

# A Discrete Elastic Model for Epitaxial Systems and the Force Field at a Step

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# A Discrete Elastic Model for Epitaxial Systems and the Force Field at a Step <sup>\*</sup>

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## Abstract

Strain has significance for both the growth characteristics and material properties of thin epitaxial films. In this work, the method of lattice statics is applied to an epitaxial system with cubic symmetry, using harmonic potentials. The energy density and force balance equations are written using a finite difference formalism that clearly shows their consistency with continuum elasticity. For simplicity, the atomic interactions are assumed to be maximally localized. For a layered material system with a material/vacuum interface and with surface steps, force balance equations are derived, and intrinsic surface stress at the material/vacuum interface is included by treating the atoms at the surface as having different elastic properties. By defining the strain relative to an appropriately chosen nonequilibrium lattice, as in the method of eigenstrains, analytic formulas in terms of microscopic parameters are found for the local force field near a step and for the macroscopic monopole and dipole moment forces due to a step. These results provide an atomistic validation of the Marchenko-Parshin formula for the dipole moment in terms of the elastic surface stress.

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# 1 Introduction

Strain has significance for both the growth and material properties of thin epitaxial films. In heteroepitaxial growth of thin films, strain is induced by mismatch between the lattice constants in the substrate and those in the epilayer; e.g., for silicon on germanium the lattice mismatch is -4%. During growth, strain changes the growth rate and surface morphology by changing the adatom diffusion coefficient [24] and other energy transition barriers. Morphological changes in a thin film, such as the growth of quantum dots (or the transition to roughening), occur in strained systems because these structures serve to relieve the strain buildup and hence lower the elastic energy. For an alloy system, strain also may lead to alloy segregation [28]. Strain also affects the electronic, optical and magnetic properties of materials, so that it is useful parameter in materials design.

In an epitaxial thin film, the effects of strain have a particular simplicity because of the ideal properties of the crystal structure. Grain boundaries and lattice defects, such as dislocations and stacking faults, are rare or absent in many systems; so that the most significant lattice inhomogeneities are steps on epitaxial surfaces and at heteroepitaxial interfaces. Continuum analysis of the strain field due to a step, under the influence of surface stress, was performed by Marchenko and Parshin [14] in terms of a multipole expansion, although Kukta and Bhattacharya [10] have found that non-multipole terms can be significant.

The method of lattice statics was developed, for example in [2, 36], to provide a simplified atomistic theory for strain in a crystalline material. See [20] for an accessible treatment. Starting from an atomistic elastic energy, the force balance equations at each atom are derived from an energy minimization criterion. Stewart, Pohland and Gibson [32] applied a lattice statics model consisting of nearest neighbor and diagonal springs to determine the monopole and dipole terms due to a step with intrinsic surface stress but no lattice mismatch. Additional lattice statics computations for interactions among steps and adatoms have been performed [7, 8, 21, 25], and the problem has been studied from other points of view, such as via embedded atom potentials [11, 27].

In this paper, we develop a harmonic lattice statics model on a simple cubic lattice that is distinct in being maximally localized: at a given point, the energy density involves only the point and its nearest neighbors,

and the force balance equations involve only the point and its nearest and next-nearest neighbors. Cubic symmetry is imposed, and a finite difference formalism is used so that consistency with continuum elasticity is clear. In the bulk, where the continuum approximation is valid, these assumptions uniquely determine the atomistic strain energy. We extend this model to systems with surfaces and interfaces under some simple assumptions that preserve the stencil for the energy density and force balance equations. In particular, intrinsic surface stress is included by changing the lattice constant at the material surface.

For a layered system with lattice misfit and intrinsic surface stress, we develop a method for isolating the effect of a surface step, by considering the strain relative to a conveniently chosen reference lattice. This method can be interpreted as a modification of the method of eigenstrains [18]. Relative to the reference lattice, we explicitly determine the force field in the neighborhood of an isolated surface step and the resulting monopole and dipole moment terms. Moreover, the monopole and dipole moment terms are independent of the choice of reference lattice, as a consequence of balance of force and torque. From these, we are able to confirm the Marchenko-Parshin relation between surface stress and dipole moment [14]. Furthermore, we extend this result to systems with misfit between the substrate and the film, for which there is a force monopole in addition to the dipole moment at the step, assuming that the center point for the dipole is properly chosen.

Partial motivation for this work has been the need for a strain model that is suitable for coupling with an epitaxial growth model. In particular, the model developed in Section 3 has been coupled to a model for motion of steps in a related work by the authors and their co-workers [26].

Most previous analysis for strain effects in thin film growth has been purely continuum. The approach of Spencer, Davis and Voorhees [29, 30, 31], who used continuum elasticity equations, is applicable to films for which the interface may be described as a smooth surface and is successful in describing morphological instabilities. It is not applicable to very thin films, such as occur in quantum wells, for which the interface would be perfectly flat on the continuum scale.

Tersoff and co-workers [13, 35] and Kukta and Bhattacharya [9] formulated a theory for the motion of step edges on a thin film, in which each step edge is described as a curve on a flat interface, and the elastic field due to a step edges is approximated by Green's function on the step. The

work of Tersoff et al [13, 35] also used the results of Marchenko and Parshin [14]. This theory is applicable for a system that is layered, but otherwise homogeneous, and in which the step height and overall height change on the interface are much smaller than the epilayer thickness. In particular, it is successful in describing interactions, such as bunching, between steps on an epitaxial surface. This approach is difficult or impossible to implement for systems with material or geometric inhomogeneities, and it is not valid for epilayers that are only a few atomic layers thick. In [10], Kukta and Bhattacharya went beyond the Green's function based methods and argued that the elastic field includes logarithmic terms that are not accounted for by the Green's function.

Lattice statics for thin films have been employed by Lam, Lee and Sander [12] and Much and Biehl [17], following earlier work by several researchers [1, 5, 19], in combination with kinetic Monte Carlo (KMC) simulations to investigate Stranski-Krastanov growth.

The quasi-continuum theory [33, 34] has been applied to material systems involving defects, such as dislocations or cracks, in the crystal lattice geometry, but not to the simpler case of thin films for which the only defects are step edges.

The equations of continuum elasticity are reviewed in Section 2, along with the use of a reference frame that may be nonequilibrium. The atomistic strain energy, including material/material and material/vacuum interfaces and intrinsic surface stress, is formulated in Section 3. In Section 4, the strain energy and the resulting force balance equations are written out for a 2D layered system with a single step at the interface with a vacuum. The force field for this step is derived in Section 5, from which the macroscopic monopole and dipole due to a step and the elastic surface stress are found, and the results of Marchenko and Parshin are confirmed. Conclusions and prospects for future developments are presented in Section 6. Appendix A contains details of the calculation of the force field around a step. Balance of force and torque and the resulting insensitivity of the monopole and dipole moment forces to the reference lattice are derived in Appendix B. The surface stress for this system is computed in Appendix C.

In performing this work, we have benefitted from many discussions with William Barvosa-Carter, Kaushik Bhattacharya, Frank Grosse, Mark Gyure, Rob Kukta, Max Petersen, Christian Ratsch, Len Sander, Alexander Schindler, Brian Spencer, Jerry Tersoff, Dimitri Vvedensky and Peter Voorhees.

## 2 Continuum Elasticity

Continuum elasticity is formulated in terms of a displacement field  $\mathbf{u} = \mathbf{u}(\mathbf{x}) = \mathbf{X}(\mathbf{x}) - \mathbf{x}$  between the equilibrium position  $\mathbf{x}$  of a material point and the elastically deformed position  $\mathbf{X}(\mathbf{x})$  of that point. The strain tensor  $\mathbf{S}$  has components defined as

$$S_{k\ell} = \frac{1}{2}(\partial_k u_\ell + \partial_\ell u_k) \quad (2.1)$$

in which  $u_k$  are the components of  $\mathbf{u}$  and  $\partial_k = \partial/\partial x_k$ . The stress tensor  $\mathbf{T}$  is defined through a constitutive law as a linear function of  $\mathbf{S}$ .

