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STRESS EFFECTS IN MULTILAYERS

by

W. A. Jesser

Department of Materials Science
School of Engineering and Applied Science
University of Virginia
Charlottesville, VA 22901

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INTRODUCTION

The research progress on calculations of interfacial stress in abrupt junctions and its effect on the defect state of the interface has yielded significant progress in the form of a series of papers. The first paper is coauthored with Professor J. H. van der Merwe and has been submitted to the Journal of Applied Physics. The second paper in the series is being completed. As the title indicates the sharp interfaces in a multilayered superlattice is treated for the case of equal elastic constants and layer thicknesses. Part II of the series is for the same case but unequal elastic constants and thicknesses. Part III of the series is not well formed but is aimed at multilayers with different misfits such as those of step graded junctions or layers of altered lattice constants by means other than composition variation e.g., variations in binding states from layer to layer. The series is expected to conclude with Part IV which will treat abrupt interfaces in mesa structures or other structures exhibiting finite width as opposed to infinite lateral extent. The following paper included in this progress report is the unreviewed part I of the series.

AN EXACTLY SOLVABLE MODEL FOR CALCULATING CRITICAL MISFIT AND THICKNESS IN EPITAXIAL SUPERLATTICES. I. LAYERS OF EQUAL ELASTIC CONSTANTS AND THICKNESSES.

Jan H. van der Merwe and W.A. Jesser[a)]

Department of Physics, University of Pretoria, Pretoria 0002, Republic of South Africa.

A parabolic interaction potential has been used to develop a model for calculating the misfit dislocation (MD) energy in the case of a superlattice of alternating layers of materials with equal elastic constants and thicknesses. The model, which is believed to be a good one for small misfits and to have some merit for covalent bonded materials, is exactly solvable for the critical thickness above which it is energetically favorable to lose coherency by the introduction of MD's into the interfaces. It was found, for a given misfit f, that the critical thickness for epitaxial superlattices free from their substrate is somewhat more than four times that for a single epilayer on a thick substrate. Furthermore, the critical thickness varies almost inversely with misfit to the power 1.22, when Poisson's ratio is 1/3. It was also shown that the critical misfit f_c obtained by equating maximal misfit strain and MD energies is a significant overestimate of f_c. The results for a superlattice are compared with those of a thin layer on a thick substrate.

a) Permanent address: Department of Materials Science, University of Virginia, Charlottesville, Va 22901, U.S.A.

I. INTRODUCTION

The concept of a limiting misfit as the upper limit of misfit below which epitaxial growth may occur, was introduced by Royer[1]. This motivated Frank and van der Merwe[2] to introduce the relevant concepts of misfit strain (MS), misfit dislocations (MD's), critical misfit f_c and critical thickness h_c. The *critical misfit* f_c is the limiting misfit below which a layer of fixed thickness is homogeneously strained into registry with the substrate and h_c is the *critical layer thickness* above which an interface of given natural misfit loses registry by the introduction of MD's.

When epitaxy became involved in the fabrication of devices needing crystals of high perfection, knowledge regarding f_c and h_c assumed great importance and calculations have been made assuming equilibrated MD densities. Although notable successes had been achieved with this approach[3,4], observed densities were frequently greatly in excess of the predicted densities[5-7]. This discrepancy has often been attributed to non-equilibrium features of the growth process and to approximations needed to facilitate the analysis. Previous calculations have employed the Volterra approximation to MD's using the concept of a "cut-off radius" to account for the dislocation core energy, the presence of other MD's and the nearby free surface[5-8] for films of finite thickness. While the reliability of these approximations has been justified[9] for the case in which the crystal thickness is of the order of the MD spacing and larger, this is not so otherwise. Furthermore an approximate procedure of energy minimization[3,8,9] has often been used too. This procedure, expressed by Eq. (42) is questionable particularly for small misfits.

The above regimes of concern, low misfit and thin crystals, are precisely those encountered in superlattice structures. It is thus of importance to resolve these issues so that confidence can be gained in the approximations adopted in calculations of f_c and h_c, particularly in the case of superlattices. At the same time one can contribute towards solving the problems associated with the equilibrium accommodation of misfit by MD's and MS for all misfits and thicknesses.

In this paper an exact solution of the "thin film-small misfit" case for superlattices is obtained using the socalled parabolic model[9]. In this model the periodic interaction potential between the crystals across an interface is modelled by a succession of parabolic arcs rather than the sinusoidal description of the Frenkel-Kontorowa[10] and Peierls Nabarro models[11,12]. Because of its sharply peaked crests it will be a more realistic representation for short ranged covalent bonding characteristic of many superlattices of semiconducting materials.

In part I of this series we deal with the simplest case of a superlattice of similar materials where the layers have equal thicknesses as well as a thin film on a thick substrate of similar materials. This will be extended and generalized in subsequent parts to the more complicated cases of a thin superlattice film on a thick substrate and to superlattices of dissimilar materials and layers of unequal thicknesses.

II. MODEL

We make the conventional assumptions (i) that the crystals A (upper) and B (lower) have simple cubic structure with lattice parameters a and b respectively[11,12,13], (ii) that a and b may be generated from a reference lattice with lattice parameter c defined by[13]

$$p = Pa = (P+1)b = (P+\tfrac{1}{2})c, \qquad (1)$$

where P is an integer and (iii) that the crystals deform under applied forces like isotropic elastic continua with shear moduli μ_a and μ_b and Poissons ratios ν_a and ν_b [11-13]. Equation (1) defines f, c and the MD spacing p as

$$p = \frac{ab}{a-b}, \quad c = \frac{ab}{(a+b)/2}, \quad f \equiv \frac{c}{p} = \frac{a-b}{(a+b)/2}. \qquad (2)$$

The interfacial atoms are subjected to two competing forces: the atomic interaction across the interface which tends to align atoms on either side and the opposing elastic forces. The former is most simply modelled as a shear stress τ having the periodicity c in the relative "displacement" U of interfacial atoms which were in registry in the reference lattice [11-12]. The two most common models for τ are the Peierls-Nabarro model[11-13] that uses a sinusoidal dependence, and the parabolic potential model[9] in which there is a piecewise linear dependence between τ and U:

$$\tau(U) = \mu_i U/d \text{ for } |U| \leq d/2 = c/2, \qquad (3)$$

where we may take the separation d of the two interfacial surfaces equal to c and the interfacial shear modulus μ_i is a measure of the bonding across the interface. The relation (3) is repeated within every period c of U to form a saw tooth pattern. For mathematical convenience we consider at first a one-dimensional sequence of saw teeth as would obtain from one-dimensional misfit as defined in Eqs.(1) and (2). Two-dimensionality will be introduced in a subsequent section.

The elastic relaxation introduced by $\tau(U)$ generates an atomic

pattern with a sequence of localized disregistries constituting a single sequence of misfit dislocations (MD's)[2,9]. They are spaced at intervals p and said to "accommodate" the misfit f. The misfit can also be partly accommodated by misfit strain $\bar{e}$, i.e. a homogeneous strain which is superimposed on the oscillatory strains of the MD's, to reduce or eliminate the misfit[2-9]. Naturally this is only possible when one or both crystals are of finite thickness, which is the case in the crystal pairs constituting a superlattice.

For mathematical simplicity the members of the pair will be assumed to have identical elastic properties. They will then be strained by equal amounts when they are equally thick. Thus, if the average lattice parameters in the strained configuration are $\bar{a}$ and $\bar{b}$, the misfit strain $\bar{e}$ will be given by

$$\bar{e} = \frac{b - \bar{b}}{b} = \frac{\bar{a} - a}{a} . \tag{4}$$

It follows that in the strained configuration the relations (2) become

$$\bar{p} = p \frac{(1 - \bar{e}^2)}{(1 - 2\bar{e}/f)} , \quad \bar{c} = c \frac{1 - \bar{e}^2}{1 - \bar{e}f/2} , \quad \bar{f} = \frac{\bar{c}}{\bar{p}} = \frac{f - 2\bar{e}}{1 - \bar{e}^2} . \tag{5}$$

It is seen that $\bar{f}$ vanishes ($\bar{p} = \infty$) when $\bar{e} = \frac{1}{2} f$, as is implicit in Eqs. (4), and that to first order

$$c = \bar{c} \quad \text{and} \quad f = \bar{f} + 2\,\bar{e}. \tag{6}$$

The second relation in Eqs. (6) is the mathematical statement that the misfit is accommodated by MD's and misfit strain (MS) jointly.

