Equilibrium theory of strained epitaxial layers

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We develop a simple theory of the equilibrium stability of strained epitaxial layers on a rigid substrate based on a generalization of the continuum theory. Each layer is treated as a continuum elastic medium while the coupling between layers is treated in a discrete manner. Using a periodic parabolic interaction between adjacent layers, we obtain exact numerical results for the stability boundary of the epitaxial phase, $\delta(N)$, expressed as a function of the misfit δ and the number of layers N. In addition, we develop a variational approach which agrees very well with the exact results. Our method interpolates between a few layers and the thick-film limit of the continuum theory, and in this limit we recover the standard result for the relation between misfit and critical thickness. Considerable deviations from continuum theory can occur in the thin-film limit. For very weak coupling to the substrate, we find $\delta(N) \propto N^{-1/2}$. The present approach has the advantage of allowing different misfits and elastic constants for each layer and arbitrary variations in the interlayer couplings.

I. INTRODUCTION

There has been a great deal of work, both theoretical and experimental, on the structure of strained epitaxial layers, which has become particularly important in recent years with the advent of molecular-beam-epitaxy (MBE) technology.[1-5] This allows the growth of artificial structures of arbitrary complexity. The main interest in these structures is in their electronic properties for device applications, but there are still fundamental questions on the stability of these structures. As the thickness of the strained adsorbed layer grows, the elastic energy eventually overcomes the commensuration energy and the adsorbed layer becomes incommensurate with the substrate. There are various estimates of the stability criteria which can be expressed as a relation between the misfit parameter δ and the number of layers, N. Conventional elasticity theory yields a relation[1]

$$\delta(N) \propto (\ln N)/N \ , \tag{1}$$

where the stability limit is taken to be the point when the energy of a misfit dislocation vanishes.

Experiments on semiconductor epitaxial layers[6,7] such as $Si_{1-x}Ge_x/Si$ seem to obey this relation when grown at high temperatures, but at lower temperatures a relation like $\delta \sim N^{-1/2}$ is a better fit to the data. The epitaxial layers in this situation correspond to a metastable configuration. Some energy barrier has to be overcome before a misfit dislocation can be nucleated.

This paper is concerned with the equilibrium thickness of an overlayer at very low temperature. Existing theoretical approaches consist of either numerical molecular-dynamics studies[8] or continuum elasticity models.[1] In our approach, we compute the energy of a single misfit dislocation as a function of thickness. The vanishing of this energy is taken to signal the critical thickness for a given misfit. We generalize the model of Frank and van der Merwe[9] to N layers, but do not use the continuum elasticity approximation in the vertical direction. The model can describe the equilibrium properties of an arbitrarily complex overlayer consisting of several parts of different elastic constants and misfits which can be used to describe a superlattice. We solve the model in a simple case of a rigid substrate and N adsorbed layers of the same type and leave extensions to more complex situations such as a superlattice to a future publication.

II. MODEL

In this section, we develop a model of N layers of adsorbate on a substrate as a generalization of the Frank and van der Merwe model of a single layer[9] in which it is assumed, for simplicity, that the overlayer can become incommensurate with the substrate in one direction only. We further assume that each layer can be described by continuum elasticity theory but the coupling between layers is treated in a discrete fashion. This allows for abrupt changes in the system in the direction normal to the substrate. The model is described by the Hamiltonian

$$E = \int dx \left[\tfrac{1}{2} \sum_{n=-N_s}^{N} K_n |(\nabla - iG_n)\rho_n(x)|^2 - \sum_{n=-N_s}^{N-1} v_{n,n+1}[\rho_n(x)\rho_{n+1}^*(x) + \text{c.c.}] \right], \tag{2}$$

