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DEFECTS, DISLOCATIONS, AND PHYSICS OF STRENGTH

Generation and Evolution of Partial Misfit Dislocations and Stacking Faults in Thin-Film Heterostructures

M. Yu. Gutkin, K. N. Mikaelyan, and I. A. Ovid'ko
Institute of Problems in Machine Science, Russian Academy of Sciences,
Vasil'evskiĭ ostrov, Bol'shoĭ pr. 61, St. Petersburg, 199178 Russia
e-mail: ovidko@def.ipme.ru

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Abstract—An analysis is made of the specific features in the generation and evolution of partial misfit dislocations at the vertices of V-shaped configurations of stacking fault bands, which terminate in the bulk of the growing film at 90° partial Shockley dislocations. The critical thicknesses h_c of an epitaxial film, at which generation of such defect configurations becomes energetically favorable, are calculated. It is shown that at small misfits, the first to be generated are perfect misfit dislocations and at large misfits, partial ones, which are located at the vertices of V-shaped stacking-fault band configurations emerging onto the film surface. Possible further evolution of stacking-fault band configurations with increasing film thickness are studied. *© 2001 MAIK "Nauka/Interperiodica".*

The generation and evolution of various defect structures in the course of growth of thin-film heteroepitaxial systems has been for many years a subject of numerous experimental and theoretical studies (see, e.g., [1–16]). In particular, one is presently witness to intense development of the concept of misfit dislocations (MDs) whose formation at the interphase boundary between the substrate and the growing epitaxial film serves as an efficient channel of removing misfit stresses caused by differences in the crystalline structure and properties between the substrate and film materials [1–6]. The role of MDs may actually be played by both perfect lattice dislocations ("perfect misfit dislocations") and partial dislocations ("partial misfit dislocations"), which are associated with stacking faults. However, nearly all of the theoretical models proposed relate to the formation and behavior of perfect MDs, although a comparative consideration of the perfect and partial MDs suggests the existence of such parameters for a heterosystem at which the formation of partial MDs is found to be energetically preferable [7, 8]. In particular, as follows from the results of a theoretical analysis from [8], if the lattice misfit between the film and the substrate is large enough (>1%), the critical thickness for the formation of partial MDs connected with V-shaped stacking fault defects becomes less than that for the appearance of perfect MDs; i.e., such partial MDs form in a heterosystem before perfect MDs do. This conclusion is of considerable interest in view of the present demand in technology for the use of heterostructures with large misfits.

However, the case considered in [8] relates to fairly simple partial MD configurations, namely, to partial MDs located at the interphase boundary at the vertices of V-shaped stacking faults. The main objective of this work is to analyze theoretically the conditions favoring generation of experimentally observed [13] partial-MD configurations of a more complex type, more specifically, of configurations made up of three partial MDs located at the interphase boundary and in the bulk of the film and connected with V-shaped stacking faults.

1. GENERATION MECHANISMS OF PARTIAL MISFIT DISLOCATIONS

Consider the possible mechanisms of formation of partial MDs at the interphase boundary between an epitaxial film and a substrate. Formation of semiloops of split dislocations at the free surface of a growing epitaxial film, followed by their slide to the interphase boundary, is one of the major mechanisms of MD generation which appears to be best studied experimentally [9–13]. For instance, the splitting of sliding perfect 60° dislocations into partial 30° and 90° Shockley dislocations (Fig. 1a) with a subsequent slide of this already split configuration to the interphase boundary, brings about the formation of a partial MD, which is connected through a stacking fault to the second partial dislocation remaining in the bulk of the film [9, 10]. A reaction between two such partial MDs near the interphase boundary gives rise to the formation of sessile partial MDs located at the vertices of V-shaped stacking faults [12], at the ends of which Shockley partial dislocations are located (Fig. 1b). Such defect configurations are similar to the Lomer–Cottrell barriers in fcc metals [17], the only difference being that, here, a partial MD acts as the stair-rod sessile dislocation. If partial MDs form even at small film thicknesses (in systems with large misfits), the formation of the second Shockley partial dislocations becomes delayed and stacking fault bands extend from the partial MD to the free film surface. As the film continues to grow, these partial dislocations will be generated on the surface and they will slide toward the vertex partial MD, after which this V-shaped defect configuration transforms (collapses) into a sessile Lomer perfect dislocation.

