Bending of a film-substrate system by epitaxy

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(Received 31 July 1995; revised manuscript received 6 December 1995)

The curvature, strains, and stresses produced by the misfit of a film-substrate system of cubic crystals in pseudomorphic epitaxy on cubic (001) faces are found by a simple general procedure which minimizes the total elastic strain energy of the system. The film thickness is not required to be small compared to the substrate thickness, but the misfit and strain are assumed to be small so that linear elasticity theory can be used. The deviations for finite film thickness from the usual limit of negligible film thickness differ from previous work. The theory in the usual limit agrees well with a recent measurement of the bending of a system of up to seven monolayers of Ge deposited on a Si(001) surface.

I. INTRODUCTION

The theory of the bending of a film-substrate system is an old problem dating back at least to 1909.[1] Two distinct cases have been studied. In case 1, which is of interest for bending of electroplated systems, it is assumed that a stress field is present in the film which forces the bending. The theory relates the radius of curvature of the system R to the stress in the film so that a measured R yields the value of that stress. Reference 1 assumes the film thickness t_f is small compared to the substrate thickness t_s. Later papers have generalized the theory to finite film thicknesses.[2,3] In case 2 the film is assumed to be crystalline and has been deposited in pseudomorphic epitaxy on a crystalline substrate. The curvature of the system is driven by the misfit between the periodic meshes of the crystal planes of the surfaces of the film and substrate. The theory then relates R to the misfit.[4–6] It is convenient to refer to curvature produced in this way as epitaxial bending.

References 1–6 all develop the theory using the force and moment balance equations of equilibrium elasticity theory. Recently a simple general method was applied to case 1 by du Trémolet and Peuzin,[7] which minimizes the total elastic energy of the system with respect to R and a parameter β which gives the position of the "neutral" layer. i.e., the layer where the bending strain vanishes. The theory of the bending in Ref. 7 again assumes t_f small compared to t_s. This paper extends the method of Ref. 7 to case 2, but does not assume that t_f/t_s is small. The development here does assume that the misfit and the consequent strains are small, so that linear elastic relations can be used, and takes account of the discontinuity in strain at the interface between film and substrate. An explicit relation is found which expresses the ratio R/t_s in terms of the misfit and the ratios t_f/t_s and Y'_f/Y'_s, where Y' is a modified Young's modulus. The relation between R and the stress in the film, which is the objective of case 1 studies, is also obtained for general t_f/t_s. The relations found here for general t_f/t_s in both case 1 and case 2 differ from previous work.

The relation developed between curvature and misfit can be verified in a system with known misfit and elastic constants. This verification is demonstrated here with a recent measurement on an epitaxial system, although just in the limit of small $r \equiv t_f/t_s$. The complete relation for non-negligible r, which will be called finite r, is not needed for the usual epitaxial system, but the derivation clarifies the theory of the bending. Clarification is needed because recent papers have found different dependences on r than that found here, due to neglect of the discontinuity in strain at the interface. The derivation also illustrates the power and simplicity of the energy-minimization procedure.

In Sec. II the total elastic energy E_{total} of the bent film-substrate system is found in terms of the properties of the film and substrate and the parameters R and β. In Sec. III E_{total} is minimized with respect to R and β. Formulas for R, β, and the strain and stress fields are derived and compared with previous work. In Sec. IV the relation between misfit and curvature is derived and shown to fit well in a recent measurement[8] of the curvature of a substrate crystal of Si(001) when a film of Ge(001) is deposited in pseudomorphic epitaxy. Section V discusses these results and their application, and also the energy-minimization method and its possible extension to more general cases of epitaxy.