An important consequence of the presence of MD's is that opposing

interfacial surfaces may undergo different displacements $w^a(x,0+)$ and $w^b(x,0-)$ normal to the interface where superscripts a and b relate to layers A and B respectively. Accordingly these displacements induce normal forces which we may, using Hooke's law, model as an interfacial normal stress

$$N[W(x)] = \frac{2\mu_i}{1-2\nu_i}\left[\frac{w^a(x,0+) - w^b(x,0-)}{d}\right] = \frac{2\mu_i}{1-2\nu_i}\frac{W(x)}{d}, \tag{7}$$

where $W(x)$ is the relative normal elastic displacement of the two opposing surfaces, ν_i an appropriate Poisson's ratio of the interface and $d = c$. Figure 1 displays one period of a superlattice of alternating A and B layers, and the coordinate axes, with origin midway between MD's.

We have introduced the simplifying assumption that A and B are elastically equivalent including the interface.

This implies that

$$\mu_i = \mu_a = \mu_b \equiv \mu, \quad \nu_i = \nu_a = \nu_b \equiv \nu \tag{8}$$

and allows us to have the layers equally thick; of thickness $2h = 2\eta c$, say. Apart from automatically satisfying the lateral force balance implied by Eq. (4), it also facilitates the simplifications in Eqs. (10) below.

The bicrystal layer between midplanes PQ and P'Q' in Fig. 1 with the interface MN may now be taken as a representative unit of the superlattice. Careful consideration of the relevant physical principles and the geometry displayed in Fig. 1 guided us to adopt the following

simplifying assumptions for the interior bicrystal unit of an extensive superlattice containing MD's:

All field quantities (stresses p_{ij}, τ and N) have the periodicity of the MD spacing p (or $\bar{p}$) e.g.

$$p_{xx}(x + p,z) = p_{xx}(x,z). \tag{9a}$$

Because of the source of antisymmetry, U(x), one also has antisymmetry in $\tau(U(x))$ of Eq. (3) and in $p_{zx}(x,0) = \tau(U(x))$, hence $p_{zx}(x,z)$ is antisymmetric in x:

$$p_{zx}(-x,z) = - p_{zx}(x,z). \tag{9b}$$

The stresses p_{zz} and p_{zx}, that act on the interface surfaces, are continuous across the interface, i.e.

$$\begin{aligned} p^{a}_{zx}(x,0+) &= p^{b}_{zx}(x,0-) = \tau[U(x)] \\ p^{a}_{zz}(x,0+) &= p^{b}_{zz}(x,0-) = N[W(x)] \ . \end{aligned} \tag{10a}$$

Because of symmetry $p_{zx}(x,z)$ and w(x,z) vanish on the midplanes PQ and P'Q', i.e.

$$p_{zx}(x,z) = 0, \quad w(x,z) = 0 \text{ at } z = \pm h. \tag{10b}$$

Three more remarks are appropriate. (i) Because the interaction energy between the homogeneous misfit strain and the oscillatory strains that are associated with the MD's vanishes they may be treated independently. This allows us, as in Eq. (9a), to use p for the MD spacing in the calculations and introduce the strained value $\bar{p}$ (see

Eq. (5)) when needed. (ii) Also, with the simple cubic crystals under consideration there will be a cross grid of MD's, rather than a single sequence. We make the simplifying approximation that the relevant energies of the MD's are additive as is expressed in Eq. (31) below. (iii) The conditions (10) strictly apply to the interior of the superlattice, "far" (possibly two to four layers) from the free surfaces and "substrate" employed to fabricate the superlattice.

III. GOVERNING EQUATION AND ITS SOLUTION

We assume that the MD's are long and straight. The related problem is accordingly one of plane strain which is normally analysed in terms of an Airy stress function $\chi(x,z)$ satisfying the biharmonic equation[14]

$$\nabla^4 \chi = 0 \tag{11}$$

and, defining the stresses in terms of the relations

$$p_{xx} = \frac{\partial^2 \chi}{\partial z^2}, \quad p_{zz} = \frac{\partial^2 \chi}{\partial x^2}, \quad p_{zx} = -\frac{\partial^2 \chi}{\partial x \partial z}. \tag{12}$$

The solutions of (11) satisfying the periodicity (9a) and having the symmetry (9b) can be expressed in Fourier transforms[9]

$$\chi^{a,b} = [(A^{a,b} + zC^{a,b}) \cosh mz + (B^{a,b} + zD^{a,b}) \sinh mz] \cos mx, \tag{13a}$$

$$m = 2\pi n/p, \quad n = 1,2, \ldots\ldots \infty \tag{13b}$$

where A, B, C and D are as yet unknown Fourier coefficients and summation is implied in all analogous subsequent expressions. By applying (12) we obtain results of the form (deleting superscripts):

$$p_{\{xx\}_{zz}} = m\left[\{{m(A+zC)+2D \atop -m(A+zC)}\}\cosh mz + \{{m(B+zD)+2C \atop -m(B+zD)}\}\sinh mz\right]\cos mx, \qquad (14)$$

$$p_{zx} = m\left[\{m(B+zD)+C\}\cosh mz + \{m(A+zC)+D\}\sinh mz\right]\sin mx.$$

In order to employ Eqs. (10) we need expressions for the x- and z-components of displacement u and w. We first obtain from Hooke's law the strains e_{ij} as

$$2\mu e_{xx} = \left[(1-\nu)p_{xx} - \nu p_{zz}\right], \quad \mu e_{zx} = p_{zx}: \qquad (15)$$

$$2\mu e_{\{xx\}_{zz}} = m\left[\{{m(A+zC)+2(1-\nu)D \atop -m(A+zC)-2\nu D}\}\cosh mz + \{{m(B+zD)+2(1-\nu)C \atop -m(B+zD)-2\nu C}\}\sinh mz\right]\cos mx,$$

$$\mu e_{zx} = m\left[\{m(B+zD)+C\}\cosh mz + \{m(A+zC)+D\}\sinh mz\right]\sin mx. \qquad (16)$$

We now calculate consecutively the rotation ω_y and the displacements u and w by path integration of the form

$$u = u_o + \int\left(\frac{\partial u}{\partial x}\,dx + \frac{\partial u}{\partial z}\,dz\right), \quad u_o = 0, \qquad (17)$$

where

$$\frac{\partial \omega_y}{\partial x} = -\frac{1}{2}\frac{\partial e_{zx}}{\partial x} + \frac{\partial e_{xx}}{\partial z}, \quad \frac{\partial \omega_y}{\partial z} = \frac{1}{2}\frac{\partial e_{zx}}{\partial z} - \frac{\partial e_{zz}}{\partial x}$$

$$\frac{\partial u}{\partial x} = e_{xx}, \quad \frac{\partial u}{\partial z} = \frac{1}{2}e_{zx} + \omega_y, \quad \frac{\partial w}{\partial x} = \frac{1}{2}e_{zx} - \omega_y, \quad \frac{\partial w}{\partial z} = e_{zz}\,. \qquad (18)$$

We obtain

$$2\mu\omega_y = 2(1-\nu)m^2[D\cosh mz + C\sinh mz]\sin mx.$$

$$2\mu u = [\{m(A+zC)+2(1-\nu)D\}\cosh mz + \{m(B+zD)+2(1-\nu)C\}\sinh mz]\sin mx \qquad (19)$$

$$2\mu w = -[\{m(B+zD)-(1-2\nu)C\}\cosh mz + \{m(A+zC)-(1-2\nu)D\}\sinh mz]\cos mx$$

and hence, at $z=0$

$$U(x) = \frac{xd}{p} + u^a - u^b = \frac{xd}{p} + [\frac{m}{2\mu}(A^a - A^b) + \frac{1-\nu}{\mu}(D^a - D^b)]\sin mx,$$

$$W(x) = \frac{1}{2\mu}[m(B^b - B^a) + (1-2\nu)(C^a - C^b)]\cos mx, \qquad (20)$$

where we had used Eqs. (8), and xd/p is the nonelastic vernier relative displacement due to the misfit.