A useful generalization of this formulation is to allow the reference configuration, that is, the configuration corresponding to zero displacement, to differ from the equilibrium configuration. Define the (nonequilibrium) reference position  $\mathbf{x}$  and the resulting displacement vector  $\mathbf{u}$  by

$$\begin{aligned} (I + \epsilon J)\mathbf{x} &= \mathbf{x}_e \\ \mathbf{u} &= \mathbf{X} - \mathbf{x} = \mathbf{u}_e + \epsilon J\mathbf{x} \end{aligned} \quad (2.2)$$

in which  $\mathbf{x}_e$  and  $\mathbf{u}_e = \mathbf{X} - \mathbf{x}_e$  are the equilibrium position and displacement vectors,  $\mathbf{I}$  is the identity matrix,  $\mathbf{J}$  is a general matrix, and  $\epsilon$  is the magnitude of the displacement. The components of the original strain tensor  $\mathbf{S}_e$  come from the matrix

$$\begin{aligned} \frac{\partial \mathbf{u}_e}{\partial \mathbf{x}_e} &= \frac{\partial \mathbf{x}}{\partial \mathbf{x}_e} \frac{\partial (\mathbf{u} - \epsilon J\mathbf{x})}{\partial \mathbf{x}} \\ &= \frac{\partial \mathbf{x}}{\partial \mathbf{x}_e} \left( \frac{\partial \mathbf{u}}{\partial \mathbf{x}} - \epsilon \mathbf{J} \right). \end{aligned} \quad (2.3)$$

Linear elasticity is consistent with replacing  $(\partial \mathbf{x}/\partial \mathbf{x}_e)$  by  $\mathbf{I}$ , to obtain the redefined strain tensor  $\mathbf{S}$ , with

$$S_{k\ell} = \frac{1}{2}(\partial_k u_\ell + \partial_\ell u_k) - \epsilon \frac{1}{2}(J_{k\ell} + J_{\ell k}). \quad (2.4)$$

Spatial dependence in  $J$  is permitted without inclusion of  $\partial \mathbf{J}/\partial x$  terms for the same reason. The transformation (2.3) is mathematically equivalent to the method of eigenstrains [18, 22].

The elastic energy density  $E$  and total energy  $\mathcal{E}$  in a domain  $\Omega$  are

$$E = \frac{1}{2} \sum_{k,\ell} S_{k\ell} T_{k\ell} \quad (2.5)$$

$$\mathcal{E} = \int_{\Omega} E d\mathbf{x}. \quad (2.6)$$

For linear elasticity with cubic symmetry, the elastic energy density  $E$  and stress tensor  $\mathbf{T}$  are

$$E = (1/2)C_{11}(S_{11}^2 + S_{22}^2 + S_{33}^2) + 2C_{44}(S_{12}^2 + S_{13}^2 + S_{23}^2) + C_{12}(S_{11}S_{22} + S_{11}S_{33} + S_{22}S_{33}) \quad (2.7)$$

$$\begin{aligned} T_{kl} &= 2C_{44}S_{kl} \quad k \neq l \\ T_{kk} &= C_{11}e_{kk} + C_{12} \sum_{j \neq k} S_{jj} \end{aligned} \quad (2.8)$$

in which  $C_{11}$ ,  $C_{44}$  and  $C_{12}$  are the cubic elastic moduli.

For linear elasticity in an isotropic material, the stress tensor  $\mathbf{T}$  and the elastic energy density  $E$  are

$$T_{kl} = \lambda \delta_{kl} \sum_m S_{mm} + 2\mu S_{kl} \quad (2.9)$$

$$E = \frac{1}{2}\lambda(\sum_k S_{kk})^2 + \mu \sum_{kl} (S_{kl})^2 \quad (2.10)$$

in which  $\lambda$  and  $\mu$  are the Lamé coefficients, with  $(C_{11}, C_{44}, C_{12}) = (\lambda + 2\mu, \mu, \lambda)$ .

The elastic equations are obtained as a stationary point for  $\mathcal{E}$ ; i.e., the displacement  $\mathbf{u}$  solves

$$\delta\mathcal{E} = 0. \quad (2.11)$$

Assuming that there are no forces on the boundary  $\partial\Omega$ , the Euler equations for this variational principle are

$$\begin{aligned} 0 &= \sum_\ell \partial_\ell \left( \frac{\partial}{\partial u_{k,\ell}} E \right) \quad k = 1, 2, 3 \quad \text{in } \Omega \\ 0 &= \sum_\ell n_\ell \left( \frac{\partial}{\partial u_{k,\ell}} E \right) \quad k = 1, 2, 3 \quad \text{on } \partial\Omega \end{aligned}$$

in which  $\mathbf{n}$  is the normal vector with components  $n_k$  and using the notation  $u_{k,\ell} = \partial_k u_\ell$ . Since

$$\frac{\partial}{\partial u_{\ell,k}} E = T_{k\ell}$$

these equations reduce to the elastic equations

$$\nabla \cdot \mathbf{T} = 0 \quad \text{in } \Omega \quad (2.12)$$

$$\mathbf{n} \cdot \mathbf{T} = 0 \quad \text{on } \partial\Omega. \quad (2.13)$$

## 3 Cubic Lattice

### 3.1 Finite Difference Notation

For a simple cubic lattice with lattice coordinates  $\mathbf{i} = (i_1, i_2, i_3)$ , the reference position  $\mathbf{x}$ , deformed position  $\mathbf{X}$  and displacement  $\mathbf{u}$  are denoted

$$\begin{aligned}\mathbf{X}(\mathbf{i}) &= (X_1(\mathbf{i}), X_2(\mathbf{i}), X_3(\mathbf{i})) \\ \mathbf{x}(\mathbf{i}) &= (x_1(\mathbf{i}), x_2(\mathbf{i}), x_3(\mathbf{i})) \\ \mathbf{u}(\mathbf{i}) &= (u_1(\mathbf{i}), u_2(\mathbf{i}), u_3(\mathbf{i})) = \mathbf{X}(\mathbf{i}) - \mathbf{x}(\mathbf{i}).\end{aligned}\tag{3.1}$$

In order to define the discrete elastic energy, denote the translation operators  $T_k^\pm$  and finite-difference operators  $D_k^\pm, D_k^0$  as follows:

$$T_k^\pm f(\mathbf{i}) = f(\mathbf{i} \pm \mathbf{e}_k)\tag{3.2}$$

$$D_k^+ f(\mathbf{i}) = h^{-1}(T_k^+ - 1)f(\mathbf{i})$$

$$D_k^- f(\mathbf{i}) = h^{-1}(1 - T_k^-)f(\mathbf{i})\tag{3.3}$$

$$D_k^0 f(\mathbf{i}) = (2h)^{-1}(T_k^+ - T_k^-)f(\mathbf{i}).$$

in which  $\mathbf{e}_k$  is the k-th unit vector. Define the bond displacement  $\mathbf{d}^{k\pm}$  at the point  $\mathbf{i}$  as

$$\mathbf{d}^{k\pm}(\mathbf{i}) = (d_1^{k\pm}, d_2^{k\pm}, d_3^{k\pm}) = D_k^\pm \mathbf{u}(\mathbf{i}) - \epsilon \mathbf{e}_k \cdot \mathbf{J}\tag{3.4}$$

For a layered epitaxial material, the parameter  $\epsilon$  will be chosen to be the relative magnitude of the lattice distortion in the film; i.e.

$$\epsilon = (a - h)/h.\tag{3.5}$$

in which  $a$  is the equilibrium lattice constant in the film and  $h$  is the lattice constant imposed by the substrate.

To form the energy for linear elasticity for a 2D cubic lattice, first form the discrete strain components, as in [2],

$$\begin{aligned}S_{kk}^\pm &= d_k^{k\pm} \\ S_{k\ell}^{pq} &= (d_k^{\ell q} + d_\ell^{kp})/2\end{aligned}\tag{3.6}$$

in which  $k$  and  $\ell$  have values 1,2, or 3 (denoting the component number of the bond) and  $p$  and  $q$  have values  $\pm$  (denoting positive or negative direction along that component).

## 3.2 Energy and Force Balance Equations

For mathematical simplicity, assume that the energy density  $E$  and force balance equations  $F$  are maximally localized; i.e., assume the following:

- A1.** The energy density  $E$  at a point  $\mathbf{x}$  is a quadratic function of displacement  $\mathbf{u}$  and involves only the point  $\mathbf{x}$  and its nearest neighbors.
- A2.** The force balance equations  $F$  at a point  $\mathbf{x}$  involve only the point  $\mathbf{x}$  and its nearest and next-nearest neighbors.

These assumptions are illustrated in Figure 1, showing the stencils for the energy density and for the force balance equations.

