Critical Reviews in Solid State and Materials Sciences
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/bsms20

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Version of record first published: 27 Sep 2006.

To cite this article: Jan H. van der Merwe (1991): Misfit dislocation generation in epitaxial layers, Critical Reviews in Solid State and Materials Sciences, 17:3, 187-209

To link to this article: http://dx.doi.org/10.1080/10408439108243751

Critical Reviews in Solid State and Materials Sciences, 17(3):187–209 (1991)

Misfit Dislocation Generation in Epitaxial Layers

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ABSTRACT: The misfit between an epilayer and a substrate may be accommodated either by misfit strain or by misfit dislocations, or by both jointly. For an epitaxial monolayer (ML) a critical misfit, depending primarily on bonding, exists below which it is stable when in registry with the substrate. When growth continues with the formation of a multilayer, misfit dislocations will enter at some critical thickness. The main objectives of this article are to critically review theoretical work aimed at explaining (1) the conditions under which an epilayer will grow in a ML-by-ML fashion to yield a uniform film and (2) the reasons why observed critical thicknesses and residual strains are often significantly in excess of the predicted ones, in terms of equilibrium and non-equilibrium concepts. Both (1) and (2) are of great fundamental and technological interest.

KEY WORDS: epilayer, misfit dislocations, critical thickness, uniform film, residual strains.

I. INTRODUCTION

Epitaxy is defined here as uniquely oriented growth of a single crystal A on the surface of a single crystal B. Of topical interest is the technological importance[1-3] of epitaxy; epitaxy being a most effective mechanism of growing thin films of highly crystalline perfection and highly uniform thickness. "Crystalline perfection" includes uniform strain to a new crystalline structure with different unit cell dimensions. Uniformity of thickness requires growth fronts (surfaces) that are more or less atomically smooth.

The atoms at the interface of a growing epilayer and substrate are subjected to the two competing lattice periodicities[4-6] a_o (overlayer) and a_s (substrate) of the two crystals. The misfit f between them has been expressed previously as[2,5]

$$f = (a_o - a_s)/\langle a \rangle \tag{1}$$

where $\langle a \rangle$ is an average or effective periodicity. For an epilayer on a thick substrate $\langle a \rangle$ is given by $\langle a \rangle = a_s$ and $\langle a \rangle = (a_s + a_o)/2$ when the epilayer is a monolayer (ML) and thick multilayer, respectively. When the misfit is accommodated by homogeneous misfit strain (MS) $\bar{e}$ and misfit dislocations (MDs) $\bar{f}$ jointly

$$f \approx \bar{f} + |\bar{e}| \tag{2}$$

$$\bar{f} = (\bar{a}_o - a_s)/\langle a \rangle \approx a_o/\bar{p} \tag{3a}$$

$$\bar{e} = (\bar{a}_o - a_o)/a_o \tag{3b}$$

where $\bar{p}$ is the MD spacing, $\bar{a}_o$ the average strained value of a_o, $f > 0$ and the approximations are valid when a_o and a_s are not very different. The limitation to the case $f > 0$ is for convenience of analytical presentation only. The generalization to include the case $f < 0$ is trivial.

The present article is primarily concerned with the problem of MS relief by the introduction of MDs, i.e., the changing distribution of f between $\bar{f}$ and $\bar{e}$ in the bicrystal during growth, and, accordingly, the technologically important goal of

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crystal perfection; a crystal without defects, of which MDs are an important category. Striving for crystal perfection also involves the absence of other dislocations, particularly threading dislocations[2] (TDs), the dislocations that thread through the growing crystal.

The other aspect of technological importance is the uniformity of film thickness that is facilitated by the smoothness of the growth front. The attainment of a smooth growth front[1-3,7] is in turn facilitated by a monolayer-by-monolayer (ML-by-ML) growth mode, also known as two-dimensional (2D) or Frank-van der Merwe (FM) growth; when compared with island (Volmer-Weber ≡ VW, 3D) growth or Stranski-Krastanov (SK: FM followed by VW) growth, with their rather rough beginnings.[3,8,9] Island growth is also undesirable because the coalescence process involved in the formation of a continuous film is conducive to the formation of TDs.[10] Relevant aspects of growth modes (shapes) are dealt with below. Specifically we are interested in the conditions that favor FM-like growth. Epilayer growth in the FM (or FM-like) mode also lends itself more simply to a description of MD generation by nucleation and motion.

The driving forces for the processes involved in shape (growth mode) formation and strain relief are the negative "gradients" of the free energies; the configurations of minimum free energy being the equilibrium configurations of the systems. In most of the present applications the free energy may be approximated by the total (internal) energy E. Both equilibration processes involve energy barriers,[2] which require thermal or other energies for their overcoming. Whereas the barriers to shape equilibration, i.e., those incurred in adatom surface migration, are more or less fixed to values of less than 1 eV, the barriers incurred in strain relief — nucleation and motion of dislocations — cover a wide range (from less than 1 eV to near 200 eV), and may also be drastically reduced by MS and other crystal defects[11,12] that act as MD sources. Whereas (substrate) temperature T and deposition rate (together they determine the super-saturation[7,13]), composition, and time scales are the important external parameters, bonding, misfit, and thickness are the dominant internal parameters.[2,5] For a given moderate bonding a coherent (pseudomorphic) ML is stable provided the misfit f is critical value f_c that depends on bonding and atomic arrangement. A multilayer of subcritical ML material becomes incoherent to the substrate by the introduction of MDs above a critical thickness. Two different critical thicknesses are envisaged: an equilibrium[2,5] one h_c^{eq} at which the pseudomorphic multilayer becomes unstable, and an observed one, defined as the thickness at which the introduction of MDs becomes observable,[14-16] for example, by the appearance of one MD within the viewing field of an electron microscope.

The problem of strain relief by the introduction of MDs has, for relative simplicity, mostly been dealt with at the equilibrium limit, using the equilibrium principle as approximated by minimum energy E,[2,5]

$$E = \min \tag{4a}$$

the implicit assumptions being that MDs would be available where and whenever they are needed for equilibration, and that the MDs form regular arrangements to minimize configurational entropy. Minimization with respect to the MS $\bar{e}$ or the MD density $\bar{f}$, could involve a formidable calculation. In some cases, the minimization calculation can be significantly simplified using the equivalent condition that the reversible work W needed to introduce one more MD vanishes,[5] i.e., that

$$W = O \tag{4b}$$

A further simplification may be accomplished if the MD is drawn in the interface from an existing (threading) dislocation through the motion of a generating threading dislocation segment (see Section III.F); equilibrium exists when the resulting force F on the generating segment vanishes[2]

$$F = O \tag{4c}$$

Existing equilibrium theories[2,5] for predicting critical quantities are briefly considered. The fact that barriers to the nucleation and motion of MDs exist implies that within the duration of an experiment, equilibrium is rarely accomplished and requires at least sufficient thermal energy (an appropriately high-temperature T) to facilitate dis-

location motion, assuming that otherwise there are MD sources that provide dislocations spontaneously. In metals the (Peierls) barriers[17,18] inhibiting dislocation motion are usually relatively small, so that equilibrium is feasible during the experiment, and at moderate T. The bonding in most semiconductors are of a covalent nature and with relatively large Peierls and nucleation barriers. The quantification of the arguments will be dealt with. The dynamics of strain relief by MD generation is a difficult problem that has not been completely solved as yet.[19-21] Commendable efforts to do so are reviewed. Misfit accommodation by MD generation in ultrathin epilayers is not only of interest in its own right, but also from a technological point of view, and, furthermore, serves as a simple introduction to the subject.

II. GROWING UNIFORM EPILAYERS

A. Equilibrium Criteria

It is technologically[3,12] and analytically desirable to have smooth growth fronts. This goal is best served by growth in the FM mode. We first consider equilibrium criteria for growth modes as formulated by Bauer[8] and Bauer and van der Merwe,[9] and subsequently considered by others.[14,22,23] To explicitly demonstrate the influence of MS and MDs in our deliberations we investigate the case in which a pseudomorphic ML (MS energy ϵ_{os} and a dislocated double layer (DL) containing MS energy ϵ_s per atomic layer and MD energy ϵ_{D2}, are separately stable and transfer material from the DL to the ML. ML-by-ML (FM) growth is energetically favored if the free energy change $\Delta\gamma$ is negative, i.e.,

$$0 \geq \Delta\gamma$$

$$\approx \Delta\gamma_o + 2\epsilon_{os} - (2\epsilon_s + \epsilon_{D2}) \quad (5a)$$

$$\approx \Delta\gamma_o \quad \text{for } \epsilon_{D2} = 0\ (\epsilon_s = \epsilon_{os}) \quad (5b)$$

$$\Delta\gamma_o \equiv \gamma_o + \gamma_i - \gamma_s \quad (6)$$

where all energies refer to unit area of interface and γ_o, γ_s, and γ_i are, respectively, the surface free energies of the overlayer, substrate, and interface. The importance of surface energies in tailoring the growth modes was also stressed by Egelhoff.[24] In Equation 5a, we approximated ML and DL properties by macroscopic ones, whereas Equation 5b represents the extreme in which the misfit is accommodated by MS ($|\bar{e}| = f$) alone. If there are MDs at the DL-substrate interface it implies that this configuration is more stable than a completely pseudomorphic one, i.e., that $2\epsilon_{os} - (2\epsilon_s + E_{D2}) > 0$.