The governing equations, i.e. the equations defining the Fourier coefficients are obtained by substituting from Eqs. (3), (7), (14), (19) and (20) into (10):

$$-m^2A^a + m^2A^b = 0 \qquad (a)$$

$$m(mB^a + C^a) - m(mB^b + C^b) = 0 \qquad (b)$$

$$m\{m(B^a + hD^a) + C^a\}c + m\{m(A^a + hC^a) + D^a\}s = 0 \qquad (c)$$

$$m\{m(B^b - hD^b) + C^b\}c - m\{m(A^b - hC^b) + D^b\}s = 0 \qquad (d)$$

$$\{m(B^a + hD^a) - (1-2\nu)C^a\}c + \{m(A^a + hC^a) - (1-2\nu)D^a\}s = 0 \qquad (e) \qquad (21)$$

$$\{m(B^b - hD^b) - (1-2\nu)C^b\}c - \{m(A^b - hC^b) - (1-2\nu)D^b\}s = 0 \qquad (f)$$

$$-m^2A^a + \frac{1}{(1-2\nu)d}\{mB^a - (1-2\nu)C^a\} - \frac{1}{(1-2\nu)d}\{mB^b - (1-2\nu)C^b\} = 0 \qquad (g)$$

$$m(mB^a + C^a) - \frac{m}{2d}(A^a - A^b) - \frac{1-\nu}{d}(D^a - D^b) = \frac{\mu(-1)^{n+1}}{\pi n}, \qquad (h)$$

where

$$c \equiv \cosh mh \quad \text{and} \quad s \equiv \sinh mh, \tag{22}$$

we had used the elastic equivalence of crystals A and B (See Eqs. (8)) and $(-1)^{n+1}d/\pi n$ for the Fourier sine coefficient of xd/p. Note that c in (21) and(22) is not the same as the reference lattice constant c in Eq. (1). The latter we also approximate by d. This system of linear equations may be solved to give

$$\begin{aligned}
&A^b = A^a = 0, \quad \Delta = -m^4(mh + sc) - 2\gamma m^3 s^2 \\
&B^b = B^a = \frac{D^b}{c^2} = -\frac{D^a}{c^2}, \quad \frac{D^a}{\Delta} = \frac{\mu(-1)^{n+1}}{\pi n(P+Q)} \\
&P = (mh + sc)m^4 c^{-2}[m(mh + sc) + 2\gamma s^2] \\
&Q = 2(1-\nu)d^{-1}m^3[m(mh + sc) + 2\gamma s^2].
\end{aligned} \tag{23}$$

where,

$$h\gamma = 2(1-\nu)h/(1-2\nu)d = 4\eta \quad \text{for } \nu = 1/3, \quad \eta \equiv h/d = h/c. \tag{24}$$

Important quantities which we need for subsequent calculations are $p_{zx}(x,0)$ and $U(x)$. We obtain by substituting from Eqs. (23) into (14) and (20)

$$p_{zx}(x,0) = \sum_{n=1}^{\infty} P_n D_n^a \sin mx, \tag{25}$$

$$U(x) = \frac{cx}{p} + \sum_{n=1}^{\infty} Q_n D_n^a \sin mx, \tag{26}$$

where P_n, Q_n and D_n^a are the P, Q and D^a in Eqs. (23).

Also the quantity Q/P plays a significant role and may be

written as

$$\phi(X) = n\beta\frac{Q(X)}{P(X)} = \frac{c^2}{cs + X} \tag{27}$$

where

$$\beta = \frac{\pi d}{(1-\nu)p} = (\frac{\pi}{1-\nu})f \quad \text{and}$$
$$X = 2\pi hn/p = 2\pi\eta fn = \zeta n \tag{28}$$

and γh is defined in Eq. (24).

The relations (23) - (28) now constitute the solution of the problem concerned with the atomic relaxations resulting from the competing interactions. A plot of U v.s. x will display the resolution of the interface into a sequence of MD's spaced at distances p[9,13]. *When MS coexists with MD's p,c and f must be replaced everywhere by the MS dependent quantities* $\bar{p}$, $\bar{c}$ and $\bar{f}$ defined in Eqs. (5).

IV. ENERGY

The energy per unit area of an interface consists of several contributions: the MD strain energies E_D^a and E_D^b in the two crystals and the energy of misfit E_m due to the residual disregistry at the interface. The homogeneous misfit strain energies $E_{\bar{e}}^a$ and $E_{\bar{e}}^b$ in the two crystals may simply be added to the above energies to yield the total energy. The sum of the latter two energies is given by the well known expression[3,15]

$$E_{\bar{e}} = 4[(1+\nu)/(1-\nu)]\mu c\eta\bar{e}^2 \tag{29}$$

which incorporates the equality of the elastic constants (Eq. (8)) and equality of MS along the interfacial cubic axes. It has also previously been

shown[9] that the energy per unit area of interface associated with the MD's i.e. $E_D = E_D^a + E_D^b + E_m$, in units of $\mu c/4\pi^2$, is given by

$$\varepsilon_D = E_D / \frac{\mu c}{4\pi^2} = \frac{1}{2p} \int_{-p/2}^{p/2} dx \, \frac{cx}{p} \, p_{zx}(x,0) / \frac{\mu c}{4\pi^2}$$

$$= \sum_{n=1}^{\infty} \frac{1}{n[n + \beta^{-1}\phi(X)]} \tag{30}$$

where the second line follows on using Eqs. (25) - (28). Since in the case of quadratic symmetry under consideration there is a cross-grid of MD's the total energy per unit area of the interface is given by

$$E = E_{\bar{e}} + 2E_D = \frac{8(1+\nu)\mu c\eta}{1-\nu} \left[\frac{\bar{e}^2}{2} + \frac{1-\nu}{16\pi^2(1+\nu)\eta} \varepsilon_D(\bar{\beta},\bar{X})\right], \tag{31}$$

where everywhere β and X should be replaced by $\bar{\beta}$ and $\bar{X}$ i.e. f by $\bar{f}$, to stress their dependence on the MS $\bar{e}$ as defined by Eqs. (5) and (6).

We can execute two consecutive approximations to the results in Eqs. (30) and (31), which are of interest. The first one is the thick ($h,\eta \to \infty$) limit E_D^∞. It follows from (27) and (28) that in this case (provided $\bar{f} \to f \neq 0$).

$$\phi(X) = 1 \qquad \text{for } \eta \to \infty, \quad \text{and} \tag{32}$$

$$\varepsilon_D^\infty \equiv E_D^\infty / \frac{\mu c}{4\pi^2} = \sum_{n=1}^{\infty} \frac{1}{n(n + 1/\beta)} \, . \tag{33}$$

This agrees with a previous[9] result and may be written in terms of derivatives of the gamma function $\Gamma(x)$[16] as

$$\varepsilon_D^\infty = \beta[\psi(1 + 1/\beta) + \gamma_o] \, , \tag{34}$$

where $\psi(x)$ is the digamma function $\Gamma'(x)/\Gamma(x)$ and $\gamma_o = 0.5772 \ldots$ is Euler's constant.

