# Structural perfection in poorly lattice matched heterostructures

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Continuum elastic theory is applied to the formation of misfit dislocations and point defects in strained layer structures. Explicit calculations of the energies of misfit dislocations in the double- and single-kink geometries yield line tensions below which strained films are stable with respect to defect formation. Our results yield a mismatch-dependent stability limit which, in the double kink case, differs from the Matthews–Blakeslee model by a geometrical factor and by the addition of a stress term associated with climb of the misfit dislocation. While our calculations yield equilibrium stability limits which may not correspond to observed critical thicknesses, the calculated stresses may be applied to descriptions of the kinetics of strain relief in films grown beyond these limits. Last, calculations of strain-related contributions to the free energy of formation of point defects suggest a contribution $|\Delta G_{\text{strain}}| \simeq 0.25$ eV for a 5% lattice mismatch. This suggests a means of suppressing or enhancing the formation of vacancies or interstitials in semiconductors favoring these defects.

## I. INTRODUCTION

The successful fabrication of devices reliant on strained-layer epitaxy[1–5] has heightened interest in the role of lattice mismatch in driving defect formation. Dislocations and point defects have been shown to have an adverse effect on the electrical and optical properties of devices.[6] In addition, many lattice-mismatched devices rely on coherent strain as a mechanism for tailoring intrinsic properties of the structure. This has fueled recent efforts to produce quantitative predictive models describing the stability limits of strained layers and the kinetics of strain relief in structures grown beyond these limits.[7,8] Most of these models have been based on continuum elastic theory, which provides a useful description of structural defects for small stress fields varying little on the scale of atomic dimensions (e.g., for regions beyond several lattice spacings of the core of a dislocation).

In this paper we present applications of continuum elastic theory to the calculation of misfit dislocation and point defect densities in the presence of a uniform elastic strain. In Sec. II we describe calculations pertaining to the stability of strained multilayer structures. In particular, we examine the dislocation line tension in the single- and double-kink geometries identified by Matthews and Blakeslee.[9] By calculating dislocation self-energies and interaction energies explicitly, we derive line tensions as a function of dislocation line orientations and layer thicknesses while avoiding the approximation of infinitely long dislocation lines. In the limit of long dislocations, our results differ from those of the Matthews–Blakeslee model by a geometrical factor and a surface traction term. Our results suggest that films are stable with respect to dislocation formation at thicknesses greater than predicted by the previous model. In addition, these results are applicable to recent quantitative descriptions of relaxation in metastable films, as increasing the stability limit can be expected to lessen the excess stress driving relaxation in a glide-limited regime. In Sec. III we estimate the contribution of the hydrostatic component of strain to the free energy of formation of vacancies and interstitials. While quantitative estimates are subject to uncertainties associated with the volumetric relaxation resulting from a point defect and with the application of linear elastic theory in regions of great stress, the results are expected to be qualitatively correct, and suggest a means of suppressing or enhancing the formation of vacancies or interstitials in semiconductors favoring these defects.

## II. DISLOCATIONS

It has been recognized for some time that overlayers break away from a substrate to which they are poorly lattice matched, at a thicknesses dependent on the differences in lattice parameters of the two materials, $f = (a_0^A - a_0^B)/a_0^B$.[10] Several theories have been proposed to describe the equilibrium limits to strained growth.[9,10] Despite the demonstration[11,12] that low-temperature epitaxial growth techniques yield films which rarely relax to equilibrium states, past equilibrium theories continue to attract attention as guides to the stability of strained films (e.g., during high-temperature processing or prolonged device operation) and to the rate of relaxation of metastable films.

