Geometrical theory of critical thickness and relaxation instrained-layer growth

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In the growth of pseudomorphic strained layers, the critical thickness is the thickness up to which relaxation does not occur and beyond which relaxation occurs by plastic deformation of the layer. Previous theories have concentrated on the strain energy and kinetics of dislocation formation. We present a purely geometrical argument which predicts critical thicknesses and also predicts how relaxation progresses with increasing thickness. We find that the critical thickness, in monolayers, is approximately the reciprocal of the strain. Some relaxation occurs abruptly at critical thickness, and further relaxation is hyperbolic with thickness. The model can also handle multilayer structures. If all the layers have the same sign of strain, the model predicts that relaxation will occur at the lowest interface. These results are found to be in good agreement with experimental observations of dislocations in epitaxial structures of InGaAs grown on GaAs.

I. INTRODUCTION

We propose a model of plastic relaxation of strained epitaxial layers and multilayer structures which is based entirely on geometrical considerations. The question of how thick such layers may be grown before plastic relaxation sets in, the critical thickness problem, has been studied for many years. The accepted models of Frank and van der Merwe,[1] Matthews and Blakeslee,[2] and People and Bean[3] are based on considerations of the strain energy of the layer, the strain energy of a dislocation, and the mechanisms whereby misfit dislocations can be generated. For an extensive review, see Ref. 4. These models consider the properties of a single dislocation; Willis, Jain and Bullough[5] develop the energy balance model by taking a periodic array of dislocations. All the models agree with experiment, to within a factor of about 2, and the key result of all the models is that the critical thickness is inversely proportional to the strain.

Much less attention has been paid to the relaxing layer above critical thickness. Thus it is not clear whether the strain will relax smoothly with increasing thickness or discontinuously at the critical thickness. Also, little attention has been paid to the prediction of relaxation in multilayer structures, although van der Merwe and Jesser[6] have considered superlattices (see also Ref. 4), and some work has been done on graded epilayers[7] and double heterostructures.[8] Successful prediction of relaxation in multilayers in agreement with experimental data[9] would provide an excellent test of critical thickness models.

Pseudomorphic strained layers, below critical thickness, are of increasing interest in the field of low-dimensional semiconductor structures, because of the possibility of electronic band structures with new properties leading to improved electronic devices. Typical examples are the growth of $In_xGa_{1-x}As$ on GaAs and Ge_xSi_{1-x} on Si; in both systems the lattice mismatch is about $0.07x$. On the other hand, single-layer and multilayer structures in which controlled plastic relaxation occurs are important for the engineering of relaxed buffer layers, where the object is to achieve a defect-free single-crystal surface with a different lattice constant from the substrate. This is necessary for the growth of GaAs on silicon substrates and for the growth of short-wavelength II-V or long-wavelength III-V laser structures on GaAs substrates.

In our model, strain energies and dislocation energies do not appear explicitly. Instead, a simple geometrical argument predicts critical thicknesses in reasonable agreement with previous models and also predicts the behavior of the relaxation above critical thickness, in good agreement with experiment, provided kinetic factors are not important. The success of the model shows that energy balance calculations are not sufficient and may not be necessary to predict critical thicknesses. We begin with an idealized version of the model, and then in Sec. III we consider the effect of various refinements, including the application of the model to multilayer structures. In Sec. IV we present some experimental results which support the predictions of the model.

II. THE IDEALIZED MODEL

We consider a perfect crystalline substrate, with a perfect epitaxial strained layer of thickness d, strain ε, and we allow misfit dislocations to form at the interface between the layer and the substrate. According to Saint-Venant's principle (see Timoshenko and Goodier)[10] and Appendix A), the strain field of a dislocation at a depth d must decay laterally within a distance of the order d. Consequently, a misfit dislocation can only relax the strain in the layer over a lateral distance md, where m is a small number, around 1 or 2, which we estimate in Appendix A. Outside this relaxed region, we approximate the relaxation to zero; within the relaxed region the relaxation averages b/md,

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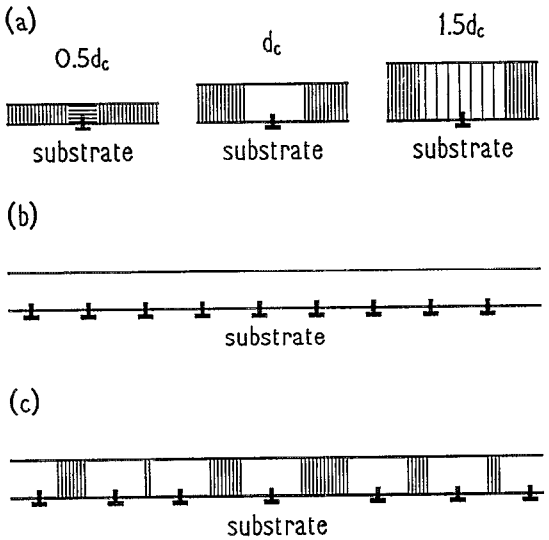

