perfect dislocation lines is decomposed into a succession of edge and screw segments moving by crystallographic translations in an underlying fcc lattice of parameter a^*. This parameter is not necessarily of atomic dimension. Its value is defined according to the characteristic scale of the problem to be treated, as discussed below. The effective stress on each segment is the sum of the stresses arising from the boundary conditions, of dislocation self-stresses, both of which are computed by the FE code, and of a local, character-dependent line tension T, which is incorporated into the DD simulation. In isotropic elasticity, use is made of an expression developed by Foreman (1967) and modified by Gomez-Garcia *et al.* (1999) to account for the geometrical specificities of the 'edge–screw' model. Within this formulation, only three quantities have to be defined: the magnitude b of the Burgers vector of the threading dislocation, the shear modulus μ which is taken as the Reuss average (for copper films, $b = 0.256$ nm and $\mu_R = 42$ GPa) and r_0, the inner cut-off radius in the dislocation line energy.

In anisotropic elasticity, the line tension takes a more complex form, which is generally not analytical. Its values were directly computed with the help of the DisDi code (Douin *et al.* 1986) and tabulated in the DD simulation.

The output of the simulation, and in particular the implementation of the line tension, has been tested in several ways. For instance, we find that, for a dislocation line emerging at a free surface, the computation of the line tension requires a specific procedure. The latter accounts for the local character and curvature of the line and is similar to that used by Schwarz (1999). In isotropic elasticity, the critical stress for the motion of a threading dislocation in a capped layer was compared with results from Schwarz and Tersoff (1996) and Gomez-Garcia *et al.* (1996). This preliminary work lead to a definition of the core radius, $r_0 = 2b$. Finally, the velocity of a dislocation segment is related to the effective stress τ^*, calculated in its centre, through $v = \tau^* b/B$, where B is a drag constant ($B_{Cu} = 5 \times 10^{-5}$ Pa s^{-1}).

The geometry of the initial configuration is shown in figure 1. In order to obtain an accurate description of the dislocation shapes irrespective of the film thickness, the underlying lattice parameter of the DD code was selected in such a way as always to satisfy $h = 2700a^*$. Two different crystallographic configurations have been studied. For (001) films, the slip system with highest Schmid factor is $[\bar{1}01](111)$, and the direction of motion of the treading dislocation is $[\bar{1}10]$. For (111) films, the active slip system is $[101](11\bar{1})$ and the direction of motion is also $[\bar{1}10]$. For both orientations, the initial and final configurations of the threading dislocation are