The second approximation to the result in Eq. (33) is to replace the sum by an integral:

$$\varepsilon_D^{\infty} = \int_{n_i}^{\infty} \frac{dn}{n(n + 1/\beta)} = \beta \ln(1 + \frac{1}{n_i\beta}). \tag{35a}$$

Both the value of the lower integration limit n_i and the accuracy of this integral in representing the sum may be assessed through a comparison of the relations in (34) and (35). As $n = 1$ for the first term in the sum of Eq. (33), the appropriate lower limit of the integral in Eq. (35a) is expected to be somewhat less than unity. We obtain the value of n_i as

$$n_i = \exp(-\gamma_o) = 0.561 \tag{35b}$$

by comparing Eqs. (34) and (35a) for large values of $1/\beta$.
In this case

$$\varepsilon_D^{\infty} = \beta \ln(e\gamma_o/\beta) \approx \beta \ln(1/n_i\beta), \tag{36}$$

which gives the result in Eq. (35b) for n_i.

We now return to the general case of Eq. (30) and adopt the approach employed for the "infinitely thick" layer in replacing the sum by an integral:

$$\varepsilon_D = \bar{\zeta} \int_{n_i\bar{\zeta}}^{\infty} \frac{d\bar{X}}{\bar{X}[\bar{X} + \alpha\phi(\bar{X})]} \equiv \bar{\zeta} I(n_i\bar{\zeta}, \alpha). \tag{37}$$

Using the transformations and definitions of Eqs. (28) we obtain

$$\bar{X} = \bar{m}h \equiv \bar{\zeta}n; \quad \bar{\zeta} = 2\pi\eta\bar{f}, \quad \eta = h/c, \quad \bar{f} = f - 2\bar{e},$$
$$\bar{\zeta}/\bar{\beta} = 2(1-\nu)\eta \equiv \alpha , \tag{38}$$

where the "bar" signals the presence of MS $\bar{e}$.

Near the critical thickness, which is presently an important regime $\bar{X} \to 0$ because $\bar{f} \to 0$ and hence $\phi(\bar{X}) \to \infty$. The series accordingly converges exceedingly slowly and the integral approximation (37) becomes more convenient. However, the integrand is rather complicated and does not lend itself to exact integration. Since $\phi(\bar{X})$ tends to unity as $\bar{X}$ becomes large and is already almost unity at $\bar{X} = 2$ it remains to find an acceptable approximation for small $\bar{X}$. Power series expansion of $\bar{c}$ ($\equiv \cosh\bar{X}$) and $\bar{s}$ suggests a sufficiently simple representation of the form $\phi(\bar{X}) = A/\bar{X} + B\bar{X}$ where A and B are rational functions of η. Numerical comparison has shown that

$$\phi(\bar{X}) = \begin{cases} \dfrac{1}{2\bar{X}}\left(1 + \dfrac{2\bar{X}^2}{3}\right) & \text{for } \bar{X} \leqslant 2 \\ 1 & \text{for } \bar{X} \geqslant 2 \end{cases} \tag{39a}$$

is an acceptable approximation. It is accordingly convenient to divide the interval $(n_i\bar{\zeta}, \infty)$ of integration into two subintervals $(n_i\bar{\zeta}, \bar{X}_t)$ and $(\bar{X}_t, \infty)$ where the transition value of $\bar{X}$ is

$$\bar{X}_t = 2 + n_i\bar{\zeta} . \tag{39b}$$

We obtain on integration

$$\varepsilon_D = \bar{\zeta} I(n_i\bar{\zeta}) = \frac{\bar{\zeta}}{\alpha}\{\frac{2}{B}\left[\arctan B\bar{X}_t - \arctan Bn_i\bar{\zeta}\right] + \ell n(1 + \frac{\alpha}{\bar{X}_t})\}, \quad (40a)$$

where

$$B = \{\frac{9 + 4\eta}{6\eta}\}^{\frac{1}{2}}, \quad \bar{\zeta} = \bar{\beta}\alpha \quad (40b)$$

and the $n_i\bar{\zeta}$ dependence of $I(n_i\bar{\zeta})$ relates only to the lower limit $n_i\bar{\zeta}$ in (37) and not $n_i\bar{\zeta}$ in (39b).

A comparison of the integrated relations (40) with the sum in Eq. (30) (summing over sufficient terms to reach $\bar{\zeta}n \equiv \bar{X} = 2$ and integrating from $\bar{X} = 2$ onwards) shows that the discrepancy does not exceed 6%. The sum is the greater of the two. Note, however that the relations (40) should be restricted to misfit values $\bar{f} \leqslant 1/\pi\eta$. Above this value Eq. (35a) should be used.

In the limit $\bar{\zeta} = 2\pi\eta\bar{f} \to 0$ $(\bar{f} \to 0)$ the thickness approaches the critical value and $I(n_i\bar{\zeta})$ in (40) becomes

$$I(0) = \frac{2}{\alpha B}\arctan 2B + \frac{1}{\alpha}\ell n(1 + \frac{\alpha}{2}). \quad (41)$$

When however, η and hence $\bar{\zeta} = 2\pi\eta\bar{f} \to 2\pi\eta f$ becomes large at nonzero f, ε_D as defined by (40a) approaches the value in Eq. (35), as it should.

V. EQUILIBRIUM: CRITICAL MISFIT AND THICKNESS

In the past the critical misfit f at which the minimum energy configuration undergoes a transition from a coherent interface to one with MD's has often been approximated by setting the energy for the coherent configuration (MS $\bar{e} = \frac{1}{2} f_c$ for a superlattice) equal

to one with only MD's, characterized by natural misfit f_c, i.e.

$$E_{\bar{e}}(f_c,\eta) = 2E_D(f_c,\eta), \tag{42}$$

the contention being that there are either no MD's or enough to accommodate practically all the misfit as in the one-dimensional Frenkel-Kontorowa model[2]. Alternatively, the critical thickness $h_c = \eta_c c$ is the thickness at which equilibrium considerations require MD's to be injected for given misfit f. Thus η_c is defined by (42) by setting $f_c = f$ and $\eta = \eta_c$.

The true criterion for the minimizing strain $\bar{e}_m$ is

$$\partial E/\partial \bar{e} = 0 \quad \text{at} \quad \bar{e} = \bar{e}_m . \tag{43}$$

Among others we wish to assess the accuracy of (42). Since the integral formulation of ε_D in Eq. (37) facilitates the numerical evaluation of ε_D we perform the minimization of E in Eq. (31) using the relation (37) rather than the series in (30). We obtain after some simplification

$$\bar{e}_m = \frac{(1-\nu)}{4\pi(1+\nu)} \left[I(\bar{X}_m,\alpha) - \{\bar{X}_m + \alpha\phi(\bar{X}_m,\alpha)\}^{-1} \right], \tag{44a}$$

where

$$\bar{X}_m = n_i \bar{\zeta}_m, \quad \bar{\zeta}_m = 2\pi\eta\bar{f}_m = 2\pi\eta(f - 2\bar{e}_m), \tag{44b}$$

as may be seen with reference to Eqs. (6) and (38). Hence, for a given thickness η, the critical misfit f_c follows by letting $\bar{e}_m \to f_c/2$ yielding

$$f_c(\eta) = \frac{(1-\nu)}{2\pi(1+\nu)} I(0,\alpha), \tag{45}$$

interface is large, one needs analytical expressions that accurately give the energy of the MD arrays per unit area per interface. Both of these regimes of interest have been satisfied through the development of Eqs. (37) - (41). It is instructive to compare the energy values obtained from this result for different misfit values, which must be small because of the approximations involved in Eq. (6).