A number of important guidelines can be deduced from Equations 5 and 6: first, the quantity $\Delta\gamma_o$ in Equation 6 may also be expressed directly in terms of "bond strengths" as[22,25-27]

$$\Delta\gamma_o = E_{oo} - E_{os} \quad (7)$$

where E_{oo} and E_{os} represent, respectively, the work (per unit area of interface) needed to separate two half-crystals (of the growing crystal) from each other and a growing half-crystal from the semiinfinite substrate. Strong bonding on the substrate, i.e., large E_{os}, is thus conducive to FM growth. In FM growth the excess energy $|\Delta\gamma_o|$ may be seen as some measure of the urge to FM growth. Second, by Equation 5b, MS alone does not affect the growth mode directly; only indirectly through contributing to the conditions for strain relief. The fact that an increase in MS, brought about by a change in alloy compositions in $In_xGa_{1-x}As$ on GaAs, enhances 3D growth[28] may as well be ascribed to a change in bonding rather than an increase in MS. However, if one argues that a surface atom contributes more or less a given amount to E_{oo}, or E_{os} in Equation 7, positive MS will reduce E_{oo} and E_{os}, possibly to a lesser extent. This means that positive and negative MS will enhance FM and VW growth,[1] respectively, but will have little effect on a transition before onset of MS relief, provided it is assumed that the interfacial force is independent of layer thickness. Berger et al.[29] have also suggested that positive/negative MS will increase/decrease the activation energy for surface migration, retard/accelerate the equilibration rate, and, accordingly, favors a pseudo 2D/3D (Stranski-Krastanov) growth mode. Growth that starts off FM-wise and reverts to island growth after one or a few MLs is known as Stranski-Krastanov (SK) growth.[8] The presence of MDs at an ov-

erlayer-substrate interface contributes positively to $\Delta\gamma$ (see Equation 5a) and may accordingly effect a transition to island growth as from the second or subsequent MLs. This will be particularly so when $\Delta\gamma_o$ is near zero, as for homoepitaxial growth in which $\gamma_s = \gamma_o$ and $\gamma_i = 0$ or, with reference to Equation 7, $E_{os} = E_{oo}$. The possibility that the introduction of MDs could effect a transition to SK growth was first recognized by Matthews[2] and subsuquently by others.[30] Indeed, Elman et al.[14] introduced the concept of a "threshold" thickness for the thickness at which the transition occurs and found that in InGaAs on GaAs this equals the critical thickness. SK growth may also be the result[26,31] of a substrate-induced change in overlayer electronic structure, as mentioned above; a change in which E_{os}, with the new composite substrate — original plus grown MLs — has fallen below the value of E_{oo} for the ML growing on top of it. Island growth can also be suppressed in alloy semiconductors by manipulating[14] the surface species and hence the bonding and surface energy.

B. Nonequilibrium Growth

The foregoing considerations suggest that continued FM growth may be a rare occurrence; more often we either have VW or SK growth.[8,32] Note that this conclusion applies when the conditions for shape equilibration are met (more or less). The technological need[3] for (atomically) smooth growth fronts (surfaces) has urged the exploitation of nonequilibrium processes[1,7,12,13,22] to achieve the desired true or pseudo-FM growth. A complete presentation of the relevant analysis is beyond the scope of this article. For the present, semiquantitative considerations will suffice.

We need to address the case in which the bonding onto the substrate is relatively weak, the growth mode is islandwise, and growth requires the nucleation of critical-sized nuclei; a process that is facilitated by a supersaturated adatom flux. A vapor that is in contact with a crystal surface is said to be supersaturated when the supersaturation ratio[22]

$$\xi = R(T)/R_e(T) \qquad (8a)$$

exceeds unity; R and R_e being, respectively, the prevailing and equilibrium deposition rates on the crystal surface at temperature T. Otherwise, the excess chemical potential $\Delta\mu$ of an atom in the vapor (μ), when compared with one in the crystal surface (μ_e), is given by

$$\Delta\gamma \equiv \mu - \mu_e = kT\,\ell n\,\xi \qquad (8b)$$

a quantity that increases as ξ increases, k being Boltzmann's constant. If the vapor is only moderately supersaturated, $\Delta\xi \equiv \xi - 1$ is small and $\Delta\mu$ may be expressed as

$$\Delta\mu \approx kT\Delta\xi \qquad (8c)$$

It also follows from the work of Markov and Kaischew[33] that the number N* of atoms constituting a critical nucleus satisfies the relation

$$N^* \propto (\Delta\mu)^{-3} \qquad (9)$$

showing that N* decreases as ξ increases. This general trend is continued even when the nucleus becomes microscopic and the supersaturation is more than moderate. In fact, it is generally accepted that critical nuclei at appropriate supersaturations is about one atom, a size that we adopt below. In this case, the suggestion that the growth mode is a nucleation phenomenon[33] is irrelevant.

The fact that the critical nucleus is only one atom allows one to grow in a pseudo-ML-by-ML mode, whereas in equilibrium the Volmer-Weber or Stranski-Krastanov mode obtains. The idea is that at an appropriate supersaturation, characterized by critical nuclei of atomic size, also the range of the adatoms on the surface is so small that only very localized equilibration is possible and not the extended equilibration that is needed for formation of equilibrium shapes. This concept can be crudely quantified by adopting the criterion that pseudo-ML-by-ML growth will obtain when the adatom diffusion range s(t) in the time t needed to deposit one ML coverage is about one or a few jump distances a. This will allow the adatoms sufficient time to move into nearby lattice points in order to grow a crystalline structure, but falls greatly short of accomplishing shape equilibration. If we identify s(t) with the root

mean square surface displacement $(\langle r^2(t)\rangle)^{1/2}$ as

$$s = \sqrt{4Dt} \tag{10a}$$

the diffusion coefficient D being given by

$$D = (a^2/2)\nu \exp(-E_D/kT) \tag{10b}$$

in terms of the activation energy E_D of surface migration, the substrate temperature T, and the frequency factor ν. The condition for the deposition of one ML is approximately

$$Rt \approx 1/a^2 \tag{10c}$$

where a^2 represents the area per atom in the surface. Combining Equations 10a–c, yields for the required deposition rate, the result

$$R \approx 4D/a^2s^2 \approx 2s^{-2}\nu \exp(-E_D/kT) \tag{10d}$$

where $s \approx a$. An implicit assumption in deriving this result is that the adatom flux is more or less uniform over the area of interest. Although the relation (Equation 10d) is certainly not accurate, it is proposed to be a useful guideline for growing a ML from adatoms, each of which constitutes a stable nucleus. Note that once one or a few MLs have been grown in this way we have returned to homoepitaxial growth in which $\Delta\gamma_o = 0$ and ML-by-ML growth can proceed spontaneously. The two-step process[32] of growing uniform films in systems that do not meet the equilibrium criterion for FM growth must be understood along these lines.

The equilibrium criteria of Bauer suffer from two shortcomings: (1) the assignment of macroscopic properties to MLs, and (2) the fact that the interfacial free energy γ_i is usually an unknown quantity. The implication is that their predictions of growth modes can only be made with some degree of uncertainty. They nevertheless provide practical guidelines for predicting growth modes and addressing the roles of MDs and MS in addition to generating understanding of the general phenomenon, as well as some foundations of the technologically important two-step process; the covering up of the substrate with a thin epilayer of practically uniform thickness to suppress the tendency to island growth so that growth can continue in the FM mode. The exact degree of supersaturation to accomplish the first step has not been quantified as yet. Such quantification would be valuable. By the appropriate supersaturation the detrimental coalescence phase is also severely suppressed provided a ML (and possibly a DL) is subcritical and the adsorption sites are unique, as on {001} cubic surfaces.

This serves the technological need of growing uniform epilayers and also justifies our consideration of MS relief by MD generation in uniform epilayers only.

III. MISFIT STRAIN RELIEF BY MISFIT DISLOCATION GENERATION

This review is primarily dedicated to the theoretical understanding of cases in which a ML is subcritical, misfit strained in registry with the substrate, and the onset of MS relief accordingly occurs at a multilayer (critical) thickness. We consecutively review: (1) the mathematical models used to calculate the energy of a dislocation, to facilitate understanding, and to provide insight into the relevant accuracies; (2) the application of the models to ultrathin (less than three MLs) epilayers, important in phase transitions in thin adsorbed layers and the initial stage of ML-by-ML growth; (3) the identification of MDs; (4) the forces driving dislocations and the important barriers to their motion; (5) the generation of MDs and the importance of sources; (6) the generation of TDs and their importance as sources of MDs; (7) some consequences of off-cutting substrates, (8) the calculation of critical thickness — equilibrium and observed values — and the time dependence of residual strain.

A. Models

In this article, the considerations are limited to analyses using phenomenological harmonic approaches. Numerical techniques using atomic potentials are not considered. The harmonic models have, although approximate and rather crude in certain respects, yielded results of surprising validity and generality, and provided indispensable guidelines for developments in tech-

nology. The harmonic models assign[2,5] isotropic or anisotropic harmonic interactions to the atoms within individual crystals A and B — model them essentially as elastic continua — and to the atoms on either side of the interface in regions where they are near continuations of both crystals (in or near registry), and unharmonic interactions where the interfacial atoms are badly out of step (in disregistry), i.e., around the dislocation line where an extra plane of atoms from one crystal terminates at the interface. In ultrathin epilayers, where pseudomorphic strains of up to 10% or more may occur, unharmonic effects[34-36] within individual crystals could be significant and could account for large differences in critical misfit in compression and extension.