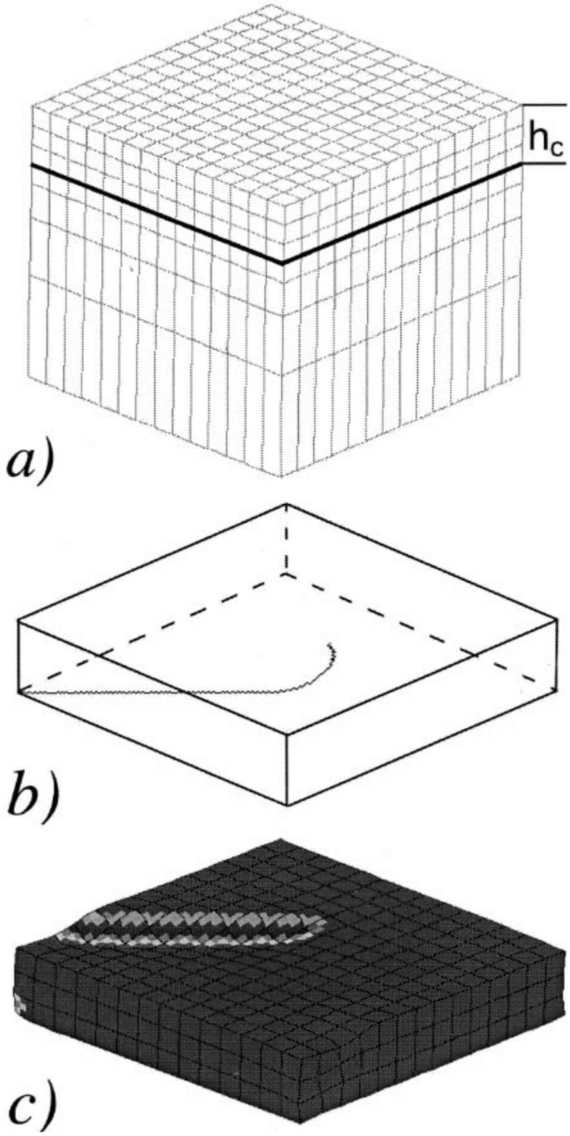

Figure 1. (*a*) Mesh geometry of the MDC simulation for the (001) interface. (*b*) A critically bowed-out shape of the threading dislocation. The latter is initially introduced by a Volterra process. It is made up of a discrete line deposited at the film–substrate interface and a straight threading segment which ends up at the surface of the film. (*c*) The resolved plastic shear strain corresponding to (*b*), $6^{1/2}(\varepsilon^{p}_{11} - \varepsilon^{p}_{33} + \varepsilon^{p}_{12} - {}^{p}_{23})$, magnified by a factor of 350.

almost crystallographically equivalent. Thus, its elastic, isotropic and anisotropic properties are nearly the same. The only difference stems from the different angles between the slip plane and the surface plane.

The (111) interface requires a specific treatment. In figure 1 (*a*) the elements of the FE mesh and of the DD lattice are oriented in the same manner, with horizontal and vertical faces parallel to $\{100\}$ directions. Thus, a (001) interface is effectively flat in the DCM. However, a (111) interface would be corrugated, which does not allow reliable computations to be performed. To bypass this problem, the procedure used is as follows. A set of coordinate axes based on the three directions [111], $[\bar{1}01]$ and $[1\bar{2}1]$ is defined. Then, without modifying the geometry in figure 1 (*a*), the material's properties, namely the crystallographic directions and the associated matrix of elastic constants, are rotated in such a way to bring the [111] direction normal to the interface. Then, a flat interface can be used in the computation with suitable values for the dislocation and thin film properties. In all the simulations, the film–substrate interfaces are supposed to be impenetrable barriers to dislocation glide and the latter are not allowed to propagate into the substrate.

2.2. *The boundary value problem*

The boundary value problem is treated by the FE code. All the results presented here were obtained with mirror boundary conditions at the side surfaces of the FE meshing (the normal displacement on the side surfaces is set to zero). One advantage of these conditions is to minimize the interactions between the threading dislocation and its periodic images. By reason of symmetry these interactions are negligible in the central area of the simulated film. Therefore, the displacements of the dislocations are restricted to that region. The top surface of the film is treated as a free surface and all the displacements on the lower surface of the substrate are set to zero. Numerical values for the elastic constants of the film and substrate are taken from Hosford (1993).

In the DCM, a FE mesh is superimposed on the DD lattice. In the present work the mesh is made up of $14 \times 4 \times 3 = 588$ cubic elements in the film and $14 \times 14 \times 4 = 784$ parallelepipedic elements in the substrate (see figure 1). It was verified that the simulation results are not affected by the use of a more refined meshing for the film ($20 \times 20 \times 3$). All elements have 20 nodes and 27 Gauss points. The ratio of the substrate thickness h_s to that of the film is set to $h_s/h = 3.5$ (larger values would necessitate too many elements to mesh the substrate). The threading dislocation is introduced by a Volterra process and moved into place from one side of the simulation box (figures 1 (*b*) and (*c*)). This displacement produces a plastic shear which is treated by the FE code as part of the boundary value problem. As this shear is localized in one slip plane of the DD simulation, it has to be homogenized over some height compatible with the FE mesh (Lemarchand *et al.* 2001). In the present case, the homogenization height is set to $3L/2$, where L is the linear dimension of the mesh elements in the film.