Figure 2 displays the functional dependence of the MD energy per unit area per interface of a superlattice free from its substrate. The thick curve labelled ∞ is a plot of Eq. (35) which represents "infinitely thick" layers. The numbered curves are plots of Eq. (40) with each number representing the thickness value. For purposes of comparison the MD energy for a thin layer on a thick substrate is also shown. The superlattice curve labelled 1 closely approximates the curve for a monolayer on a thick substrate up to values of $f \leqslant 0.1$. The thick curve labelled ∞ also represents the asymptotic value of the thin layer on an infinitely thick substrate for the layer thickness being large. Because of the choice of a representative section of the superlattice for purposes of calculation, a monolayered superlattice corresponds to $\eta = \frac{1}{2}$ (see Fig. 1) and is labelled by this thickness value. Only for the infinite layer is the slope of the curve infinite at the origin. In all cases the slopes decrease with increasing misfit at constant thickness and also decrease at zero misfit as the thickness value is decreased. The nearly linear rise of the energy with misfit for a very thin layered superlattice

can be understood from the arrays of MD's which act nearly independently of their in-plane spacing and therefore contribute to the superlattice energy essentially in proportion to their number density.

One notices that there are regions of f for which the value of ε_D exceeds that value ε_D^∞ for the infinitely thick layered superlattice. The misfit values for which this occurs are near $\eta f = 1/\pi$ which is also near the transition value $\bar{X}_t$ of Eq. (39). The rise of ε_D over ε_D^∞ is not caused by the approximations involved in Eq. (39) but is also found in the exact representation Eq. (30). Mathematically it occurs because $\phi(X)$ in Eq. (30) falls below unity near $\bar{X}_t$ while $\phi(\bar{X})$ = unity for all $\bar{X}$ when $\eta \to \infty$ (Eq. (33)). Physically this result can be understood as a consequence of the boundary conditions for the superlattice case. There is the constraint of zero displacement at the midplanes of a superlattice layer while the free surface of the thin layer on a thick substrate is stress free.

A comparison of the MD energy of a superlattice with that of a single layer on a thick substrate shows that when the layer thickness of the superlattice is small, strong cancellation of the stress fields of the MD's in adjacent layers occurs provided the misfit is not too large. The magnitude of this cancellation

reduces the MD energy by about 20% in a monolayered superlattice of small misfit as compared to a single monolayer on a thick substrate.

Also shown in Fig. 2 is a graphical comparison of the two methods for determining at a fixed thickness η, the critical misfit f_c above which it is energetically favorable to introduce MD's into the interface of a superlattice. This pair of misfit-thickness values is exactly equivalent to giving the critical thickness $\eta_c(=\eta)$ for loss of coherency in a superlattice of fixed misfit $f(=f_c)$. The one method of equating the homogeneous strain (MS) energy of a coherent superlattice to the MD energy when all the misfit is accommodated by MD's is given analytically by Eq. (42) and graphically by the intersection point of the homogeneous strain energy (plotted against $f = 2\bar{e}$) with the MD energy curve. Plots of this situation are shown for two thickness values. The homogeneous strain energy curves A and B (dotted parabolas) correspond respectively to half-layer thickness values of η equal to 10 and 1. The intersection points are near misfit values respectively of 0.0315 and 0.154 which are also the calculated values from Eq. (42). The second and proper method of calculating the critical misfit-(critical) thickness pair of values is equivalent to equating the slope of the MD energy curve at the origin (all of the misfit is accommodated by MS) to the slope of the same value on the homogeneous strain energy curve. This is the condition expressed by Eq. (43) for $\bar{e}_m = \frac{1}{2} f$ and is shown in Fig. 2 for the case $\eta = 1$ by the two (dashed) tangents T. One tangent touches the MD energy curve at the origin to determine its slope, and the other tangent of the same slope is placed in contact with the homogeneous strain energy curve at the unique point of the same slope labelled i.

This point is at the misfit value 0.131 which is also the calculated value from Eq. (45). Notice that the misfit values given by the two methods, one proper and labelled i, the other approximate and labelled ii are rather different (0.131 versus 0.154); ii is too high by about 17%. Clearly the proper method is preferred and offers an improvement over the approximate one.[3,8,9,17]

An exploration of how the magnitude of this overestimate varies with thickness revealed that it varied from about 17% for a monolayered superlattice to about 35% for large values of η, i.e. over a thousand monolayers. A similar comparison of the estimated critical thickness for a given misfit showed that the estimate exceeded the proper value by about 30% when the layer thickness is small and by about 40% when η is large. This result suggests that one could "correct" the estimated value of critical thickness by multiplying it with a factor of about 0.75.

The main objective of the present considerations is to find an exact expression for calculating the critical thickness η_c above which loss of coherency at a given misfit is energetically favorable (Eq. (45)). The evaluation of this expression for the case of uniform elastic constants ($\mu_a = \mu_b = \mu_i = \mu$) and $\nu = \frac{1}{3}$ is displayed in the curves of Fig. 3. Here one sees a strong dependence of η_c on natural misfit f for small values of f. From a log-log plot (inset on Fig. 3) of the thickness-misfit values a nearly straight line emerges so that over a range of values a power law models the dependence fairly accurately. It follows from the figure that

$$\eta_c \approx 0.114\ f^{-1.22}\ , \tag{46a}$$

or equivalently

$$f_c \approx 0.17\ \eta^{-0.82}. \tag{46b}$$

These expressions describe the equilibrium case for which there are no barriers to the acquisition of MD's. In practice barriers exist and therefore one expects significant departures from these equilibrium values when comparisons with experimental values are made. These differences between experiment and theory are common with the experimental values of MD densities exceeding the theoretical ones particularly in the case of semiconductor materials where the frictional force opposing the motion and nucleation of MD's can be quite large. One can see the magnitude of these differences for example in the work of Matthews[3] and People and Bean[8].

It is of interest to compare the results of the present development for superlattices of individual layer thickness 2η to the same parabolic-potential model but for an infinite substrate and a single epitaxial film of equivalent thickness 2η (Appendix). There are two differences between these two cases. The first difference is that for the case of superlattices, the parallel MD arrays in adjacent interfaces strongly interact when the layer is thin and lower the energy of the MD array in comparison to that of the single-interface case on the infinite

substrate. The second and more important difference lies in the accommodation of misfit by homogeneous elastic strain. For the superlattice each layer accommodates half the misfit so that the N interfaces and N+1 layers can become coherent with one half of the elastic strain that is required to produce a coherent interface in the infinite-substrate case. Because of the square dependence of the homogeneous strain energy on strain, this introduces a factor of four between the two cases. The combined effect on critical thickness of these two differences is displayed in the Table.

The thickness of the single layer is compared to twice the half-thickness of each superlattice layer. The ratio of layer thickness for loss of coherency in the case of a superlattice, as compared to that of a single layer on a thick substrate is about five for small layer thicknesses and approaches four for large thicknesses. This result agrees with factor of four argued for superlattices by Matthews and Blakeslee[18]. The ratio of critical misfits for these two cases also approaches four for thick layers but starts at a factor of about three for a thin layer.

The ratio of critical thicknesses greater than the factor four introduced by the homogeneous elastic strain term can be understood in terms of the slope of the MD energy as a function of misfit. The MD energy for the superlattice case is less than that for the case of an infinite substrate. Correspondingly the slope of this curve is also less at the common value of misfit at the origin. In satisfying the parallel tangent condition this results in an overall shift in critical thickness values by a factor somewhat more than four when comparing the superlattice case to the case of an infinitely thick substrate.

VII. CONCLUSIONS

A parabolic interaction potential has been applied to the case of a free standing superlattice of many layers to obtain an exact solution for the energy of the arrays of misfit dislocations at the interfaces. An analytic expression for this energy as a function of misfit and layer thickness is provided in Eqs. (37) and (40). The main results of this theoretical development are:

1. The energetically favored critical thickness for loss of coherency depends approximately inversely on misfit to the power 1.22 for the case of uniform elastic constants and a Poisson's ratio of 1/3.

2. A comparison of the critical thickness in a superlattice with that of a single layer on a thick substrate shows that for a fixed misfit, the critical thickness of the superlattice is between four and five times that of the single layer. This result occurs because for the superlattice case each layer accommodates half the misfit and the derivative $\partial\varepsilon_D/\partial f$ of the MD energy, ε_D is somewhat smaller than that of the thick-substrate case at $f \to 0$, except for large layer thicknesses where the values of ε_D approach one another.