In principle, stability of a multilayer structure during growth requires that each part of the structure be stable with respect to defect formation (i.e., for a film of thickness $h$, the areal strain energy density between any two film depths must lie below that required for formation of a single misfit dislocation, $\int_{z_1}^{z_2} dE_s < E_d$ for $0 \leqslant (z_1, z_2) \leqslant h$). For periodic $ABAB\cdots$-type multilayer structures, this reduces to the constraint that each individual layer $A$ and $B$ be stable with respect to misfit defect formation and that the structure viewed as a whole be stable. In practice, however, stability of the film during growth has not proven to be as great a concern as subsequent stability of the structure, as it has been possible to inhibit dislocation formation during the relative-

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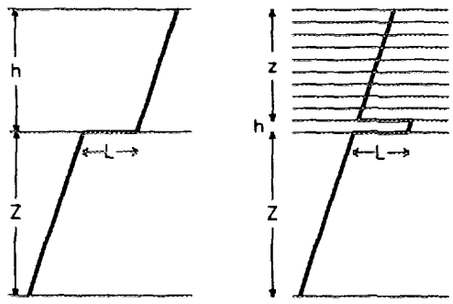


FIG. 1. Threading dislocations in the (a) single- and (b) double-kink geometries.

ly short duration of film growth. Slow relaxation during growth can be attributed variously to a paucity of dislocation sources, the magnitude of barriers against spontaneous loop formation, and the slow rate of glide at low growth temperatures.

Conditions for relaxation of a multilayer structure subsequent to growth differ from those applied during growth. While the condition that the overall film be stable with respect to formation of an isolated misfit dislocation remains the same, individual layers must now relax by formation of a "double-kink" or "hairpin" dislocation, rather than a single dislocation line. These relaxation mechanisms are illustrated in Figs. 1(a) and 1(b), which depict single- and double-misfit dislocation kinks in a dislocation threading through the film. Although the dislocation threading through the substrate is not a requisite for relaxation of the film, the appearance of misfit dislocations in the geometries depicted is a general result. [A misfit dislocation is an interfacial dislocation which relieves lattice mismatch by virtue of a Burger's vector having an edge component inclined with respect to the interface normal; $\mathbf{b}_{edge} \times \mathbf{n} \neq 0$, where $\mathbf{b}_{edge} = (\xi \times \mathbf{b}) \times \xi$, for Burger's vector $\mathbf{b}$, unit vector $\xi$ in the direction of the misfit dislocation line, and interface normal $\mathbf{n}$.]

Relaxation of a film in the geometries depicted requires both that dislocation sources be present and that conditions for glide and/or climb be favorable (i.e., nonzero glide velocities and a lowering of the energy of the system upon appearance of misfit dislocations.) There is increasing evidence of a wealth of complex nucleation and multiplication mechanisms dependent on specifics of the materials system involved and the conditions of film growth.[14,15] In this paper, we turn our attention exclusively to the stability of films with respect to the elongation of misfit dislocation lines originating from preexisting sources.

We have derived conditions under which misfit dislocation elongation is favorable by balancing a dislocation line tension resisting elongation against a force due to lattice mismatch. Although our treatment of this balance is conceptually identical to that developed by Matthews and Blakeslee,[9] our derivation of line tension is different and yields a somewhat different result. By considerating the energetics of specific dislocation geometries we examine the approximation of infinitely long dislocations inherent in the previous calculations. In addition, we incorporate a geometrical factor and a term specific to dislocation climb which was neglected in the previous treatment.[9]

The calculations briefly summarized here are presented elsewhere in greater detail.[16] The energy of a set of piecewise straight dislocation lines $C_i$ may be described as a sum of self- and interaction energies[17]

$$W = \sum_i W_i + \sum_{i<j} W_{ij}.$$

A line tension may then be derived by considering the change in configurational energy of the system under elongation of the misfit dislocation lines(s)[17]

$$S = \delta W / \delta L.$$

As in the Matthews–Blakeslee model, by equating this line tension with a force deriving from the resolved shear stress associated with lattic mismatch, $F = hb\sigma$, we derive a mismatch-dependent stability limit to the film thickness $h$. (We avoid the term critical thickness since, as noted by Tsao *et al.*,[18] the term has been used variously to describe the film thickness at which lattice relaxation becomes measurable by a given technique, that at which the first misfit dislocation appears on a wafer, and the thickness at which a film is no longer stable with respect to the elongation of misfit dislocation lines.)