The mismatch strain between the film and the substrate is introduced by imposing a differential thermal strain between the two materials. Specifically, the substrate is assumed to have no thermal dilatation and the mismatch strain ε_0 is obtained by applying a temperature change ΔT to a film with a thermal expansion coefficient α_f such that $\varepsilon_0 = -\alpha_f \Delta T$. As a result, the film is elastically deformed in plane-stress conditions and there is no deformation in the substrate. Thus, the loading imposed on a threading dislocation is identical with that obtained when $h_s/h \gg 1$.

§ 3. Isotropic and anisotropic critical thicknesses

The critical thicknesses are computed as follows. Five values of the film thickness, ranging from $10b$ to $10^3 b$, are selected, thus defining the dimension of the FE mesh and of the DD lattice. For each thickness, the mismatch strain is progressively incremented and the plastic strain produced by the threading dislocation as well as the resolved stresses on it is monitored. For a critical value of the mismatch strain, the threading dislocation starts to glide forwards, which defines a couple of critical values for the mismatch strain and the film thickness. In such conditions, h_c is measured within an accuracy of 3%.

In a first step, results of the simulation in isotropic elasticity are validated with respect to the Matthews *et al.* criterion. Figure 2 shows the critical thickness for a (001) interface in the Cu/Cu system, as yielded by the MDC. These results perfectly agree with the values predicted by equation (1). One can notice that, as mentioned above, the core radius used in the simulations is $r_0 = 2b$, whereas $r_0 = b$ in equation (1). This factor of two is attributed to differences in the cut-off procedures for the elastic energy.

In a second step, the influence of elastic anisotropy is investigated. It is split into two contributions. The anisotropic elastic stresses in the film, keeping the local line tension of the dislocation isotropic, are considered first. Then, the additional effect of an anisotropic line tension is introduced. As expected from plane-stress conditions, the mismatch stress in a dislocation-free film is uniform but depends on the orientation (*hkl*) of the interface. The two non-zero components of the stress tensor are of the form

$$\sigma^a = Y^{hkl}\varepsilon_0, \tag{2}$$

where Y^{hkl} is a biaxial modulus which reduces to $E/(1-\nu)$ in isotropic elasticity. For Cu at room temperature, $Y^{001} = 115\,\mathrm{GPa}$, $Y^{111} = 261\,\mathrm{GPa}$ and $E = 112\,\mathrm{GPa}$.

The strong influence of an anisotropic treatment of the stresses is illustrated in figure 3 for a Cu film on different substrates and a (001) interface. The prediction of

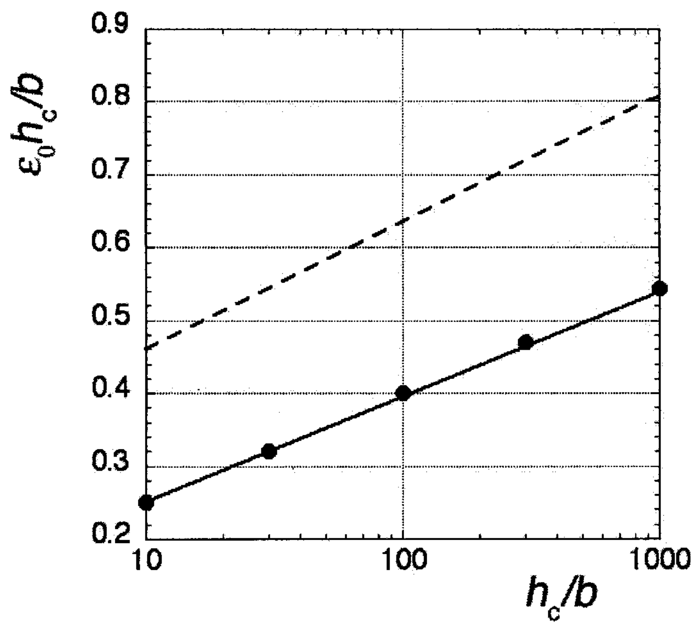

Figure 2. Semilogarithmic plot of the reduced misfit $\varepsilon_0 h_c/b$ as a function of the reduced critical film thickness h_c/b for the Cu/Cu system in isotropic elasticity and with a (001) interface: (——), prediction of the Matthews *et al.* criterion; (- - - -), prediction of the modified model by Freund (1990); (●), simulation results.