3. Estimating the critical thickness and critical misfit by equating the maximum strain energy ($\bar{e} = f/2$) to the maximum misfit dislocation energy ($\bar{e} = 0$) was shown to be rather crude; the estimated critical misfit for given thickness is too high by about 25% for all thicknesses. Similarly the estimated critical thickness for given misfit is too high by about 35%.

4. The equilibrium elastic strain and hence the lattice constants of

the superlattice vary nearly inversely with thickness once the critical thickness for loss of coherency has been exceeded.

5. The pointed high crests of the parabolic potential, which is the main objection to the model has on the one hand little impact when the misfit is small (MD's far apart) and otherwise may have merit for short ranged covalently bonded materials. Its main advantage is that it yields an exactly solvable model for the critical misfit and critical thickness.

6. The MD energy per unit area per interface for a thin layered superlattice can rise slightly above that for an infinitely thick layered superlattice when ηf is near $1/\pi$.

7. The analysis applies to the interior of the superlattice far from the free surfaces.

ACKNOWLEDGEMENTS

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APPENDIX: THIN EPILAYER ON A THICK SUBSTRATE

A comparison of the thin epilayer - thick-substrate case with the superlattice had always been of great interest. This interest still persists. The former can be dealt with by some modification of the superlattice analysis. Although this had been dealt with previously the results needed for the present comparison have not been given and can be derived rather compactly from the foregoing calculations.

Let A be the thin layer of thickness h and B by a semiinfinite substrate. The main modification in the model is that the midplane boundary conditions (10b) need be replaced by

$$p^a_{zx}(x,z) = 0, \quad p^a_{zz}(x,z) = 0 \quad \text{at } z = h \tag{A.1}$$

for the free boundary of A and

$$p_{ij}(x,z) \to 0 \text{ as } z \to \infty \tag{A.2}$$

for the vanishing of the stresses in B far from the interface; i (and j) being either x or z.

The condition (A.2) can be incorporated by deleting the e^{-mz} parts of χ^b, (Eq. (13a)) and in subsequent expressions relating to B. This is most simply handled by putting

$$A^b = B^b, \quad C^b = D^b. \tag{A.3}$$

We may thus write down the quantities

$$p^b_{xz} = m[\,m(A^b + zC^b) + C^b]\,e^{mz}\sin mx$$

$$p^b_{zz} = -\,m^2(A^b + zC^b)e^{mz}\cos mx$$

$$u^b(x,z) = \frac{1}{2\mu}\,[\,m(A^b + zC^b) + 2(1-\nu)C^b]\,e^{mz}\sin mx \qquad (A.4)$$

$$w^b(x,z) = -\,\frac{1}{2\mu}[\,m(A^b + zC^b) - (1-2\nu)C^b]\,e^{mz}\cos mx$$

which we need explicitly below and in which we had used the elastic equivalence in Eqs. (7). It now follows from Eqs. (19) and (A.4) that

$$U(x) = xd/p + \{mA^a + 2(1-\nu)D^a - mA^b + 2(1-\nu)C^b\}/2\mu$$

$$W(x) = \{-mB^a + (1-2\nu)C^a + mA^b - (1-2\nu)C^b\}/\mu\,. \qquad (A.5)$$

Substitution from Eqs. (14), (A.4) and (A.5) into (10a) and from (A.4) into (A .1) shows that Eqs. (21) (a) - (c) and (h) are unchanged and that otherwise we obtain for $p^a_{zz}(x,h) = 0$ in (A.1) and $p^a_{zz}(x,0+) = N[W(x)]$ in (10a) the relations

$$-m(A^a + hC^a)c - m(B^a + hD^a)s = 0$$
$$-m^2A^a + \frac{1}{(1-2\nu)d}\,[\,mB^a - (1-2\nu)C^a - mB^b + (1-2\nu)C^b] = 0. \qquad (A.6)$$

(A.6) and (21) (a) - (c) and (h) are six equations needed to solve for the six unknown Fourier coefficients. Our main interest is to calculate ε_D using the integral in Eq. (30). Hence we only need the values of B^a and C^a in

$$p^a_{zx} = m[\,mB^a + C^a]\,\sin mx. \qquad (A.7)$$

We obtain

$$
\begin{aligned}
B^a &= -(m^3h^2 + \delta m^2h^2)R/\Delta, \\
C^a &= [\, m^2s^2 + \delta m(sc + s^2 + mh)]R/\Delta, \\
\Delta &= m(P + Q), \quad R = (\mu/\pi n)(-1)^{n+1}, \\
P &= m^3(s^2 - m^2h^2) + m^2\delta(s^2 + sc + mh - m^2h^2), \\
Q &= \lambda m^2(s^2 + cs - mh - m^2h^2) + m\lambda\delta\,(c+s)^2, \qquad \text{(A.8)} \\
\lambda &= (1-\nu)/d, \quad \delta = \lambda/(1-2\nu), \quad \alpha = \bar{\zeta}/\bar{\beta}\,, \\
p_{zx}\,(x,0) &= R/(1 + QP^{-1}), \\
\varepsilon_D &= \sum_1^{\infty} \frac{1}{n[\,n + \phi(\bar{X})/\beta]} \simeq \bar{\zeta} \int_{n_i\bar{\zeta}}^{\infty} \frac{d\bar{X}}{\bar{X}[\,\bar{X} + \alpha\phi(\bar{X})]}\,, \\
\phi(\bar{X}) &= \frac{mQ}{2\lambda P} = \frac{\bar{\beta}nhQ}{hP} = \frac{1}{2}\,\frac{\bar{X}(\bar{s}^2 + \bar{c}\bar{s} - \bar{X} - \bar{X}^2) + \delta h(\bar{c}+\bar{s})^2}{\bar{X}(\bar{s}^2 - \bar{X}^2) + \delta h(\bar{s}^2 + \bar{s}\bar{c} + \bar{X} - \bar{X}^2)}\,,
\end{aligned}
$$

where $\bar{c}$, $\bar{s}$, and $\bar{X}$ have been defined in Eqs. (22) and (28). At this point it is of interest to note that $\phi(\bar{X}) \to 1$ as $\bar{X} \to \infty$ $(\eta \to \infty)$ as before so that the same result as in Eq. (33) is obtained for large thicknesses but that no simple expression like (39) for small $\bar{X}$, could be obtained that connects accurately enough to $\phi(\bar{X}) = 1$.

With respect to energy minimization we obtain, instead of the relations (6), (31), (38), (44a) and (45):

$$
\begin{aligned}
f^t &= \bar{f}^t + \bar{e}^t, \quad \bar{\zeta}^t = 2\pi\eta^t(f^t - \bar{e}), \quad \bar{X}^t = n\bar{\zeta}^t, \quad \bar{X}_m^t = n_i\bar{\zeta}_m, \quad \alpha^t = 2(1-\nu)\eta^t \\
E &= \frac{4(1+\nu)\mu c\eta^t}{1-\nu}\left[\left(\frac{\bar{e}^t}{2}\right)^2 + \frac{(1-\nu)}{8\pi^2(1+\nu)\eta^t}\,\bar{\zeta}^t I(\bar{X}^t, \alpha^t)\right] \qquad \text{(A.9)} \\
\bar{e}_m^t &= \frac{(1-\nu)}{4\pi(1+\nu)}\left[\, I(\bar{X}_m^t, \alpha^t) - \{\bar{X}_m^t + \alpha^t\phi^t(\bar{X}_m^t, \alpha^t)\}^{-1}\right] \\
f_c^t(\eta^t) &= \frac{1-\nu}{4\pi(1+\nu)}\, I(0, \alpha^t),
\end{aligned}
$$

with $I(\bar{X}_m^t, \alpha^t)$ and $I(0, \alpha^t)$ given by Eq. (37) not by Eqs. (40a) and (41),

where the letter t designates (t)hin film-(t)hick substrate. It is notable that the expression for $\bar{e}_m^t$ in (A.9) is of the same form as $\bar{e}_m$ in Eq. (44a) but that the expression for f_c^t in (A.9) differs from that for f_c in Eq. (45) by a factor of two; that is apart from the fact that $\phi^t \equiv \phi$ in Eq. (A.8) is a different function and that we usually make a comparison where the layers in the superlattice have the same thickness as the thin film, i.e. $\eta = \frac{1}{2}\eta^t$.