FIG. 1. In (a) the relaxed region around a misfit dislocation is shown for three layer thicknesses, in the idealized model of Sec. II. The strain is indicated by the hatching: Vertical hatching corresponds to strain in the grown-in direction, and horizontal hatching indicates strain of the opposite sign. The density of hatching is proportional to the strain. In the thinnest layer, drawn for half the critical thickness, relaxation induces an equal and opposite strain in the region around the dislocation. The next layer is at critical thickness, and the strain is fully relieved around the dislocation. In the thickest layer, the strain is only partially relieved. Full relaxation at critical thickness is shown in (b), by a periodic array of dislocations. A random distribution of dislocations at critical thickness is shown in (c); the gaps between the unstrained regions are all less than md wide.

where b is the Burgers vector of the dislocation. We approximate this to a uniform relaxation of $\Delta\varepsilon = b/md$ throughout the relaxed region [Fig. 1(a)].

The model is then based on the following key observations: (1) A dislocation will not form if the relaxation b/md exceeds the strain ε in the layer. (2) If a dislocation forms within a region of width md, translational symmetry demands that dislocations will form in every other available region of width md in the crystal.

The first observation is due to the fact that relaxation to a state of opposite strain should not occur. The condition can be weakened by allowing some opposite strain to be developed; we consider this point below (Sec. III C). It is still a geometrical constraint, for although we are aware that relaxation occurs in order to reduce the energy of the system, we are limiting the amount of relaxation simply by observing that large opposite strains are no improvement on the original large grown-in strain. The second observation expresses the fact that the model does not include any assumptions about mechanisms of dislocation generation, but does assume that a perfect crystal would have the same critical thickness as a real crystal. That is, although real crystals contain defects which act as dislocation sources and which break the translational symmetry, we assume that the value of the critical thickness is not affected, only the mechanism of relaxation. If this were not so, any theory of critical thickness should be dominated by details of substrate and epilayer defects.

Thus the layer is prevented from relaxing at small thicknesses simply because the relaxation $\Delta\varepsilon = b/md$ exceeds the strain ε; it may relax when $b/md = \varepsilon$, and if sufficient strain energy is available, the layer will relax when this condition is met. Rearranging, we obtain a prediction for the critical thickness of

$$d_c = b/m\varepsilon. \tag{1}$$

If we take a Burgers vector of one atomic separation and put $m \sim 1$, this becomes

$$d_c \sim 1/\varepsilon, \tag{2}$$

where d is in units of monolayers. This result is in fair agreement with other models and with experiment.

The relaxation induced by a periodic array of dislocations at the separation md_c is b/md_c; from Eq. (1) this is equal to ε. Consequently, the idealized model predicts that relaxation occurs discontinuously and completely at the critical thickness [Fig. 1(b)]. Discontinuous relaxation was also found by Frank and van der Merwe in the one-dimensional monolayer model.[1,4] Refinements to our model, however, reduce or eliminate the discontinuity, as we shall see in the next section.

III. REFINEMENTS TO THE MODEL

A. Random dislocation generation

We are considering here the relaxation of a perfect crystal, without localized dislocation sources. This means that dislocations may form anywhere, independently. It follows that the regions of width md_c containing a dislocation will not normally be contiguous: There will be gaps between them of unrelaxed material [Fig. 1(c)]. These gaps may be of any width up to md_c, but not larger because then another dislocation would form. The analysis of the statistical distribution of gap widths is given in Appendix B. It is approximately a triangular distribution, so that the average gap width is a third of md_c. This means that at the critical thickness only three-quarters of the initial strain is relieved.

There are two approaches to the subsequent relief of strain above critical thickness. We may take an interface containing misfit dislocations (a partially relaxed interface) to be no different from an unrelaxed interface. A layer in which three-quarters of the strain has been relieved is then equivalent to a layer with a uniform strain of $\varepsilon/4$, and Eq. (1) then predicts a new critical thickness four times as large. Relaxation then proceeds in a stepwise way, with the strain being reduced by a factor of 4 when the thickness is increased by the same factor (see Fig. 2). Alternatively, we may note that the strain after initial relaxation is not uniform since the gaps are distributed statistically. Larger gaps will tend to induce further relaxation before narrow gaps do. In particular, the larger gaps nearly md_c in width should relax at thicknesses not much greater than d_c. This effect is expected to smooth the steps after the initial relaxation at d_c (see Fig. 2); a full statistical analysis is, however, outside the scope of this paper. It may readily be seen, however, that if the steps are fully smoothed, the