where $\rho_n(x)=e^{i\theta_n(x)}$. In Eq. (2), $2\pi/(d\theta/dx)$ has the meaning of local spacing between atoms. This can be seen as follows. When the nth overlayer assumes its natural spacing a_n, $\theta_n(x)=G_n x$, where $G_n=2\pi/a_n$ is the basic reciprocal-lattice vector for the nth overlayer. In this case, $2\pi/(d\theta/dx)\equiv a_n$. When the spacing of the particles in the overlayer is not uniform, then $d\theta_n/dx$ is no longer constant and $2\pi/(d\theta_n/dx)$ has the meaning of a local spacing $a_n(x)$. The deviation from natural spacing a_n would cause an elastic energy proportional to $|\nabla\theta_n(x)-G_n|^2$ which is the origin of the first term in (2). The second term in Eq. (2) is the epitaxial energy. It is finite and negative when adjacent layers are in registry but vanishes when they are out of registry. The competition of the two terms in the energy expression (2) determines whether the lowest energy of the film corresponds to an epitaxial configuration or not. The summations are taken over the N_s+1 substrate layers and the N adsorbed layers. Displacements are allowed only in the x direction—the direction of mismatch. This is a somewhat unrealistic assumption which is equivalent to the constraint that the spacing between layers is held fixed which could be relaxed at the expense of introducing extra phases into $\rho_n(x)$ with the associated extra mathematical complexity. However, the model of Eq. (1) captures the essence of the epitaxy as a function of misfit and film thickness. In this work we do not consider surface effects. Accounting for both mismatch and surface tension can lead to an instability giving rise to droplet formation.[10] Finite-temperature effects also leads to additional mathematical problems. Even for the simplest system, consisting only of two coupled layers in the absence of a substrate, the resulting phase diagram as a function of temperature and misfit differences has a rich structure.[11] These effects will not be considered here. This model is suitable if all the G_n are almost equal and the ratios $G_n/G_m\neq p/q$. This is the situation commonly occurring in strained epitaxial layers where the natural periodicities typically differ at most 5%, and the ground state for thin layers is the epitaxial (commensurate) configuration. This justifies the neglect of higher harmonics in the free energy of the form $\mathrm{Re}(\rho_n^p\rho_m^{*q})$ which would be important if the ground state were a higher-order commensurate state. When written in terms of the phase variables $\theta_n(x)$, the energy becomes

$$E=\int dx\left[\frac{1}{2}\sum_{n=-N_s}^{N}K_n(\nabla\theta_n-G_n)^2-\sum_{n=-N_s}^{N-1}v_{n+1,n}\cos(\theta_{n+1}-\theta_n)\right]. \tag{3}$$

This model is still very general despite all the simplifications, allowing for the loss of registry between any pair of layers, arbitrary misfits between layers, an elastic substrate, and the study of arbitrary superlattice configurations. For the purposes of this paper which is an initial study of this model, we assume a rigid substrate which is modeled by

$$K_n=\infty, \quad -N_s\leq n\leq 0\ . \tag{4}$$

This is not a serious approximation provided the substrate is much thicker than the overlayer ($N_s\gg N$). With this approximation, the energy is minimized for the substrate layers by the choice

$$\theta(x)=G_s x, \quad -N_s\leq n\leq 0 \tag{5}$$

where G_s is the substrate reciprocal-lattice vector. Defining for the adsorbed layers

$$\theta_n(x)=G_s x-\phi_n(x), \quad 1\leq n\leq N \tag{6}$$

where ϕ_n is a measure of the displacement of the nth layer from perfect registry, we obtain

$$E-E_0=\int dx\left[\frac{1}{2}\sum_{n=1}^{N}K_n(\nabla\phi_n-\delta_n)^2+\sum_{n=0}^{N-1}v_{n,n+1}[1-\cos(\phi_{n+1}-\phi_n)]-\frac{1}{2}\sum_{n=1}^{N}K_n\delta_n^2\right], \tag{7}$$

where $\delta_n=G_s-G_n$ is the usual misfit parameter measuring the mismatch between the lattice spacing of the substrate and the nth adsorbed layer. With this definition, $\delta_n>0$ implies that the natural spacing of the nth layer is larger than the substrate period. Throughout the paper we will consider the $\delta>0$ case. The other one can be treated in a completely equivalent manner. This form can be used to study the stability of an arbitrary superlattice on a rigid substrate by choosing the mismatches δ_n appropriately, but in this paper we make the further simplification to a system of N identical layers so that $K_n=K$, $\delta_n=\delta$, $v_{n,n+1}=v$ ($n\geq 1$) is the coupling between adjacent layers of the adsorbate and $v_{01}=h$ is the coupling of the bottom layer to the substrate (note that $\phi_0=0$).