References

[1] L. Royer, Bull. Soc. Fr. Mineral. 51, 7 (1928).

[2] F.C. Frank and J.H. van der Merwe, Proc. Roy. Soc. Ser. A198, 205, 216 (1949).

[3] J.W. Matthews, Dislocations in Solids, Ed. F.R.N. Nabarro, (North Holland Pub. Co. 1979), p.461; Epitaxial Growth, Ed. J.W. Matthews, (Academic Press, New York 1975), p.559.

[4] M. Shinohara, T. Ito, K. Yamada, and Y. Imamura. Jap. J. Appl. Phys. 24, L711 (1985).

[5] J.C. Bean, L.C. Feldman, A.T. Fiory, S. Nakahara, and I.K. Robinson, J. Vac. Sci. Technol. A2, 436 (1984).

[6] P.M.J. Mareé, R.I.J. Olthof, J.W.M. Frenken, and J.F. van der Veen, J. Appl. Phys. 58, 3097 (1985).

[7] E.J. Fantner, H. Clemens and G. Bauer, in Advances in X-ray analysis, Vol. 27, edited by Cohen, Russ, Leuden, Barrett and Predecki (Plenum Publishing Corporation, 1984) p.171.

[8] R. People and J.C. Bean, Appl. Phys. Lett. 47, 322 (1985); 49, 229 (1986).

[9] J.H. van der Merwe, J. Appl. Phys. 34, 117, 123 (1963).

[10] J. Frenkel and T. Kontorowa, Phys. Z. Sowjetunion 13, 1 (1938).

[11] R.E. Peierls, Proc. Phys. Soc. London, 52, 34 (1940).

[12] F.R.N. Nabarro, Proc. Phys. Soc. London, 52, 90 (1940).

[13] J.H. van der Merwe, Proc. Phys. Soc. London, A63, 616 (1950).

[14] S. Timoshenko, Theory of Elasticity (McGraw-Hill, New York, 1934) pp. 12-134.

[15] W.A. Jesser and D. Kuhlmann-Wilsdorf, Phys. Stat. Sol.19, 95 (1967).

[16] Handbook of Mathematical Functions, Eds. M. Abramowitz and I.A. Segun (Dover Publications, New York, 1968) pp.259, 267-276.

[17] J.H. van der Merwe, J. Woltersdorf and W.A. Jesser, Mater. Sci. & Eng., 81, 1 (1986).

[18] J.W. Matthews and A.E. Blakeslee, J. Cryst. Growth 27, 118 (1974); 29, 273 (1975); 32, 265 (1976).

TABLE. Comparison of the critical thickness η_c^t of a single layer on a thick substrate and $2\eta_c$ of a layer in a superlattice when the natural misfit f is the same in both; similarly the critical misfits f_c and f_c^t respectively are compared for equivalent thicknesses $\eta_c^t = 2\eta_c$.

f^t	η_c^t	$2\eta_c$	$2\eta_c/\eta_c^t$	f_c/f_c^t
.07143	1	5.09	5.09	2.78
.04395	2	10.08	5.04	2.99
.01283	10	49.3	4.93	3.45
.001955	100	460	4.60	3.66

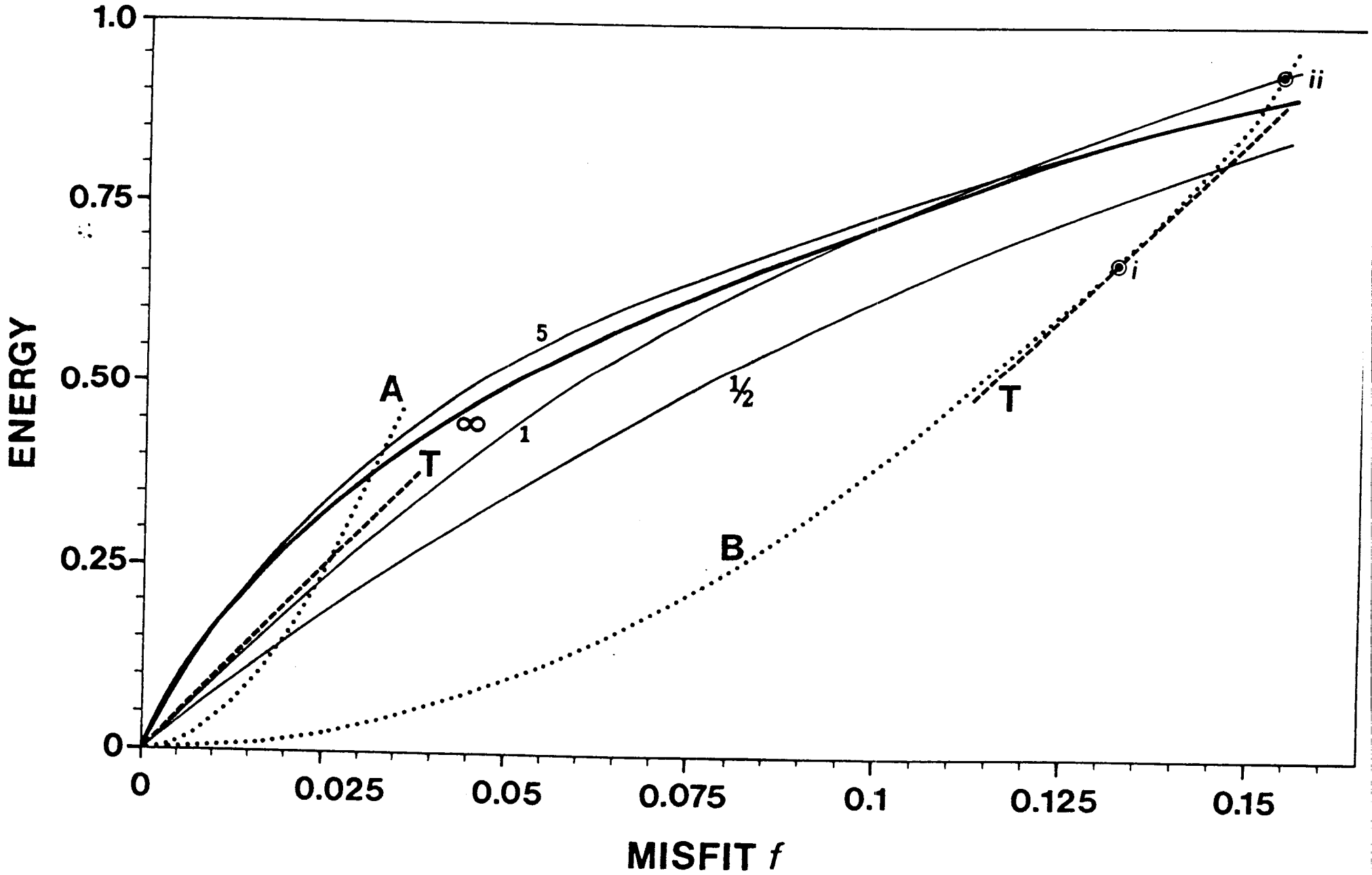
Figure Captions

Fig.1. Schematic representation of a superlattice of alternating layers A and B of equal thickness $2h = 2\eta c$. The AB and BA interfaces are represented by solid lines and contain planar arrays of MD's of alternating sign as shown. The coordinate origin is in an interface and lies midway between MD's with the z-axis normal to the interface planes and the y-axis along the axis of the MD's shown. A representative section of the superlattice is given by the mid planes P'Q' in layer A and PQ in layer B each lying at a distance $h = \eta c$ on either side of the reference interface MN that contains the origin and is located in the interior of the stack of layers.