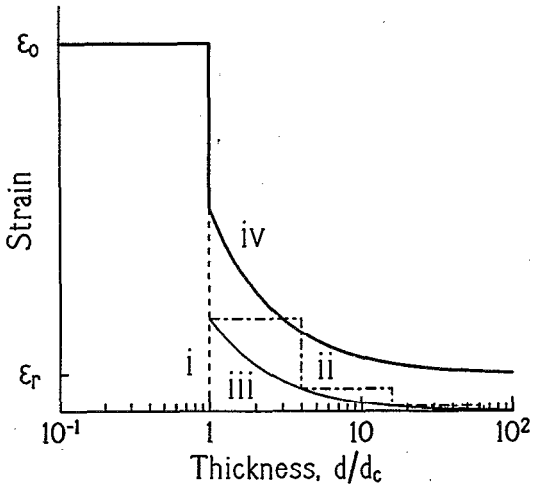

FIG. 2. Relaxation is shown as a function of layer thickness as described in the text. The dashed line (i) shows the discontinuous, complete relaxation predicted by the idealized model and shown in Fig. 1(b). Taking the random generation of dislocations into account, as in Fig. 1(c) the dot-dashed line (ii) shows the stepwise relaxation by factors of 4 if the layer is assumed to be homogeneous after each step. The dotted line (iii) shows schematically the smoothing effect of the layer inhomogeneity. Finally, the solid line (iv) shows in addition the effect of softening the edges of the relaxed regions around each dislocation, together with the effect of residual strain. Note that in all cases the critical thickness is the same.

state of strain of a layer above critical thickness will be independent of the original strain and will be given by the thickness alone:

$$\varepsilon(d)=\varepsilon_0, \quad d<d_c,$$
$$\varepsilon(d)=f\varepsilon_0 d_c/d, \quad d\geqslant d_c, \tag{3}$$

where ε_0 is the mismatch and $(1-f)$ is the fraction of the strain which is relieved abruptly at critical thickness.

B. Softening the edges of the relaxed regions

We may improve upon the approximation that the relaxed regions are entirely relaxed and that the relaxation then falls discontinuously to zero. Since the relaxation falls away exponentially (actually as ze^{-z}) with a characteristic length of approximately d outside the region of width md (see Appendix A), a dislocation will discourage the formation of other dislocations over a region of width say about $2md$ or more. This does not affect the estimate of critical thickness given by the idealized model, but it does reduce the initial density of dislocations by a corresponding factor of about 2 or more. Thus, instead of three-quarters complete relaxation at d_c, we expect relaxation only of a third or less of the initial strain (Fig. 2), followed by continuous or stepwise relaxation according to the arguments of Sec. III A.

C. Overrelaxation

All we have needed to know about the energies is that sufficient energy is available to induce relaxation at $d_c=b/m\varepsilon$. It is interesting to use the geometrical model to demonstrate the *insensitivity* of the critical thickness to the energy available. If in fact much more energy than necessary is available, it is possible that the layer will relax earlier, so that the regions around each dislocation will acquire strain of the opposite sign. This is not a violation of our premises, however, as we shall see that the geometrical constraint is still the most important determinant of the critical thickness and the subsequent plastic relaxation.

The strain energy before relaxation in the region of width md around a dislocation is proportional to the volume and to the square of the strain:

$$E\propto md^2\varepsilon^2. \tag{4}$$

If relaxation occurs at a thickness $d<d_c$, the resulting strain in the relaxed regions will be $\varepsilon-b/md$, and this implies a strain energy after relaxation of

$$E_1\propto md^2(\varepsilon-b/md)^2. \tag{5}$$

If only a fraction g of the strain energy at the critical thickness of Eq. (1) is required for plastic relaxation and relaxation therefore occurs at $d<d_c$, conservation of energy gives

$$gmd_c^2\varepsilon^2+E_1=md^2\varepsilon^2. \tag{6}$$

If we write x for d/d_c and recall that $d_c=b/m\varepsilon$, so that $b/md=\varepsilon/x$, then, substituting from Eqs. (4) and (5) into Eq. (6) we have

$$x=\tfrac{1}{2}(1+g). \tag{7}$$

For $g=1$, relaxation occurs at the critical thickness d_c as defined by Eq. (1), while at the other extreme of $g=0$, relaxation occurs at $d=d_c/2$. That is, even if dislocation creation required no energy whatsoever, the critical thickness would only be reduced by a factor of 2. In contrast, in the models in the literature, the critical thickness would be reduced to zero. This is a very important result, since generally there is enough energy available for relaxation at the critical thickness, and so it follows that the critical thickness is in fact determined by the geometrical constraints discussed here, with energy balance criteria providing only a minor correction.