III. STABILITY ANALYSIS

The criterion for loss of registry we shall use follows the standard theory of the commensurate-incommensurate transition at zero temperature in which one searches for the point at which the energy of a misfit dislocation vanishes.[12] The aim of this paper is to find the stability boundary, $\delta(N)$, at which the overlayer loses complete registry with the substrate and to investigate where in the system the misfit dislocations first appear. This type of analysis is relevant to systems in which the energy barrier to misfit dislocation formation is very low. However, many experimental systems such as Si-Ge alloys grown on a clean Si substrate at low temperatures are metastable configurations presumably due to a large energy barrier. This is an extremely interesting and important problem, but it is outside the scope of this paper.

The analysis follows the standard route by minimization of the energy with respect to ϕ_n, but this leads to a system of coupled sine-Gordon equations which are somewhat intractable even when $N=2$, so we replace the cosine interaction by a periodic parabolic interaction

$$(1-\cos\phi)\rightarrow V(\phi)=\tfrac{1}{2}\phi^2, \quad -\pi<\phi<\pi$$
$$V(\phi+2\pi)=V(\phi)\ . \tag{8}$$

This approximation has also been used in other problems.[13]

With this replacement and a rescaling of $x\rightarrow x(K/v)^{1/2}$, we can write the energy of the system of length L in the x direction as

$$E-E_0=(Kv)^{1/2}\int_0^{L(v/K)^{1/2}}dx\left[\tfrac{1}{2}\sum_{n=1}^{N}(\nabla\phi-\bar{\delta})^2+\sum_{n=1}^{N-1}V(\phi_{n+1}-\phi_n)+\bar{h}V(\phi_1)\right], \tag{9}$$

where $\bar{h}=h/v$ and $\bar{\delta}=\delta(K/v)^{1/2}$.

Again, this approximation will not have serious qualitative effects since the curvature of the cosine potential and $V(\phi)$ are identical. The main difference between the two is in the maxima of the potential at $\phi=(2n+1)\pi$, but this potential barrier has only a small effect on the energy since the phase difference between layers $\phi_{n+1}-\phi_n$ is small in most of the system and it is these regions which give the main contribution to the elastic energy. Also, the interaction potential is not too well known and there are many uncertainties in the energy barrier even in more realistic models.

Performing the minimization leads to the following set of linear equations of motion for ϕ_n ($-\pi\leq\phi_n\leq\pi$):

$$\begin{aligned}&\phi_n''=2\phi_n-\phi_{n+1}-\phi_{n-1}, \quad 2\leq n\leq N-1\\ &\phi_1''=(1+\bar{h})\phi_1-\phi_2\ ,\\ &\phi_N''=\phi_N-\phi_{N-1}\ ,\end{aligned} \tag{10}$$

which have solutions, for a system of length L, of the form

$$\phi_i(x)=\sum_{j=1}^{N}(a_{ij}e^{k_jx}+b_{ij}e^{-k_jx}), \quad i=1,2,\ldots,N\ . \tag{11}$$

There are two possibilities here: either there is a soliton in $\phi_i(x)$ which corresponds to the removal or addition of a single atom to the ith layer or there is not. The former case corresponds to a solution of the equations with a boundary condition

$$\phi_i(0)=0, \quad \phi_i(L)=2\pi \tag{12a}$$

and

$$\phi_i(x)=\begin{cases}\pi\displaystyle\sum_{j=1}^{N}A_{ij}\frac{\sinh(k_jx)}{\sinh(k_jL/2)}, & 0<x<L/2\\ \pi\left[2-\displaystyle\sum_{j=1}^{N}A_{ij}\frac{\sinh[k_j(L-x)]}{\sinh(k_jL/2)}\right], & L/2<x<L\end{cases} \tag{12b}$$