There are different models within the class of harmonic approaches. They differ essentially in the representation of the unharmonicity around the dislocation. Crudely, there are two main models. One is the Frenkel-Kontorowa model (and its generalizations)[3,5,7] that adopts an interfacial force between the atoms on either side of the interface and varies periodically with the disregistry — the relative tangential displacement. In this context, the Frenkel-Kontorowa (FK) model is most simply understood for a system in which crystal B is a ML with perfect matching in one direction. The authors adopted a Fourier series, truncated[38] at the first harmonic term, to represent the periodic force in the perpendicular misfitting direction. This model was subsequently extended by Nabarro[39] and van der Merwe[37(a)] to the case where A and B are both semiinfinite and by Frank and van der Merwe[5] to a ML with anisotropic interfacial misfit.

The other main model is the Volterra model, exploited extensively by Matthews[2] and subsequently by others. In this model the two crystal halves, taken as elastic continua, are "glued" together at the interface; in registry on both sides of the dislocation but displaced by one lattice period (Burgers vector) on one side of the dislocation line, which itself is replaced by a hole of radius r_o. This inner "cut-off" radius r_o is of atomic dimensions. It is an adjustable parameter introduced for convenience;[40] it eliminates, in the mathematical description, the singularity at the dislocation line and its value is selected to provide for the "core" energy of the dislocation.[11,40-42] The values usually adopted for r_o are

$$r_o \approx \begin{cases} b & \text{for metals} \\ b/2 \text{ to } b/4 & \text{for semiconductors}^{15,42} \\ & (b/e;\ \text{Matthews}^2) \end{cases} \tag{11}$$

where b is the Burgers vector and $e = 2.718\ldots$ the naperian logarithmic base. An outer cut-off radius R is also introduced to allow for the cancellation of stress fields[2] by other neighboring dislocations and/or the presence of free surfaces.

The Frenkel-Kontorowa model has proven its usefulness in the case of ultrathin epilayers, for example, in the description of phase transitions in adsorbed layers on crystalline surfaces[25] and in understanding the principles underlying epitaxy.[5] The Volterra model has proven its value for the description of misfit accommodation and strain relief in intermediate to thick epilayers, where the governing equations of the Frenkel-Kontorowa model are not solvable (except for the parabolic approximation). Under these conditions, the Volterra model still retains its mathematical simplicity. The two models are complimentary rather than exclusive. In both models the total energy E can be expressed as the sum of the MS energy E_ε and the MD energy E_D, i.e.,

$$E = E_D + E_\varepsilon \tag{12}$$

An expression for the E_ε in the harmonic approximation is uniquely defined by isotropic (or anisotropic) elasticity theory. The practice of using bulk elastic constants in calculations seems to be justified except perhaps in the ultrathin (e.g., ML) stage of growth. Also in ultrathin epilayers, pseudomorphic strains may be so large that unharmonic effects[34-36,43-47] become important. We shall not deal with attempts at refining the theory to incorporate these effects, except to say (1) that reliable calculations of MS energy for pseudomorphic strains up to 20% should certainly provide for unharmonicity, and (2) that unharmonicity introduces asymmetries in critical quantities for epilayers in tension and compression. Pseudomorphic MLs may, of course, also behave differently in compression and tension for reasons other than unharmonicity, e.g., for geometrical

reasons.[43] Also, large pseudomorphic strains may deform an epicrystal into a structure regime where a metastable phase exists.[48-50] In such a case, large homogeneous "strains" outside the harmonic range can be sustained up to large thicknesses.[48]

A simple expression for $E_{\bar{e}}$, applicable to an isotropic elastic epilayer of thickness h and rectangular interfacial symmetry can be written as[37(c),45]

$$E_e^- = \mu_0 h(\bar{e}_x^2 + \bar{e}_y^2 + 2\nu\bar{e}_x\bar{e}_y)/(1 - \nu_0) \quad (13)$$

per unit area of interface, when the surface is free and the shears in planes normal to the interface can be neglected, μ_o being the shear modulus of the epilayer and ν_o its Poisson's ratio. When the interfacial symmetry is quadratic, as is often the case, the strain is isotropic: $\bar{e}_x = \bar{e}_y \equiv \bar{e}$.

The derivation of an expression for the MD energy E_D is less straightforward. There are essentially two approaches, one of Volterra type and one of Frenkel-Kontorowa type. In both calculations the MDs are assumed to be long and straight, to be arranged in two regular orthogonal sequences, and it is also assumed that the interactions at the crossings are negligible. In the Volterra approach, E_D is usually expressed[2] as

$$E_D = \frac{1}{2} B \, \ell n(R/r_0) \quad (14a)$$

$$B = \frac{\Gamma b^2 \bar{f}}{\pi}; \frac{1}{\Gamma} = \frac{1 - \nu_0}{\mu_0} + \frac{1 - \nu_s}{\mu_s} \quad (14b)$$

$$R = \begin{cases} \bar{p}/2 & \text{for } h \geq \bar{p}/2 \\ h & \text{for } h \leq \bar{p}/2 \end{cases} \quad (14c)$$

for pure edge type MDs, where subscripts o and s refer to overlayer and substrate, respectively, $\bar{p}$ is the MD spacing and some conventional values of r_o are specified in Equation 11. Analytically, the onset of strain relief is most simply obtained from the limiting relation

$$\bar{f} = 0 \quad (15)$$

For the injection of the first MD, $\bar{p}$ is of the order of the interface "length", which is usually much greater than h. This implies that R = h is the appropriate outer cut-off at onset of strain relief. Also, normally it is assumed[2] that $\nu_o = \nu_s \equiv \nu$, which seems acceptable for alloy semiconductors that are elastically very much the same. In cases where the relevant materials are significantly different, use of the appropriate values of the μs and particularly the νs (Voigts averages if appropriate) may have a profound effect on the values of the calculated energies.

In the Frenkel-Kontorowa model, simple energy expressions have been obtained only for the two extreme cases: the ultrathin epilayer[5,37(c)] (specifically a ML) and the thick epilayer. It follows from this theory that the energy of an epilayer of finite thickness h on an infinite substrate is within 2% of the same as when both crystals are infinite, provided $h > \bar{p}/2$. To a good approximation we may therefore declare an epilayer "thick" when

$$h \geq \bar{p}/2 \quad (16a)$$

This result is justification for the concept of an outer cut-off radius. The energy of a thick epilayer is expressed in terms of a parameter

$$\beta = 2\pi\Gamma d/\mu\bar{p} \quad (16b)$$

μ being an interfacial shear modulus. In the limit when MDs are far apart ($\beta \ll 1$), i.e.,

$$\bar{p} \gg 2\pi\Gamma d/\mu \quad (16c)$$

for example, when strain relief commences, the expression for the thick epilayer has the asymptotic form

$$E_D \approx \frac{1}{2} B \, \ell n\left(\frac{e\mu\bar{p}}{4\pi\Gamma b}\right); \quad h \geq \bar{p}/2 \quad (17)$$

This means that in the thickness regime $h \geq \bar{p}/2 \gg 2\pi\Gamma d/\mu$, Equations 14a and 17 would be identical provided we take

$$r_0 = 2\pi b\Gamma/e\mu, \quad R = \bar{p}/2 \quad (18a)$$

When the bonding in the crystal halves and

the interface are about the same, i.e., $\nu_o \approx \nu_s \approx 1/3$, $\mu_o \approx \mu_s \approx \mu$

$$r_0 \approx 2b, \quad h \geq \bar{p} \gg 8b \tag{18b}$$

The value of r_o is seen to be somewhat larger than the more conventional ones in Equation 14a, which is based partly on the supposition that a single sinusoidal term represents the periodic interaction potential adequately. Nevertheless, the considerations related to Equations 16 to 18 provide some quantitative justification for the introduction of inner and outer cut-off radii r_o and R, respectively. Calculations of critical thickness for epilayers with perfect MDs have been carried out by Matthews.[2] Of particular interest is the case with imperfect MDs dealt with in Section III.F.

B. Ultrathin Epilayers

Although strain relief in intermediate to thick epilayers is the most challenging problem at present, strain relief in ultrathin layers is also important; if only for the fact that most epilayers are ultrathin initially and accordingly have an influence on the ultimate result. It is appropriate to briefly present the Frank-van der Merwe theory;[5] an equilibrium theory that has gained universal acceptance for a lucid qualitative, and to some extent quantitative, understanding of the pseudomorphic growth of a deposit on a crystalline substrate of different lattice parameter below a critical misfit and the subsequent relaxation of strains by the introduction of MDs as the thickness increases.[46] The theory also addresses the important role of bonding and the barriers to the introduction of MDs. The Frank-van der Merwe theory is based on the Frenkel-Kontorowa[6] model; a one-dimensional model in which the overlayer is represented by a regular linear chain of particles (atoms) subjected to the competing periodicities of identical connecting elastic (harmonic) springs (force constant $\bar{\mu}$ and natural length a_o) and a "rigid" periodic substrate potential, represented by a Fourier series truncated at the first harmonic, i.e.,

$$V = \frac{1}{2} V_0[1 - \cos(2\pi x/a_s)] \tag{19}$$

with overall amplitude V_o, periodicity a_s, and minima at $x = 0, a_s, \ldots$ of value zero. In this model $\bar{\mu}$ and V_o have physical meanings and may, respectively, be regarded as measures of atom-atom and atom-substrate bond strengths. Numerical calculations, using atomic potentials, have confirmed that the Fourier coefficients decay rapidly with harmonic order and that such truncations are accordingly justified.[38]

The governing equation for the equilibrium positions of the particles reduces in the continuum approximation to a sine-Gordon equation by which the resolution of the chain of particles into a regular sequence of MDs of density $\bar{f} = a_o/\bar{p}$ is a natural consequence of the analysis and the average total energy E consisting of MS energy $E_{\bar{e}}$ and MD energy E_D can be calculated. MDs can be introduced by displacing (gliding) the free end of the chain from a stable equilibrium position x_o to the next at $x_o + a_s$. The minimization of E can be accomplished by setting the work W, needed to introduce an additional MD, to zero (see Equation 4b). This determines the equilibrium misfit $f = f^{eq}$. Also, the activation energy W_{AC} for the versible formation of the MD by glide can be calculated as the work done in a displacement of the free end from x_o to the nearest position $a_s - x_o$ of unstable equilibrium.