II. THE TOTAL ELASTIC ENERGY OF THE BENT SYSTEM

The elastic energy density of a strained cubic material of volume V is given by[9]

$$\frac{E_{\text{el}}}{V} = \frac{c_{11}}{2}(\varepsilon_1^2+\varepsilon_2^2+\varepsilon_3^2)+c_{12}(\varepsilon_2\varepsilon_3+\varepsilon_3\varepsilon_1+\varepsilon_1\varepsilon_2) + \frac{c_{44}}{2}(\varepsilon_4^2+\varepsilon_5^2+\varepsilon_6^2). \tag{1}$$

The ε_i, $i=1-6$ are the strain components and the c_{ij}, $i,j=1-6$, are the elastic constants in the reduced index form defined by

$$\varepsilon_1=\varepsilon_{xx}, \quad \varepsilon_2=\varepsilon_{yy}, \quad \varepsilon_3=\varepsilon_{zz},$$
$$\varepsilon_4=2\varepsilon_{yz}, \quad \varepsilon_5=2\varepsilon_{zx}, \quad \varepsilon_6=2\varepsilon_{xy}. \tag{2}$$

In the system to be studied there are no shear components of strain; hence

$$\varepsilon_4=\varepsilon_5=\varepsilon_6=0. \tag{3}$$

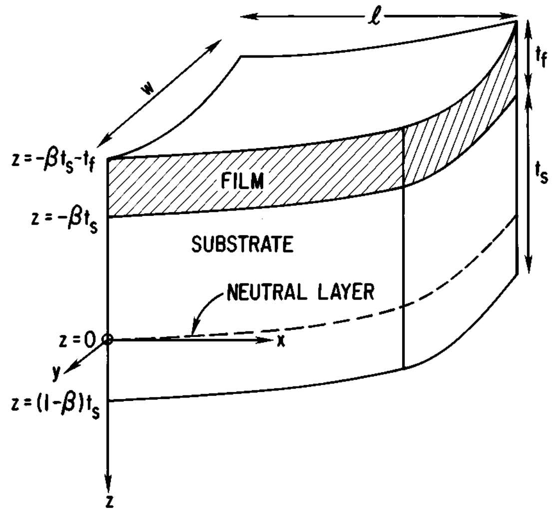

FIG. 1. A film-substrate system with cubic (001) surfaces of length l, width w, film thickness t_f, substrate thickness t_s, bent with negative radius of curvature in the x and y directions, x, y, and z axes in crystal axis directions. The origin of coordinates is in the neutral layer (dashed), which is at a distance βt_s from the interface.

The system consists of a rectangular film on a rectangular substrate both of length l and width w with cubic (001) crystal surfaces; the surfaces are in the x-y plane and x, y, and z are along the crystal axes, as shown in Fig. 1.

Since there are no applied forces in the z direction, the stress in the z direction vanishes, and gives the linear elastic relation

$$\sigma_3=\sigma_{zz}=c_{12}(\varepsilon_1+\varepsilon_2)+c_{11}\varepsilon_3=0; \tag{4}$$

hence

$$\varepsilon_3=-\frac{c_{12}}{c_{11}}(\varepsilon_1+\varepsilon_2). \tag{5}$$

There will be stresses in the x and y directions because the film and substrate will exert in-plane forces on each other. Putting (5) into (1) and dropping the shear terms gives

$$E_{\rm el}=V\left[\frac{c_{11}^2-c_{12}^2}{2c_{11}}(\varepsilon_1+\varepsilon_2)^2-(c_{11}-c_{12})\varepsilon_1\varepsilon_2\right]. \tag{6}$$

If we now use the symmetry of cubic (001) surfaces so that the x and y directions are equivalent and note that epitaxy will act symmetrically, i.e., isotropically, in these two directions, then

$$\varepsilon_1=\varepsilon_2; \tag{7}$$

hence the elastic energy can be written

$$E_{\rm el}=\frac{V(c_{11}-c_{12})(c_{11}+2c_{12})}{c_{11}}\,\varepsilon_1^2=V\,\frac{Y}{1-\nu}\,\varepsilon_1^2\equiv VY'\varepsilon_1^2, \tag{8}$$

where Y is Young's modulus and ν is Poisson's ratio, both along cubic axes. The abbreviation Y' is conveniently introduced for the modified Young's modulus $Y/(1-\nu)$.

Figure 1 shows symmetric bending in both the x and y directions. The origin of coordinates is in the neutral layer, drawn dashed in the figure. The z axis points downward, so the radius of curvature R shown in the figure is negative. The neutral layer lies a fraction β of t_s from the interface, so the interface is at $z=-\beta t_s$.