with $\sum_{j=1}^{N}A_{ij}=1$. The latter condition corresponds to a boundary condition

$$\phi_i(0)=\phi_i(L)=0 \tag{13a}$$

and

$$\begin{aligned}&\phi_i(x)=\pi\sum_{j=1}^{N}A_{ij}\frac{\sinh(k_jx)}{\sinh(k_jL/2)}, \quad 0<x<L/2\\ &\phi_i(L-x)=-\phi_i(x), \quad L/2<x<L\end{aligned} \tag{13b}$$

with $\sum_{j=1}^{N}A_{ij}=0$. Note that an isolated soliton in the ith layer corresponds to a pair of elementary misfit dislocations of equal but opposite Burgers vectors, one just above and one just below the ith layer. In our formalism, it is more convenient to parametrize the configurations of the layers in terms of solitons rather than misfit dislocations.

These solutions are quite natural. Suppose we have two layers on a substrate with the soliton in the second layer. In an atomic picture, the expected displacements are shown in Fig. 1. In terms of the phases ϕ_1 and ϕ_2, corresponding to the displacements, ϕ_2 has a solution $\phi_2(0)=0$ and $\phi_2(L)=2\pi$, whereas $\phi_1(x)$ has a twist or elastic displacement which is matching up as well as possible with the second layer and substrate so that $\phi_1(0)=\phi_1(L/2)=\phi_1(L)=0$ and $\phi_1(L-x)=-\phi_1(x)$ corresponding to displacements to the right in the left-hand part of the layer and to the left in the other part.

The general program to find the condition at which a misfit-dislocation formation energy first vanishes is now clear. We specify our selected misfit-dislocation configuration, allowing, at most, one soliton in a given layer, and compute the energy from Eq. (9) and compare the energies for all possible configurations. This involves calculating the N^2 quantities A_{ij} from the equations of motion and the boundary conditions specifying the soliton configuration. The N different k_j are evaluated from the Nth-order polynomial equation for k^2:

$$\det\begin{vmatrix}k^2-1-\bar{h} & 1 & 0 & 0 & 0 & 0\\ 1 & k^2-2 & 1 & 0 & 0 & 0\\ 0 & 1 & k^2-2 & 1 & 0 & 0\\ & & & & & 1\\ 0 & & & & 1 & k^2-1\end{vmatrix}=0\ . \tag{14}$$

It is easily shown that all roots of this are real and positive so that the k_i are real and may be chosen positive.

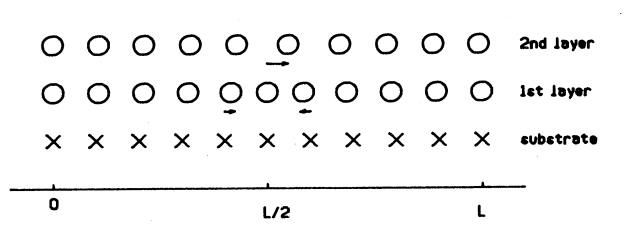

FIG. 1. Atomistic view of one of the solutions to Eq. (10) in which there is a soliton in the second layer and a twist in the first one.

Note that there are $N(N-1)$ linearly independent equations of motion for the A_{ij} and the remaining N equations are given by the boundary conditions. Note also that there are 2^N soliton configurations to be investigated. This can be carried out analytically for small values of N, but rapidly becomes extremely tedious.