D. Structure of a misfit dislocation

In layers of small strain and large critical thickness, our model is insensitive to the structure of the misfit dislocations. When the strain is large and the critical thickness is only a few monolayers, the structure of the misfit dislocation may be the dominant factor. This is seen most clearly with small soap bubbles, which have an interbubble potential very close to the Lennard–Jones interatomic potential[11] and therefore simulate metallic structures. Bragg and Nye created misfit dislocations in a bubble raft and showed that they extend over about ten bubbles.[12] For strains much over 0.05, therefore, there is no geometrical constraint and critical thicknesses may be as little as a monolayer, depending on energy considerations. For smaller strains, dislocations will not be created until they can relax material outside the ten bubbles width and our geometrical model applies.

E. Residual strain

Previous models predict that the critical thickness diverges to infinity as the grown-in strain tends to zero. This also implies that as the thickness of a relaxing layer is increased, the strain tends to zero. Experimentally, a residual strain of the order of 0.01%–0.1% is usually found, even in very thick layers. This is caused by the bulk elastic properties of the material of the layer. A solid material will support a finite tensile or compressive strain up to its elastic limit; only for strains above the elastic limit will plastic deformation occur. (Surface defects can of course induce cracking or brittle fracture in layers under tension below the elastic limit.) Consequently, plastic relaxation of a single strained layer will relieve elastic strain only to the elastic limit and not beyond. The critical thickness therefore diverges to infinity as the strain tends to the elastic limit or as the stress tends to the compressive strength of the material under growth conditions (Fig. 3). Multilayer structures are more complicated and can be designed to eliminate residual strain; this is discussed below.

It is difficult to predict the residual strain ε_r. Perfect single crystals are very weak at temperatures sufficient for dislocations to be mobile, and this is generally the case at growth temperature. However, at low growth temperatures, the strength will be greater. Also, if a layer has undergone much plastic deformation, there may be a significant amount of work hardening, and this will increase the residual strain. However, we are not aware of any detailed studies of the mechanical strength of semiconductors as a function of temperature and deformation during growth.

Taking all the factors into account that have been discussed in this section, our predictions for critical thickness and for relaxation above critical thickness may be approximated by the following expressions:

$$\begin{aligned} &\varepsilon(d)=\varepsilon_0, \quad d<1/(\varepsilon_0-\varepsilon_r), \\ &\varepsilon(d)=1/d+\varepsilon_r, \quad d\geqslant 1/(\varepsilon_0-\varepsilon_r). \end{aligned} \tag{8}$$

F. Multilayer structures

Many epitaxial structures require a change of lattice constant from the substrate to the epilayer of interest, and so relaxed buffer layers are required. The control of dislocations usually requires that the relaxed buffers have several layers of different compositions; sometimes superlattices are used. It is then important to know not only how a single homogeneous layer will relax during its own growth, but also whether subsequent layers grown on top will induce or prevent further relaxation.

Analysis of multilayer structures begins with the observation that any combination of layers will relax in the same way as a single layer of the same total thickness and with a strain equal to the average strain of the multilayer structure. This is because the stress-strain relationships of the usual crystals are approximately linear, so that strain fields may be superposed. Internal strains within a structure consequently do not affect the elastic properties of the structure. Thus, during growth of a structure with n layers, one may consider separately the top layer and the top i layers ($i = 1$–n) at any stage of growth. If any one of these combinations is beyond the critical thickness of the equivalent single layer, relaxation will occur at the bottom interface of that combination. (Exceptions to this statement will occur if the internal structure of a multilayer combination can obstruct dislocation creation or movement; this is a kinetic problem and so outside the scope of this paper.)

It is interesting to note that if the strains are all of the same signs, relaxation will always start at the deepest interface. This may be seen by considering a structure of two layers. We ignore residual strain, for simplicity, and use Eq. (4) to obtain critical thicknesses and relaxation. A subcritical layer with a mismatch of ε_1 to the substrate is grown first, to a thickness d_1. A layer of mismatch $\varepsilon_2 > \varepsilon_1$ is then grown on top, to a thickness d_2. The top layer has a critical thickness of $1/\varepsilon_2$ with respect to the interface between the two layers, so that the relaxation will occur at this interface at the total growth thickness

$$d_{c2}=d_1+1/\varepsilon_2.$$

However, the structure has an average strain given by

$$\varepsilon_{\rm av}=(d_1\varepsilon_1+d_2\varepsilon_2)/(d_1+d_2),$$

and a critical thickness with respect to the lower interface of $d_{c1} = 1/\varepsilon_{\rm av}$. Since $d_{c1} = d_1 + d_2$ at relaxation, by rearrangement we obtain

$$d_{c1}=d_1+1/\varepsilon_2-d_1\varepsilon_1/\varepsilon_2,$$

which is always less than d_{c2} when the two strains have the same sign.