The discrete energy density is formed to be consistent with the continuum energy (2.7), using the discrete strains  $S_{k\ell}^{pq}$  as

$$E = \alpha \sum_{k,p} (S_{kk}^p)^2 + \sum_{k \neq \ell, p, q} \{2\beta (S_{k\ell}^{pq})^2 + \gamma S_{kk}^p S_{\ell\ell}^q\}. \quad (3.7)$$

This can be considered to be a finite difference version of the continuum energy density, with

$$(\alpha, \beta, \gamma) = (C_{11}, C_{44}, C_{12})/4. \quad (3.8)$$

In the continuum case,  $E = E(x, y, z)$  is a function of continuous variables, whereas, in (3.7)  $E = E(\mathbf{i})$  is a lattice function, and so, it can be interpreted as an energy per atom. The total energy, analogous to (2.6) in the continuum case is

$$\mathcal{E} = \sum_{\mathbf{i}} E(\mathbf{i})$$

Note that (3.7) is an average over the discrete strain components in different directions. In fact, (3.7) is the unique finite difference form of the energy that satisfies assumptions A1 and A2, that is a second order (in the lattice spacing  $h$ ) finite difference approximation to the continuum energy (2.7) and that is invariant under the cubic symmetry group.

Although this derivation of (3.7) is based on discretization of the continuum energy, the energy is identical to that of a harmonic lattice statics model, with nearest neighbor interactions. The specific form (3.7) can be derived by starting from a general (nonharmonic) lattice statics model with two

and three body nearest neighbor interactions and with translational and rotational invariance. The energy (3.7) is realized as the leading order (quadratic) approximation for small displacements from equilibrium. A similar procedure is partially carried out in [2]. Alternatively, the energy (3.7) is equivalent to that of a cubic system with springs and bond bending terms [26].

The atomistic displacements  $\mathbf{u}$  are determined by minimizing the total discrete energy  $\mathcal{E}$ , resulting in the discrete variational problem  $\delta\mathcal{E}[\mathbf{u}] = 0$ ; i.e.,

$$\frac{\partial\mathcal{E}}{\partial u_k(\mathbf{i})} = 0 \quad k = 1, 2, 3 \quad (3.9)$$

for all  $\mathbf{i}$ . The conditions (3.9) are force balance laws for each of the atoms. With this explicit form of the energy Eq. (3.7), the force balance equations (3.9) are

$$4\alpha D_k^+ D_k^- u_k + 4\beta \sum_{\ell \neq k} D_\ell^+ D_\ell^- u_k + 4(\gamma + \beta) \sum_{\ell \neq k} D_k^0 D_\ell^0 u_\ell = 0 \quad (3.10)$$

for  $k = 1, 2, 3$  and for each point  $\mathbf{i}$ . In the continuum limit this is consistent with the continuum elastic equation Eq. (2.12).

### 3.3 Interfaces

For problems in which the underlying lattice has cubic symmetry but the material geometry includes interfaces (either between different materials, or between material and vacuum), the energy should only involve bond interactions that are consistent with cubic symmetry but with no symmetry constraint on the coefficients. In other words, if the local geometry is not fully cubic symmetric, we assume that no new interactions between particles are introduced, but we relax the requirement that the energy itself is invariant under any symmetries that are missing. This allows different force constants  $\alpha, \beta, \gamma$  for different bonds emanating from the same point near an interface. The resulting generalization of (3.7) is

$$E = \sum_{k,p} \alpha_k^p (S_{kk}^p)^2 + \sum_{k \neq \ell, p, q} \{2\beta_{k\ell}^{pq} (S_{k\ell}^{pq})^2 + \gamma_{k\ell}^{pq} S_{kk}^p S_{\ell\ell}^q\} \quad (3.11)$$

in which  $k$  and  $\ell$  have values 1,2, or 3 and  $p$  and  $q$  have values  $\pm$ .

Each coefficient  $\alpha_k^p$ , as well as the lattice mismatch parameter  $\epsilon$  (defined as in (3.5)), corresponds to a bond between two atoms; each of the coefficients  $\beta_{k\ell}^{pq}$  and  $\gamma_{k\ell}^{pq}$  corresponds to the interaction of two bonds in orthogonal directions from a central point, which defines a square “cell”. We assume that the values of  $\alpha_k^\pm$  and  $\epsilon$  depend only on the material type of the two atoms at the endpoints of the corresponding bond, and that  $\beta_{k\ell}^{pq}$  and  $\gamma_{k\ell}^{pq}$  depend only on the material type of the four atoms at the endpoints of the corresponding cell.

Consider a system consisting of two materials with elastic parameters  $\alpha^m, \beta^m, \gamma^m, \epsilon^m$  for  $m = 1, 2$ . Denote a cell or bond to be “pure” if all of its vertices are of a single material type and “mixed” otherwise. For maximal simplicity, we make the following assumptions:

- A3.** For pure bonds (pure cells) in material  $m$ ,  $\alpha_k^p = \alpha^m$  and  $\epsilon = \epsilon^m$ , (respectively,  $\beta^{pq} = \beta^m$  and  $\gamma^{pq} = \gamma^m$ ).
- A4.** For mixed bonds (mixed cells) in a two-material system,  $\alpha_k^p = \frac{1}{2}(\alpha^1 + \alpha^2)$  and  $\epsilon = \frac{1}{2}(\epsilon^1 + \epsilon^2)$  (respectively,  $\beta^{pq} = \frac{1}{2}(\beta^1 + \beta^2)$  and  $\gamma^{pq} = \frac{1}{2}(\gamma^1 + \gamma^2)$ ).
- A5.** For a bond (cell) in which one of the vertices is in the vacuum,  $\alpha_k^p = 0$  (respectively,  $\beta^{pq} = \gamma^{pq} = 0$ ).
- A6.** Intrinsic surface stress is included at a material/vacuum interface by considering bonds between two interface sites as having different values of  $\epsilon_I$ , without changing the properties of bonds between interface and bulk sites or of cells involving interface and bulk sites.

Assumption A6 could be modified to change the elastic moduli  $\alpha_I$  for the surface bonds as well, and this may be a more realistic model, but it is doubtful that this would significantly change our results, and in the present study we have only changed the lattice parameter of the surface bonds.

Assumption A5 has appealing simplicity; in particular, it implies that along a flat boundary adjacent to a step the force balance equations are formally the same at points neighboring the step as they are at points away from the step. On the other hand, it implies that an adatom has no elastic energy, which is insufficient for some applications. Intrinsic surface stress as in A6 has been used for example by [32].

Assumptions A3-A6 allow determination of the energy and solution of the force balance equations to be automated, by the following algorithm: From

Assumptions A3-A6 determine all of the elastic coefficients and lattice mismatch parameters, so that the energy (3.11) can be calculated for a specified displacement field. For this quadratic energy, the derivative (3.9) at point  $\mathbf{i}$  is a linear function of  $\mathbf{u}(\mathbf{i}')$  over values of  $\mathbf{i}'$  that are equal to  $\mathbf{i}$ , nearest neighbors of  $\mathbf{i}$ , or next-nearest neighbors of  $\mathbf{i}$ . The coefficients of the linear function can be exactly determined as a finite difference of  $\mathcal{E}$  with respect to  $\mathbf{u}(\mathbf{i})$  and  $\mathbf{u}(\mathbf{i}')$ . Then a linear equation solver is used to find  $\mathbf{u}$  by solving (3.9). This procedure does not require analytic determination of the force balance equations, which is advantageous since the force balance equations at an interface with a step require many separate cases, as seen in Section 4.

## 4 2D Layered Material with Intrinsic Surface Stress

Consider a two-dimensional epitaxial thin film with parallel steps on its surface and with lattice mismatch  $\epsilon_1$  relative to the substrate. Set the coordinate  $x$  to be normal to the steps and  $y$  to be the growth direction. The interface between substrate and epilayer is always assumed to be horizontal ( $y = y_0$ ).

Along the interface between epilayer and vacuum, the lattice mismatch of the interface atoms (relative to the substrate) is  $\epsilon_2$ , so that the lattice mismatch of the interface relative to the film is the difference  $\delta = \epsilon_2 - \epsilon_1$ . For simplicity the elastic coefficients  $\alpha$ ,  $\beta$  and  $\gamma$  are assumed to be uniform throughout the material system (substrate, epilayer and surface layer). Illustrations for a system consisting of substrate and epilayer without intrinsic surface stress are in Figure 2 with no step and Figure 3 with a step. Figure 4 shows a system with substrate and epilayer, and with intrinsic surface stress. The lattice plotted in each of these figures is the reference lattice used in the subsequent analysis. The corresponding shift  $\epsilon J$  in the strain tensor is taken to be  $diag(\epsilon_1, \rho_1 \epsilon_1)$  in the bulk and  $diag(\epsilon_2, \rho_{21} \epsilon_1 + \rho_{22} \epsilon_2)$  at the interface.