The energy of the system relative to its registered state is given by

$$\frac{\Delta E}{\sqrt{vK}} = \pi^2 \sum_{i,j}^{N} P_{ij} \int_0^{L/2} dx \frac{\cosh(k_i x)\cosh(k_j x)}{\sinh(k_i L/2)\sinh(k_j L/2)} + \pi^2 \sum_{i,j}^{N} Q_{ij} \int_0^{L/2} dx \frac{\sinh(k_i x)\sinh(k_j x)}{\sinh(k_i L/2)\sinh(k_j L/2)} - 2\pi\bar{\delta} \sum_{i,j}^{N} A_{ij} k_j \int_0^{L/2} dx \frac{\cosh(k_j x)}{\sinh(k_j L/2)} . \quad (15)$$

In the limit $L \to \infty$, this reduces to

$$\frac{\Delta E}{\sqrt{vK}} = \pi^2 \sum_{i,j}^{N} \frac{P_{ij}+Q_{ij}}{k_i+k_j} - 2\pi\bar{\delta} \sum_{i,j}^{N} A_{ij} , \quad (16)$$

where

$$P_{ij} = \sum_{l=1}^{N} k_i k_j A_{li} A_{lj} ,$$
$$Q_{ij} = \sum_{l=1}^{N-1} (A_{li} - A_{l+1,i})(A_{lj} - A_{l+1,j}) + \bar{h} A_{1i} A_{1j} . \quad (17)$$

The equations determining the A_{ij} are the $N(N-1)$ linearly independent members of the equations of motion

$$A_{1j}(k_j^2 - 1 - \bar{h}) + A_{2j} = 0 ,$$
$$A_{ij}(k_j^2 - 2) + A_{i+1,j} + A_{i-1,j} = 0, \quad 2 \le i \le N-1 \quad (18)$$
$$A_{Nj}(k_j^2 - 1) + A_{N-1,j} = 0, \quad j = 1, \ldots, N$$

together with the 2^N possible boundary conditions

$$\sum_{j=1}^{N} A_{ij} = \begin{cases} 0 & \text{if no soliton in layer } i , \\ 1 & \text{if there is a soliton in layer } i . \end{cases} \quad (19)$$

We have evaluated the energy difference of the various configurations from the registered state analytically for $N = 1,2$ and numerically for $N = 3,4$, investigating in detail all 2^N possibilities, and we find that the lowest-energy configurations always fall into two classes. For $\bar{h} = h/v$ sufficiently small (≤ 1.2), the lowest-energy configuration is one with a soliton in every layer corresponding to a conventional misfit dislocation between the substrate and first layer. For $h/v > 1.2$, we find that the first layer remains essentially commensurate with the substrate except for elastic distortions of the twist type. The remaining $N-1$ layers each have a soliton which corresponds to a misfit dislocation starting from the second layer. Note that the soliton width increases with distance from the substrate (see Fig. 2).

Guided by these calculations we have also evaluated the critical stability boundary, $\bar{\delta}(N) = \sqrt{K/v}\,\delta(N)$, for large N by finding the roots of Eq. (14) numerically and evaluating ΔE numerically. The results of this are plotted in Fig. 3. For large N, this method becomes rather cumbersome so we have also performed a variational calculation assuming the misfit dislocation starts from the first layer.

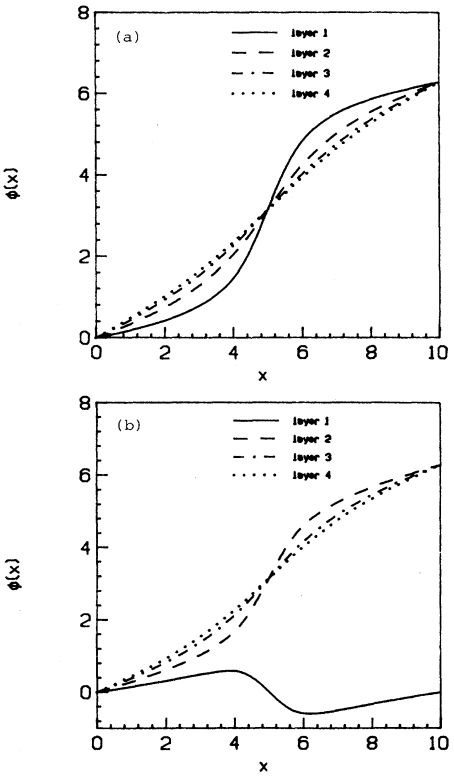

FIG. 2. Solutions of Eq. (10) for a system consisting of four layers with $L/a = 10$ and $h/v = 1$. (a) With a soliton in each layer and (b) with no soliton in the 1st layer.