The following results have been obtained:

$$W(k) = 2V_o\ell_0(f(k) - f^{eq}), \tag{20a}$$

$$f^{eq} \equiv f(k) = \frac{2E(k)}{\pi k \ell_0} \tag{20b}$$

$$\bar{f}(k) = \frac{\pi}{2\ell_0 k K(k)}$$

$$\bar{f} = 0, \quad f_c^{eq} \equiv f_c \tag{21}$$

$$= 2/\pi\ell_0 \ (k = 1) \tag{22}$$

$$E = E_e^- + E_D \tag{23}$$

$$W_{AC} = (4V_0\ell_0/\pi) \times [(1 - f^2\ell_0^2)^{1/2} - f\ell_0 \cos^{-1}(f\ell_0)] \tag{24}$$

$$\ell_0^2 = \bar{\mu}a_s^2/2V_o$$

where K(k) and E(k) are elliptic integrals of the First and Second kinds with parameter k, the given value of W_{AC} is for the pseudomorphic configuration, and f_c is the equilibrium critical misfit. It follows from Equation 24 that W_{AC} changes sign at a misfit

$$f_s = 1/\ell_0 \qquad (25)$$

which means that MDs will enter spontaneously for misfits exceeding f_s. Frank and van der Merwe have estimated $\ell_0 \approx 7$ using Lennard-Jones pair potentials. This yields the estimates $f_c = 9\%$, $f_s = 14\%$, and $W_{AC} = 1.7\ V_o$.

The dependences of the equilibrium MD density $\bar{f}$ and of W_{AC} on f are illustrated in Figures 1 and 2. Figure 1 shows that in the equilibrium configuration there are no MDs up to a critical misfit f_c, whereafter $\bar{f}$ increases rapidly to the configuration where, in equilibrium, $\bar{f}$ and f approaches each other. The main message of Figure 2 is that the activation energy for MS relief by the generation of MDs in a pseudomorphic ML is reduced by the pseudomorphic strain and only vanishes at a misfit $f = f_s$, which is significantly greater than f_c.

Also, of great significance is the fact that both W and W_{AC} vary with the MD density $\bar{f}(k)$. From the properties of elliptic integrals it follows that K(k) decreases from infinity, so that $f(\bar{k})$ decreases, as k decreases from one downward, whereas the displacement x_o of the free end of the chain decreases, and W_{AC} accordingly increases, as k decreases. If now in a given case $f > f_c$, W for MD injection in a pseudomorphic configuration will be negative, i.e., there exists a thermodynamic force that drives MS relief by the injection of MDs. However, while W tends to zero as the equilibrium configuration $f^{eq} = f(k)$ is approached, the activation energy W_{AC} increases. The implication is that the rate of equilibration will decrease as the equilibrium configuration is approached and vanishes in the limit when W becomes zero.

These results carry important messages. Although the equilibrium configuration is one with MDs, not only does the equilibration driving force tend to zero as the equilibrium configuration is

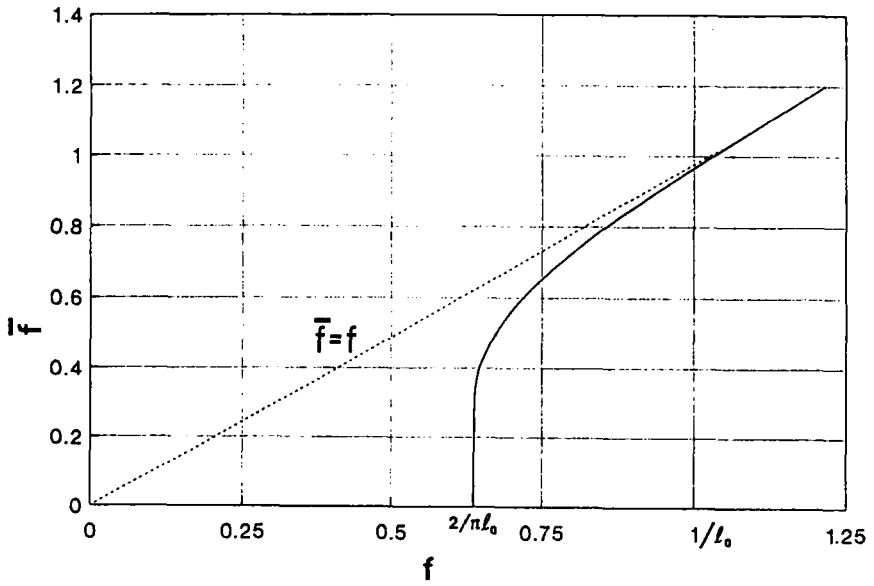

FIGURE 1. Curve displaying the equilibrium dependence of the misfit dislocation (MD) density $\bar{f}$ on misfit f; $\bar{f}$ is zero until $f = f_c \equiv 2/\pi\ell_0$ at which point there is an abrupt increase, approaching the configuration in which $\bar{f} = f$. In a monolayer (two-dimensional system), the transition is rapid though continuous. Note that for $f > f_c$ MD generation still requires an activation energy (see Figure 2), which only vanishes at $f = f_s \equiv 1/\ell_0$.

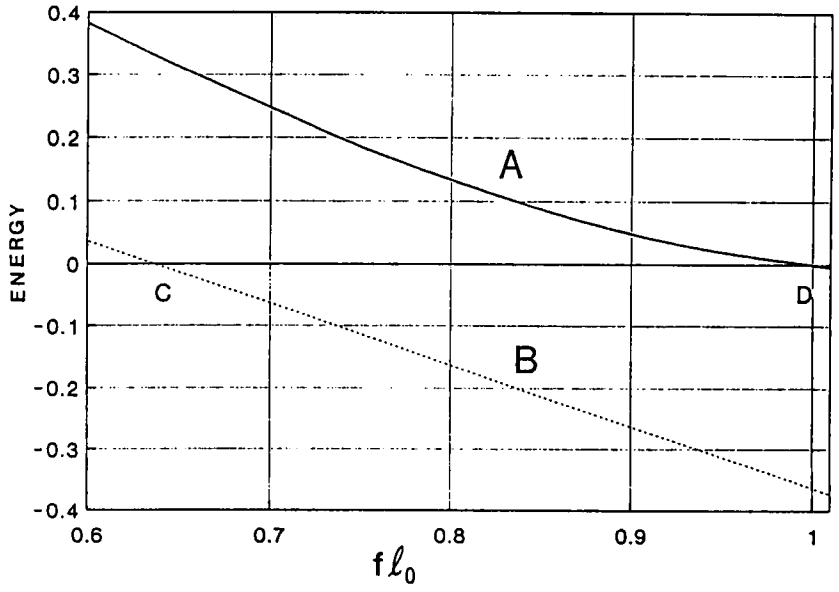

FIGURE 2. Curves showing the dependence on misfit f (in units of $1/\ell_o$) of (A) the activation energy W_{AC} (in units of $2V_o\ell_o$) for a coherent to noncoherent configuration, and (B) the work of formation W (in units of $2V_o\ell_o$) of the first misfit dislocation (MD). Note that the transition is accompanied by an energy gain ($W < 0$) for $f > 2/\pi\ell_o$ (point C) and a positive W_{AC} that decreases as the coherency strain $\bar{e} = f$ increases and vanishes when $f = f_s \equiv 1/\ell_o$ (point D).

approached, but also the activation energy for overcoming the barriers increases. The activation energy for onset of MS relief is reduced by the pseudomorphic MS $\bar{e} = f$ and vanishes if $f = f_s$.

The foregoing considerations have been extended to more realistic models, two-dimensional MLs of rectangular[5,37(c)] and rhombic[37(d)] symmetries. The main contribution emanating from the extension to the case with 2D rectangular symmetry is to highlight the influence of Poisson's phenomenon (ratio ν), for example, for the equilibrium critical misfit in one direction (coherency fixed in the other direction)

$$f_c^{(2)} = \frac{2}{\pi(1 + \nu)\ell}; \quad \ell^2 = \frac{\mu a_s^2 a_0}{V_0(1 - \nu)} \qquad (26)$$

where μ is the shear modulus of the ML usually approximated by that of the bulk. This introduces a significant reduction of the critical misfit when compared with the one-dimensional model.

Frank and van der Merwe[5] also noted that a growing epitaxial film that is below critical at the ML stage will become critical (unstable) at a certain thickness h_c^{eq}, which may be estimated very crudely by assigning a force constant $n\mu$ to a n-fold layer. It follows from Equation 26 that

$$h_c^{eq} \sim a_0 \left[\frac{2}{\pi\ell(1 + \nu)f}\right]^2 \qquad (27)$$

a result that demonstrates the principle, but is otherwise of little quantitative significance. As in the case of a ML above a critical misfit, one may anticipate that the onset of strain relief in a multilayer (above a critical thickness; $h > h_c^{eq}$), involves an energy of activation that decreases with increasing excess $h - h_c^{eq}$.