Line tensions for the double- and single-kink geometries of Fig. 1 are presented in Fig. 2 as a function of misfit dislocation line length. A film thickness of 100 $a_0$ was assumed for the case shown. The results are appropriate to the commonly observed 60° dislocations on (100) zinc blende semiconductors. As shown by Matthews and Blakeslee,[9] these 60° dislocations are characterized by Burger's vectors of $\frac{1}{2}[011]$, interfacial [110]-oriented dislocation lines, and $(1\bar{1}1)$ glide planes. We have assumed that threading components of the dislocations lie along the $[\bar{1}12]$ direction. Although the exact orientation of the threading component is only approximated by this assumption, the qualitative results we derive are independent of this assumption, and the limiting line tension for long misfit dislocation lines is independent of the

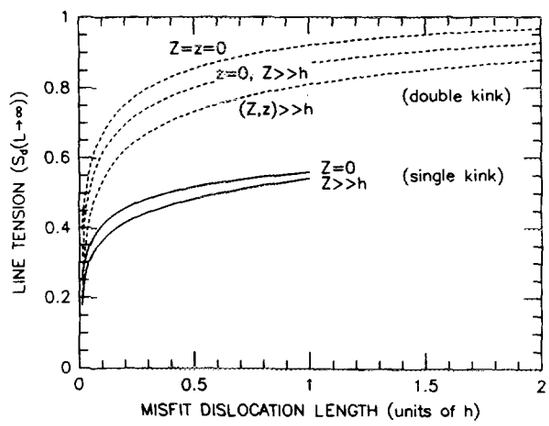


FIG. 2. Dislocation line tension in the double-kink (dashed lines) and single-kink (solid lines) geometries. Calculations pertain to 60° dislocations lying in (100) interfaces in elastically isotropic materials. Film thickness $h$ was chosen to be 100 $a_0$. Tension $S$ is plotted as a function of kink length $L$. Tension is scaled to the double-kink asymptotic limit for $L \to \infty$.

geometry of the threading component. The results of Fig. 2 are calculated on the assumption of elastic isotropy, which is a reasonable approximation for covalently bonded semiconductors such as Si and Ge, but worsens substantially from the group III–V's to the II–VI's. The model of Matthews and Blakeslee has been extended by Hirth for anisotropic elastic constants for one particular geometry.[19] For the III–V case of GaAs on GaP, Hirth derives a 27% increase in the stability limit when elastic anisotropy is included, comparable in magnitude to the correction described here for elongation in the glide plane. While the anisotropic case clearly represents a substantial increase over the isotropic case in the example considered by Hirth, it is difficult to generalize this result as the magnitude of the increase depends greatly on the particular materials system and geometry under consideration. A more complete treatment of anisotropy is beyond the scope of the present paper but will be presented elsewhere.

Our results can be summarized as follows. For both the single- and double-kink cases, the line tension rises monotonically to an asymptotic limit. For the double-kink case, the asymptotic limit is given by the Matthews–Blakeslee model, with the exceptions that the film thickness is replaced by the spacing between dislocations and that an additional line tension term is inserted[17] when elongation of the dislocation occurs out of the glide plane. Hirth has previously noted the geometrical correction to the film thickness.[19] We derive the limit

$$S_{L\to\infty}(h) = 2\left[S_{M-B}\left(\frac{h}{\xi\cdot\mathbf{n}}\right) + \frac{\mu b^2 \sin^2\theta}{4\pi(1-\nu)}\right],$$

where $\theta$ is the angle between the glide plane of the misfit dislocation and the plane containing the misfit and threading dislocations [$\sin\theta = |(\xi\times\xi_t)\times(\mathbf{b}\times\xi)|/|\xi\times\xi_t|$, for misfit line $\xi$ and threading dislocation line $\xi_t$], $\mu$ is the bulk shear modulus, and $\nu$ is Poisson's ratio. The line tension of Matthews and Blakeslee, $S_{M-B}(h)$, is given in this case by