IV. VARIATIONAL CALCULATION

Using the information gleaned from the calculations of the preceding section that either N or $N-1$ layers have solitons, we can perform a variational calculation to estimate $\delta(N)$ for arbitrary N. We ignore the difference between the two possible situations since we are principally interested in $\delta_c(N)$ for large N, so for convenience we assume a soliton in each layer centered at $x = L/2$ and in the limit $L \to \infty$ the phase ϕ_n is assumed to have the variational form

$$\phi_n(x) = \begin{cases} \pi e^{k_n(x-L/2)}, & 0 < x < L/2 \\ 2\pi - \pi e^{-k_n(x-L/2)}, & L/2 < x < L . \end{cases} \quad (20)$$

By symmetry, the energy of the system with $x < L/2$ is the same as for $x > L/2$, so that, when $L \to \infty$, we get

$$\frac{\Delta E}{\sqrt{Kv}} = \varepsilon_N - 2\pi N\bar{\delta} , \quad (21)$$

where

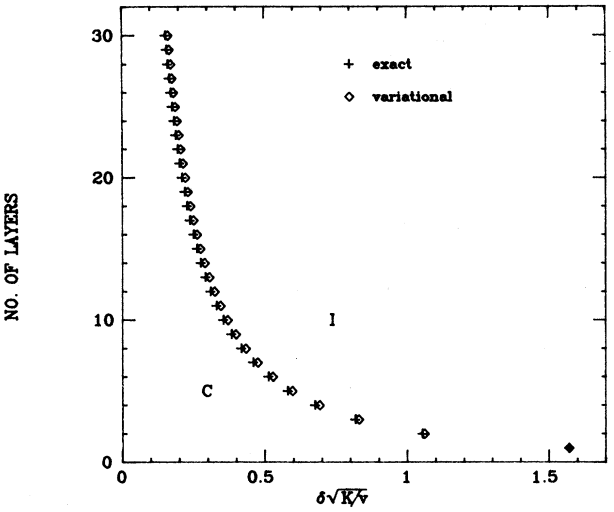

FIG. 3. Stability boundary for $h/v=1$, according to the exact calculations of Sec. III and the variational calculations of Sec. IV. C labels the commensurate (epitaxial phase) and I labels the incommensurate phase.

$$\varepsilon_N=\frac{\pi^2}{2}\left[\sum_{n=1}^{N-1}k_n+\frac{1}{k_n}+\frac{1}{k_{n+1}}-\frac{4}{k_n+k_{n+1}}+k_N+\frac{h}{k_1}\right]. \tag{22}$$

The critical boundary is given by $\Delta E=0$, or

$$\bar{\delta}(N)=\frac{1}{2\pi N}\varepsilon_N\ . \tag{23}$$

We now make the additional ansatz that, to minimize ε_N,

$$k_n=\lambda n^{-\alpha}\ , \tag{24}$$

which is a convenient variational form for numerical calculation, with the result that

$$\varepsilon_N=\frac{\pi^2}{2}(\lambda A_N+\lambda^{-1}B_N)\ , \tag{25}$$

where

$$A_N=\sum_{n=1}^{N}n^{-\alpha}\ , \tag{26a}$$

$$B_N=\sum_{n=1}^{N-1}\frac{[(n+1)^\alpha-n^\alpha]^2}{(n+1)^\alpha+n^\alpha}+\bar{h}\ . \tag{26b}$$

Minimizing $\varepsilon_N(\alpha,\lambda)$ with respect to λ gives

$$\lambda=(B_N/A_N)^{1/2} \tag{27}$$

and

$$\varepsilon_N=\pi^2(A_NB_N)^{1/2}\ . \tag{28}$$

In order to check the accuracy of the variational ansatz against the exact solution described in the preceding section, we have calculated the critical thickness for a given misfit, using Eq. (23), by direct numerical minimization of Eq. (28) with respect to α and find very good agreement (see Fig. 3). Note that for $N=1$ the agreement is perfect because the number of variational parameters in Eq. (24) is sufficient to completely determine the solution of Eq. (10).