The main shortcomings of the Frank-van der Merwe ML theory are (1) that little is known about the equilibrium of free MLs and their elastic and lattice constants — the practice of approximating these by bulk values is risky, particularly for MLs, which are not (even nearly) close-packed and (2) the lack of values for the appropriate Fourier coefficients. Useful attempts at calculating the latter have been initiated, though.[38]

C. Misfit Dislocations (MDs)

A dislocation qualifies as MD provided its Burgers vector has a nonzero component in the interface plane normal to the dislocation line. Only this component can accommodate misfit. Accordingly, MDs are most efficient in accommodating misfit when they are perfect (efficient), i.e., in edge orientation with their Burgers vector in the interface.[2] Perfect MDs can be generated by glide, if the interface is a glide plane and the crystal boundary normal to the interface is free, as is usually the case in island growth[45,51-53] and in the case of a finite ML, or by climb from the free surface of a continuous film in a process that involves migration of vacancies or interstials.[54]

Imperfect (inefficient) MDs are acquired by glide in glide planes that are inclined to the interface. The most prominent[2,11,17,55,56] of these are the 60° MDs — their Burgers vector is at 60° to the MD line — on {111} glide planes of face-centered cubic (fcc) metals and diamond-structured semiconductors. The 60° MDs may furthermore split into partials[2] with a stacking fault in between.

Sessile perfect (Lomer) MDs may also be generated by a reaction[55,57] between two 60° dislocations. Such a MD is normally created outside the interface, but may get there by climb. Dregia and Hirth[56] recently proposed the rebound mechanism that avoids the climb process in that the oncoming 60° dislocation reacts at the interface to yield a Lomer MD there and another 60° dislocation that glides toward the surface or other interface.

D. Motion of Dislocations

A dislocation segment within a stressed region of a crystal experiences a force from the field and has both climb and glide components. The glide motion, which is normally much faster than climb (climb requires material transport) is opposed, also in a perfect crystal, by the so-called Peierls barriers,[2,17,18,42,58,59] which exist because of the discrete periodic nature of the crystals. The Peierls barriers to dislocation glide on {111} fcc planes of most metals are small when compared with those on equivalent planes in covalently bonded semiconductors. Accordingly, in many metals dislocations move at infinitesimal stresses. When the stress is too small to overcome the barriers, the dislocations can still migrate by thermal creation and migration of kinks[12,17,59] in them, or simply by an appropriate diffusion mechanism. For the migration of 60° MDs in $Ge_{0.25}Si_{0.75}/S_i(001)$ the activation energy for MD migration was measured as (1.1 ± 0.2) eV. Of course, MDs also experience interactions from other dislocations and MDs, or crystal defects[40,59-62] that may pin them at their crossings, while the segment in between bows out to an extent determined by the stresses and the MD line tension.

E. Misfit Dislocation Sources

We define a MD source (MDS) as a defect where MDs are more easily generated than within the perfect crystal. The creation of a MD is (1) opposed by an energy barrier characteristic of the source; the energy of nucleation Q_n of a critical-"sized" MD, and (2) facilitated by thermal energy depending on the substrate temperature T. Q_n is reduced by MS, for example (see Equation 23) W_{AC}, which is the 1D equivalent of Q_n, decreases from 1.7 V_o to 0 as the pseudomorphic MS increases from $f_c^{eq} = 2/\pi 1_o$ to $f_s = 1/1_o$ (see Equations 21 and 25).

A variety of MDSs, depending on the size, shape, and structure of an epicrystal, have been proposed. Frank and van der Merwe[5] have taken the free edge of a ML as the source and suggested that a perfect MD be generated by displacing the edge parallel to the substrate surface by one atomic spacing, i.e., by a glide mechanism. The nucleation energy per atom length of a long straight MD thus generated at a long straight edge is given by[37(c)] Equation 23, but with ℓ_o replaced by the ℓ of Equation 26.

As with other approaches,[63,64] the foregoing estimates the nucleation energy per atom length of a long straight MD. If we assume that the critical length is about four atoms and that V_o can be identified with the activation energy of surface migration of adatoms as 0.6 eV, the nucleation energy for glide from the free edge of a ML is approximately 4 eV and requires a sig-

nificant substrate temperature for its overcoming. One expects this nucleation mechanism to occur in island growth.[52]

When a ML or multilayer covers the substrate completely, perfect MDs can still be generated by climb of adatoms to or from the free surface — particularly so with a coherent ML in tension (negative misfit) when excess adatoms[43,65] are available during deposition. Vacancy loops, leading to perfect MDs, could also form within an epilayer, by aggregation of vacancies.[44,45] In fact, it has been shown[66] that the critical MD size is only about one interstitial or vacancy. This implies that interstitials or vacancies that have been incorporated in the growing film would constitute perfect sources in a ML. Preliminary calculations[67] using simple pair potentials also suggest that the activation energy for injecting an adatom into a pseudomorphic ML in tension, i.e., generating a critical MD nucleus, becomes vanishing small at the equilibrium critical misfit f_c^{eq}. It would seem that the introduction of MDs by climb in a pseudomorphic ML in tension is energetically favored, and more so because it does not involve the Peierls barriers.

The MDSs discussed above are more or less limited to ultrathin (near ML) epilayers. They nevertheless provide good guidelines for the identification of MDSs in intermediate to thick layers. In this case the free surface is the most obvious position for nucleating MDs by glide (on an inclined glide plane though), and by climb. As with MLs, climb is believed to be an important mechanism of formation of MDs. Of particular interest are finite half loops or finite loop segments that can be generated with the aid of thermal energies and can constitute true MD nuclei. As for MLs, it may be anticipated that MS $\bar{e}$ and MD density $\bar{f}$ will have important consequences for their nucleation energies. Strictly speaking, it is a TD nucleus that is formed at the surface; a MD is only subsequently generated at the interface by the TD.

The onset of strain relief by the injection of MDs in coherently strained multilayer structures through nucleation of interior loops, surface half loops, and by the bowing out of TDs, has been studied by Kamat and Hirth.[68] The authors proposed an "observability" criterion to quantify the practical onset of MD injection. The criterion requires critical-sized nuclei to be formed at a rate of one nucleation event every few thousand seconds, or equivalently, one event in a volume of 10^{-15} to 10^{-18} cc. This volume is typically the region in the view of an electron microscope. Using standard rate theory, the authors have written down expressions for the concentration n* of critical nuclei and the nucleation rate J as

$$n^* = n_1 \exp(-W_c/kT) \tag{28a}$$

$$J = Z\omega n^* \simeq 10^{36} \exp(-W_c/kT) \tag{28b}$$

where $n_1 \approx b^{-3} \approx 10^{22}$ cm^{-3}, W_c is the energy of a critical sized loop, $Z \approx 0.1$ is the Zeldovich factor and $\omega = (8\pi r_c/b)\nu_o \approx 10^{15}$ s^{-1} is the frequency factor, r_c being the radius of the critical-sized loop and ν_o the Debye frequency. With these estimates the observability criterion simplified to

$$W_c \lesssim 37kT \tag{29}$$

The authors have taken the loops to be circular, neglecting the variations in line tension associated with screw and edge character, and used a Volterra dislocation model in linear elasticity, accounting for core energies and free surface image effects by adjusting inner and outer cut-off radii, to derive relations for the critical radii r_c and nucleation energies W_c. Using these relations in conjunction with the observability criterion (Equation 29) the critical radii and critical misfits f_c^* for observable onset of misfit strain relief could be calculated at any given temperature.

Although Kamat and Hirth have designed their calculations for applications to {001} interfaces of crystals with diamond cubic or metallic structures, the predicted tendencies will have wide validity. Their approach can be most simply demonstrated for the formation of an interior loop of perfect dislocation $\frac{1}{2}\langle 011\rangle$ on an inclined $\{11\bar{1}\}$ glide plane. The self-energy of a circular loop of radius r is given by[68,69]

$$W_\ell = \frac{(2-\nu)\mu b^2 r}{4(1-\nu)} \ell n\left(\frac{24r}{be^2}\right) \tag{30a}$$

where μ is the shear modulus, ν is Poisson's ratio, b the magnitude of the Burger's vector, e

the Naperian logarithmic base, and the inner cutoff radius is taken as $r_o = b/3$, a value accepted for semiconductors. The coherency strain energy released by the formation of the loop is given by

$$W_e = -\tau b\pi r^2 = -\pi(1+\nu)\mu b r^2 f/\sqrt{6}(1-\nu) \quad (30b)$$

where the misfit f is defined in Equation 1 and τ is the resolved shear stress due to the misfit strain $\bar{e} = f$. Maximizing the total energy of formation $W = W_\ell + W_e$ with respect to r yields, for the radius r_c of the critical nucleus, the equation

$$r_c = \frac{3(2-\nu)b}{4\sqrt{6}\pi(1+\nu)f}\,\ell n\left(\frac{24r_c}{be}\right) \quad (31a)$$

and for the (nucleation) energy W_c of the critical-sized loop, the value

$$W_c = \frac{(2-\nu)\mu b^2 r_c}{8(1+\nu)}\,\ell n\left(\frac{24r_c}{be^3}\right) \quad (31b)$$

Equations 29, 31a, and 31b constitute three equations from which we can solve for the three unknowns: the nucleation energy W_c, the radius r_c of a critical-sized loop, and the critical misfit f_c^* needed for its formation, treating the temperature T as a parameter.