Once relaxation has occurred at an interface, it may be taken to continue smoothly or to go stepwise (Fig. 3). In either case, if critical thickness criteria still apply to the other interfaces in the structure, relaxation will not occur elsewhere until the layer above the relaxing interface has been driven to the opposite sign of strain. However, it is not clear to what extent random strain fields in the vicinity of misfit dislocations in an interface may reduce critical thicknesses in other nearby interfaces. Further experimental work is required in this area.

IV. DISCUSSION AND EXPERIMENTAL RESULTS

A. Geometrical models

The model presented here shows that Saint-Venant's principle is sufficient to account quantitatively for critical thicknesses in strained-layer growth. It predicts the critical thickness itself, the extent of relaxation at critical thickness, and the way in which relaxation proceeds as the layer thickness increases further. It shows that the geometry of the problem is at least as important as the strain energies of the layer and of dislocations.

Obviously, a complete calculation of energy balance for random and ordered arrays of misfit dislocations will also give a correct prediction—and, indeed, would be equivalent to a fully refined version of the present model. However, the models in the literature include geometrical factors only in the calculation of the energy of a dislocation

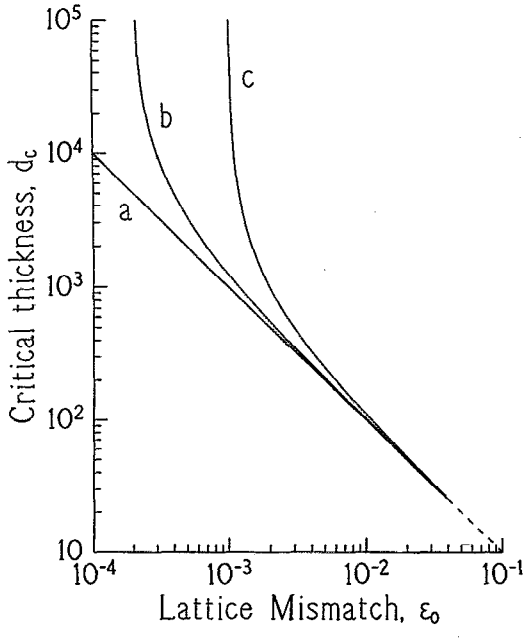

FIG. 3. The critical thickness predicted by the geometric model is shown as a function of the lattice mismatch (a) neglecting residual strain and for residual strain due to the elastic strength of the layer with values of (b) $\varepsilon_r = 2.10^{-4}$ and (c) $\varepsilon_r = 10^{-3}$. At high values of mismatch, the structure of the misfit dislocation may need to be considered, and in this region the predictions are shown by dashed lines.

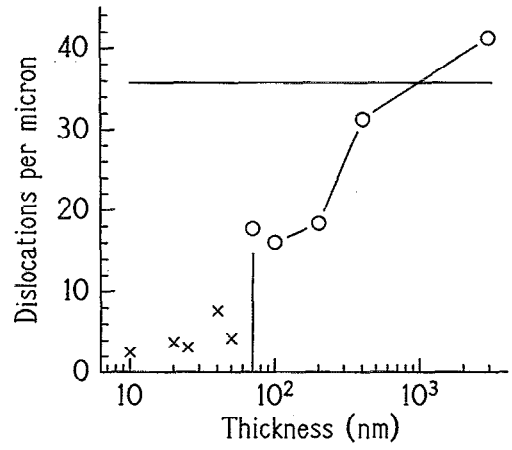

FIG. 4. Dislocation densities measured by plan-view TEM are shown for $In_{0.2}Ga_{0.8}As$ layers of various thicknesses grown on GaAs. These values are averages of the densities in the (110) and (1$\bar{1}$0) directions. Most of the dislocations in thin unrelaxed layers below critical thickness are found to be 60° partials and are ineffective in relieving strain; these data points are marked by crosses. The majority of dislocations in relaxing layers are effective in relieving strain, and their densities are marked by circles. The horizontal straight line indicates the density of pure edge dislocations required to relieve the strain completely; the other lines are a guide to the eye.

at a distance d from the free surface; once this energy is obtained, the geometrical information is discarded.

The value of a geometrical model was summarized by Jesser and van der Merwe as being simple and useful.[4] If the model gives critical thicknesses and relaxation in as good agreement with experiment as more sophisticated models, that is already a sufficient justification. In addition, the geometrical model, we believe, indicates that attention should be concentrated on the important contribution to the energy, the long-range strain fields of individual dislocations and their interaction. Clearly, this implies that the approximations of a single dislocation or of a periodic array of dislocations are unlikely to be adequate.