### 4.1 Energy Density

At an interior point, the energy density is

$$E = \alpha[(d_1^{1+})^2 + (d_1^{1-})^2 + (d_2^{2+})^2 + (d_2^{2-})^2] \quad (4.1)$$

$$\begin{aligned}
& + \frac{\beta}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2-})^2 + (d_2^{1+} + d_1^{2+})^2] \\
& + \gamma[d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2+} + d_1^{1-}d_2^{2-} + d_1^{1+}d_2^{2+}].
\end{aligned}$$

Consider a point  $(i, j)$  on the horizontal interface at the upper edge of the material. The bonds with  $(i \pm 1, j)$  and  $(i, j - 1)$  are interior bonds and the bond with  $(i, j + 1)$  is an empty space bond. The cells corresponding to  $+-$  and  $--$  are interior cells, and those corresponding to  $++$  and  $-+$  are empty space cells. From Assumption A5, the energy contribution for a horizontal edge point is

$$\begin{aligned}
E & = \alpha[(d_1^{1+})^2 + (d_1^{1-})^2 + (d_2^{2-})^2] + \frac{\beta}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2-})^2] \\
& + \gamma[d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2-}].
\end{aligned} \tag{4.2}$$

The two types of corners are convex corners, as in the upper corner point of a step in Figure 3, and concave corners, as in the lower corner point of a step in Figure 3. For  $(i, j)$  a convex corner point, the energy is

$$E = \alpha[(d_1^{1-})^2 + (d_2^{2-})^2] + \frac{\beta}{2}(d_2^{1-} + d_1^{2-})^2 + \gamma d_1^{1-}d_2^{2-}. \tag{4.3}$$

As in the case of the edge energies, this energy can be obtained from the full energy (3.7) by discarding all terms that involve bonds that are outside the material.

At a concave corner point  $(i, j)$ , all 4 bonds from  $(i, j)$  exist in the material, so that the full set of  $\alpha$  coefficients are present. The  $++$  cell at  $(i, j)$  is an empty space cell, however, so that  $\beta^{++}(i, j) = \gamma^{++}(i, j) = 0$ . The resulting energy for a concave corner is

$$\begin{aligned}
E & = \alpha[(d_1^{1+})^2 + (d_1^{1-})^2 + (d_2^{2+})^2 + (d_2^{2-})^2] \\
& + \frac{\beta}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2-})^2] \\
& + \gamma[d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2+} + d_1^{1-}d_2^{2-}].
\end{aligned} \tag{4.4}$$

## 4.2 Force balance equations

The force balance equations Eq. (3.9) come from energy minimization. In the interior, the elastic energy is given by (3.7), the force balance equations are

Eq. (3.10) and the continuum limit is identical to the continuum elasticity equations. Near the epilayer/vacuum surface, there are 9 types of points as indicated in Figure 5: (1) edge points away from the step; (2) points on the row below the edge and away from the step; (3) the point to the left of the convex corner; (4) the convex corner; (5) the point to the left of the concave corner; (6) the concave corner; (7) the point to the right of the concave corner; (8) the point below the concave corner; (9) the point to the right of point 8. At each of these point types, the force balance equations consist of finite differences of the displacement, defined relative to the reference lattice, and forces that come from the shift to the reference lattice. Points that are not labeled in Figure 5 are those for which the interior form Eq. (3.10) of the force balance equations is valid.

At a horizontal edge (point types  $i=1,3,7$ ), the force balance equations are

$$F_{i1} = -h(4\alpha D_1^+ D_1^- u_1 + 2\gamma D_1^0 D_2^- u_2) + 4\beta D_2^- u_1 + 2\beta(1 + T_2^-) D_1^0 u_2 \quad (4.5)$$

$$F_{i2} = -h(2\beta D_1^+ D_1^- u_2 + 2\beta D_1^0 D_2^- u_1) + 4\alpha D_2^- u_2 + 2\gamma(1 + T_2^-) D_1^0 u_1 \quad (4.6)$$

The lattice parameter  $h$  occurs since these equations are a mixture of first and second order finite differences. The leading order part of these equations is a discretization of the usual vanishing normal stress condition (2.13).

At a convex corner ( $i = 4$ ), the force balance equations are

$$F_{41} = 4\alpha D_1^- u_1 + 2\beta D_2^- u_1 + \gamma(1 + T_1^-) D_2^- u_2 + \beta(1 + T_2^-) D_1^- u_2 \quad (4.7)$$

$$F_{42} = 4\alpha D_2^- u_2 + 2\beta D_1^- u_2 + \gamma(1 + T_2^-) D_1^- u_1 + \beta(1 + T_1^-) D_2^- u_1. \quad (4.8)$$

At a concave corner ( $i = 6$ ), the equations are

$$F_{61} = -4h\alpha D_1^+ D_1^- u_1 - 2h\beta D_2^+ D_2^- u_1 + 2\beta D_2^- u_1 \quad (4.9)$$

$$+ \gamma(D_2^+ u_2 - T_1^+ D_2^- u_2 + 2T_1^- D_2^0 u_2) + \beta(D_1^+ u_2 - T_2^+ D_1^- u_2 + 2T_2^- D_1^0 u_2)$$

$$F_{62} = -4h\alpha D_2^+ D_2^- u_2 - 2h\beta D_1^+ D_1^- u_2 + 2\beta D_1^- u_2 \quad (4.10)$$

$$+ \gamma(D_1^+ u_1 - T_2^+ D_1^- u_1 + 2T_2^- D_1^0 u_1) + \beta(D_2^+ u_1 - T_1^+ D_2^- u_1 + 2T_1^- D_2^0 u_1).$$

At points of type  $i=2,5,8$  or  $9$ , the force balance equations are

$$F_{i1} = -h(4\alpha D_1^+ D_1^- u_1 + 4\beta D_2^+ D_2^- u_1 + 4(\gamma + \beta) D_1^0 D_2^0 u_2) \quad (4.11)$$

$$F_{i2} = -h(4\alpha D_2^+ D_2^- u_2 + 4\beta D_1^+ D_1^- u_2 + 4(\gamma + \beta) D_1^0 D_2^0 u_1) \quad (4.12)$$

In these equations, the forces due to the shift to a nonequilibrium reference lattice are

$$\begin{aligned}
\mathbf{F}_1 &= (0, \quad 2\gamma(\epsilon_1 + \epsilon_2) - 4\alpha(\rho_{21}\epsilon_1 + \rho_{22}\epsilon_2)) \\
\mathbf{F}_2 &= (0, \quad 2\gamma\delta - 4\alpha\Delta) \\
\mathbf{F}_3 &= \mathbf{F}_1 + (\gamma\delta, \quad 0) \\
\mathbf{F}_4 &= (4\alpha\epsilon_2 - \gamma(\delta + 2(\rho_{21}\epsilon_1 + \rho_{22}\epsilon_2)), \quad \gamma(\epsilon_1 + \epsilon_2) - 4\alpha(\delta + (\rho_{21}\epsilon_1 + \rho_{22}\epsilon_2))) \\
\mathbf{F}_5 &= \mathbf{F}_2 + (\gamma\delta, \quad 0) \\
\mathbf{F}_6 &= (4\alpha\delta - \gamma(\delta + \rho_1\epsilon_1 + (\rho_{21}\epsilon_1 + \rho_{22}\epsilon_2)) + \beta\Delta, \quad 2\gamma\epsilon_1 - 4\alpha(\Delta - \delta) - 2\beta\Delta) \\
\mathbf{F}_7 &= \mathbf{F}_1 + ((\beta - \gamma)\Delta, 2\beta\Delta) \\
\mathbf{F}_8 &= (-(\gamma + \beta)\Delta, \quad \gamma\delta) \\
\mathbf{F}_9 &= \mathbf{F}_2 + (-(\gamma + \beta)\Delta, \quad 0)
\end{aligned} \tag{4.13}$$

in which

$$\begin{aligned}
\delta &= (\epsilon_1 - \epsilon_2) \\
\Delta &= \rho_1\epsilon_1 - (\rho_{21}\epsilon_1 + \rho_{22}\epsilon_2).
\end{aligned}$$

The force balance equations at a corner do *not* admit interpretations as  $\mathbf{n} \cdot \mathbf{T} = 0$ , for any vector  $\mathbf{n}$ .

## 5 Force Field at a Step

In this section, by proper choice of the parameter  $\rho$  in the shift of the strain tensor, we compute the force field in the neighborhood of a step, from which formulas for the monopole and dipole torque due to a step are derived.