The authors have calculated the "observable" critical misfits f_c^* for dislocation loop nucleation in GaAs and Ag. The magnitudes of these critical misfits f_c^*, when compared with characteristic misfits of GaAs and Ag on various substrates, determine the likelihoods that MDs are generated in such coherently strained epicrystals. The calculations confirmed the expectation that nucleation of MDs are more likely at higher than at lower temperatures and at vicinal (stepped) rather than singular surfaces. The calculations in fact revealed that the nucleation of MDs is highly unlikely at perfect singular surfaces and even at vicinal surfaces; for example, the misfits involved in the epigrowth of GaAs are typically less than 1%, whereas the predicted critical misfit for nucleation of MDs by loop formation at vicinal surfaces is about 9% at temperatures as high as 1000 K. The authors, furthermore, stressed the fact that their calculations ignored the barriers — e.g., the Peierls barriers — to the motion of dislocations, which implies that their results represent lower limits. Kamat and Hirth also calculated the critical thickness at which MDs would be generated from TDs and obtained a result that agrees with the Mathews-Blakeslee prediction and accordingly confirms the perception that TDs constitute the softest MD sources. Their results furthermore showed that the nucleation of MDs in Ag is significantly easier — takes place at a lower misfit — than in GaAs. This result is believed to be generally true for semiconductors and metals.

The work of Kamat and Hirth[68] addressed very important issues and carries the following messages: (1) the nucleation of MDs within, or at the surface of, a perfect semiconductor crystal is highly unlikely, even at fairly high temperatures; (2) the existence of sources (crystal defects) that facilitate the nucleation of MDs is probably a prerequisite; (3) TDs are probably the softest sources; and (4) the nucleation of MDs is easier in metals than in semiconductors. The origin of TDs will be considered in more detail in Section III.G.

Thus far, we have limited the discussion to sources that provide MDs for the onset and early stages of strain relief. While we naturally expect that identical sources will continue to operate during the subsequent multiplication stages, other sources or mechanisms have been identified. Of these, the Hagen-Strunk[12,61,62] mechanism seems to be generally accepted. This source is formed on a {001} interface plane in thin films from the perpendicular crossing of two 60° MDs whose Burgers vectors are parallel. At the crossing point, an annihilation reaction leads to two angular dislocations in an asymmetric configuration. One angular dislocation is attracted toward the free surface where it disconnects, forming two separate dislocations (TDs), each of which generates a MD under the action of the MS stress in a process involving cross-slip. The existence of this source has been confirmed for small misfit systems and is believed also to operate in large misfit systems where it is, unfortunately, difficult to observe.[61]

The "rebound mechanism" proposed by Dregia and Hirth,[56] a mechanism in which an incoming 60° dislocation rebounds at the inter-

face to form a Lomer-type MD there and a receding 60° dislocation, can also act as a multiplication mechanism if the rebounded 60° dislocation acquires sufficient kinetic energy to be reflected from the surface, as was suggested by F. C. Frank many years ago.

Cherns and Stowell[11] have proposed the trigon as a mechanism for MS relief in Pd films grown on {111} Au substrates. The trigon is an extended three-dimensional defect with faulted hexagonal base (parallel to the interface) bounded by three Shockley dislocations (having small Burgers vectors), three stair-rod dislocations, and three inclined faulted {111} planes. No evidence for the widespread occurrence of this mechanism has been presented as yet.

F. Critical Thickness and Residual Strain

In this section we deal with the critical quantities, critical misfit f_c, and critical thickness h_c, mainly with the latter. Critical misfit has been adequately dealt with in Section III.B. Existing calculations of h_c have been summarized previously, for example, by Wagner et al.[71] The name "critical misfit" will be reserved for the equilibrium (minimum energy) critical misfit of a ML; $f_c \equiv f_c^{eq}$. Hence, any epicrystal system having $f < f_c$ will only become unstable with respect to the introduction of MDs at a critical (equilibrium) thickness[2,5] $h_c^{eq} > 1$ ML. Because of the energy barrier to nucleation and motion of MDs an *"observed"* critical thickness for a given system will depend on temperature T, time scale t, and the resolution of the apparatus. Hence, whereas h_c^{eq} is uniquely defined by the properties of the perfect epicrystal system, any h_c^{obs} will not only depend on T, t, and the apparatus, but also on the nature of the MD sources. Accordingly, h_c^{obs} for a given system could be very different from h_c^{eq}.[14,16,20,21,72-74] Obviously, $h_c^{obs} \geq h_c^{eq}$, and possibly $h_c^{obs} \gg h_c^{eq}$, in some instances.

We first consider approaches to calculating the equilibrium critical thickness h_c^{eq}. We classify all calculations based on energy minimization and balancing forces, in this category, the contention being that MDs would be available where and when they are needed for equilibration, or that adequate time for equilibration is allowed. Various attempts had been made to measure h_c^{eq}. Houghton and collaborators[15,75,76] have concluded, on the basis of careful experiments involving extensive annealing of $Si_{1-x}Ge_x/Si$, that the onset of MS relief occurs at the equilibrium critical thickness predicted by Matthews and Blakeslee[70] on the basis of the blowing out of TDs (see Equation 35).

Most existing calculations are facilitated by the fact that the total energy can be expressed as the sum of the energy $E_{\bar{e}}$ of MS and the energy E_D of the MDs, as was revealed by the result in Equation 22. It has been proposed previously[37(b)] that the minimization calculation can be simplified by the approximate criterion that strain relief will commence at a critical thickness for which the pseudomorphic ($|\bar{e}| = f$) MS energy $E_{\bar{e}}$ becomes equal to the MD energy E_D of fully relaxed ($\bar{f} = f$) MS. An analysis has shown[77] that this approximation may introduce discrepancies of up to 25%. The main reason for this is that at slightly supercritical misfit only part, and not all, of the MS is converted into MDs.

Much effort[20,21,73,78,79] has been dedicated recently to attempts at understanding why predictions of critical thickness and residual MS in epilayers do not correlate satisfactorily with observations, and why this discrepancy is larger for semiconductors than in metals, particulary for {111} fcc interfaces. The answers to these questions were essentially given by Matthews[2] and Matthews and Blakeslee.[70] Recent attempts went somewhat further in quantifying critical thickness and the time dependence of strain relief, e.g., those of Dodson and Tsao,[20] Fox and Jesser,[78] and Houghton.[21] An important concept introduced by these authors is that of "excess" or "effective" stress to describe the resultant driving forces for MS relief and their decay as relief progresses. The work of Fox and Jesser is specifically aimed at MDs generated from TDs in epilayers of finite thickness on a thick substrate. Since TDs constitute the most sensitive and abundant sources of MDs, brief reviews of the related theories are justified. The theories also yield, as a limiting case, the equilibrium results of Matthews.[2]

When MDs are generated from TDs, which are usually 60° (mixed) dislocations, the energy minimization calculation is greatly facilitated by

application of the equivalent vanishing of forces, Equation 4c, now given by

$$0 = F = F_e^- - F_\ell - F_f \tag{32}$$

$$F_e^- = Dh\bar{e},$$

$$D = [2\mu_0(1+\nu_0)b \cos \lambda]/(1 - \nu_0) \tag{33a}$$

$$F_\ell = C\, \ell n(R/r_0),$$

$$C = \Gamma b^2(1 - \nu \cos^2 \psi)/2\pi,$$

$$R = h,\ r_0 = b/e \tag{33b}$$

$$F_f = Ahv \exp[U_i/kT] + Bvh \exp[Q_i/kT] + \Delta Eh \exp[W_i/kT] \tag{33c}$$

The apparent absence of a resemblance between Equations 13 and 14a on the one hand, and 33a and 33b on the other, is due to the fact that the former corresponds to energies of pure edge type MDs, whereas the latter corresponds to forces on 60° (mixed) MDs.

In Equation 32, F is the resultant glide force on the mobile segment LB of the TD in Figure 3 — the generating segment whose motion (glide) draws the MD KL in the interface — $F_{\bar{e}}$ is the Peach Koehler MS force, F_ℓ the force exerted by the line tension of the MD,[2,70] and F_f the frictional force. The symbols in Equations 33a to c represent: Poisson's ratio ν for the interface (for convenience usually approximated as $\nu = \nu_o \approx \nu_s$); λ the angle between the Burgers vector b and that normal on the trace of the slip plane and interface that lies in the interface plane; and ψ the angle between b and the MD line. The three terms in F_f represent frictional resistances: consecutively due to Peierls barriers, to scattering of electrons and phonons, and to pinning by impurity atmospheres. A and B are constants, E is a factor depending on impurity concentration, $\Delta = 0$ or 1, depending on whether the dislocation has already escaped the impurity atmosphere or not, U_i is an activation energy for a dislocation (of type i) in overcoming the Peierls barriers, Q_i is an activation energy related to the scattering

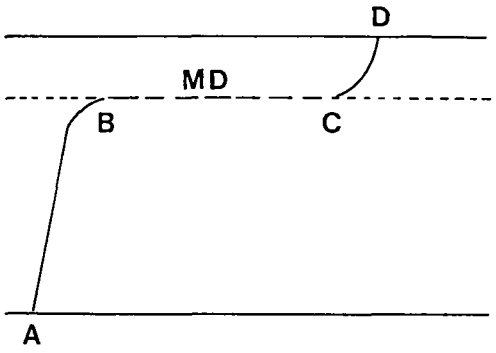

FIGURE 3. Diagram illustrating the generation of a misfit dislocation (MD) BC by the glide motion of the generating segment CD of the threading dislocation ABCD.

resistance experienced by the dislocation (type i) when moving at velocity v, and W_i is an activation energy for diffusion of the atmosphere. Note that the value R = h of the outer cut-off radius R (compare Equation 14c to Equation 33b) applies to the initial stages of MS relief when $\bar{p} > 2$ h; subsequently when $\bar{p}$ falls below 2 h the radius is taken as R = p/2. The term

$$F_p = Avh \exp(U_i/kt) \tag{34}$$

representing the Peierls resistance, has been altered here, as compared to the one of Fox and Jesser, by inclusion of the TD velocity v in order to agree with that of the reference[80] cited by the authors in deriving their result (see Equation 11 of Reference 78). Actually it has been suggested that the force obeys a power law F_p^m (m = 1 to 1.5). The linear dependence in Equation 34 is an approximation introduced[78] for solvability.