In [8], we considered the first case in detail, where stacking fault bands always reached the surface of the film as the film grew. When applied to the GaAs/Si(001) heterosystem, where such partial MDs were observed to exist at the vertices of V-shaped stacking faults [12], it is implied that each sessile 90° partial MD is formed of two partial 30° dislocations sliding toward each other to merge at the interphase boundary and that the 90° partial MDs, which should terminate the stacking fault bands, had no time to nucleate.

The present work considers the second, more general case, where partial 90° dislocations also slide from the film surface after the 30° partials, but stop at a certain distance from the surface (Fig. 1b). Thus, the V-shaped stacking fault is now bounded from below by a 90° partial MD at its vertex and from above by two 90° partial dislocations residing in the bulk of the film. Note that such defect configurations were observed experimentally [13], but have not been treated theoretically.

In the subsequent sections, we are going to calculate the critical parameters for the formation of partial MDs connected through V-shaped stacking faults with partial dislocations in the bulk of the growing film and analyze the further evolution of such defect configurations in the course of epitaxial growth. The analysis will be illustrated by GaAs/Si heteroepitaxial structures.

2. CRITICAL PARAMETERS OF THIN-FILM HETEROSTRUCTURES WITH PARTIAL MISFIT DISLOCATIONS

One of the important parameters characterizing a heteroepitaxial system is the critical film thickness h_c, above which the formation of MDs becomes energetically favorable [1–6]. The appearance of the first MDs alone determines the magnitude of h_c; therefore, it is sufficient in itself for study of a system consisting of one partial MD connected through a V-shaped stacking fault with two partial 90° dislocations in the bulk of the film (Fig. 1b).

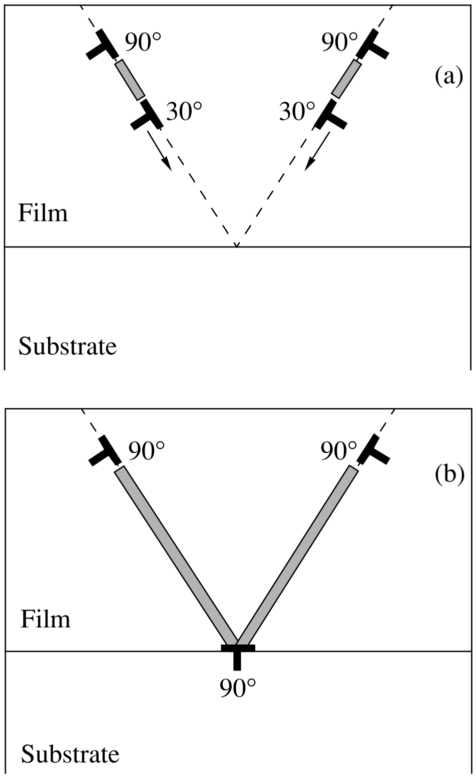

Fig. 1. Formation of partial misfit dislocations. (a) Slide of 60° dislocations split into Shockley partial 30° and 90° dislocations. (b) Formation of a sessile partial 90° MD connected through stacking fault bands with Shockley partial 90° dislocations in the bulk of the film.

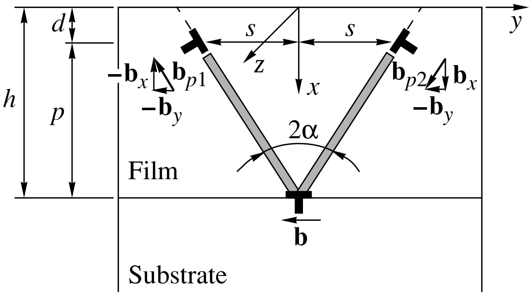

Fig. 2. Model of a V-shaped configuration of stacking fault bands with a partial 90° MD at the vertex and two Shockley partial 90° dislocations at the band ends.

Consider a model heteroepitaxial system in the form of a thin elastically isotropic film of thickness h, which is grown epitaxially on a semi-infinite elastically isotropic substrate (Fig. 2). The elastic constants, the shear modulus G, and the Poisson ratio ν will be considered the same for the materials of the film and of the substrate. The original coherent state of the system is characterized by the elastic strain of the film $\varepsilon = -f$, where $f = (a_2 - a_1)/a_1 > 0$ is the original two-dimensional lattice misfit between the substrate and film whose lattice parameters are a_1 and a_2, respectively. We place a partial MD with the Burgers vector $\mathbf{b}$ at the point $(h, 0)$ at the interface and partial 90° dislocations with Burgers vectors $\mathbf{b}_{p1} = -\mathbf{b}_x - \mathbf{b}_y$ and $\mathbf{b}_{p2} = \mathbf{b}_x - \mathbf{b}_y$ at points $(d, \pm s)$ in the bulk of the film. The partial MD connects with these dislocations through the stacking fault bands making up a V-shaped configuration with an opening angle 2α. For convenience, we present each of these partial 90° dislocations as a superposition of two edge dislocations with Burgers vectors $\pm\mathbf{b}_x$ and $\mathbf{b}_y$ (Fig. 2).

