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Equilibrium theory of the Stranski–Krastanov epitaxial morphology

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We present a theory of the equilibrium morphology adopted by $\mathcal{N}$ atoms of one material when they crystallize epitaxially onto the surface of a dissimilar material. The discussion is limited to the case of the so-called Stranski–Krastanov morphology where a strongly bound but elastically strained wetting layer coats the substrate. The arrangement of atoms atop this layer is determined by minimizing an approximate total energy expression derived for a set of vertically coupled Frenkel–Kontorova chains of finite yet variable length. In this way, both elastic and plastic strain accommodation are treated with a common formalism. Our semi-analytic treatment permits us to compare very rapidly the energy of essentially all configurations of $\mathcal{N}$ atoms (up to about $\mathcal{N} = 5000$) including uniform films, coherent islands and dislocated islands. The results are presented in the form of a morphological phase diagram as a function of misfit, surface energy and total particle number for the case of diamond structure materials. Coherent islands are found to be stable in a non-negligible portion of the phase diagram and the relevant phase boundaries are well predicted by simple analytic expressions. A kinetic interpretation of the results is possible when the variable $\mathcal{N}$ is redefined appropriately.

1. Introduction and background

The morphology adopted by the atoms of one material when they crystallize onto the surface of a dissimilar material is one of the fundamental issues of heteroepitaxy [1]. The question clearly is a matter of constant concern for practical crystal growth where one generally seeks to maintain a uniform flat surface during deposition. Unfortunately, this proves to be the exception rather than the rule and numerous experiments [2] reveal the existence of three distinct morphologies for small volumes of deposited material. Adopting conventional terminology [3], these are: the Frank–van der Merwe (FM) morphology (flat single crystal films consisting of successive complete layers); the Volmer–Weber (VW) morphology (three-dimensional islands that leave portions of the substrate exposed); and the Stranski–Krastanov (SK) morphology (three-dimensional islands atop a very thin flat film that completely covers the substrate).

Of these three, the FM and VW morphologies are easily understood on the basis of macroscopic wetting arguments that involve only interfacial free energies [3]. By contrast, the existence of the SK morphology is intimately related to the accommodation of elastic strain associated with epitaxial lattice misfit. Over the years, this point has been made many times by many authors using theoretical models of varying degrees of sophistication [3–8]. In all these treatments, the first monolayer (or so) of film material is strongly bound yet strained to match the substrate lattice constant. Subsequent deposited material collects into islands that are regarded as essentially bulk-like due to the presumed existence of interfacial misfit dislocations (MD) to relieve the strain.

The foregoing model prediction definitely occurs in many heteroepitaxial systems [2]. But another scenario apparently can occur as well: the SK morphology with *dislocation-free* islands. To date, this phenomenon has been documented most thoroughly for the Ge/Si(100) system [9,10] and the $In_xGa_{1-x}As/GaAs(100)$ system [11,12]. The question naturally arises whether these observations represent equilibrium structures or simply reflect slow kinetics associated with MD nucleation. The latter seems unlikely here because, unlike the "critical height" issue associated with strained-layer epitaxy [13], there is no obvious motivation for islanding if not for the strain relief afforded by MDs. One anyway expects kinetic barriers to island formation even in the absence of MDs [8,29].

As it happens, well before the experimental evidence became available, a hint to the equilibrium nature of such *coherent* islands was present in the theoretical discovery that a small-amplitude corrugation wave lowers the energy of a dislocation-free elastic medium with an epitaxially strained surface [15,16]. Subsequent theoretical work has confirmed the notion (already recognized long ago [17] in connection with the VW morphology) that *lateral* strain relief at the free surface of the islands is the principal mechanism of strain relief. This may be seen directly both in atomistic simulations using realistic interatomic forces [18] and in simulations based on a harmonic solid-on-solid model [19]. Particularly noteworthy for present purposes is the two-dimensional elasticity calculation of Vanderbilt and Wickham [20] who computed numerically the dependence of lateral relaxation on the aspect ratio of truncated pyramidal islands. Using this information and a crude estimate of the cost of MDs, these authors produced a phase diagram that yields stable coherent islands as the ground state morphology for certain ranges of the parameters.