$$S_{M-B}\left(\frac{h}{\xi\cdot\mathbf{n}}\right) = \frac{\mu}{4\pi}\left[(\mathbf{b}\cdot\xi)^2 + \frac{|\mathbf{b}\times\xi|^2}{1-\nu}\right]\ln\left[\frac{\alpha h}{b(\xi\cdot\mathbf{n})}\right],$$

where $b/\alpha$ is the core radius at which the energy integrals start. The calculations of Matthews and Blakeslee assumed $\alpha = e$; we assume $\alpha = 3$, which is typical of dislocations in materials having primarily covalent bonding.[19] For the single kink case, image forces not treated in our model can be expected to substantially affect the line tension for $L > h$. The appropriate limit in this case, with image forces approximated by terminating the energies at the free surface, is

$$S_{L\to\infty}(h) = S_{M-B}(h) + \frac{\mu b^2 \sin\theta}{4\pi(1-\nu)}.$$

As there are no local maxima in the dislocation line tensions, these asymptotes provide tensions beyond which it is energetically favorable for dislocation lines to elongate.

It is important to note that the double-kink line tension is always greater than the single-tension $S_d(h) > S_s(h)$. Consequently, individual strained layers grown dislocation-free beyond the single-kink stability limit but below that of the double kink may be stabilized by growth of an overlayer of opposite or lesser strain. As a result of this, low-temperature growth techniques may be applied to grow structures which, although metastable during growth, are ultimately stable with respect to dislocation formation.

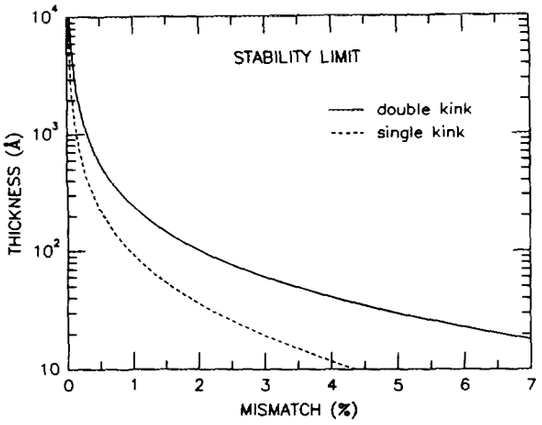


FIG. 3. Stability limits in the double- and single-kink geometries, based on the single-kink model of Matthews and Blakeslee (Ref. 9) (dashed line) and on the limiting line tension derived in the present work (solid line).

Stability limits for films in the double- and single-kink geometries are plotted in Fig. 3. The results assume misfit dislocations of the 60°-type in an elastically isotropic material, with the lattice constant of Si chosen as a length scale. The single-kink result is that due to Matthews and Blakeslee, whereas the double-kink limit is determined by the limiting line tension with the geometrical factor included. As can be seen from the figure, the double-kink limit substantially exceeds that of the single kink, yielding a window in which films metastable during growth may subsequently be stabilized.

## III. POINT DEFECTS

While much effort has been devoted to structural studies of strained layers, to date this work has focused on characterization of the extended dislocations which result when a strained film is grown beyond a critical thickness. However, substantial changes in the equilibrium densities of point defects can be expected in layers strained to the levels presently attainable. These defects could be expected to alter characteristics of strained devices, directly though the introduction of deep levels, and indirectly through enhanced or reduced diffusion rates and dopant incorporation.

As the introduction of vacancies or interstitials strains a crystal, hydrostatic stresses act as driving forces to the creation of these defects. The contribution of hydrostatic pressure $p = 1/3\ \mathrm{Tr}\{\sigma\}$ ($\sigma$ is the stress tenor) to the Gibbs free energy of formation of a vacancy or interstitial can be modeled[17] to first order as a $pdV$-type term:

$$G = G_i + p\Delta V,$$

for a change in crystal volume $\Delta V$ in response to removing or adding an atom. This has the effect of changing $C^0_{I,V}$, the unstrained equilibrium concentration of defects, according to a Boltzmann factor:

$$C_{I,V} = C^0_{I,V} \exp\left(\frac{-\sum_i \sigma_{ii}\Delta V_{I,V}}{3k_B T}\right).$$