Because of the bending, the lengths of the layers change. Between two layers Δz apart in either film or substrate we have a change in the length of the layer of $\theta\Delta z$, where θ is the angle subtended by the specimen at the center of curvature, compared to the length $R\theta$, so that the strain is

$$\Delta\varepsilon_1=-\frac{\Delta z}{R}. \tag{9}$$

Thus in Fig. 1 with $R<0$, ε_1 increases as in (9) as z increases in both substrate and film.

At the interface there is a discontinuity in ε_1 since the strain in the film ε_1^f refers to the equilibrium state of the film, whereas in the substrate ε_1^s refers to the substrate equilibrium. The condition for pseudomorphic epitaxy, which forces the square mesh cells of film and substrate to coincide, can be written

$$a_0^f(1+\varepsilon_1^{fi})=a_0^s(1+\varepsilon_1^{si}), \tag{10}$$

where a_0^f and a_0^s are the sides of the equilibrium mesh cell of film and substrate, respectively, and ε_1^{fi} and ε_1^{si} are the strains at the interface indicated by the superscript i. Then (10) can be written

$$\varepsilon_1^{fi}-(1+m)\varepsilon_1^{si}=m\equiv\frac{a_0^s-a_0^f}{a_0^f}, \tag{11}$$

where m is the misfit between film and substrate. Assuming that $m\ll 1$, which corresponds to the strains being small and linear elastic theory applicable, we write the discontinuous strain at the interface as

$$\varepsilon_1^{fi}=\varepsilon_1^{si}+m. \tag{12}$$

The total strain in film and substrate is the strain produced by the misfit when the system is constrained to be flat plus the strain due to bending. Thus

$$\varepsilon_1^f(z)=m_f-z/R,\quad \varepsilon_1^s(z)=m_s-z/R, \tag{13}$$

where m_f and m_s are the homogeneous strains due to misfit in the flat system. Then from (12) at $z=-\beta t_s$

$$m_f-m_s=\varepsilon_1^{fi}-\varepsilon_1^{si}=m. \tag{14}$$

Minimization of the energy in the flat system

$$E_{\rm total}^{\rm (flat)}=V_fY_f'(\varepsilon_1^{f\rm (flat)})^2+V_sY_s'(\varepsilon_1^{s\rm (flat)})^2=V_fY_f'm_f^2+V_sY_s'm_s^2$$

with respect to m_f using (14) gives

$$\frac{m_s}{m_f}=-\frac{V_fY_f'}{V_sY_s'}=-\gamma r, \tag{15}$$

where $\gamma\equiv Y_f'/Y_s'$ and $r\equiv t_f/t_s=V_f/V_s$. Hence from (14) and (15)

$$m_f = \frac{m}{1+\gamma r}, \quad m_s = -\frac{m\gamma r}{1+\gamma r}. \tag{16}$$

The total elastic energy E_{total} of the bent system can be found by integrating (8) over z using (13):

$$\begin{aligned} E_{\text{total}} &= lw\left[Y_f' \int_{-\beta t_s - t_f}^{-\beta t_s} dz \left(m_f - \frac{z}{R} \right)^2 \right. \\ &\quad \left. + Y_s' \int_{-\beta t_s}^{(1-\beta)t_s} dz \left(m_s - \frac{z}{R} \right)^2 \right] \\ &= V_f Y_f' [(m_f + \alpha\beta)^2 + (m_f + \alpha\beta)\alpha r + \alpha^2 r^2/3] \\ &\quad + V_s Y_s' [(m_s + \alpha\beta)^2 - (m_s + \alpha\beta)\alpha + \alpha^2/3], \end{aligned} \tag{17}$$

where $\alpha \equiv t_s/R$.

From (17)

$$\frac{\partial E_{\text{total}}}{\partial m_f} = \frac{1}{\alpha} \frac{\partial E_{\text{total}}}{\partial \beta}; \tag{18}$$

hence at the minimum of E_{total}, where $\partial E_{\text{total}}/\partial\beta = 0$, $\partial E_{\text{total}}/\partial m_f$ also vanishes. Thus the minimum of E_{total} is independent of the individual values of m_f and m_s provided (14) holds, but depends only on m. It is convenient to put $m_f = m$ and $m_s = 0$ in (17) for purposes of evaluating β, α and E_{total} at the minimum, which will depend only on γ, r, and m.