### 5.1 Choice of Reference Lattice

The choice  $J = I$ , in which  $I$  is the identity matrix, corresponds to use of a single lattice whose spacing is that of the substrate. At the atomistic level, this means that zero displacement corresponds to a homogeneous strain such that the lattice constant has been changed from its equilibrium value  $a$  to a new value  $h$  throughout the material. This formulation was used in [29] following [6] in a study of morphological stability in heteroepitaxy.

On the other hand, when the epilayer is compressed (or stretched) in the  $x$ -direction to match the substrate, it will contract (or expand) in the  $y$ -direction because of the Poisson ratio. The resulting non-cubic lattice is a more physically meaningful choice of reference lattice and corresponds to the choice  $J = \text{diag}(1, -\rho, 0)$ , for suitable choice of  $\rho$  so that there is no force along the surface away from any steps.

For an epilayer with lattice misfit on top of a substrate, but without a step, as in Figure 2, there is no strain relative to this lattice. For systems with a step, but with no surface layer (i.e. no intrinsic surface stress), we will use this relaxed state as the reference state; i.e., we use  $\epsilon = \epsilon_1$  and  $J = \text{diag}(1, -\rho)$  through the epilayer, as illustrated in Figure 3.

If a surface layer is included, as a model of intrinsic surface stress (but no step), then there is a different displacement in the top layer than that in the rest of the film, as illustrated in Figure 6 away from the step. For systems with a surface layer, the value of  $\epsilon$  should be different in the top layer. If the system has a step, then the surface layer is vertically displaced on the left of the step, relative to the right of the step. The matrix  $J = \text{diag}(1, -\rho, 0)$  may be used throughout the epilayer, but the value of  $\rho$  for the top layer from its value in the remainder of the epilayer. This choice of reference lattice is illustrated in Figure 6. Note that in this reference lattice, the row below the top of the step does not line up horizontally, but the next row down does line up.

Two multipole coefficients of the resulting force field have macroscopic significance. Because of balance of forces and torques, the monopole term  $\mathbf{M}$  and torque component  $\mathbf{D}_T$  of the dipole for the microscopic force field are the same as those for the macroscopic force field, as described in Appendix B.

## 5.2 Monopole and Dipole Moment

The choice  $\rho_1 = \gamma/\alpha$ , which is the Poisson ratio in two-dimensions, and  $\rho_{21} = \rho_{22} = \gamma/(2\alpha)$  makes  $\mathbf{F}_1 = \mathbf{F}_2 = 0$ . The remaining forces are

$$\begin{aligned}
 \mathbf{F}_3 &= (\gamma\delta, \quad 0) \\
 \mathbf{F}_4 &= \left( 4\alpha\epsilon_2 - \gamma\delta - (\gamma^2/\alpha)(\epsilon_1 + \epsilon_2), \quad -\gamma(\epsilon_1 + \epsilon_2) - 4\alpha\delta \right) \\
 \mathbf{F}_5 &= (\gamma\delta, \quad 0)
 \end{aligned} \tag{5.1}$$

$$\begin{aligned}
\mathbf{F}_6 &= \left( (4\alpha - \gamma)\delta - (\gamma^2/2\alpha)(3\epsilon_1 + \epsilon_2) + \beta\gamma\delta/2\alpha, \quad (4\alpha - 2\gamma)\delta + 2\gamma\epsilon_1 - \beta\gamma\delta/\alpha \right) \\
\mathbf{F}_7 &= \left( (\beta - \gamma)\gamma\delta/2\alpha, \quad \beta\gamma\delta/\alpha \right) \\
\mathbf{F}_8 &= \left( -(\gamma + \beta)\gamma\delta/2\alpha, \quad \gamma\delta \right) \\
\mathbf{F}_9 &= \left( -(\gamma + \beta)\gamma\delta/2\alpha, \quad 0 \right)
\end{aligned}$$

It follows that the monopole force is the sum of these 7 forces; i.e.,

$$\mathbf{M} = h \left( 4(\alpha^2 - \gamma^2)\alpha^{-1}\epsilon_1, \quad 0 \right). \quad (5.2)$$

The torque component of the dipole term, computed around the convex corner point of the step (i.e. point # 4) is

$$\mathbf{D}_T = h(4\alpha(\epsilon_1 - \epsilon_2) - (\gamma^2/\alpha)(4\epsilon_1 - 2\epsilon_2)). \quad (5.3)$$

In Appendix C, we show that the elastic surface stress  $g$  for this system is

$$g = -4\alpha(\epsilon_1 - \epsilon_2) + (\gamma^2/\alpha)(4\epsilon_1 - 2\epsilon_2). \quad (5.4)$$

This confirms the result from continuum elasticity [14] that

$$\mathbf{D}_T = -hg \quad (5.5)$$

for elastic surface stress  $g$ . The result Eq. (5.5) is new, since previous treatments [14] were restricted to the case of no misfit strain in the film, i.e.,  $\epsilon_1 = 0$ , so that the monopole term is  $\mathbf{M} = 0$ . Note that this result is dependent on the choice of center point for the dipole.

The force distribution Eq. (5.1) depends on the specific elastic model from which it was derived, but the method of derivation should be applicable to a wide range of models. On the other hand, the formulas Eq. (5.2), Eq. (5.3), Eq. (5.4) and Eq. (5.5) for force monopole, dipole moment, elastic surface stress and the relation between them are somewhat insensitive to the elastic model. A direct calculation shows that these formulas are not changed by the addition of any terms proportional to  $S_{11}^+ S_{11}^-$  and  $(S_{12}^{++})^2$  at the concave corner.

Our confirmation of Eq. (5.5) is in contrast to the results of Shilkrot and Srolovitz [27]. For an embedded atom potential, they determined the dipole term by matching the resulting displacement to that of a Green's function and found that it disagrees with Eq. (5.5). The difference between our result and that of [27] could be due to the difference in the elastic model or it could be due to the difficulty in going from multipole expansion to displacements that was found by [10].

## 6 Conclusions and Future Directions

Although the connection between a lattice statics model and finite difference equations for the continuum elastic energy has been discussed before (e.g. [2]), the finite difference formulation for the force balance equations Eq. (3.10) and Eq. (4.7)-Eq. (4.12) of lattice statics appears to be new and is well suited for computation. In application to three-dimensional problems with material interfaces, we expect to employ adaptive mesh refinement (AMR), with an atomistic grid near the interface and a coarse-grained grid away from the interface. Since the atomistic strain model is a finite difference of a continuum strain model, application of AMR to this problem is a numerical analysis problem that should not require additional physics.

The lattice statics model used here can be generalized to more complex geometries, such as simple cubic, face-centered cubic, body-centered cubic and zinc-blende in three dimensions. The principal complication of this extension is the wider class of possible geometries at a material interface and the necessity for inner relaxation for models which lack inversion symmetry (cubic lattices do not). This inner relaxation should occur automatically when the elastic energy is minimized, and extra displacement is not seen at the macroscopic level. In addition, the relation between the continuum elastic coefficients and the atomistic coefficients must include the effects of the inner relaxation, as discussed in [3, 4, 15, 16].

The model could also be generalized to involve nonlinear elastic interactions. Nonlinearity is necessary for extension to include lattice defects such as dislocations; it may also have significance at steps where the strain energy is larger than in the bulk.

We have used this lattice statics model for simulation of strain effects in epitaxial growth. In a companion paper [26] with several collaborators, we have performed numerical simulation of step interactions on a two-dimensional, vicinal, epitaxial interface, including the interactions with buried steps at the interface between substrate and epilayer. Extensions to include intrinsic surface stress and three-dimensionality are currently underway.