the Matthews *et al.* criterion (see figure 2) is also shown for comparison. Considering first the two sets of results obtained for the Cu/Cu system, the two curves are approximatively parallel but, for a given thickness, the critical misfit strain is increased by a factor ranging between 2.3 for $h_c/b = 10$ and 1.7 for $h_c/b = 10^3$. This relative hardening can be compared with the value of 1.6 yielded by the isotropic model given by Freund (1990), which considers the interactions of threading and misfit dislocations (see figure 2).

The small dependence of the above results on the film thickness is thought to originate in the increasing influence of the image forces from the free surface when the film thickness decreases. Unfortunately, this feature cannot be investigated directly with the MDC since the latter does not allow one to differentiate between the different stress contributions.

The influence of the elastic properties of the substrate is shown in figure 3, where results are plotted for two materials other than Cu: Au ($Y^{001} = 78$ GPa, $Y^{111} = 189$ GPa and $E = 64$ GPa) and Ni ($Y^{001} = 210$ GPa, $Y^{111} = 394$ GPa and $E = 202$ GPa). Note that Au is on average substantially more compliant than Cu and that Ni is substantially stiffer.

Changing the nature of the substrate slightly modifies the critical conditions for the motion of the threading dislocations. The influence of the anisotropy of the Cu film discussed above is thus predominant. Nevertheless, second-order effects manifest themselves in figure 3, in the form of small shifts between the results obtained for different systems. It was checked that, as expected, the substrate is not deformed by the mismatch stresses. However, some local deformation should be induced in it by the self-stress field of the dislocation. In other terms, the threading dislocation sees

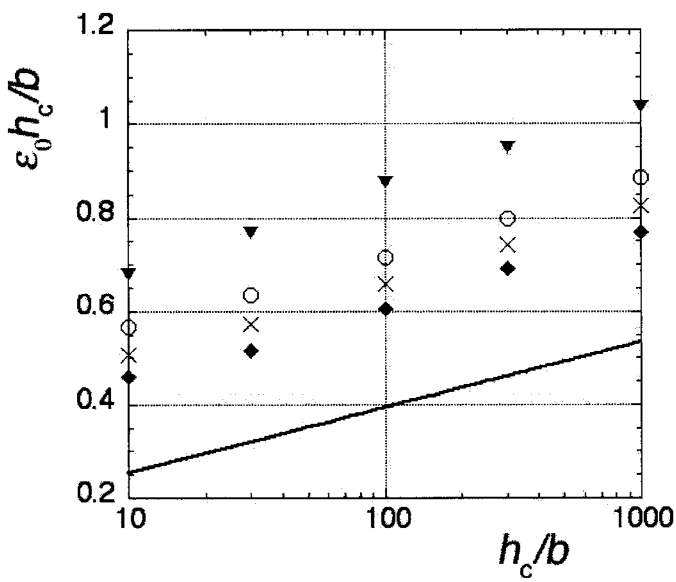

Figure 3. Influence of elastic anisotropy on the critical thickness for a Cu film on various substrates and with a (001) interface. (——), for comparison the prediction of the Matthews *et al.* criterion for the isotropic Cu/Cu system; (×), (◆), (○), the results for anisotropic mismatch stresses and isotropic line tension for the threading dislocation for Cu/Cu (×), Cu/Au (◆) and Cu/Ni (○); (▼) the additional effect of an anisotropic line tension in the case of the Cu/Ni system.

an image force from the substrate that is attractive for compliant substrates and repulsive for stiff substrates. The present results indicate that this effect cannot be simply rationalized, as is sometimes done, by considering an average modulus (Fitzgerald 1991).