III. MINIMIZATION OF THE TOTAL ENERGY

A. Solution for α and β

From (17), setting the derivative of E_{total} with respect to α to 0 gives

$$\begin{aligned} \frac{\partial E_{\text{total}}}{\partial \alpha} &= V_f Y_f' \left[2(m+\alpha\beta)\beta + (m+2\alpha\beta)r + \frac{2\alpha r^2}{3} \right] \\ &\quad + V_s Y_s' 2\alpha[\beta^2 - \beta + \tfrac{1}{3}] = 0; \end{aligned} \tag{19}$$

hence

$$\alpha = -\frac{r\gamma m(\beta + r/2)}{r\gamma(\beta^2 + \beta r + r^2/3) + (\beta^2 - \beta + 1/3)}, \quad r \equiv \frac{t_f}{t_s},$$

$$\gamma \equiv \frac{Y_f'}{Y_s'}. \tag{20}$$

Equations (19) and (20) are identical with the moment balance equation around the neutral axis. Setting the derivative of E_{total} with respect to β to 0 gives

$$\frac{\partial E_{\text{total}}}{\partial \beta} = V_f Y_f' [2(m+\alpha\beta)\alpha + \alpha^2 r] + V_s Y_s' \alpha^2 (2\beta - 1) = 0; \tag{21}$$

hence

$$\alpha = -\frac{r\gamma m}{(\beta + r/2)\gamma r + (\beta - 1/2)}. \tag{22}$$

Equations (21) and (22) are identical with a force balance equation. Equating (20) and (22) and solving for β gives

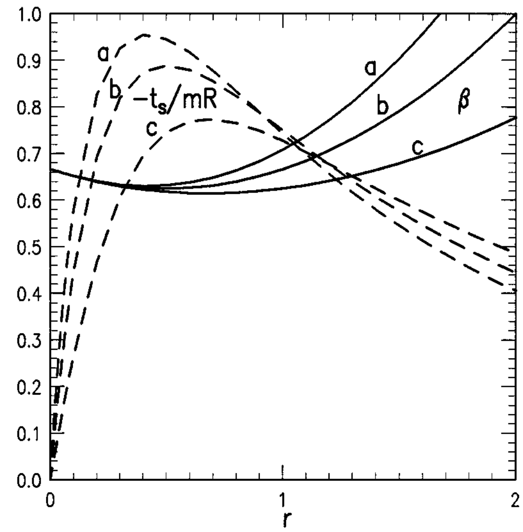

FIG. 2. Plots of β (full lines) and $-t_s/mR$ (dashed lines) as functions of r for γ=1.5 (marked *a*), γ=1.0 (marked *b*), and γ=0.5 (marked *c*) from (23) and (24).

$$\beta = \frac{2}{3} \frac{[1 + (r/4)(3 + \gamma r^2)]}{1+r}, \tag{23}$$

and putting (23) into (22) gives

$$\alpha \equiv \frac{t_s}{R} = -\frac{6\gamma m r(1+r)}{1 + 4\gamma r + 6\gamma r^2 + 4\gamma r^3 + \gamma^2 r^4}. \tag{24}$$

Keeping just the first-order correction in r to the values of β and α in the limit of small r, (23) and (24) become