Our interest in this problem was stimulated largely by a scanning tunnelling microscopy (STM) study of Ge/Si(100) by Mo et al. [10]. Therein, one finds a striking image of a very large (presumably dislocated) three-dimensional Ge island in coexistence with a very large number of small (presumably coherent) Ge "hut" clusters. The latter are three-dimensional prismatic islands that expose four equivalent {105} facets – a finding that has been reproduced by others [21]. The authors of ref. [10] suggest that the small islands are an intermediate metastable phase that ultimately coarsens to the final large-island morphology. Our long-range aim is to test this hypothesis with a kinetic model of heteroepitaxial growth. Such a model must have the capacity to: (i) provide a reasonable characterization of misfit accommodation by both elastic and plastic strain relaxation; (ii) account for atomistic effects such as bond breaking and surface reconstruction; and (iii) be computationally efficient enough to deal with hundreds (perhaps thousands) of atoms over laboratory time scales. To our knowledge, no model that satisfies all these requirements has been described in the literature.

The purpose of this paper is to introduce such a model that we believe is capable of a realistic description of heteroepitaxial growth. Here, discussion is limited to a presentation of its equilibrium morphological phase diagram at $T=0$; kinetic results will be presented elsewhere. Our principal result is that coherent islands are indeed ground state structures for certain values of lattice misfit, surface energy and total particle number. Dislocated islands are energetically favored in the thermodynamic limit. Numerical estimates using model parameters appropriate to semiconductor systems yield coherent island *sizes* in good accord with the results of STM experiments. The *shape* of coherent islands is found to be a very sensitive function of the surface energy of reconstructed facets.

2. Preliminary considerations

Our theory of epitaxial morphology is based on the Frenkel–Kontorova model [22]. This model of a linear chain of harmonically coupled atoms in contact with a rigid sinusoidal potential has the great virtue that it captures the competition between elastic strain and plastic deformation (misfit dislocation generation) as mechanisms of misfit accommodation within a single theoretical framework. Applications to monolayer epitaxy began over forty years ago [23] and have been in continuous use ever since – particularly by van der Merwe and coworkers [24]. The basic model can be generalized to a film of finite thickness by stacking such chains one atop another [25] and to islands by stacking chains of finite length [26]. For the case of a double layer system, an approximate solution for an island with true two-dimensional misfit is available as well [27]. Regrettably, all of these analytic calculations are very demanding and we deem their generalization to arbitrary island shapes and sizes neither useful nor warranted.

Our approach to evaluating the energy of an arbitrary arrangement of $\mathcal{N}$ atoms involves several approximations that permit repetitive use of an analytic solution to the one-dimensional finite chain Frenkel–Kontorova model obtained by Niedermayer [28]. First, we suppose that misfit accommodation in the two orthogonal directions in the plane of the substrate occurs independently. Detailed calculations by Snyman and van der Merwe [29] for monolayer islands demonstrate that this approximation can be surprisingly good. Accordingly, we analyze only a 1 + 1 dimensional model (substrate + height) in this paper. Second, we assume that each layer of atoms presents a rigid sinusoidal potential to the layer of atoms above it. More precisely, the chain of atoms in layer p interacts with a potential whose periodicity is fixed at the *average* value a_{p-1} of the inhomogeneous atomic spacings obtained from the Niedermayer solution for the chain of atoms in layer $p-1$ (fig. 1). In this way, the lateral strain relief achieved at the free ends of each chain is propagated to the layer above. As we shall see, this relaxation mechanism at the free surface of the island can compete successfully with MD formation in certain circumstances.