Another result is shown in figure 3, still for a (001) interface. It is concerned with a full anisotropic calculation for the Cu/Ni system, that is including the anisotropic local line tension. The critical mismatch strain is then further increased by about 20%. This additional effect is explained as follows. The critical stress is mainly governed by the dragging effect of the misfit dislocation through its line tension. This effect is accounted for in the simulation through the anisotropic long-range interactions between segments. The additional effect of the anisotropic local line tension is therefore restricted to the bowed-out part of the line. The anisotropic line tension of Cu is a maximum for the screw orientation and a minimum near the edge orientation. The ratio of the maximum to minimum values is about 3, twice the corresponding value in isotropic elasticity: $1/(1-\nu)=3/2$. In the geometry of a [001] interface, a threading dislocation bows out towards the screw direction. Thus, the enhancement in line tension near the screw orientation in the anisotropic case is partly translated into an increase in critical stress to move the dislocation or, equivalently, into an increase in the critical thickness. Similar qualitative considerations would apply for other interface orientations and character dependencies of the line tension.

Figure 4 shows the results obtained for the Cu/Ni system with a (111) interface. For a given thickness, the critical misfit strain increases by a factor of between two

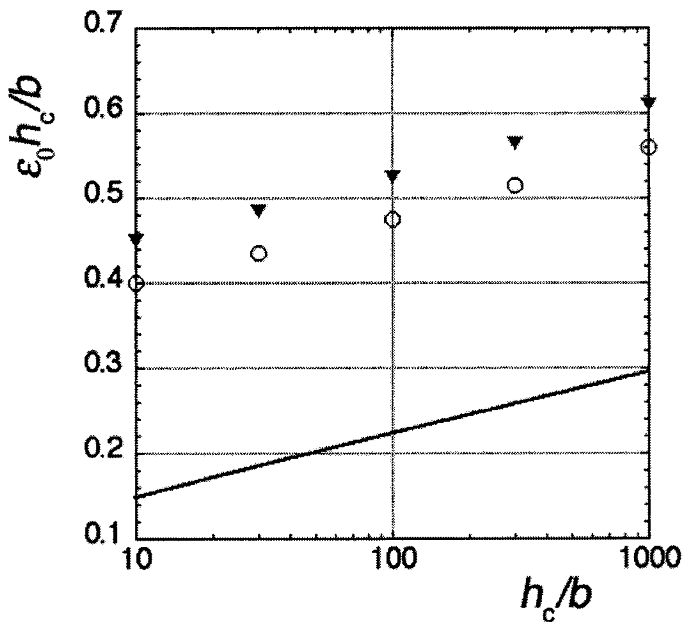

Figure 4. Influence of the elastic anisotropy on the critical thickness for the Cu/Ni system with a (111) interface: (——), the prediction of the Matthews criterion for the isotropic Cu/Cu system, as applied to a (111) interface; (○), (▼), the results for anisotropic mismatch stresses and isotropic line tension for the threading dislocation (○) and for the full anisotropic calculation (▼).

Table 1. Ratios of the critical properties of Cu/Ni films for (001) and (111) interfaces and two different thicknesses in anisotropic elasticity: mismatch strains from figures 3 and 4, stresses, resolved stresses and resolved stresses per unit line length.

Thickness	$\varepsilon_0^{111}/\varepsilon_0^{001}$	$\sigma_c^{111}/\sigma_c^{001}$	$\tau_c^{111}/\tau_c^{001}$	$\tau_c^{111}l^{001}/\tau_c^{001}l^{111}$
$10b$	0.661	1.500	0.922	1.065
$1000b$	0.588	1.335	0.821	0.948

and three when going from the isotropic prediction to the fully anisotropic calculation. When the line tension of the dislocation is isotropic, this increase is slightly smaller, a factor of between 1.85 and 2.65.