B. Comparison with experiment

A considerable amount of data in the literature supports the conclusion that the critical thickness is close to inversely proportional to the strain. For example, Cibert *et al.*[13] give data for CdTe on (001) CdZnTe, grown with lattice mismatches from 0.15% up to 6%. Over this range, the critical thickness varies from 1000 monolayers to 5 monolayers, deviating by at most a factor of 2 from

$$d_c = 1/\varepsilon,$$

except at the highest strains.

There are also data to support the hyperbolic relaxation we predict above critical thickness. In Fig. 4 we show experimental data on the dislocation density observed by plan-view transmission electron microscopy (TEM) of $In_{0.2}Ga_{0.8}As$ layers grown on GaAs to various thicknesses. Misfit dislocations are observed at the InGaAs/GaAs interface. At small thicknesses, a low density of 60° dislocations is observed, which varies randomly from sample to sample, but shows no significant correlation with sample thickness. These, we believe, are due to the turning over of threading screw dislocations from the substrate and are not treated by the present model. The onset of significant relaxation and the critical thickness treated here are marked by the generation of high densities of new misfit dislocations. These, from the figure, follow approximately the behavior required by the model: a jump to about half the density required for full relaxation, followed by a smooth increase to full relaxation at many times the critical thickness. Similar behavior has been observed by Moore *et al.*,[14] who measured the strain in layers of $In_{0.05}Ga_{0.95}As$ grown on GaAs to thicknesses up to 6 μm. Other authors, however, report kinetically controlled relaxation (e.g., Whaley and Cohen;[15]); in this case the present model is not applicable (except for putting a lower limit on critical thicknesses and an upper limit on the extent of relaxation at any given thickness). The kinetics of relaxation have been discussed by Dodson and Tsao.[16]

The prediction that relaxation will always occur first at the lowest interface of a structure in which strains are all of the same sign is illustrated by the micrographs shown in Figs. 5 and 6. A stack of multiple quantum wells of $In_{0.2}Ga_{0.8}As$ in GaAs barriers on GaAs was grown, with the thinnest well at the bottom. The strain for this system is compressive, with a mismatch of about 1.4%. A detailed TEM study of this sample has been reported elsewhere.[17] Figure 5(a) shows a cross-sectional TEM picture of the stack, tilted so that the misfit dislocations are seen in projection (the short black lines). Only the top three wells are above critical thickness for this material combination, and

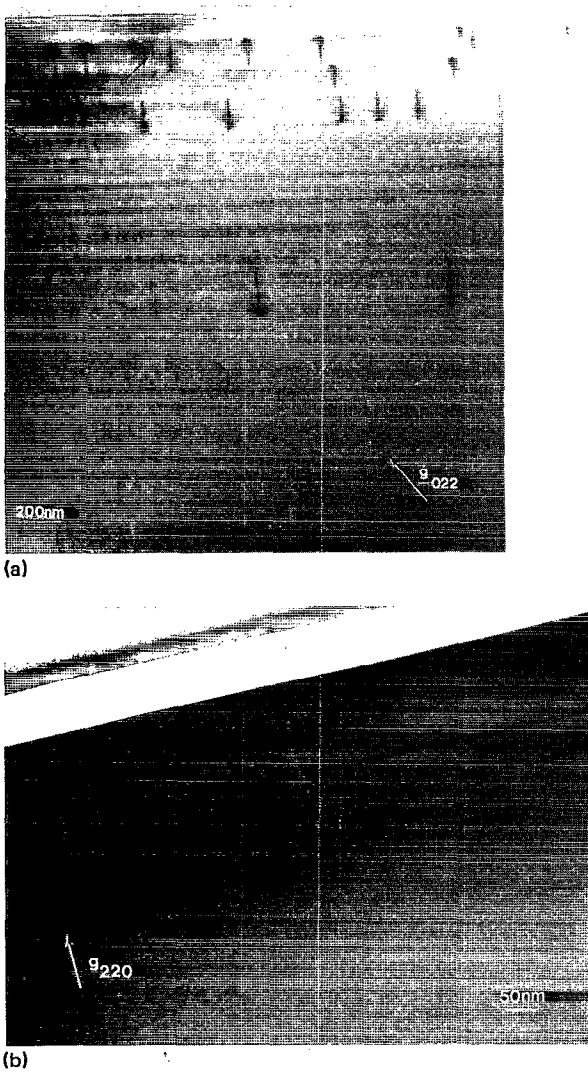

FIG. 5. (a) A cross-sectional TEM micrograph of a multiple-quantum-well (MQW) sample of $In_{0.2}Ga_{0.8}As/GaAs$. There are ten wells, with the thinnest at the bottom of the stack, of thicknesses 40, 60, 80, 100, 120, 140, 160, 180, 200, and 220 Å, with barriers of 1000 Å of GaAs between them. The sample was tilted so that the misfit dislocations are seen in projection, as the black lines seen in the top three wells and in the bottom well; two other dislocations are indicated by the arrows. The wells are spread out by the projection. (b) A micrograph of a similar $In_{0.2}Ga_{0.8}As/GaAs$ MQW sample, containing only four wells of thicknesses 30, 40, 60, and 120 Å. Note the complete absence of any misfit dislocations.