$$\beta \simeq \frac{2}{3}\left(1 - \frac{r}{4}\right), \tag{25}$$

$$\frac{t_s}{R} \simeq -6\gamma m r[1 + (1 - 4\gamma)r]. \tag{26}$$

Figure 2 plots β and the reduced curvature α/m as functions of r for several values of γ from (23) and (24). The curvature is small for r large and r small, while β remains near 2/3 up to $r=1$, and then rises and becomes greater than 1, which means there is no neutral layer in the substrate. However, β from (23) is always positive and the neutral layer never moves into the film, which would correspond to negative β. But one expects that at some large r the neutral layer must be in the film, since now greater reduction of energy is achieved by reducing the average strain in the film. Clearly there is a second solution to the curvature calculation, which can be found by interchanging film and substrate in the above calculation. The results of this calculation at γ=0.5 are shown in Fig. 3, where β_1 is the first solution and β_2 is the second solution. We define β_2 such that $\beta_2 t_s$ is the distance from the interface to the neutral layer. Hence $\beta_2 < 0$ means that the neutral layer is now on the film side of the interface. The reduced energies $E_i/(m^2 V_s Y_s')$, $i=1,2$, for the two solutions are also plotted in Fig. 3, showing that the first solution is more stable at small r, but at $r > 2.44$ ($1/r < 0.41$) the second solution becomes more stable, as expected. How-

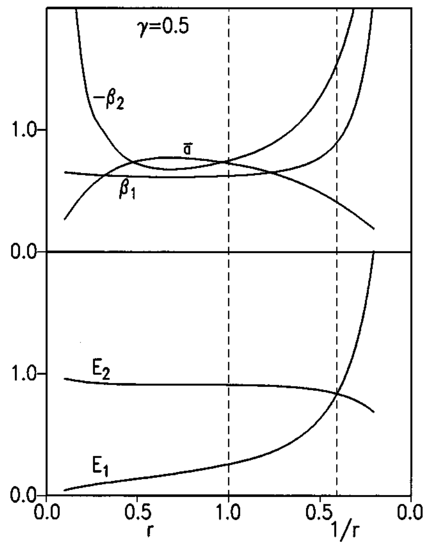

FIG. 3. Plots of the parameter β, of the reduced curvature $\overline{\alpha}\equiv\alpha/m\equiv t_s/mR$, and of the reduced total energy $E_{\mathrm{total}}/(m^2V_sY_s')$ for the two solutions for bending of a film-substrate system at $\gamma=0.5$. These three quantities are plotted against r up to $r=1$ (dashed line) and then against $1/r$ for $r=1$ to ∞. The negative values of β_2 mean the neutral layer is in the film. The first solution is more stable up to $r=2.44$ ($1/r=0.41$) (dashed line), when the second solution becomes the stable state. The reduced curvature $\overline{\alpha}$ is the same for both solutions.

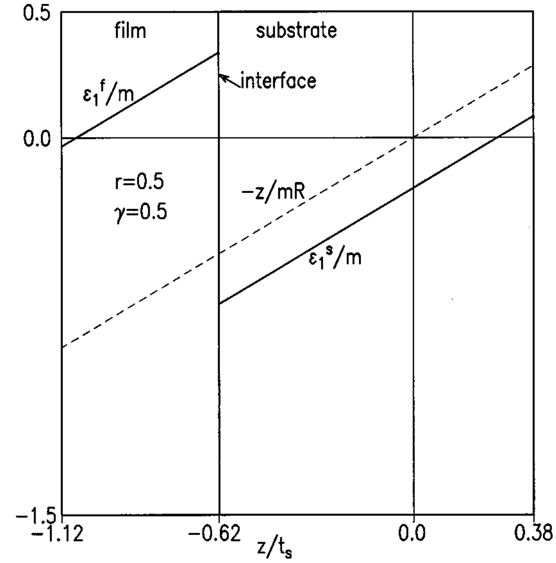

FIG. 4. Cross section of film-substrate system at $r=0.5$ and $\gamma=0.5$ with origin of z at the neutral axis and $\beta=0.62$. The reduced total strains ε_1^f/m in the film and ε_1^s/m in the substrate (solid lines) and the reduced bending strain $-z/mR$ (dashed line) are shown. The reduced total strains show a unit discontinuity at the interface and show unstrained layers at $z/t_s=-1.07$ and 0.27; the bending strain vanishes at $z=0$.

ever, the curvatures of both solutions are the same, as shown by the single curve for $\overline{\alpha}=t_s/mR$.

In Fig. 4 the reduced total strains (ε_1/m) in film and substrate for the first solution mentioned above at $r=0.5$ and $\gamma=0.5$ are shown over the cross section, along with the bending strain (dashed). From Fig. 4 we see the unit discontinuity in the reduced total strains at the interface, and that the neutral layer, where the bending strain vanishes, is different from the unstrained layers, of which there are two in this case.