## A Calculation of Force Field at a Step

The force field computation was performed in several steps. First, we analytically calculated the force balance equations  $\delta\mathcal{E} = 0$  in which the displacement is measured relative to the lattice of the substrate. The resulting equations are identical to (4.5)-(4.12) but with the forces on the left replaced by forces  $\mathbf{F}^s$  defined as

$$\begin{aligned}
 \mathbf{F}_1^s &= (0, \quad 2\gamma(\epsilon_1 + \epsilon_2) + 4\alpha\epsilon_1) \\
 \mathbf{F}_2^s &= (0, \quad 2\gamma\delta) \\
 \mathbf{F}_3^s &= \mathbf{F}_1^s + (\gamma\delta, \quad 0) \\
 \mathbf{F}_4^s &= (4\alpha\epsilon_2 + \gamma(\epsilon_1 + \epsilon_2), \quad 4\alpha\epsilon_2 + \gamma(\epsilon_1 + \epsilon_2)) \\
 \mathbf{F}_5^s &= \mathbf{F}_2^s + (\gamma\delta, \quad 0) \\
 \mathbf{F}_6^s &= (\gamma(\epsilon_1 + \epsilon_2) + 4\alpha\delta, \quad 2\gamma\epsilon_1 + 4\alpha\delta) \\
 \mathbf{F}_7^s &= (0, \quad 2\gamma(\epsilon_1 + \epsilon_2) + 4\alpha\epsilon_1) \\
 \mathbf{F}_8^s &= (0, \quad \gamma\delta) \\
 \mathbf{F}_9^s &= \mathbf{F}_2^s
 \end{aligned} \tag{A.1}$$

This result was validated computationally as follows: Our numerical method starts from the energy  $\mathcal{E}$  and determines the matrix  $M$  and the external forces  $F_i^s$  by numerical finite differencing of  $\mathcal{E}$ . The numerical results agree with Eq. (A.1).

The second step was to compute the difference between the substrate lattice  $x^s$  and the reference lattice  $x^p$  of Section 5 that is based on the Poisson ratio. This is conveniently expressed in terms of the displacements  $u^s$  and  $u^p$  relative to each lattice, as

$$\begin{aligned}
 x^p &= x^s - (u^p - u^s) \\
 u^p &= u^s - (1 + \rho_1)\epsilon_1 x_2 \hat{e}_2 - \begin{cases} ((\rho_{21}\epsilon_1 + \rho_{22}\epsilon_2) - \rho_1\epsilon_1)h\hat{e}_2 & \text{if } x_2 = 0, x_1 > 0 \\ \text{or } x_2 = h, x_1 \leq 0 \\ 0 & \text{otherwise} \end{cases}
 \end{aligned} \tag{A.2}$$

This difference is easily characterized in terms of finite differences across bonds; i.e. using the labels in Figure 6,

$$D_i(u^p - u^s)_1 = 0 \quad \text{for } i = 1, 2 \tag{A.3}$$

$$D_1(u^p - u^s)_2 = \begin{cases} -((\rho_{21}\epsilon_1 + \rho_{22}\epsilon_2) - \rho_1\epsilon_1) & \text{on bond labeled "c"} \\ 0 & \text{otherwise} \end{cases} \quad (\text{A.4})$$

$$D_2(u^p - u^s)_2 = \begin{cases} -(1 + \rho_1)\epsilon_1 & \text{on bonds labeled "a"} \\ -(1 + \rho_{21})\epsilon_1 - \rho_{22}\epsilon_2 & \text{on bonds labeled "b"} \end{cases} \quad (\text{A.5})$$

The force balance equations in terms of the displacement  $u^p$  is the matrix equation

$$Mu^p = F^p = F^s + M(u^p - u^s) \quad (\text{A.6})$$

We numerically calculated  $F^p$  from this formula, to verify the formulas in Eq. (4.13).

## B Discrete Balance of Force and Torque

Because of translation invariance of the elastic energy  $\mathcal{E}$ , it depends only on differences between the positions of the particles; i.e.

$$\mathcal{E} = \mathcal{E}(\{\mathbf{w}_{ij}\}) \quad (\text{B.1})$$

in which  $\mathbf{w}_{ij} = \mathbf{u}_i - \mathbf{u}_j$  is the difference in the displacements at points  $i$  and  $j$ . The notation in Eq. (B.1) is intended to mean that  $\mathcal{E}$  can depend on all such differences. Define the force  $\mathbf{F}_{ij}$  of particle  $j$  on particle  $i$  as

$$\mathbf{F}_{ij} = \partial\mathcal{E}/\partial\mathbf{w}_{ij}. \quad (\text{B.2})$$

It follows that forces between  $i$  and  $j$  are equal and opposite; i.e.,

$$\mathbf{F}_{ij} = -\mathbf{F}_{ji}. \quad (\text{B.3})$$

The elastic equations are  $\mathbf{F}_i = -\mathbf{F}_i^{ext}$ , in which  $\mathbf{F}_i = \partial\mathcal{E}/\partial\mathbf{u}_i = \sum_j \mathbf{F}_{ij}$  is the total elastic force on  $i$  and  $\mathbf{F}_i^{ext}$  is the external force on point  $i$ . For any subset  $\Omega$  of points,

$$\begin{aligned} -\sum_{i \in \Omega} \mathbf{F}_i^{ext} &= \sum_{i \in \Omega} \mathbf{F}_i \\ &= \sum_{i \in \Omega} \sum_j \mathbf{F}_{ij} \\ &= \sum_{i \in \Omega} \sum_{j \notin \Omega} \mathbf{F}_{ij} \end{aligned} \quad (\text{B.4})$$

in which the last equality is due to cancelation of  $\mathbf{F}_{ij}$  and  $\mathbf{F}_{ji}$  if both  $i \in \Omega$  and  $j \in \Omega$ . Since the last term on the right in Eq. (B.4) is the force on points in  $\Omega$  from points outside  $\Omega$ , this shows that the total external force on points inside a set is balanced by the force across the boundary of the set. In particular, this shows that the force monopole (the sum of the external forces) is well-defined, if the external forces are constrained to a finite set.

Because of rotational invariance of the elastic energy  $\mathcal{E}$ , it depends only on inner products of differences between the positions of the particles; i.e.

$$\begin{aligned}\mathcal{E} &= \mathcal{E}(\{a_{ijkl}\}) \\ a_{ijkl} &= (\mathbf{X}_i - \mathbf{X}_j) \cdot (\mathbf{X}_k - \mathbf{X}_l).\end{aligned}\tag{B.5}$$

Since  $(\mathbf{X}_i - \mathbf{X}_j) = \mathbf{e}_{ij} + (\mathbf{u}_i - \mathbf{u}_j)$  in which  $\mathbf{e}_{ij} = (\mathbf{x}_i - \mathbf{x}_j)$  is the vector between the reference positions for points  $i$  and  $j$ , the linearized version of Eq. (B.5) is

$$\begin{aligned}\mathcal{E} &= \mathcal{E}(\{b_{ijkl}\}) \\ b_{ijkl} &= \mathbf{e}_{kl} \cdot \mathbf{w}_{ij} + \mathbf{e}_{ij} \cdot \mathbf{w}_{kl} \quad .\end{aligned}\tag{B.6}$$

The torque on point  $i$  is

$$\begin{aligned}\mathbf{T}_i &= \mathbf{x}_i \times \mathbf{F}_i \\ &= \mathbf{x}_i \times (\partial\mathcal{E}/\partial\mathbf{u}_i) \\ &= \sum_{jkl} \mathbf{T}_{ijkl} \\ \mathbf{T}_{ijkl} &= c_{ijkl}(\mathbf{x}_i \times \mathbf{e}_{kl}) \\ c_{ijkl} &= \partial\mathcal{E}/\partial b_{ijkl} \quad .\end{aligned}\tag{B.7}$$

It follows that

$$\begin{aligned}\mathbf{T}_{ijkl} + \mathbf{T}_{jikl} &= c_{ijkl}(\mathbf{x}_i - \mathbf{x}_j) \times \mathbf{e}_{kl} \\ &= c_{ijkl}(\mathbf{e}_{ij} \times \mathbf{e}_{kl}) \\ &= -(\mathbf{T}_{klij} + \mathbf{T}_{lkij})\end{aligned}$$

so that

$$\mathbf{T}_{ijkl} + \mathbf{T}_{jikl} + \mathbf{T}_{klij} + \mathbf{T}_{lkij} = 0.\tag{B.8}$$

For any subset  $\Omega$  of points,

$$\begin{aligned}
-\sum_{i \in \Omega} \mathbf{T}_i^{ext} &= \sum_{i \in \Omega} \mathbf{T}_i \\
&= \sum_{i \in \Omega} \sum_{jkl} \mathbf{T}_{ijkl} \\
&= \sum_{i \in \Omega} \sum_{(j,k,l) \notin \Omega \times \Omega \times \Omega} \mathbf{T}_{ijkl}.
\end{aligned} \tag{B.9}$$

Since the last term on the right in Eq. (B.9) is the torque on points in  $\Omega$  from points outside  $\Omega$ , this shows that the total external torque on points inside a set is balanced by the torque across the boundary of the set. In particular, this shows if the external torques are constrained to a finite set, then the force dipole moment (the sum of the external torques) is well-defined.