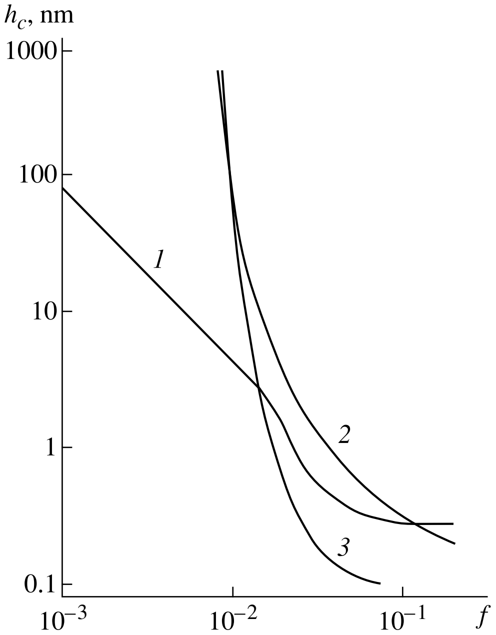

Fig. 3. *f*–*h* diagram (*1*) for a perfect MD, (*2*) for a partial MD with stacking fault bands and Shockley partial 90° dislocations at the band ends, and (*3*) for a partial MD with stacking fault bands reaching the surface of the growing film.

The total energy of the system per unit dislocation length, W^t, can be presented as

$$W^t = W^f + W^n + W^{fd} + W^{\gamma} + W^d, \tag{1}$$

where W^f is the elastic energy of the original misfit, $W^n = G(b^2 + 2b_p^2)/[4\pi(1-\nu)]$ is the total energy of the dislocation cores, $b_p^2 = b_{p1}^2 = b_{p2}^2$, $W^{fd} = -2Gf(bh + 2b_y d)(1+\nu)/(1-\nu)$ is the total interaction energy between dislocations and the elastic original-misfit stress field, $W^{\gamma} = 2\gamma(h-d)/\cos\alpha$ is the stacking-fault band energy, γ is the stacking fault energy, and W^d is the elastic energy of the dislocation subsystem including the interaction of dislocations with the free film surface and with one another. The last term is calculated using the relations for the stress fields of an edge dislocation located near a free surface [18], which finally yields (in units of $G/[4\pi(1-\nu)]$)

$$\begin{aligned}
W^d = & -b^2\left(\ln\frac{b}{2h-b} + \frac{2h(h-b)}{(2h-b)^2}\right) - \frac{4b_x b_y s d^3}{(d^2+s^2)^2} \\
& - 2bb_y\left(\ln\frac{(h-d)^2+s^2}{(h+d)^2+s^2} - \frac{2s^2}{(h-d)^2+s^2}\right. \\
& \left. + \frac{2(s^2+2dh)}{(h+d)^2+s^2} - \frac{8dhs^2}{[(h+d)^2+s^2]^2}\right) \\
& + 2bb_x s\left(\frac{2(h-d)}{(h-d)^2+s^2} - \frac{2(h-d)}{(h+d)^2+s^2} - \frac{8dh(h+d)}{[(h+d)^2+s^2]^2}\right) \\
& + b_y^2\left(\ln\frac{b_y^2 s^2}{(d^2+s^2)(2d-b_y)^2} + \frac{4d(d-b_y)}{(2d-b_y)^2} - \frac{d^2(d^2+3s^2)}{(d^2+s^2)^2}\right) \\
& - b_x^2\left(\ln\frac{b_x^2(d^2+s^2)}{s^2(2d-b_x)^2} + \frac{4d(d-b_x)}{(2d-b_x)^2} - \frac{d^2(3d^2+s^2)}{(d^2+s^2)^2}\right).
\end{aligned} \tag{2}$$