A central ingredient to our calculations is the energy of a finite Frenkel–Kontorova chain. For an N-atom chain, this can be written

$$E(N) = W\ell_0^2 \sum_{n=1}^{N-1} [\xi(n+1) - \xi(n) - f]^2 + \tfrac{1}{2}W \sum_{n=1}^{N} [1 - \cos 2\pi\xi(n)], \tag{1}$$

where $\xi(n)$ is the displacement of the nth atom of the chain from the bottom of the nth substrate well (measured in units of the substrate periodicity a_0), $f = (b - a_0)/a_0$ is the misfit between the substrate and the chain (natural lattice constant b), and $\ell_0 = \sqrt{\mu a_0^2/2W}$ is a dimensionless material parameter defined in terms of the spring constant μ and the amplitude of the sinusoidal substrate potential $W/2$. It is straightforward to minimize this expression with respect to the $\xi(n)$ subject to the boundary condition that the atoms on the ends of the chain feel no net force. For definiteness, suppose that N is odd. Then, for a chain that contains an even number of misfit dislocations m, the final result for the relative displacement of the nth atom can be written [28, 30]

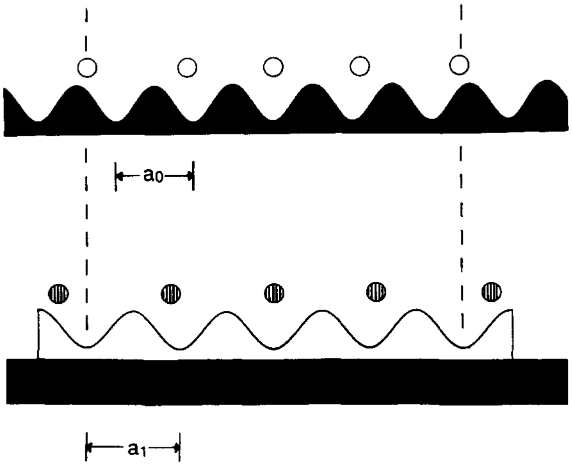

Fig. 1. Schematic representation of the relaxation algorithm used in this paper to vertically couple linear Frenkel–Kontorova chains. Top panel: The first layer of film atoms (open circles) arrange themselves on a substrate of lattice constant a_0 (solid corrugation) to minimize the total energy of the system. This yields non-uniform spacings between the atoms. Bottom panel: The second layer of film atoms (cross-hatched circles) arrange themselves non-uniformly on a "substrate" of finite length (white corrugation) with a *uniform* lattice constant a_1 equal to the *average* of the true inhomogeneous atom spacings in the first film layer. The algorithm repeats for every subsequent layer so that lateral relaxation propagates to the top of the film.

$$\xi(n) = \frac{1}{2} + \frac{1}{\pi}\mathrm{am}\left[\frac{\pi}{k\ell_0}\left(n - \frac{N+1}{2}\right) + F(k, -\tfrac{1}{2}\pi)\right], \tag{2}$$

where $F(k, \phi)$ denotes the incomplete elliptic integral of the first kind and am$[u]$ is its ampli-

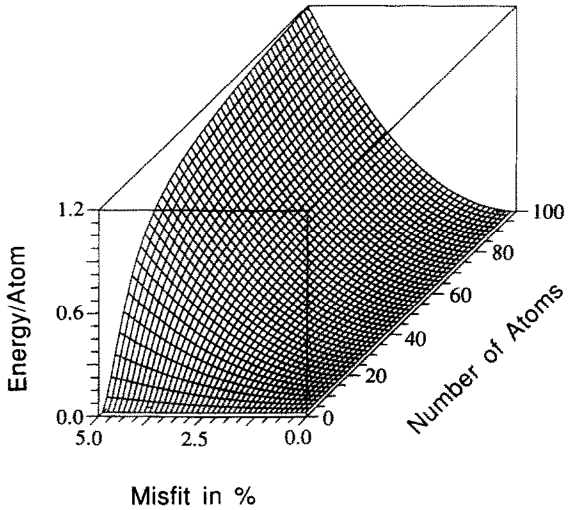

Fig. 2. The average energy per atom of a finite, dislocation-free Frenkel–Kontorova chain $E(N)/N$ as a function of misfit and total particle number N. The energy is given in units of the amplitude W.