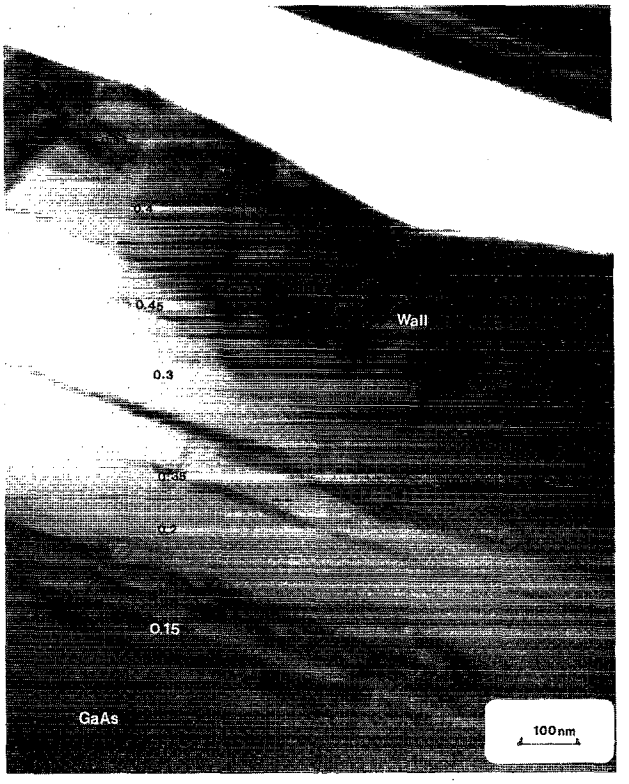

FIG. 6. The multilayer structure described in the text is shown in cross-sectional TEM. The 2000 Å layers of $In_xGa_{1-x}As$ (values of x marked) each contain a 70-Å quantum well with an indium content of $x + 0.15$ (marked), 500 Å below the top of the layer. The lowest quantum well is 70 Å of $In_{0.15}Ga_{0.85}As$ in GaAs, 500 Å below the $In_{0.2}Ga_{0.8}As/GaAs$ interface. Although this quantum well is well below critical thickness, dislocations can be seen in it. A dislocation wall (marked) is seen in the $In_{0.4}Ga_{0.6}As$ layer.

a large density of misfit dislocations is seen in them. Dislocations are also seen in the lowest well, indicating that during growth of the top wells the entire stack went supercritical with respect to relaxation at the bottom interface. Clearly, only a little relaxation would be required to change the average strain of the stack of wells and barriers into tension, after which further relaxation occurs at the interfaces of the top wells only. To confirm that the dislocations under the bottom well are due to the growth of the last few wells, we show for comparison in Fig. 5(b) a sample grown under the same conditions, but with only four quantum wells. No dislocations are found. Zou *et al.*[9] have reported similar behavior in multilayer stacks.

In Fig. 6 we show a cross-sectional TEM picture of a more complicated structure, in which successive 2000-Å layers of, respectively, $In_{0.2}Ga_{0.8}As$, $In_{0.3}Ga_{0.7}As$, and $In_{0.4}Ga_{0.6}As$ were grown on a GaAs substrate. These thicknesses are well above critical, so that these layers are partially relaxed. Each layer contains a 70-Å quantum well as a probe for optical quality. In addition, a 70-Å quantum well was grown in the underlying GaAs. Each well had an indium content 0.15 higher than its barriers. Normally, a 70-Å well of $In_{0.15}Ga_{0.85}As$ in GaAs shows no evidence of relaxation at all, whether by TEM or from its optical properties; for example, low-temperature photoluminescence linewidths of 1–2 meV are typical. However, this well, beneath the relaxed material, shows evidence of damage: The TEM micrograph (Fig. 6) shows several dislocations in it, and the photoluminescence (PL) linewidth was broadened to about 20 meV. Thus the unstrained GaAs above it has not protected the well from relaxation in higher layers, consistent with the theory put forward here.

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here were obtained. This work was funded by the Science and Engineering Research Council.

APPENDIX A: SAINT-VENANT'S PRINCIPLE AND THE EXPONENTIAL DECAY OF A STRAIN FIELD

Consider a system of forces statically equivalent to a zero force and zero couple, applied to a small part of the surface of a body. Saint-Venant's principle states that such a system gives rise to local stress and strain only.