To find the critical film thickness h_c at which the formation of even the first partial MD alone becomes energetically favorable, we equate the change in energy that is associated with the formation of a partial MD connected through a V-shaped stacking fault with two partial 90° dislocations to zero,

$$\Delta W = W^t - W^f = 0, \tag{3}$$

and obtain a transcendental equation for h_c:

$$\begin{aligned}
& 2b_p^2 - 8\pi f(1+\nu)(bh + 2b_y d) + \frac{8\pi\gamma(1-\nu)(h-d)}{G\cos\alpha} \\
& + b^2\left(1 - \ln\frac{b}{2h-b} - \frac{2h(h-b)}{(2h-b)^2}\right) \\
& - 2bb_y\left(\ln\frac{(h-d)^2+s^2}{(h+d)^2+s^2} - \frac{2s^2}{(h-d)^2+s^2}\right. \\
& \left. + \frac{2(s^2+2dh)}{(h+d)^2+s^2} - \frac{8dhs^2}{[(h+d)^2+s^2]^2}\right) \\
& + 2bb_x s\left(\frac{2(h-d)}{(h-d)^2+s^2} - \frac{2(h-d)}{(h+d)^2+s^2}\right. \\
& \left. - \frac{8dh(h+d)}{[(h+d)^2+s^2]^2}\right) - \frac{4b_x b_y s d^3}{(d^2+s^2)^2} \\
& - b_y^2\left(\ln\frac{b_y^2 s^2}{(d^2+s^2)(2d-b_y)^2} + \frac{4d(d-b_y)}{(2d-b_y)^2}\right. \\
& \left. - \frac{d^2(d^2+3s^2)}{(d^2+s^2)^2}\right) - b_x^2\left(\ln\frac{b_x^2(d^2+s^2)}{s^2(2d-b_x)^2}\right. \\
& \left. + \frac{4d(d-b_x)}{(2d-b_x)^2} - \frac{d^2(3d^2+s^2)}{(d^2+s^2)^2}\right) = 0.
\end{aligned} \tag{4}$$

Using Eq. (4),we consider the dependence of h_c on the original misfit f for the case where the partial dislocations are located at a depth d. We use, as before [8], the parameters characteristic of the GaAs/Si(001) heterosystem [7, 19]: $G = 32.5$ GPa, $\nu = 0.31$, $b = 0.133$ nm, $b_p = 0.231$ nm, $b_x = 0.19$ nm, $b_y = 0.133$ nm, $2\alpha \approx 70°$, and $\gamma = 0.06$ J m^{-2}.

Figure 3 presents the $h_c(f)$ dependences for a perfect MD (curve *1*, $b = 0.398$ nm, $\gamma = 0$), for a partial MD at the vertex of a V-shaped configuration of stacking-fault bands terminated by two partial 90° dislocations in the bulk of the film at a minimal depth $d = b_x = 0.19$ nm (curve *2*), and for a partial MD at the vertex of the same configuration for the case where the stacking-fault bands reach the free surface (curve *3*, $d = 0$, $b = 0.133$ nm). As seen from the plots, perfect MDs can be generated at any misfits f (provided the film is thick enough), whereas for a partial MD, in both cases, there exists a limiting minimal misfit f_l below which their generation is energetically unfavorable. The values of f_l in the latter two cases are approximately equal, $f_l \approx 0.009$. It was also found that the formation of a partial MD with $d = 0$ is always more probable than that with $d = b_x$ (curve *3* passes below curve *2*). Consider now what happens as d increases. Figure 4 presents the dependence of h_c on d for a fixed misfit $f = 0.02$. As seen from the figure, for small d, the critical film thickness h_c increases with d to reach a maximum at $d \approx 4b_x \approx 0.76$ nm, after which it falls off while remaining substantially larger than the critical thicknesses for perfect MDs (≈0.14 nm) and partial MDs with $d = 0$ (≈0.12 nm). Thus, one can conclude that for small misfits ($f < 0.01$), the first to be generated are perfect MDs, whereas for large misfits ($f > 0.01$), partial MDs are generated first, with the stacking-fault bands reaching the surface of the growing film.

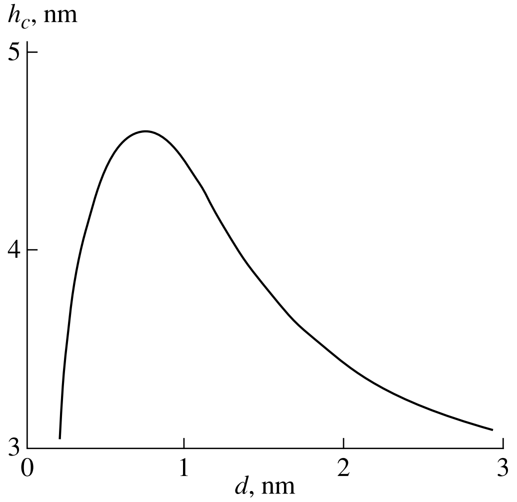

Fig. 4. Dependence of the critical thickness h_c on depth d of Shockley partial 90° dislocations, calculated for a misfit $f = 0.02$.