The equilibrium critical thickness h_c^{eq}, as calculated by Matthews,[2] follows from the equilibrium Equation 32, by deleting F_f and putting $\bar{e} = f$, while subsequently, when h exceeds h_c^{eq}, we put $\bar{e} = \bar{e}_{eq} < f$; we obtain

$$h = (C/Df)\ell n(eh/b) \quad \text{for } h = h_c^{eq},\ \bar{p}/2 > h_c^{eq} \tag{35a}$$

$$\bar{e}_{eq} = (C/Dh)\ell n(eh/b) \quad \text{for } \bar{p}/2 > h > h_c^{eq} \tag{35b}$$

$$= \frac{C}{Dh}\, \ell n\left[\frac{e}{2(f - \bar{e}_{eq})}\right] \quad \text{for } \bar{p}/2 < h \tag{35c}$$

where we have written, for convenience, $\bar{e}$ instead of $|\bar{e}|$ for the residual strain.

When frictional forces are taken into account we have for the onset ($v = 0$, $\bar{e} = f$) of MS relief, the same equilibrium results as in Equation 35 except that in Equation 35a f must be replaced by $f - \bar{e}_a$;

$$\bar{e}_a = (E/D)\exp(W_i/kT) \tag{36a}$$

to yield a somewhat larger critical thickness due to the resistance of the impurity atmosphere.
In neglecting the velocity dependence of F_p in Equation 34, the authors obtained, instead of $f - \bar{e}_a$, the factor $f - \bar{e}_a - \bar{e}_u$;

$$\bar{e}_u = (E/D)\exp(U_i/kT) \tag{36b}$$

as well as an additional term $\bar{e}_u$ on the right-hand side of Equation 35b. This has led[78] to erroneous predictions of unduly high critical thickness and residual strain, which meant that even at infinite thickness the residual strain ($\bar{e}_u$) is nonzero. This violates the principle that, at nonzero Kelvin, the barrier will be overcome by thermal fluctuations provided one waits long enough.

Fox and Jesser[78] have also attempted a calculation of the rate of MS relief, expressed as the time dependence $\bar{f}(t)$ of the misfit accommodated by MDs at a given supercritical thickness. The authors introduced an equilibrium critical MD density (per atom)

$$\bar{f}_{eq} = f - \bar{e}_{eq} \tag{37}$$

and expressed the TD velocity as

$$v(t) = \kappa[\bar{f}_{eq} - \bar{f}(t)] \tag{38a}$$

$$\frac{1}{\kappa} = \frac{B}{D}\exp\left(\frac{Q_i}{kT}\right) + \frac{A}{B}\exp\left(\frac{U_i}{kT}\right) \tag{38b}$$

where the occurrence of the Peierls term (the second one) is a consequence of having the TD velocity v included in the Peierls resistance, as was done in Equation 34.

The authors adopted a one-to-one correspondence between TDs — being driven by the effective stress — and MDs that they create, and related the linear density

$$N_L(t) = \bar{f}(t)/b\cos\lambda \tag{39}$$

of MDs *per unit length* to the areal density $N_A(t)$ of TDs per unit area at time t, as

$$N_L(t) = \frac{1}{q}\int_0^t N_A(\xi)v(\xi)\,d\xi \tag{40a}$$

$$\approx \frac{1}{q} N_A v t \tag{40b}$$

The approximation in Equation 40b is due to the authors and implies that N_A and v are independent of time; alternatively, that it approximates the rate of MS relief immediately after onset. The quantity q designates the number of slip plane traces on the interface, for example, $q = 2$ for {111} slip plane traces on a {001} interface.
It follows from Equations 38, 39, and 40a that

$$\frac{d\bar{f}}{dt} = \frac{b\cos\lambda}{q} N_A(t)\kappa[\bar{f}_{eq} - \bar{f}(t)] \tag{41}$$

The areal density N_A of TDs can vary with time for at least two reasons: (1) by elimination of TDs on reaching the crystal boundary, and (2) by creation of new TDs at TD sources. If we ignore both mechanisms, as Fox and Jesser have done, we obtain, on integration, the result

$$\bar{f}(t) = \bar{f}_{eq}(1 - e^{-\alpha t}) \tag{42a}$$

$$\alpha = \frac{\kappa b\cos\lambda}{q} \tag{42b}$$

$$= N_A \frac{b\cos\lambda}{q} \Big/ \left[\frac{B}{D} e^{Q_i/kT} + \frac{A}{D} e^{U_i/kT}\right]$$

where N_A is now the initial density.

The additional Peierls term is prominent again. Although this result is rather crude, it does exhibit the anticipated reason for the rate of equilibration being slower in the case of semiconductors as compared to metals, namely, that α is smaller for the latter because of the domination

of the exponential factor in the Peierls term. In the limit of small t Equation 42 reduces to

$$\bar{f}(t) \approx \bar{f}_{eq} \frac{N_A t\, b \cos\lambda}{q} \Big/ \left[\frac{B}{D} e^{Q_i/kT} + \frac{A}{D} e^{U_i/kT}\right] \quad (42c)$$

Fox and Jesser[78] have also considered the creation of additional (multiplication) TDs, but could not take the analysis to a final conclusion, because the multiplication rate is still an unknown quantity. They endeavored though to derive a criterion for equilibration by MS relief through the creation of MDs. They do not state the physical basis for the criterion clearly. It would seem that it is based on the empirical fact that the slope of the observed variation $\bar{f}(h)$ is less than that of the predicted equilibrium variation $\bar{f}_{eq}(h)$, i.e., that $\partial\bar{f}(h)/\partial h < \partial\bar{f}_{eq}(h)/\partial h$. This yields the result

$$r \leq r_c \equiv \frac{Dvh^2 N_A b \cos\lambda}{q\, C\, \ell n(h/b)} \quad (43a)$$

where the growth rate r is defined by

$$h - h_c = rt \quad (43b)$$

and the right-hand side of Equation 43a contains a correction for a typographical error in the original result.[78] Although this is a crude result, it is qualitatively consistent with the expectation that the critical rate r_c will be higher (1) the larger the TD velocity v, i.e., the larger the effective stress; (2) the larger the thickness, i.e., the larger the MS driving force; (3) the larger N_A, i.e., the more abundant the TDs; and (4) the more effective the accommodation of misfit as expressed by $b\cos\lambda$, whereas r_c will be retarded by the line tension embodied in the factor $\ell n(h/b)$.

The variation of plastic strain $\bar{f}(t) = f - e(t)$ with time t for the generation of MDs by TDs nucleated from sources was calculated by Houghton[21] for the initial low dislocation (TD) density regime. The author used the semiempirical expression

$$v(t) = v_0 \left(\frac{\tau_{eff}(t)}{\mu}\right)^m \exp\left(-\frac{Q_v}{kT}\right); \quad m = 1\text{–}1.5 \quad (44)$$

to relate the TD velocity v at temperature T and time t to the effective stress τ_{eff}, an activation energy Q_v involved in TD motion, and a material constant v_o. Note that this is the same relation (with m = 1) that Fox and Jesser[78] had used to write down the expression (34) for the Peierls resistance, and that the time dependence of v originates in the time dependence of τ_{eff}; τ_{eff} decreases with anneal time as plastic strain proceeds by the injection of MDs. Otherwise, the author used the semiempirical relation

$$\frac{dN(t)}{dt} = BN_0 \left(\frac{\tau_{eff}(t)}{\mu}\right)^n \exp\left(-\frac{Q_n}{kT}\right); \quad n \sim 2.5 \quad (45)$$

for the rate of nucleation of TDs, B and n being material constants, N_o the density of incipient TD sources at time t, N(t) the number of activated sources — the supposition being that each source provides just one TD — and Q_n the activation energy for nucleation. The authors assumed that τ_{eff} is time independent and confirmed it experimentally for the regime of interest. This also meant that the TD velocity v could be taken as constant and that the fraction of TDs that escapes is negligible. Under these conditions both Equation 45 and the plastic strain rate equation

$$\frac{d\bar{f}(t)}{dt} = N(t)vb\cos\lambda \quad (46)$$

could be integrated to yield the time dependence of plastic strain as

$$\bar{f}(t) = \frac{1}{2} B\nu_0 N_0 t^2 b \cos\lambda \left(\frac{\tau_{eff}}{\mu}\right)^{n+m} \exp\left(-\frac{Q_n + Q_v}{kT}\right) \quad (47)$$

This result differs, for understandable reasons, in important features from that in Equation 42c: (1) the time dependence in which the former and the latter are proportional, respectively, to t^2 and t, which are, respectively, due to the need to create TDs and to their preexistence, and (2) the activation barrier dependence where, for the former, the barriers to nucleation and motion are in "series", whereas for the latter, the Peierls (U_i) and scattering barriers Q_i are effectively in "parallel".

G. Threading Dislocations and Buffer Layers

A threading dislocation (TD) is a dislocation that threads through the thickness of an epilayer[2] and is a line defect that is most detrimental to the performance and lifetime of a device, for example, by providing an easy diffusion path for dopants and by being a soft source of MDs. Its presence is, accordingly, most undesirable.

Threading dislocations often originate[2] from substrate dislocations that have continued into the epilayer during growth, but may also be generated from dislocation[81] half-loops that are nucleated either at dislocation sources in the epilayer surface by the Peach-Koehler MS stresses, or in an epilayer of critical or near critical misfit that grows in the island mode so that the islands themselves are of supercritical size with high density of MDs — mostly efficient ones in pure edge orientation — when they coalesce.[82-85] Misfit dislocations from adjacent islands that do not form part of a perfect interfacial MD arrangement, and, accordingly, do not connect at the trace of the island-island boundary and the interface, continue as TDs in the growing epilayer.