There are two special limits in which one can easily find the values of α which minimize the energy in Eq. (28). First, when $\bar{h}=0$, ε_N is clearly minimized when $\alpha=0$, so for $h\to 0$

$$\bar{\delta}(N)=\frac{\pi}{2}\left[\frac{\bar{h}}{N}\right]^{1/2}\ . \tag{29}$$

In the other limit $N\gg 1$, but $\bar{h}$ not too small, we can approximately replace the summations by integrals in Eqs. (26a) and (26b), which gives

$$A_N\simeq\frac{1}{1-\alpha}(N^{1-\alpha}-1)+C_1\ , \tag{30a}$$

$$B_N\simeq\frac{\alpha^2}{2(\alpha-1)}(N^{\alpha-1}-1)+C_2+\bar{h}\ , \tag{30b}$$

where C_1, C_2 are constants. Now, if $\alpha>1$, $B_N\sim N^{\alpha-1}$ and $A_N\sim C_1$, while if $\alpha<1$, $B_N\simeq C_2+\bar{h}$ and $A_N\simeq N^{1-\alpha}$, so that

$$\varepsilon_N\simeq N^{|\alpha-1|/2}\ . \tag{31}$$

Clearly, within this approximation ε_N is minimized by $\alpha=1$ when both A_N and B_N behave like $\ln N$ so that

$$\lambda=1/\sqrt{2} \tag{32}$$

and

$$\bar{\delta}(N)=\frac{\pi}{2\sqrt{2}}\frac{\ln N}{N}\ . \tag{33}$$

This is the same N dependence as the more conventional theory of misfit dislocations. In the Appendix we show how the same results can be obtained, without making use of Eq. (24), by directly minimizing Eq. (22). The crossover between these two regimes is roughly given by $N\bar{h}\sim 4$.

The two limiting cases have a simple physical interpretation. As shown in the Appendix, when $\bar{h}N$ is small, the soliton width in the first layer is $\simeq\bar{h}^{-1/2}$. Although the width increases linearly with the layer index n, the layer is too thin for this increase in width to affect the energy. One may then regard all solitons as having the same width l. Minimizing ε_N with this ansatz yields $\varepsilon_N\simeq(N\bar{h})^{1/2}$. When $\bar{h}N$ is large, the energy is dominated by the layers with index $n\gg 1/\bar{h}$ in which the soliton width increases linearly with n, leading to the standard linear elasticity result.

The result for the $\bar{h}N\to 0$ limit fits some of the experimental data quite well, but this is probably fortuitous since the treatment in this paper assumes thermal equilibrium, whereas it is believed that many of the systems studied experimentally are in metastable states. However, we note that in some molecular-dynamics studies,[8] the

critical thickness N has been found to fall more rapidly with misfit than $1/\delta$ for large δ, in agreement with our weak-coupling or thin-film limit.

V. CONCLUSIONS

In this paper we have developed a simple theory of the equilibrium stability of strained epitaxial layers on a rigid substrate assuming that loss of registry occurs only in one direction. We have used a generalization of the Frank–van der Merwe model[9] to N layers with a periodic potential between adjacent layers. Each layer is treated as a continuum elastic medium, while the coupling between layers is treated in a discrete manner. Using a periodic parabolic interaction between layers, we obtained exact numerical results for the stability boundary $\delta(N)$. In addition, we developed a variational approach which agrees well with the exact results. Our method interpolates between a few layers and the thick-film limit of standard dislocation theory and in this limit the standard results are obtained. Considerable deviations from continuum elasticity theory occur in the thin-film limit. For very weak coupling to the substrate, or sufficiently thin films, we found that $\delta(N)\sim N^{-1/2}$. The advantage of our method over previous ones is that we can allow for arbitrary variations in the misfits with the substrate δ_n, the coupling constants $v_{n,n+1}$, and elastic constants K_n. This will allow us to perform stability analyses of arbitrary superlattice configurations containing, for example, thick layers of one material and thin layers of another. Also, it should be possible to investigate the stability of a film separated from the substrate by an incommensurate buffer layer, and the effects of an elastic substrate. Such situations will be considered in a future publication.