Fig.2. Misfit dislocation energy per unit area ϵ_D (numbered solid curves in units of $\mu c/4\pi^2$) as a function of misfit f and homogeneous elastic strain energy per unit area $E_{\bar{e}}/(\mu c/2\pi^2)$, (lettered dotted curves) as a function of $\bar{e} = f/2$. For calculational purposes $\mu_a = \mu_b = \mu_i = \mu$ and $\nu = 1/3$. The thick curve labelled ∞ corresponds to Eq. (35) while the rest of the numbered curves are given by equation (40) with the numbers referring to the half-thickness $\eta = h/c$. Strain-energy curves A and B refer respectively to $\eta = 10$ and 1. The two linear tangents T are drawn by dashes for the case $\eta = 1$ and define the critical misfit f_c by $\partial(2E_D + E_{\bar{e}})/\partial\bar{e} = 0$ at $\bar{e}_m = f_c/2$ given by point i. Point ii represents an approximation to the critical misfit as calculated by $2E_D(f_c) = E_{\bar{e}}(\bar{e}_m = f_c/2)$. Note that the value of critical

misfit at i ($f_c \sim 0.131$) is rather different from that of point ii ($f_c \sim 0.154$).

Fig.3. Graph of the relationship between critical thickness η_c and the corresponding critical misfit f_c. Note from the inserted log-log plot that the critical thickness is reasonably approximated by a power law with an exponent near 1.22.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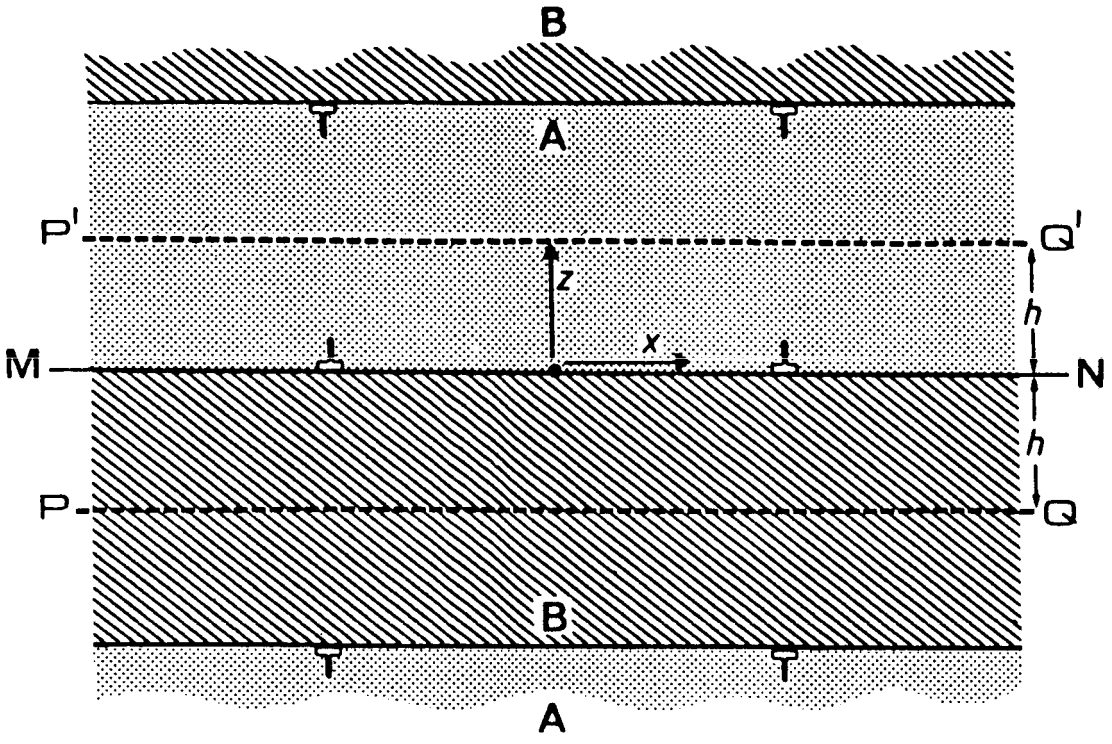
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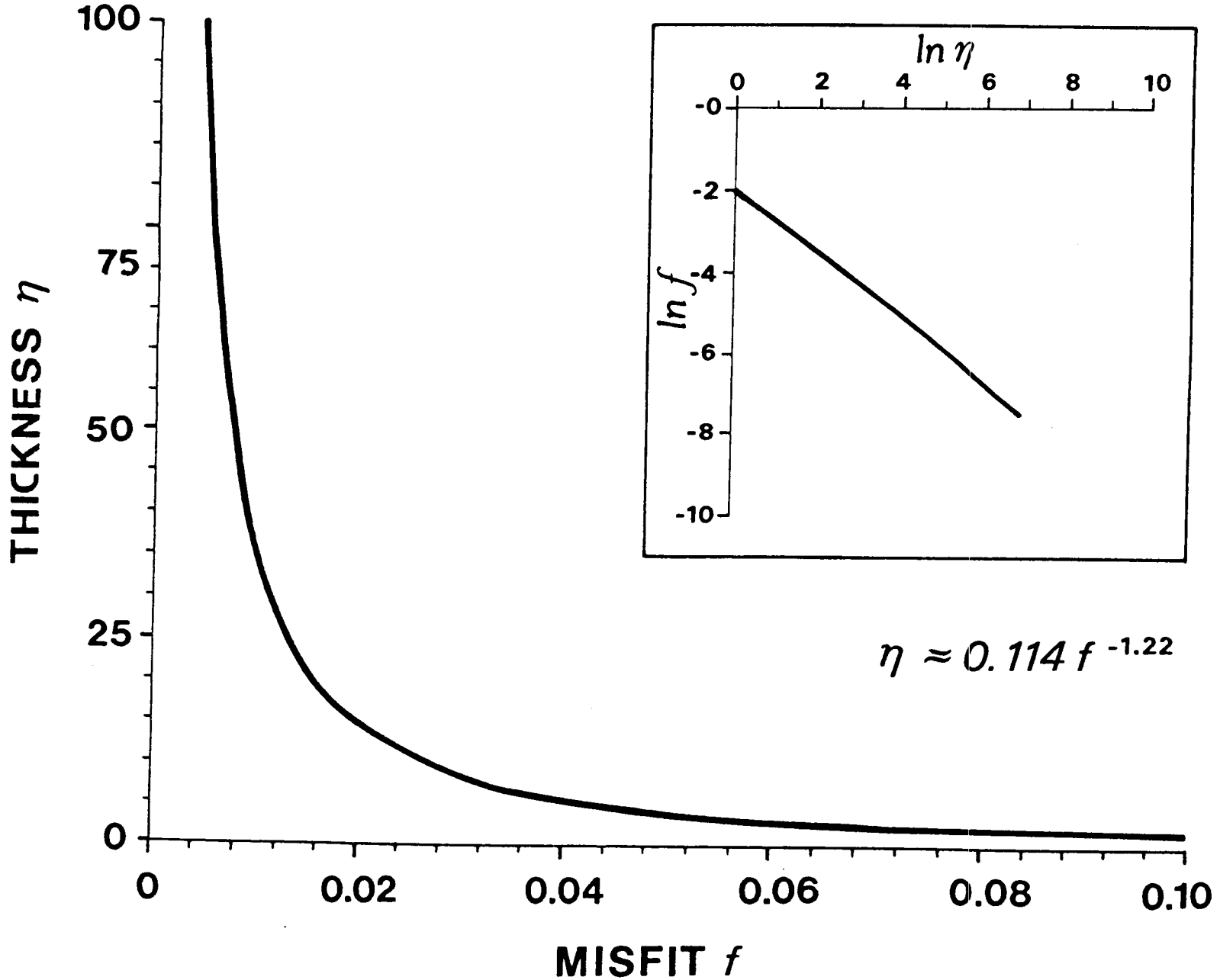
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