The conventional way of eliminating TDs is by means of a buffer layer[2,70,84,85] — a misfit strained epilayer of supercritical thickness in which the TDs are bent by the Peach-Koehler MS forces into the interface, where they become MDs — the objective being either to free an active epilayer from TDs, or to generate a substrate (the buffer layer) free of TD sources of MDs. The theory on which the mechanism is based is essentially the Matthews-Blakeslee theory of critical thickness, briefly presented in Section III.F.

The term "buffer layer" also characterizes (1) a thin uniform epilayer grown in the pseudo-ML-by-ML mode at an appropriately high supersaturation — a procedure employed in the "two-step" process — the objective being to grow an epilayer with the desired smoothness of surface[10,86,87] (see Section II.B), and (2) epilayers that are designed to accommodate thermal misfit, for example, a buffer layer of CaF_2 on Si{111} to facilitate the growth of high-quality GaAs.[88]

H. Geometrical Theory of Critical Thickness

A geometrical theory of critical thickness and strain relaxation has been proposed recently by Dunstan et al.,[89] an undertaking that was presumably meant to yield a simplifying approximation of existing theories, and that this author wishes to think of as a zero*th* order approximation, although the authors probably would not agree. The theory is based on a concept of "strain relaxation" that the authors link to the Saint Venants principle and that has some similarity to the concept of an "outer cut-off" radius as is used in the Volterra model of a dislocation. The authors propose that a MD lying at a distance h below the surface can relax MS within a distance mh ($1 < m < 2$) to an amount of $\bar{e} = b/mh$, and none outside, b being the Burgers vector. Ideally, therefore, complete relaxation of the pseudomorphic MS f will be accomplished at a critical thickness h_c with a MD spacing mh_c, such that

$$f = b/mh_c \tag{48}$$

The authors cite the prediction of the one-dimensional Frenkel-Kontorowa model to justify their supposition that at the critical thickness h_c there is an abrupt transition to a relaxed configuration with nearly enough MDs to accommodate all the misfit f. The authors proceed, though, to refine their model by allowing only for a fraction δ of the pseudomorphic MS f to be relieved at $h = h_c$

$$\bar{e}(h) = \begin{cases} f & \text{for } h < h_c \\ \delta f h_c/h & \text{for } h \geq h_c \end{cases} \tag{49}$$

It was also argued that, as the MS decreases, the Peach-Koehler driving stress will eventually fall below the yield limit and that no further plastic deformation (MS relief) will occur. There then exists a fixed residual strain $\bar{e}_r$, even though the thickness increases indefinitely. The authors suggest a dependence of MS strain $\bar{e}$ on thickness h as

$$\bar{e}(h) = \begin{cases} f & \text{for } h < 1/f - \bar{e}_r) \\ 1/2h + \bar{e}_r & h \geq 1/f - \bar{e}_r) \end{cases} \tag{50}$$

Since the theory only invokes physical principles in an indirect and qualitative manner, it cannot be widely reliable and will not be pursued further, even though it may yield useful rule of thumb criteria.

I. Tilted Substrates

Convincing evidence[87,90-92] exists in support of the claim that adequately cut-off substrates — usually Si{001} — facilitate the epigrowth of good-quality compound semiconductors. The full role of the steps is still somewhat unclear. One proposal is that the steps inhibit the formation of antiphase (inversion) domain boundaries — a very undesirable defect — during growth. The theory is partly based on the fact that an inclined surface has an abundance of steps of one sign ("up" or "down") when compared with a surface that is fairly accurate in {001} orientation — in the latter the step density is normally low and the steps occur more or less in pairs of opposite sign — and partly on the assumption that pairs of steps combine into steps of double height, the supposition being that this configuration is energetically more favorable than two separated steps of monotomic height. On a perfect {001} substrate, monatomic steps would be greatly in excess of double-height steps. Monatomic steps are conducive to the formation of antiphase domain boundaries between islands (or overlayers) that have nucleated on neighboring terraces, whereas double steps are not.

Another proposal is based on the observation that epilayers that grow on inclined substrates become tilted themselves,[93] and more so above the critical thickness (or size) when MS is relieved by the introduction of 60° MDs generated from dislocations arriving on parallel {111} glide planes. The tilt is generated by the Burgers vector component normal to the interface. The direction of tilt depends on the sign of the misfit and is such as to reduce the mismatch at the interface and accordingly the need for strain relief, and to enhance the tendency to epitaxy. The tilt of the epilayer generates a tension across the interface on one side of the tilt axis and a compression on the other, a situation that is most favorably accommodated by an appropriate sequence of terrace-step combinations. Alternatively, given the off-cut, the sequence of steps may be conducive to the formation of a given set of 60° MDs. Likewise, with a perfect {001} substrate, the tilt may be avoided by the formation of alternate 60° MDs on different {111} glide planes.

It has also been suggested that efficient Lomer MDs nucleate at the double steps,[92,94] as at edges of supercritical islands, and that the Lomer MDs are less inclined to generate defects, particularly when they are generated in a continuous film.

IV. SUMMARY

The main objective of this critical review is to assess the success of existing theories that have been developed with the view to guiding endeavors at growing perfect crystalline epilayers of uniform thickness. Uniformity is a problem of tailoring the growth mode. This is dealt with in Section II. Section III is dedicated to the understanding of deviations from crystalline perfection by the generation of misfit dislocations (MDs). An important issue has been the accomplished degree of equilibration.

Although the equilibrium criteria of growth modes by Bauer,[8] outlined in Section II.A, are not fully applicable to most practical epigrowth cases, they have become widely accepted for providing useful guidelines in designing epigrowth procedures. The main shortcomings of their application are the lack of knowledge of interface energies and the assignment of thermodynamic properties to ultrathin films.

In Section II.A we have concluded that an island growth stage is almost inevitable in a quasi-equilibrium epigrowth process. In Section II.B it is shown that careful application of nonequilibrium procedures can be employed to "suppress" this undesirable stage and grow in a ML-by-ML fashion, the most effective growth mode for accomplishing thickness uniformity.

This review has been limited to phenomenological theories, the justification being that, although crude, they have accomplished surprising qualitative and quantitative successes. A few comments are appropriate. First, the problem of unharmonicity associated with large pseudomorphic strains cannot be handled within the har-

monic models. Second, the Frenkel-Kontorowa (FK) model expresses the breakdown of linear elasticity at the dislocation in terms of physically meaningful quantities — the coefficients of an optimum Fourier truncation of the periodic interfacial interaction — whereas the Volterra model deals with this breakdown by the introduction of the inner cut-off radius r_o, essentially an adjustable parameter. It is true though, that the Fourier coefficients can be calculated fairly uniquely only for an isolated adatom and less so for epimonolayers and epimultilayers. The FK model is nevertheless recommendable for ultrathin epilayers where bond strength is important. The effect of bond strength decays, though, with thickness and the Volterra model becomes superior for thickening films also because of its mathematical simplicity in handling even MDs of mixed nature (60° MDs).

In Section III.B we have briefly reviewed the application of the Frenkel-Kontorowa model to a monolayer by Frank and van der Merwe. The main assets of the exercise are that the relevant problems can be solved more or less exactly and that the model displays all the topical features of epitaxy: misfit accommodation by misfit strain (MS) and MDs, critical misfit and thickness, activation barriers to MS relief — the generation of MDs — and the reduction of the barrier heights by MS (Peach-Koehler) stresses.

After brief introductions to the types of misfit dislocations that occur and the nature of the forces experienced by dislocations, the important subject of MD sources is dealt with in Section III.E. The essential messages of this section, specifically the work of Kamat and Hirth,[68] are that the observed critical thickness exceeds the predicted equilibrium value and that normally sources are needed for the generation of MDs; dislocation (half) loops that are nucleated at the sources expand to form TDs that bow out under the Peach-Koehler MS stresses to lay the MDs at the interface. TDs constitute the softest sources of MDs. The acquisition of TDs are more fully considered in Section III.B.

Fox and Jesser[78] and Houghton[21] have analyzed the onset (equilibrium critical thickness) and the time dependence (continued generation of MDs) of MS relief (see Section III.F). Whereas Fox and Jesser have taken existing TDs directly as sources, Houghton has considered the nucleation of TDs from prefabricated sources. Both approaches include the effect of Peierls barriers and solve the governing equations for the initial stage (near onset) of MS relief only, the main constraint being the lack of knowledge regarding TD multiplication rates. The results nevertheless clearly display the retarding effect of Peierls barriers, confirming the anticipated reason for time-dependent differences in MS relief for semiconductors and metals. A measurement of "equilibrium" critical thickness agreed with the theory, as was also predicted by Matthews and Blakeslee.[70]

In a geometrical theory of critical thickness, Dunstan and co-workers[89] proposed that a MD lying at a distance h below the surface relaxes MS to an amount b/mh ($1 < m < 2$) and none outside. On the basis of this concept, they proposed a critical thickness dependence on misfit and a thickness dependence of residual strain. This theory, which is justified by handwaving arguments, could be greatly in error in specific cases.

Tilt mechanisms of MS relief are briefly and superficially dealt with.

It is evident that many important topics have not been considered, and that much still needs to be done before the chapter on growing epilayers of uniform thickness and perfect crystalline structure is completed.

ACKNOWLEDGMENT

The Foundation for Research Development is gratefully acknowledged.

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