Finally we show that the force monopole and force dipole moment are well defined and do not depend on the specific choice of reference lattice. Far from the step, the film surface is flat, so that the correct reference lattice has vertical spacing determined by the Poisson ratio, as seen in Figure 4 away from the step. The lattice on the far right does not match the lattice on the far left, so that near the step a choice must be made in how to piece these two together. Figure 4 displays the choice made in Section 5, but other choices would be possible. The various choices differ only by localized changes near the step. We now show that localized changes in the reference lattice do not change the monopole or dipole moment. For localized changes, the elastic forces  $\mathbf{F}'$  and torques  $\mathbf{T}'$  due to the change in reference lattice are confined to a finite set. For forces confined to a finite set, the balance laws Eq. (B.3) and Eq. (B.8) imply

$$\begin{aligned}
\sum_i \mathbf{F}'_i &= \sum_{ij} \mathbf{F}'_{ij} = 0 \\
\sum_i \mathbf{T}'_i &= \sum_{ijkl} \mathbf{T}'_{ijkl} = 0
\end{aligned} \tag{B.10}$$

i.e., that the sum of forces and torques are both 0. So the change of reference lattice does not change the total force monopole and dipole moment.

Note that if the displacement due to a change of reference lattice or due to external forces is not localized, then the multiple sums in Eq. (B.10) are not absolutely convergent and cannot be rearranged to get 0.

Because the differences  $w_{ij}$  are linearly independent (i.e. the sum around a loop adds to 0), the form Eq. (B.1) for the energy is not unique, so that the formula Eq. (B.2) for the force on particle  $i$  due to particle  $j$  is not unique. Nevertheless, the force and torque across the boundary of a domain are unique, since Eq. (B.4) and Eq. (B.9) show that they are a sum of external forces and torques.

## C Calculation of Surface Stress

Using the results of Appendix B, the surface stress can be calculated for this system, as in Appendix M of [23]. Consider a film that is strained due to lattice mismatch  $\epsilon_1$ , having an interface with lattice mismatch  $\epsilon_2$ . Label the bonds as in Figure 8, and consider the stress and strain components relative to the equilibrium lattice.

As defined in Section 3, the strain components for the bonds are

$$\begin{aligned}
 S_{11}^a &= \epsilon_2 \\
 S_{11}^b &= S_{11}^c = \epsilon_1 \\
 S_{22}^d &= -(\rho_{21}\epsilon_1 + \rho_{22}\epsilon_2) \\
 S_{22}^e &= -\rho_1\epsilon_1
 \end{aligned}
 \tag{C.1}$$

In order to compute the corresponding stress tensor, we mimic continuum elasticity, and derive constitutive laws for the stress tensor by differentiating the discrete elastic energy density with respect to the corresponding strain component. That is, we will define a discrete stress tensor  $T_{kl}$  by

$$T_{kl} = \frac{\partial E}{\partial S_{kl}}$$

The resulting stress tensor, then, is

$$\begin{aligned}
 T_{11}^a &= 4\alpha S_{11}^a + 2\gamma S_{22}^d \\
 &= 4\alpha\epsilon_2 - 2\gamma(\rho_{21}\epsilon_1 + \rho_{22}\epsilon_2) \\
 T_{11}^b &= 4\alpha S_{11}^b + 2\gamma(S_{22}^d + S_{22}^e) \\
 &= 4\alpha\epsilon_1 - 2\gamma(\rho_1\epsilon_1 + \rho_{21}\epsilon_1 + \rho_{22}\epsilon_2) \\
 T_{11}^c &= 4\alpha S_{11}^c + 4\gamma S_{22}^e
 \end{aligned}
 \tag{C.2}$$

$$\begin{aligned}
&= 4\alpha\epsilon_1 - 4\gamma\rho_1\epsilon_1 \\
T_{22}^d &= 4\alpha S_{22}^d + 2\gamma(S_{11}^a + S_{11}^b) \\
&= -4\alpha(\rho_{21}\epsilon_1 + \rho_{22}\epsilon_2) + 2\gamma(\epsilon_1 + \epsilon_2) \\
T_{22}^e &= 4\alpha S_{22}^e + 4\gamma S_{11}^c \\
&= 4\alpha\rho_1\epsilon_1 + 4\gamma\epsilon_1
\end{aligned}$$

The equation for  $T_{22}^e$  for some of the bonds depends on the equality  $S_{11}^b = S_{11}^c$ . The remaining components  $S_{12}$  and  $T_{12}$  are all zero. These are equivalent to the forces, as calculated in the Appendix B.

From the choice of  $\rho_1$ ,  $\rho_{21}$  and  $\rho_{22}$ , it follows that  $T_{22} = 0$ . The surface stress is defined as the net defect in stress one-dimension along the surface. By “defect”, we mean the difference between the stress on the top and in the bulk. Since this stress component varies over both the top and the next to top layer, we add these together to get the surface stress  $g$  as

$$\begin{aligned}
g &= T_{11}^a + T_{11}^b - 2T_{11}^c \\
&= -4\alpha(\epsilon_1 - \epsilon_2) - 4\gamma(\rho_{21}\epsilon_1 + \rho_{22}\epsilon_2) + 6\gamma\rho_1\epsilon_1 \\
&= -4\alpha(\epsilon_1 - \epsilon_2) + (\gamma^2/\alpha)(4\epsilon_1 - 2\epsilon_2)
\end{aligned} \tag{C.3}$$

This formula provides a microscopic determination of the elastic surface stress, or alternatively a method for calibrating a microscopic model if the elastic surface stress is known. As shown in Appendix B, the computed value of the elastic surface stress does not depend on the choice of reference lattice. Also as in Appendix B the surface stress is well-defined, even though the forces between particles may be nonunique.

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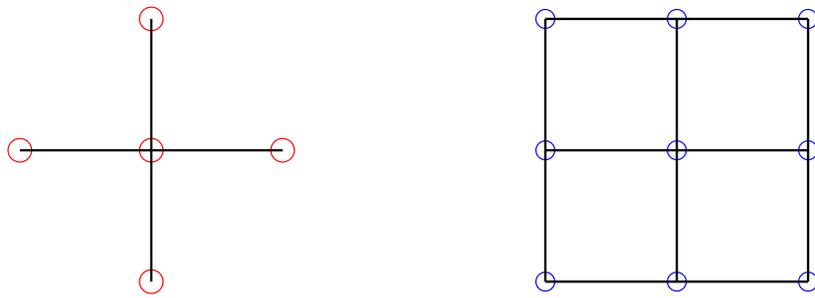


Figure 1: 5-point stencil for energy (left) and 9-point stencil for force balance equations (right) in 2D.

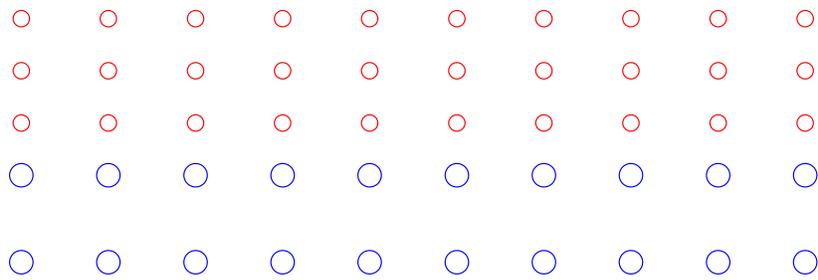


Figure 2: Reference lattice for an epilayer on a substrate, with lattice misfit in the epilayer. The large and small circles are substrate and epilayer atoms, respectively.

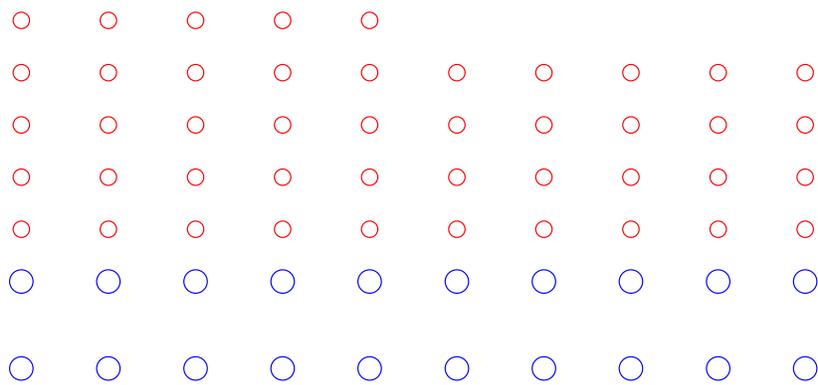


Figure 3: Reference lattice for an epilayer with a step on a substrate, with lattice misfit in the epilayer. The large and small circles are substrate and epilayer atoms, respectively.