We can now compare the values of β and R found here to the values found in Refs. 4–6. Those references all use the values of β found in Ref. 4 by a moment balance equation. In the present notation this value is

$$\beta=\tfrac{1}{2}-\frac{\gamma r(1+r)}{2(1+\gamma r)}\simeq\tfrac{1}{2}(1-\gamma r) \tag{27}$$

[Ref. 4, Eq. (7); Ref. 5, Eq. (7)] to compare with (23) and (25). The formulas are quite different, even for small r. However, the value $\beta=\frac{2}{3}$ from (25) in the limit $r\rightarrow 0$ is in agreement with Refs. 1 and 7. The error in the derivation of (27) in Ref. 4 can be traced to the assumption that the strain in the film is determined just by the curvature and hence overlooks the discontinuity of m in the strain at the interface as in (14).

The value of t_s/R in Refs. 5 and 6 is different from (24) and is given by the following formula (m has been dropped compared to 1):

$$\frac{t_s}{R}=-\frac{6\gamma mr(1+r)}{1+7\gamma r+6\gamma r^2+3\gamma r^3+3\gamma^2r^2}$$
$$\simeq-6\gamma mr[1+(1-7\gamma)r] \tag{28}$$

[Ref. 5, Eq. (16); Ref. 6, Eq. (16a)]. The value in the limit $r=0$ is the same as (26), but the first-order correction in r is different. In the moment balance equation around the midlayer of the substrate for $r\simeq 0$ β drops out, and the limiting value of t_s/R is obtained directly without knowledge of β. Hence Refs. 5 and 6 find the correct limiting value in (28) with a wrong equation for β.

B. Strains due to misfit

At the interface, to first order in r,

$$\varepsilon_1^{fi}=m_f+\frac{\beta t_s}{R}=\frac{m}{1+\gamma r}+\alpha\beta\simeq m(1-5\gamma r), \tag{29}$$

$$\varepsilon_1^{si}=m_s+\frac{\beta t_s}{R}=-\frac{\gamma mr}{1+\gamma r}+\alpha\beta\simeq-5\gamma rm. \tag{30}$$

The ratio of the strains at the interface to first order in r is

$$\frac{\varepsilon_1^{fi}}{\varepsilon_1^{si}}=-\frac{1}{5\gamma r}. \tag{31}$$

From (29)–(31) it follows that when $r\rightarrow 0$, $R\rightarrow\infty$, and all the strain is in the film.

C. Stresses in the film

The general solution with finite r for the in-plane strain can be used to find the in-plane stress in the film, and hence gives a general solution for the case 1 problem, which seeks to relate stress and R. The solution can then be compared to previous work on case 1. Thus, from (6), (7), and (29),

$$\sigma_1^{fi}=\frac{\partial(E_{\rm total}/V)}{\partial\varepsilon_1^f}=Y_f'\varepsilon_1^{fi}=Y_f'\left(m_f+\frac{\beta t_s}{R}\right). \tag{32}$$

The relation (32) can be transformed using (23) and (24), which give

$$\frac{m_fR}{t_s}+\beta=-\frac{[1+3\gamma r^2+4\gamma r^3-\gamma^2r^2(4+3r+\gamma r^3)]}{6\gamma r(1+r)(1+\gamma r)},$$

and (32) takes the form

$$\sigma_1^{fi}=-\frac{Y_s't_s}{6rR}\frac{[1+3\gamma r^2+4\gamma r^3-\gamma^2r^2(4+3r+\gamma r^3)]}{(1+r)(1+\gamma r)}$$

$$\simeq-\frac{Y_s't_s}{6rR}[1-(1+\gamma)r]. \tag{33}$$

The form (33) can be compared with the results of Refs. 1, 2, and 7, which solve case 1 for the relation between σ_1^{fi} and R. Reference 1 finds, in the notation used here,