tude [31]. The modulus k is determined from the condition

$$\frac{\pi(N-1)}{2k\ell_0} = (m+1)F\left(k, \tfrac{1}{2}\pi\right) - F(k, \phi), \quad (3)$$

where $\sin^2\phi = k^{-1} - \ell_0^2 f^2$. Similar formulae apply when m is odd and for all m when N is even. Although an analytic expression for the average energy/atom, $E(N)/N$, is available [28,30], it is simpler to substitute eq. (2) into eq. (1) and evaluate the result numerically. One finds that this quantity exhibits both a quadratic dependence on misfit f and a rapid saturation with particle number N (fig. 2). A simple parameterization thus renders the results readily amenable to rapid numerical evaluation.

We turn now to the construction an explicit expression for the total energy of an epitaxial island composed of $\mathscr{N}$ atoms in accordance with the model assumptions outlined above. Let N_p denote the number of atoms in the pth layer of an island formed by a vertical stacking of h linear chains of atoms. The island configurations we consider correspond to all values of N_p and h such that $\Sigma_{p=1}^{h} N_p = \mathscr{N}$ subject to the restriction that $0 \le N_p - N_{p+1} = \text{const.}$, i.e., there are no overhangs and the island sidewalls form single crystallographic facets. The total relaxed island energy is

$$\mathscr{E}_\mathrm{R} = \sum_{p=1}^{h} E(N_p, a_{p-1}). \quad (4)$$

We have displayed the dependence of the chain energy on the substrate lattice constant explicitly because, according to the prescription sketched in fig. 1, the chain in layer $p+1$ is imagined to interact with a rigid "substrate" with lattice constant

$$a_p = a_{p-1}\left(1 + \frac{\xi_p(N_p) - \xi_p(1)}{N_p - 1}\right), \quad (5)$$

where $\xi_p(n)$ is the relative displacement of the nth atom of the chain in layer p.

Let us consider strain relaxation in *dislocation-free* islands as a first application of eqs. (4) and (5). A useful figure of merit for this purpose is the relative relaxation,

$$\mathscr{S} \equiv \frac{\mathscr{E}_\mathrm{U} - \mathscr{E}_\mathrm{R}}{\mathscr{E}_\mathrm{U}}, \quad (6)$$

where $\mathscr{E}_\mathrm{U}$ is the total energy of the unrelaxed island, i.e., an island where every constitutent atom is commensurate with the underlying substrate and $a_p = a_0$. For the case of rectangular islands, the calculated relaxation turns out to depend strongly only on the height-to-width aspect ratio h/w of the island. In particular, the numerical results for $\mathscr{S}$ are *independent* of misfit. Fig. 3 illustrates this quantity for a typical choice of the model parameters. Our results for $\mathscr{S}(h/w)$ compare well with those obtained in ref. [20] with a finite-element elasticity computation. On the other hand, our atomistic model permits us to calculate an approximate *analytic* expression for the behavior of $\mathscr{S}$ for all but the smallest values of $\mathscr{N}$.

To this end, we note that the computed values of $\xi_p(n)$ reveal the behavior one expects on intuitive grounds: in each layer, the relaxation occurs predominantly at the ends of each chain. Thus, as a crude model, we suppose that in every layer of a rectangular island exactly $\Lambda/2$ atoms at each end are relaxed completely while the remaining

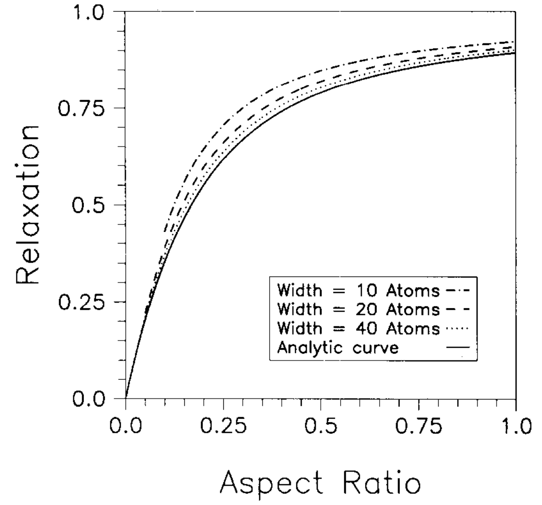

Fig. 3. The relative relaxation (6) of a rectangular coherent island as a function of its height-to-width aspect ratio h/w. Each curve corresponds to an island with a fixed width. For $w > 100$, the numerical results are coincident with the analytic formula (9).