The stress and strain due to localized loading on an extended body diminishes with distance on account of geometrical divergence (in simple cases, by the inverse square law) whether or not the resultants are zero. The localization required by Saint-Venant's principle is stronger than this, and we show here that it is essentially exponential. Any continuous stress or strain field may be decomposed into Fourier components. Accordingly, we consider a stress imposed on the surface of a semi-infinite solid, given by

$$\sigma(x)=\sin \alpha x$$

which has zero resultant, and we consider how the stress decays into the solid, in the negative z direction. The general equation for the stress function, in two dimensions, is

$$\frac{\partial^4\phi}{\partial x^4}+\frac{\partial^4\phi}{\partial x^2\partial y^2}+\frac{\partial^4\phi}{\partial y^4}=0,$$

for which the solutions are

$$\phi(x,z)=\sin \alpha x(A\cosh \alpha z+B\sinh \alpha z + Cz\cosh \alpha z+Dz\sinh \alpha z),$$

giving[10]

$$\sigma_x(x,z)=\sin \alpha x(A\alpha^2\cosh \alpha z+B\alpha^2\sinh \alpha z + C\alpha(2\sinh \alpha z+\alpha z\cosh \alpha z) + D\alpha(2\cosh \alpha z+\alpha z\sinh \alpha z),$$

$$\sigma_z(x,z)=-\alpha^2\sin \alpha x(A\cosh \alpha z+B\sinh \alpha z + Cz\cosh \alpha z+Dz\sinh \alpha z),$$

$$\tau_{xz}(x,z)=-\cos \alpha x(A\alpha\sinh \alpha z+B\alpha\cosh \alpha z + C\alpha(\cosh \alpha z+\alpha z\sinh \alpha z) + D(\sinh \alpha z+\alpha z\cosh \alpha z),$$

in the usual notation. The boundary conditions are the applied sinusoidal stress at $z=0$, vanishing stress at $z=-\infty$, and of course $\tau_{xz}(x,0)=0$; applying these conditions, we obtain

$$A=B=-1/\alpha^2,$$

$$C=D=1/\alpha,$$

so that

$$\sigma_x(x,z)=e^z\sin \alpha x,$$

$$\sigma_z(x,z)=(1-\alpha z)e^z\sin \alpha x,$$

$$\tau_{xz}(x,z)=\alpha z e^z\cos \alpha x,$$

giving the decay of all stress components away from the surface as approximately exponential.

This result may be applied to the misfit dislocation as follows. We consider now an infinite solid and insert an extra plane of atoms in the x-y plane at $z=0$, between $x=-d$ and $x=d$, and from $y=-\infty$ to $y=\infty$. The stress pattern set up will consist of a long-range resultant which will decay geometrically $(1/r)$ with cylindrical symmetry about the y axis, together with a local field which has Fourier components with wavelengths shorter than and of the order of d. This local field will decay rapidly with radius. The slowest decaying components of the local field are those of longest wavelength, decaying as $r\exp(-r/\lambda d)$, where λ is of the order of unity. The local field is, however, similar to those components of the strain field of a misfit dislocation which are effective in relieving misfit strain, as may be seen by cutting the infinite solid in half to make the y-z plane the free surface and letting the region $-d<x\leqslant 0$ constitute a pseudomorphic layer under biaxial stress. The misfit dislocation at $z=0$, $x=-d$ therefore relieves strain in the strained layer only between $z\sim\pm d$.

APPENDIX B: DISTRIBUTION OF RANDOMLY PLACED NONOVERLAPPING LINE SEGMENTS

If a density ρ of points are placed at random on a line, it is well known that the distribution of intervals between them is exponential, so that the probability that an interval is of width w is given by the probability density function

$$P(w)=\rho e^{-\rho w}.$$

A dislocation in our model, however, prevents another dislocation forming within a certain width around it. This is equivalent to placing nonoverlapping line segments at random on a line. If the segments are of length unity, then for densities much less than unity the requirement that the segments do not overlap will scarcely change the distribution of intervals between them. However, as further segments are added, a higher proportion of the line becomes unavailable, and there is a limiting density when all the intervals are of width less than unity, and no further segments may be placed on the line.

We have performed Monte Carlo calculations in which random numbers between 0 and L are generated, and points are discarded if they are within unity of a previously accepted point. In several runs, with values of L up to 1000, the limiting density was found to average 0.75. A histogram of the resulting intervals showed a triangular distribution. These results are consistent with a distribution given by

$$P(w)=2(1-w),\quad w\leqslant 1,$$

$$P(w)=0,\quad w\geqslant 1.$$

An analytic solution for the average crack spacing in reinforced brittle matrix composite materials (which is mathematically the same problem) has been given by Kimber and Keer.[18] They obtain a limiting density of 0.748, to

which our Monte Carlo result approximates closely. Kimber has also obtained an analytic solution for $P(w)$, to which our Monte Carlo triangular distribution is a rather poor approximation.[19]

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