$$\sigma_1^{fi}=-\frac{Y_st_s}{6rR} \tag{34}$$

(Ref. 1), which may be called the Stoney formula for bending due to stress. The relation (34) is the limit of (33) with $r\to0$, but makes the error of using Y_s in place of Y_s'. Reference 7, which minimizes the total elastic energy to solve case 1, finds for r negligible the corrected Stoney formula

$$\sigma_1^{fi}=-\frac{Y_s't_s}{6rR} \tag{35}$$

(Ref. 7, Eq. 11), which replaces Y_s by Y_s'. Reference 2 does not correct the error in the elastic constant, but makes a correction for finite film thickness in the form

$$\sigma_1^{fi}=-\frac{Y_st_s}{6rR}\frac{1+4\gamma r+6\gamma r^2+4\gamma r^3+\gamma r^4}{1+r} \tag{36}$$

(Ref. 2, Eq. 33). The result (36) again gives the Ref. 1 result for $r\to0$, but gives corrections for finite r which are different from (33).

IV. APPLICATION TO A MEASURED EPITAXIAL BENDING

A recent experiment on an epitaxial system by Schell-Sorokin and Tromp[8] provides an opportunity to test the theory of epitaxial bending in the limit of small r. The bending of a Ge(001)-Si(001) film-substrate system in pseudomorphic epitaxy for up to seven monolayers (ML) of Ge was measured optically. The experiment measured the change in an angle θ between two laser beams reflected from the specimen at points a distance b apart as the Ge film was deposited. Equation (24) or (26) in the limit of small r can be applied. Thus, using (26),

$$\theta=\frac{b}{R}=-\frac{6\gamma mt_fb}{t_s^2}, \tag{37}$$

$$\frac{d\theta}{dt}=-\frac{6\gamma mb}{t_s^2}\frac{dt_f}{dt}, \tag{38}$$

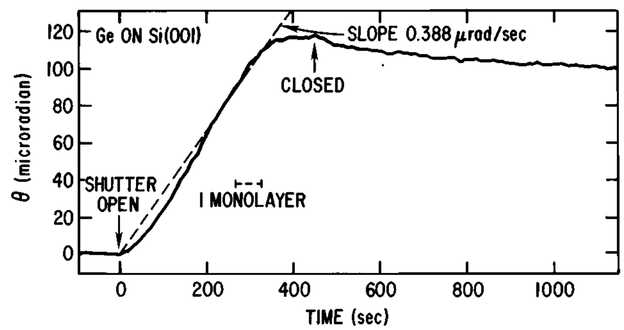

FIG. 5. Measured bending (Ref. 8) produced by steady deposit of Ge on a Si(001) crystal at 500 °C. The change in the angular separation of two laser beams reflected from the surface at points 0.84 Å apart is plotted in μrad as a function of deposition time in sec. The line with the theoretical slope 0.388 μrad/sec (dashed) is drawn through the origin of the deposition.

where t is time. We estimate $d\theta/dt$ using the following values of the parameters (b, m, t_s, and dt_f/dt are taken from Ref. 8):

$$b=0.84\ \ \text{cm},$$

$$\gamma=0.774\quad(Y_{\rm Ge}'=1.41\ \ \text{Mbar},\ \ Y_{\rm Si}'=1.82\ \ \text{Mbar}),$$

$$m=-0.043, \tag{39}$$

$$t_s=10^{-2}\ \ \text{cm},$$

$$\frac{dt_f}{dt}=\frac{1\ \ \text{ML}}{6.13\ \ \text{sec}}=\frac{1.414\ \ \text{Å}}{61.3\ \ \text{sec}}=0.023\times10^{-8}\ \ \text{cm/sec};$$

hence (38) gives

$$\frac{d\theta}{dt}=0.388\ \frac{\mu\text{rad}}{\text{sec}}. \tag{40}$$

In Fig. 5 the line with slope given by (40) is drawn on the experimental plot of $\theta(t)$. The line follows the measured curve, especially for the thicker films of up to 7 ML. A model that assumes bulk behavior of the film, as is done here, should be more accurate for the thicker films. Above 7 ML the pseudomorphic epitaxy breaks down.