$N_p - \Lambda$ atoms remain locally unrelaxed, i.e, locked to the template established by the layer beneath. From eq. (5), one easily verifies that the effective misfit f_p in layer p is related to the original misfit f by

$$f_p = \frac{b - a_{p-1}}{a_{p-1}} \simeq f\left(1 - \frac{\Lambda}{w}\right)^{p-1} \simeq f\,\mathrm{e}^{-\Lambda(p-1)/w} \qquad (7)$$

to lowest order in Λ/w. Accordingly, the relaxed energy of a coherent island is

$$\begin{aligned}\mathscr{E}_{\mathrm{R}} &\simeq Aw \sum_{p=1}^{h} f_p^2 \\ &\simeq Awf^2 \sum_{p=0}^{h-1} \exp\left(-\frac{2p\Lambda}{w}\right) \\ &\simeq \frac{w^2 f^2}{2\Lambda}\left[1 - \exp\left(-\frac{2\Lambda h}{w}\right)\right],\end{aligned} \qquad (8)$$

where A is proportional to an elastic constant. Since $\mathscr{E}_{\mathrm{U}} \simeq Awhf^2$ in this approximation we find that

$$\mathscr{E}(h/w) = 1 - \frac{1}{2\Lambda}\frac{w}{h}\left[1 - \exp\left(-2\Lambda\frac{h}{w}\right)\right]. \qquad (9)$$

The solid curve in fig. 3 is eq. (9) with the (fitted) choice $\Lambda = 3\pi/2$. This number is independent of misfit but presumably depends on ℓ_0, i.e., the material parameters. We note that formulae similar to eq. (9) have appeared in the literature of this problem previously [32,33]. However, despite the claim in ref. [32], the stated result does not follow from a proper solution to the corresponding elastic boundary value problem [34]. Similarly, the formula cited in ref. [33] is introduced as an empirical fit to numerical elasticity calculations.

3. Results and discussion

We turn next to the application of our model to the zero temperature morphological phase diagram of a Stranski–Krastanov system with the diamond structure and a (100) substrate. To treat the problem in $1+1$ dimensions, we consider only island configurations where the height is a multiple of a double-layer (fig. 4). The total island energy is computed as the sum of several contributions. Since $\mathscr{E}_{\mathrm{R}}$ (eq. (4)) counts all misfit-induced contributions to the energy, the proper unrelaxed energy is obtained by adding to this a value $-E_{\mathrm{bond}}$ for every saturated bulk bond. In addition, a term $-\frac{1}{2}E_{\mathrm{dimer}}$ is added for every exposed surface atom on a (100) facet. We thereby incorporate a simple dimer reconstruction energy for the (100) facet [35]. The surface energies of all other facets are presumed equal to their unreconstructed broken bond values [36].

To be more precise, the total island energy

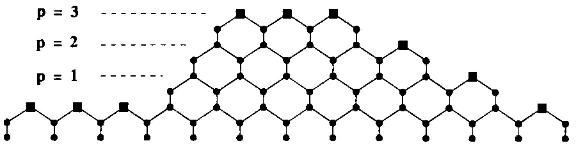

Fig. 4. Side view of an island with the diamond structure. Only islands with heights equal to an integer number of double layers are considered. Surface atoms marked as squares form dimers with atoms one plane behind. Here, the left island sidewall corresponds to a (111) facet and the right to a (311) facet.