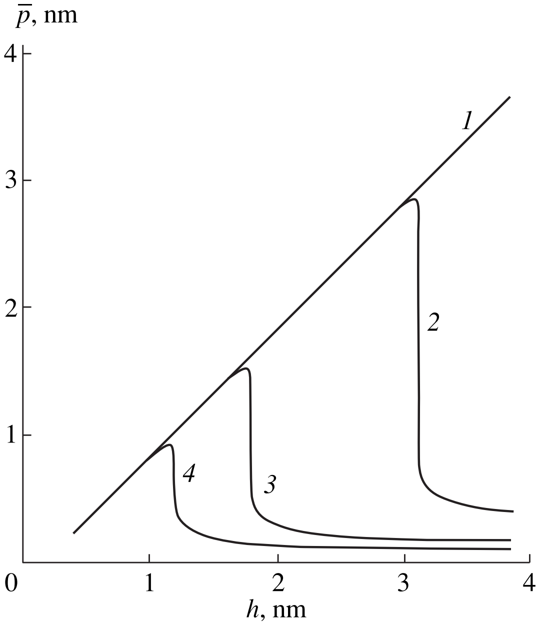

Fig. 5. Variation of the equilibrium distance $\bar{p}$ between Shockley partial 90° dislocations and the interphase boundary with increasing film thickness, calculated for the misfits f (*1*) 0.02, (*2*) 0.04, (*3*) 0.07, and (*4*) 0.10.

3. EVOLUTION OF PARTIAL MISFIT-DISLOCATION CONFIGURATIONS IN THE COURSE OF FILM GROWTH

Consider the development of the situation as the film continues to grow in the case of large misfits ($f > 0.01$). We calculate the equilibrium position of the partial 90° dislocations terminating the stacking-fault bands in the bulk of the film (Fig. 2) using Eqs. (1) and (2). One can determine the change in the equilibrium distance $\bar{p}$ (i.e., corresponding to the maximum gain in energy ΔW) as the film thickness h increases with the misfit f kept fixed. The results of the calculation are plotted in Fig. 5 as $\bar{p}(h)$ functions for $f = 0.02$, 0.04, 0.07, and 0.10 (curves *1*–*4*, respectively). It is readily seen that, as long as the thickness h is small ($h < 1$ nm), we have $\bar{p}(h) = h - b_x$ for any of these misfits; i.e., the stacking-fault bands grow as the film grows to finally reach (to within b_x) the free surface. At the instant h reaches a critical value h'_c, $\bar{p}$ exhibits a sharp drop, which can be treated as a fast displacement of 90° partial dislocations to the interface separating the film from the substrate; the drop is accompanied by a shortening of the stacking-fault bands until they disappear altogether and the V-shaped configuration collapses, with the partials transforming to perfect MDs. For instance, to the misfits $f = 0.02$, 0.04, 0.07, and 0.10 correspond now “new” critical thicknesses, $h'_c \approx 5.7$, 3.1, 1.9, and 1.3 nm, at which the partials become perfect MDs. The collapse of the V-shaped configurations of stacking-fault bands with partial MDs at their vertices, resulting in the formation of perfect MDs, confirms the conclusion [8] that a decrease in partial MD density and an increase in perfect MD density in the course of film growth inevitably occur and suggests that a natural mechanism is involved in the transformation of partial to perfect MDs. A decrease in the partial MD density and an increase in the perfect MD density with increasing thickness of the growing film were observed in the experiments in [13].

Thus, our theoretical consideration of partial MDs located at the vertices of V-shaped configurations of stacking-fault bands, which terminate at Shockley partial 90° dislocations in the bulk of the film, permits the following conclusions. At small misfits, the first to be generated are perfect MDs, while at large ones, partial MDs are generated at the vertices of the V-shaped configurations of stacking-fault bands emerging onto the film surface. In the latter case, as the film grows in thickness, the stacking-fault bands first grow longer and reach, as before, the film surface, but after the thickness has attained a critical value h'_c, which decreases with increasing misfit, they shorten rapidly through the generation of Shockley partial 90° dislocations and their slide to the interphase boundary. As these dislocations approach the interface, the V-shaped configuration collapses and the partial MDs transform into perfect MDs. This mechanism of transformation of partial to perfect MDs accounts for the decrease in partial MD density and the increase in perfect MD density during the growth of nanolayer heterosystems, which is well known from experiments (see, for instance, [13]).

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