Within the framework of anisotropic elasticity, the quantitative influence of the interface orientation can be rationalized as follows. For a given value of the misfit strain ε_0, σ_c denotes the critical stress to move an isolated threading dislocation on a slip system with Schmid factor S and τ_c is the corresponding resolved shear stress. Then, making use of equation (2), we have

$$\tau_c = S^{hkl}\sigma_c^{hkl} = S^{hkl}Y^{hkl}\varepsilon_0. \tag{3}$$

Table 1 shows the ratios of the critical mismatch stresses and strains for (111) and (100) interfaces in Cu/Ni, for the smallest and largest thicknesses investigated. From figures 3 and 4, it appears that the critical mismatch strain is always smaller for the (111) interface than for the (100) interface. There is a compensating effect of the Schmid factors ($S^{001} = 0.408$ and $S^{111} = 0.251$; hence $S^{111}/S^{001} = 0.615$) and of the biaxial moduli ($Y^{111}/Y^{001} = 2.270$), so that the critical resolved stresses are not very different for the two orientations (cf. equation (3) and table 1). Taking into account the difference in initial dislocation length between the two orientations ($l^{111}/l^{001} = 3^{1/2}/2$), the two critical resolved stresses per unit length become almost identical. This simply results from the crystallographic similarity between the two configurations mentioned in §2.1. Regarding the critical non-resolved stresses (equations (2) and (3)), the effect of the biaxial moduli reverses the trend observed on the mismatch strains, so that the (111) interface is the 'hardest' (table 1). This non-trivial result cannot be simply guessed from figures 3 and 4.

Thus, the dependence of the critical stress on interface orientation is sensitive to elastic anisotropy. In fact, the Matthews *et al.* isotropic criterion leads to a prediction opposite to the present criterion. This can be checked from figures 3 and 4, where the critical mismatch strain (or stress) is the largest for the (100) orientation.

§ 4. Concluding remarks

The influence of elastic anisotropy on the critical conditions for plastic relaxation was investigated numerically for Cu films deposited on various substrates with two interface orientations. With respect to the isotropic prediction of Matthews *et al.*, the critical thickness is found to be substantially larger. This hardening effect is mainly due to the influence of anisotropic elasticity on mismatch stresses. To a smaller extent it depends on other factors such as the anisotropy of dislocation line tension and the elastic properties of the substrate.

Models including dislocation–dislocation hardening effects have been proposed to improve the predictions yielded by the Matthews *et al.* criterion, which are too small in comparison with experiments. However, the present results show that the influence of interface orientation is opposite to the predictions of these models.

A similar question is met in thin polycrystalline metallic films. Their surprisingly large plastic strength is thought to result from a combination of several contributions to dislocation glide:

(i) line tension forces;
(ii) image forces arising from the condition of strain continuity at the film–substrate interface and at the free surface of the film;
(iii) interactions between dislocations with same Burgers vector;
(iv) interactions of threading dislocations with other dislocations intersecting their glide plane.

Recent experimental investigations on metallic systems suggest that the last two contributions may be the most important ones in a grain of given orientation (Baker *et al.* 2001, Kobrinsky *et al.* 2001, Weihnacht and Bruckner 2001). There are, however, marked orientation effects in Cu films, where the texture is made up of columnar (001) and (111) grains. For instance, Hommel and Kraft (2001) found that the flow stress of (111) grains at 0.1 and 0.5% strain is about twice that of (001) grains. As illustrated above, the present numerical model qualitatively reproduces this important experimental fact. The ratio $\sigma_c^{111}/\sigma_c^{001}$ reproduced by the simulation goes from 1.5 to 1.35 when the film thickness is increased. It is suggested that the difference between simulation and experiment can be explained by the absence of strain hardening in the present simulations.

In conclusion, elastic anisotropy appears to affect dislocation behaviour significantly in confined systems. The results presented here deal only with a few model situations. A wealth of types of behaviour is expected to arise from the consideration of a wider spectrum of materials and textures.

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