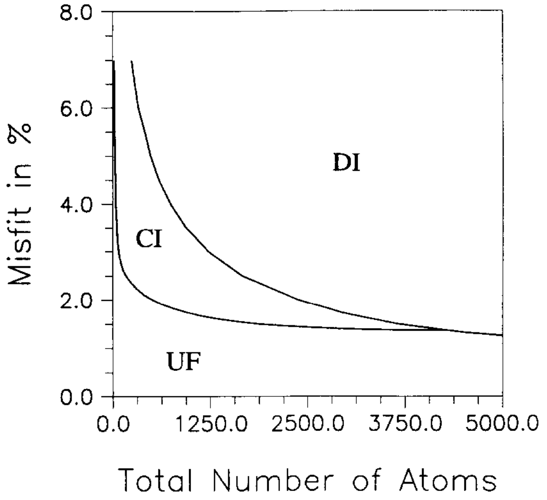

Fig. 5. Equilibrium morphological phase diagram as a function of lattice misfit and total particle number as determined from minimization of eq. (10). Phase fields are found for uniform films (UF), coherent islands (CI) and dislocated islands (DI). $E_{\rm dimer} \approx 1.7$ eV in this example.

(relative to that of the dimerized SK wetting layer) is written

$$E_{\rm tot} = \mathscr{E}_{\rm R} - \sum_{p=1}^{h} (4N_p + 2)E_{\rm bond} + \tfrac{1}{2}hE_{\rm dimer}, \tag{10}$$

where h now denotes the total number of double layers (fig. 4) and N_p is the number of atoms in the top layer of the pth double layer. As a numerical example, we choose parameter values typical of semiconductors: $W \approx 2.0$ eV, $\ell_0 \approx 7$, $E_{\rm bond} \approx 1.9$ eV, and $E_{\rm dimer} \approx 1.7$ eV. A phase diagram (fig. 5) is produced by minimizing eq. (10) with respect to island shape and the number of misfit dislocations for $\mathscr{N} \leq 5000$ and $0 \leq f \leq 0.07$. Because the model is so simple, only about half an hour of computing time is required on an IBM RISC 6000/530 workstation to compare the energy of $\sim 10^8$ different island configurations.

As expected, the uniform flat (UF) film is the $T = 0$ ground state for small values of misfit or small atom mumbers. Island configurations with (111) sidewall facets are preferred as the number of atoms or the misfit increases. Coherent islands (CI) occupy a distinct phase field when $\mathscr{N}$ is not too large and f is not too small. Large values of $\mathscr{N}$ favor a dislocated island (DI) ground state. From a computation of the chemical potential we have verified that large islands are stable against break up into smaller islands. It is interesting to note that the calculated coherent island widths just at the CI–DI phase boundary are in reasonably good agreement with those observed in scanning tunnelling microscopy studies of the Ge/Si(100) [10] and $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{As}$/GaAs(100) [12] SK systems at the appropriate values of misfit. For example, we find an island width of ~ 170 Å at $f = 3\%$, whereas the islands imaged by Snyder et al. [12] exhibit an average width of ~ 200 Å for $f = 2.9\%$.

On the other hand, the islands observed by STM do not expose (111) sidewall facets as we find. Our model produces (111) facets simply because the resulting island shape possesses the largest aspect ratio and hence the largest elastic relaxation (cf. fig. 3). If the islands seen in experiment indeed represent quasi-equilibrium structures (see below), we can speculate that higher index sidewall facets (such as (105) for Si/Ge(100)) occur because such facets may contribute an energy gain due to reconstruction ignored by us. It is easy to experiment with this idea within our model and it turns out that the equilibrium island shape is a *very* sensitive function of these facet energies. We conclude that, unlike the distinction between coherent islands and dislocated islands, our model is too crude to predict island shapes with reliability.