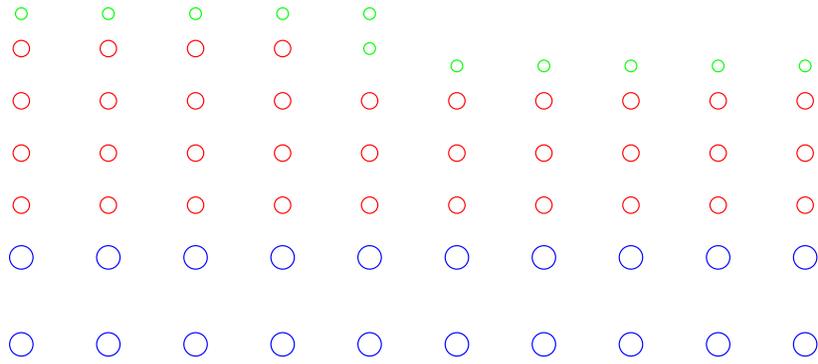


Figure 4: Reference lattice for an epilayer with a step on a substrate, with lattice misfit in the epilayer and intrinsic surface stress in a surface layer. The large, medium and small circles are substrate, epilayer and surface atoms, respectively.

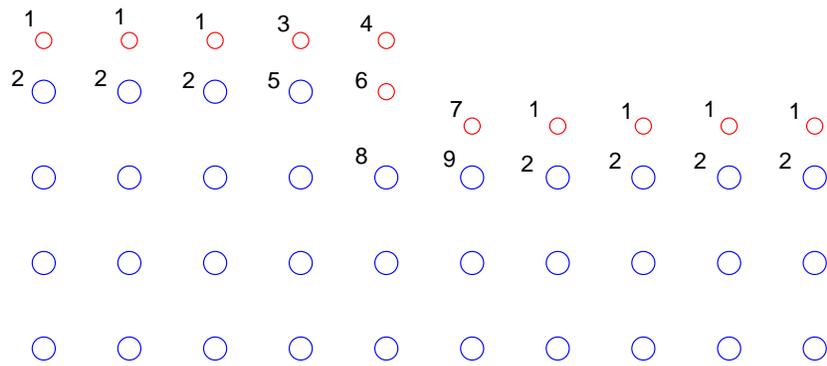


Figure 5: Points in the reference lattice for a single material (the epilayer) with lattice misfit in the epilayer, a step on a substrate, and intrinsic surface stress in a surface layer. The numerical labels refer to types of points near the interface and step, as discussed in the text. The large and small circles are bulk and interface atoms, respectively, in the epilayer.

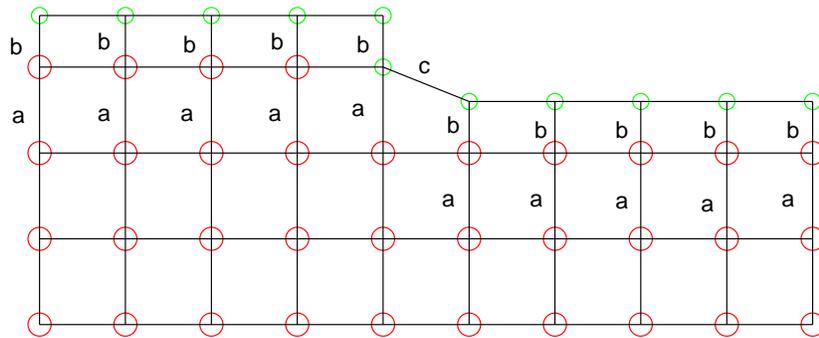


Figure 6: Bonds in the reference lattice for a single material (the epilayer) with lattice misfit in the epilayer, a step on a substrate, and intrinsic surface stress in a surface layer. Letters on the bonds refer to the bond differences in Eq. (A.4). Bonds ‘a’ and ‘b’ are vertical; bond ‘c’ is horizontal; all unlabeled vertical bonds are of type ‘a’. The large and small circles are bulk and interface atoms, respectively, in the epilayer.

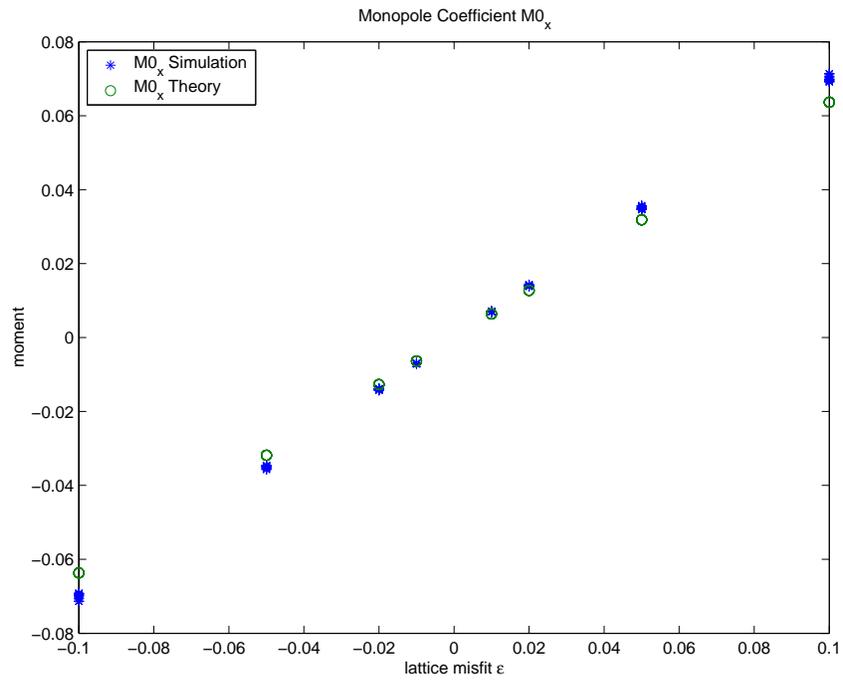


Figure 7: Monopole coefficient  $MO_x$  for the  $x$  component of the displacement along the surface. Plotted as a function of lattice misfit  $\epsilon$  for 128 values of elastic coefficients  $\lambda$ ,  $\mu$  and  $\epsilon$ . Values from the simulation (\*) and from theory (o) are plotted.

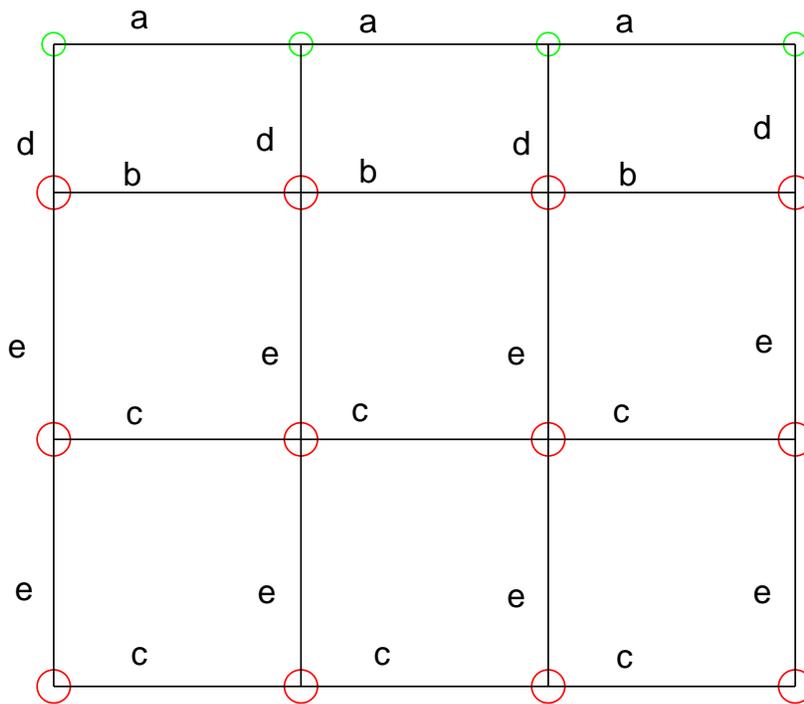


Figure 8: Bonds in the lattice for a single material (the epilayer) with lattice misfit in the epilayer, and intrinsic surface stress in a surface layer. Letters on the bonds refer to the bond differences in Eq. (C.1)-Eq. (C.2). Bonds 'a', 'b' and 'c' are vertical; bonds 'd' and 'e' are horizontal. The large and small circles are bulk and interface atoms, respectively, in the epilayer.