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APPENDIX

Except in the special limits discussed in Sec. IV, analytical results for different $\bar{h}$ and N are difficult to obtain using the variational assumption of Eq. (24). However, within the basic variational ansatz of Eq. (20), one can obtained analytic results for $N=1,2$ by direct minimization. It is also possible to obtain results for $N\gg 1$ and arbitrary $\bar{h}$ by assuming that k_n varies smoothly with n. By defining $l_n=1/k_n$, which is the width of the soliton in the nth layer, and replacing the summations by integrals, we have

$$\varepsilon_N \simeq \frac{\pi^2}{2}\int_1^N dn\left[l^{-1}+\tfrac{1}{2}l^{-1}\left[\frac{dl}{dn}\right]^2\right]+\frac{\pi^2}{2}\bar{h}l_1 . \tag{A1}$$

To derive Eq. (A1), we have assumed that $d^2l/dn^2 \ll dl/dn \ll l$ and kept only the leading terms. As can be checked, this is valid for $N\gg 1$, so is a reasonable approximation. For $n>1$, the extremum condition is

$$l\frac{d^2l}{dn^2}-\frac{1}{2}\left[\frac{dl}{dn}\right]^2+1=0 . \tag{A2}$$

The most general solution of Eq. (A2) is

$$l(n)=a_0+a_1n+a_2n^2 , \tag{A3}$$

where $a_2=(a_1^2-2)/4a_0$. When $a_2=0$, the integral in Eq. (A1) is proportional to $\ln N$, whereas for $a_2\neq 0$ it increases as N. So when the second term in Eq. (A1), $\bar{h}l_1$, is finite, the latter solution has higher energy. We then take $a_2=0$ and so $a_1=\sqrt{2}$. The lower-energy solution has a soliton width which increases linearly with distance from the substrate, exactly like a standard misfit dislocation. Substituting this form into the energy, we find

$$\varepsilon_N(a_0)\simeq\frac{\pi^2}{\sqrt{2}}\left[\ln\left[\frac{\sqrt{2}N+a_0}{\sqrt{2}+a_0}\right]+\bar{h}(\sqrt{2}+a_0)\right] , \tag{A4}$$

where we have matched $l_1=\sqrt{2}+a_0$. The constant a_0 has the interpretation of the width of the soliton in the first layer. Minimizing $\varepsilon_N(a_0)$ with respect to a_0 yields a quadratic equation for a_0 with the solution

$$l_1=a_0+\sqrt{2}=\frac{\sqrt{2}}{2}(N-1)\left[\left[1+\frac{4}{\bar{h}(N-1)}\right]^{1/2}-1\right] . \tag{A5}$$

For a stronger coupling to the substrate $\bar{h}=O(1)$, or very thick films such that $\bar{h}N\gg 4$, Eq. (A5) gives $l_1\simeq 1/\bar{h}$ and so we obtain the conventional result of linear elasticity theory,

$$\varepsilon_N=\frac{\pi^2}{\sqrt{2}}\{\ln[\bar{h}(N-1)+1]+1\} , \tag{A6}$$

and

$$\bar{\delta}(N)=\frac{\pi}{2\sqrt{2}}\frac{\ln(\bar{h}N+1)+1}{N} . \tag{A7}$$

However, for very weak coupling to the substrate, $\bar{h}(N-1)\ll 4$, we find, from Eq. (A5), $l_1\propto(N/\bar{h})^{1/2}$. In this case the second term in Eq. (A1) is proportional to $(\bar{h}N)^{1/2}$ and the energy is now minimized when $a_2\neq 0$. After minimizing with respect to a_1 and a_0, to leading order $l_1\simeq(N/\bar{h})$ results, and we recover the result $\bar{\delta}(N)\propto N^{-1/2}$ as given in Eq. (29).

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