Many of the strained structures examined to date display stresses with a substantial hydrostatic component. Cases of particular interest are those in which a semiconductor with cubic symmetry (prior to the application of strain) is grown upon a (100)- or (111)-oriented cubic substrate. For growth of a (100) thin film on a similarly oriented substrate, the hydrostatic stress is given by

$$\sigma_H = \frac{2}{3}(C_{11} + 2C_{12})\left(\frac{C_{11} - C_{12}}{C_{11}}\right)\epsilon$$

for elastic constants $C$ and in-plane strain $\epsilon$ (where $\epsilon = f$, the lattice mismatch, for coherently strained growth). Similarly, for (111)-oriented growth on a (111) substrate this stress is

$$\sigma_H = \frac{4C_{44}(C_{11} + 2C_{12})}{C_{11} + 2C_{12} + 4C_{44}}\epsilon.$$

In the case of isotropic media, the hydrostatic pressure is given by

$$\sigma_H = \frac{4}{3}\mu\left(\frac{1+\nu}{1-\nu}\right)\epsilon,$$

for Poisson's ratio $\nu$ and shear modulus $\mu$.

The volumetric contraction or expansion of a lattice in response to removing or adding an atom, respectively, is uncertain for semiconductors. Results in metals show a total (atom conserving) change in volume smaller than, but of the order of, the atomic volume, with values spanning the range $(0.25\text{–}0.8)v_a$.[20] In the absence of experimental data we calculate contributions to the free energy based on the assumption of a total change in volume $\Delta V = (1/2)v_a$, assigning $v_a = \frac{1}{8}a_0^3$ for the zinc blende semiconductors.

Table I lists the contributions to the free energy for a biaxial strain commensurate with a 5% lattice mismatch. Although the strains resulting from this large a mismatch are substantial, much greater mismatches have been accommodated elastically in films grown by low temperature techniques.[21] Approximate contributions for different strains are readily determined by scaling the 5% strain values linearly with lattice mismatch (e.g., a 480 meV contribution for a 5% strain in Si becomes approximately a 100 meV contribution for a 1% strain). Larger hydrostatic strains for growth in the (111) orientation increase contributions to the free energy of formation substantially over the (100) case, with differences increasing for the more anisotropic II-VI's. While these contributions might not be expected to greatly perturb the low densities of point defects found in high quality Si or Ge, the effect on materials such as HgTe, which favor these defects, could be significant. In addition to modulating the density of deep levels, perturbing the population of vacancies substantially might be expected to alter diffusion mechanisms dependent upon these defects, as well as dopant incorporation onto substitutional, rather than interstitial, sites.

TABLE I. Contributions to the energy of formation of a point defect arising from a 5% strain.

| | $\Delta G_{strain}$ (meV) | |
|---|---|---|
| Material | (100) | (111) |
| Si | 380 | 480 |
| Ge | 330 | 430 |
| GaAs | 280 | 400 |
| InAs | 250 | 370 |
| CdTe | 140 | 260 |
| ZnTe | 190 | 310 |
| HgTe | 150 | 290 |

## IV. CONCLUSIONS

We have presented applications of continuum elastic theory to the problems of dislocation and point defect formation in the presence of stress due to lattice mismatch. Explicit calculations of dislocation configurational energies show that the line tension in the double-kink geometry exceeds that in the single-kink geometry, providing a window in which films metastable during growth may be stabilized by subsequent deposition of an overlayer of lesser or opposite strain. Dislocation tension is shown to rise monotonically to an asymptote exceeding that of the Matthews–Blakeslee model. Our result suggest that films are stable with respect to dislocation formation at thicknesses somewhat greater than previously thought, and that metastable films should relax more slowly than would be expected from the previous stability limits.

Last, we have considered the consequences of a several-percent strain for the formation of point defects. While the contributions to the free energy of formation of vacancies and interstitials may not warrant attention in semiconductors such as Si and Ge which display exceedingly low point defect densities in equilibrium unstrained conditions, they suggest a means of suppressing or enhancing defect formation in semiconductors such as HgTe, which favors vacancy formation.

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