The shape of all the phase boundaries in fig. 5 can be predicted by applying the methodology of Orr and coworkers [19] (used by them for the UF–CI transition) to the conventional continuum model of the UF–DI transition [4]. In particular, we write the energies of a uniform film $E_{\rm UF}$, rectangular coherent islands $E_{\rm CI}$, and rectangular dislocated islands $E_{\rm DI}$ as:

$$E_{\rm UF} = \mu f^2 \mathscr{N} + w\gamma_1, \tag{11}$$

$$E_{\rm CI} = \mu f^2 \mathscr{N} \mathscr{G}(x) + w\gamma_1 + 2h\gamma_2, \tag{12}$$

$$E_{\rm DI} = \mu \varepsilon^2 \mathscr{N} \mathscr{G}(x) + w\gamma_1 + 2h\gamma_2 + B(f - \varepsilon)\sqrt{\mathscr{N}/x}, \tag{13}$$

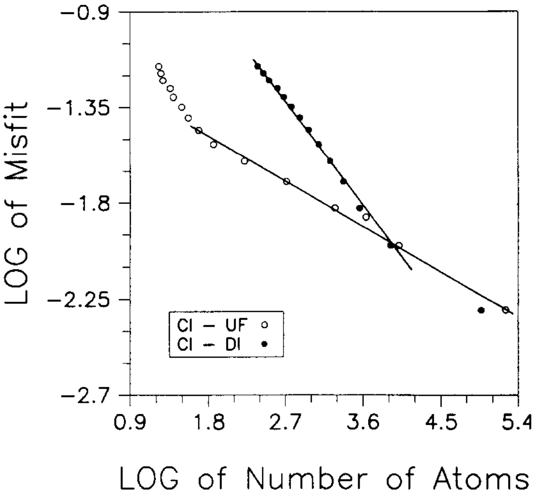

Fig. 6. Log–log plot of the phase boundaries in fig. 5 (circles). Solid curves denote the prediction of the continuum theory discussed in the text.

where $x = h/w$, γ_1 and γ_2 respectively denote the surface energies of the (100) and (vertical) sidewall facet, ε is the strain and B is a constant [37]. As a first step, minimize eq. (12) with respect to x and eq. (13) with respect to x and ε. The UF–CI phase boundary is found by setting $E_{\mathrm{UF}} = E_{\mathrm{CI}}$ and the CI–DI phase boundary is found by setting $E_{\mathrm{CI}} = E_{\mathrm{DI}}$. Our microscopic calculations show that $x_{\mathrm{CI}} > x_{\mathrm{DI}}$ by a small amount. But if we neglect this difference, the phase boundaries are predicted to be $f^{\mathrm{UF-CI}} \sim \mathscr{N}^{-1/4}$ and $f^{\mathrm{CI-DI}} \sim \mathscr{N}^{-1/2}$. A logarithmic plot of our computed phase boundaries (fig. 6) shows that the continuum predictions (11)–(13) are valid for large values of $\mathscr{N}$.

It is instructive to consider the morphological effect of variations in the dimer energy when all other material parameters are held fixed. In the laboratory, this can be effected by the addition of surfactants [38] or, for alloy systems simply by varying growth conditions [39]. Fig. 7 illustrates a typical result for the case of 3% misfit [40]. The UF phase field expands as the dimer energy increases – a conclusion readily obtained from the continuum modelling sketched above [39] – simply because large values of E_{dimer} favor the exposure of more (100) surface. Nonetheless, strain relaxation ultimately favors island formation when $\mathscr{N}$ is large enough. From eq. (10) one sees that large dimer energy favors dislocated islands over coherent islands (for fixed $\mathscr{N}$) due to the aspect ratio difference noted just above.

The results discussed so far formally pertain solely to equilibrium results. But since we specify the total particle number $\mathscr{N}$ (rather than the number density of particles), the favorable comparison made above between the largest coherent islands observed by STM and our CI–DI phase boundary strongly suggests that there must be a natural *kinetic* interpretation of our results. One possibility was discussed by Pintus et al. [41] and later by Snyder and coworkers [42]. These authors introduce a diffusion length $L = \sqrt{D\tau}$, where D is the surface diffusivity and τ is the time to deposit a monolayer. If one argues that only atoms from a substrate segment of length L are available to form either a uniform film or a coherent island, the total volume of material is Lt, where t is the thickness of a film. Figs. 5 and 7 then may be read as a kinetic phase diagram with Lt substituted for $\mathscr{N}$.