The fit shown in Fig. 5 between measured bending and the bending predicted by elasticity theory has also been noted in Ref. 8. The stress measured by applying the corrected Stoney formula (35) to the measured curvature (800 dyn/cm ML) is compared to the stress required (845 dyn/cm ML) to strain a Ge(001) film by the misfit to Si(001) (−0.043) using the bulk elastic constants of Ge. This comparison is equivalent to deriving the epitaxial relation (26) by putting $\sigma_1^f=Y_f'm$ from (32) into (35). Then (26) can be applied as above to find $d\theta/dt$.

V. DISCUSSION AND CONCLUSIONS

The principal result of this energy-minimization analysis is the relation (24) [or (26) for small r] between the radius of curvature R and the misfit m in epitaxial bending, which is derived under the assumption of small misfit, and hence small strain, so that linear elasticity theory applies. The relation (24) for general r differs from previous work[4–6] because that work makes an error in the formula for β due to neglect of the discontinuity in strain at the interface. The relation in the limit of small r (the Stoney formula for bending due to epitaxy) is contained in Ref. 5 as corrected in Ref. 6, but is not clearly exhibited there because the form given for small r [their Eq. (17a)] omits the important elastic factor γ. The experiment in Ref. 8 provides verification of the relation for small r, including the factor γ, since the misfit is known independently from crystal structure measurements. Application of the Stoney formula for bending due to stress determines the stress in the film from the bending, but does not verify the relation unless an independent evaluation of the stress has been made.

The corrections for finite r are of practical importance in the calculation of the bending of a bimetallic strip, which is a problem equivalent to the calculation of bending by epitaxial misfit. Such strips are produced, for example, by electroplating and develop a misfit when changes in temperature act on the different coefficients of thermal expansion of the two metals. In these systems film and substrate are frequently comparable in thickness and the finite-r corrections are needed, as discussed in Ref. 2.

It is possible but difficult to produce epitaxial films with finite r if the mismatch is small, in which case the relation for curvature would require finite-r corrections. Such an experiment does not appear to have been done at this time. However, it is easy to produce epitaxial films with a substantial number of atomic layers, e.g., more than ten, whose bending in surely dominated by bulk elastic coefficients. The bulk relation (26) between mismatch and curvature would apply quantitatively and could be used with confidence to evaluate the product of the mismatch and the elastic constant of the film Y'_f from the measured curvature. The application to the seven-atomic-layer film in Sec. IV is probably at the lower limit of applicability of bulk elastic theory, since surface relaxation effects generally extend two layers deep.

The solution of the epitaxial bending problem (case 2) for finite r provides also a new solution for the old problem of bending due to stress in the film (case 1) when r is not small. The corrected Stoney formula for bending due to stress, where the correction is the replacement of Y_s by Y'_s, has been found in many papers (e.g., in Refs. 3, 7, 8, and 10). However, the corrections for finite r found here differ from those in previous work, e.g., compare (33) with (36).

The energy-minimization method used here not only leads easily to the curvature formula for finite r, but also permits immediate determination of the more stable state between the two solutions for the curvature at a given r and γ. The method is applied here to the simplest case of epitaxy [on cubic (001) surfaces], but the method is simple enough to be readily applicable to more general types of pseudomorphic epitaxy. Thus the method could be applied to epitaxial curvature by a film epitaxial on an arbitrary surface of an arbitrary crystal structure when the film grows with a surface mesh similar in shape to the substrate surface mesh. Among the complications in treating this more general epitaxy is the need to use the elastic constant matrix of that surface in that structure. The strains could first be calculated by the methods of Ref. 11, which finds the strains in epitaxial films in cases of general epitaxy when the substrate is so thick that it remains unstrained and flat. However, the methods must be generalized to consider strains in the finite-thickness flat substrate as well as in the film. Three components of out-of-plane strain will generally appear, including two shear strains. Then the strains due to anisotropic bending must be calculated with the elastic constants of that surface. In the linear approximation the bending strain can be superposed on the misfit strain for the flat substrate. The total energy with that superposed strain would then have to be minimized with respect to anisotropic R and β.

ACKNOWLEDGMENTS

The author thanks Erik Klokholm for bringing this problem to his attention and thanks him and A. J. Schell-Sorokin for discussions about it.

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