An alternative kinetic interpretation of our results follows if we accept the proposal of Mo and coworkers [10] that there exist long-lived metastable epitaxial configurations that may be

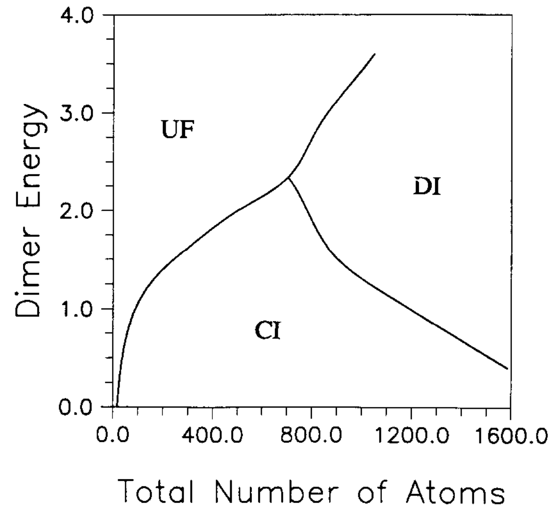

Fig. 7. Equilibrium morphological phase diagram as a function of dimer (surface) energy (in units of E_{bond}) and total particle number. The misfit $f = 3\%$ in this example.

separated from the true equilibrium state by substantial energy barriers. In that case, the effect of aspects of the true problem neglected by us, e.g., elastic interactions between islands, may be sufficient to permit us to identify our equilibrium results with groups of $\mathcal{N}$ atoms in portions of the sample kinetically isolated from other groups of atoms by such barriers. Indeed, this interpretation of the STM experiments seems most likely to us.

4. Summary and conclusion

We have introduced an approximate model for the $T=0$ energetics of Stranski–Krastanov heteroepitaxial films and islands based on a set of vertically coupled Frenkel–Kontorova chains of finite yet variable length. In the interest of high computational speed (for later application to real-time kinetics simulations) a number of approximations to reality have been accepted, e.g., the complete neglect of strain non-uniformity in the direction parallel to the substrate. Nonetheless, elastic strain and plastic deformation are treated on an equal footing. Some confidence in our methods may be gained from the fact that, when comparison has been possible, we have found good agreement with previous elasticity calculations and phenomenological treatments of the energetics of dislocations.

The phenomenon of lateral strain relaxation at the free surface of a dislocation-free island was demonstrated and an analytic expression for the energy gain derived. The simplicity of the theory then permitted energetic comparisons of up to 10^8 diamond structure configurations for islands with up to 5000 atoms with and without misfit dislocations. The final results were reported in the form of equilibrium morphological phase diagrams as a function of misfit and surface energy versus total particle number. Coherent (dislocation-free) islands were found to be ground state structure for a significant portion of the phase diagram and thus provides support for speculations to this effect in various experimental reports. For a fixed misfit, the maximum width of stable islands computed with this model agrees surprisingly well with STM observations. The shapes of the computed islands do not agree with experiment due to the extreme sensitivity of the model to facet surface energies. Dislocated islands always appear in the thermodynamic limit.

As in previous related work, our results can be re-interpreted kinetically if the total number of atoms we employ is regarded instead as the number of atoms within a characteristic diffusion length or otherwise accessible to one another without excessive free energy cost. The equilibrium phase diagrams then can be read as kinetic phase diagrams.

The model used here possesses many of the features needed to create a truly time-dependent theory of morphological evolution during heteroepitaxy. Significant challenges clearly remain, e.g., a realistic treatment of dislocation injection. But, since there is presently no reliable kinetic theory available that can incorporate misfit dislocations during island coarsening and/or growth in *any* manner, we believe our results represent a useful step forward.

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