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The elastic field of a surface step: The Marchenko–Parshin formula in the linear case[☆]

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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.

Keywords: Marchenko–Parshin formula; Elasticity; Epitaxial growth

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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% (the significance of the minus sign is that the germanium is under compression). During growth, strain changes the growth rate and surface morphology by changing the adatom diffusion coefficient [10] and other energy transition barriers. Morphological changes in a thin film, such as the growth

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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 [14–16]. Strain also affects the electronic, optical and magnetic properties of materials, so that it is a 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.

The problem of the elastic field of a surface step has been considered by many authors over the last 20 years. The study originated with the work of Marchenko and Parshin in [7], a reference which has been regarded as the definitive work on the subject. Marchenko and Parshin considered simply a surface step of atomic height on an otherwise flat and infinite surface, without lattice mismatch, in the context of continuum elasticity. They proposed that the induced elastic field of a surface step should be that of a dipole traction with normal component gh where g is the surface stress and h is the lattice spacing, and therefore also the step height, as well as an unspecified tangential component f; i.e., the effective traction at the surface is

$$\begin{pmatrix} f \\ gh \end{pmatrix} \delta'(x), \tag{1.1}$$

assuming the step is located at $x = 0$. Here, δ' is the derivative of the Dirac delta function. Its presence in (1.1) has the effect of concentrating the dipole traction at the location of the step. Moreover, the first two terms of the multipole expansion of the elastic field induced by (1.1) are completely determined. The monopole coefficient M (i.e., the total force) and the dipole coefficient D (i.e., the moment) are

$$\mathbf{M} = \mathbf{0}, \tag{1.2}$$

$$D = -gh \tag{1.3}$$

(note: The $-$ in the formula for D arises from δ').

The formula has an intuitive appeal, and Marchenko and Parshin proposed it without any derivation. Indeed, as pointed out in [6] the true multipole expansion of the elastic field of a surface step can never be calculated fully without some microscopic model of the step. Continuum elasticity cannot, by itself, capture the physics of the step. Nevertheless, formula (1.1) is widely believed to be accurate.

In [17] the problem was considered more systematically, but the analysis was still based on continuum elasticity. Then in [12] Shilkrot and Srolovitz tested prediction (1.1) using data from embedded atom simulations. The displacement field from EAM simulations was fit to the displacement field of a point dipole source, as in (1.1), assuming it was accurate to use the half space Green's function for the displacement, in spite of the stepped geometry, a very commonly used approximation. The effective dipole was backed out of this fitting, and compared with (1.1). Discrepancies, on the order of 100% were found, and the authors questioned the validity of the Marchenko–Parshin result.

In [6], however, Kukta and Bhattacharya proposed that the entire idea of using the half space Green's function and its multipole expansion for the stepped surface is invalid. They proposed that there were logarithmic terms in the far field expansion of the elastic field, the first of which being of lower order than the dipole term of (1.1), and that whether or not (1.1) was a valid formula, one could not find the true elastic field using the half space Green's function.

The primary purpose of this paper is to validate (1.1), the Marchenko–Parshin traction for a step. This derivation will be accomplished by developing a harmonic lattice statics model [2,18] on a 2D simple cubic lattice. In the body of the text, the model is built in a finite difference formalism which emphasizes the structural similarity to continuum elasticity. A rigorous atomistic justification is given in Appendix B.

A layered epitaxial system is considered representing a thin film growing on a (possibly) lattice mismatched substrate, and with an atomic sized step on its surface. The effective traction of the step is isolated from the total elastic field by a judicious choice of reference lattice and special half space solutions for the displacement. The result is a localized force distribution $\mathscr{F}(i, j)$ (with (i, j) representing the lattice coordinates of the atom the force is applied to). The explicit formulas for $\mathscr{F}$ are found at the beginning of Section 5.3. The effective monopole and dipole terms can then be calculated as

$$M=\sum_{i,j}\mathscr{F}(i,j), \tag{1.4}$$

$$D=\sum_{i,j}\mathbf{r}\times\mathscr{F}(i,j). \tag{1.5}$$

The force distribution vanishes except for atoms that are within two atoms of the step, so these sums are finite. The principal result of this paper is to show that (1.4) and (1.5) agree with (1.2) and (1.3), showing that our atomistic traction is "statically equivalent" to the Marchenko–Parshin traction (1.1). In fact, our full result is more general than Marchenko and Parshin's in that we extend this calculation 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.

Our result supports the conclusions of Kukta and Bhattacharya, and suggests that the discrepancies of Shilkrot and Srolovitz are not due to the inaccuracy of the Marchenko/Parshin formula, but rather to their use of the half space Green's function for a stepped surface.

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.

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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 $\mathbf{e}$ has components defined as

$$e_{k\ell}=\tfrac{1}{2}(\partial_k u_\ell+\partial_\ell u_k), \tag{2.1}$$

where u_k are the components of $\mathbf{u}$ and $\partial_k=\partial/\partial x_k$.

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. In order to formulate the effect of this change of coordinates on the strain tensor properly, it is best to work at the level of nonlinear elasticity to derive the relationship between the two different strain tensors, and then impose the assumption of small displacements. We consider two different configurations of the material, a reference configuration, measured in coordinates $\{x_i\}_{i=1}^3$, and an equilibrium configuration, measured in coordinates $\{y_i\}_{i=1}^3$. The equilibrium configuration corresponds to a local minimum of the elastic energy. We assume there is a diffeomorphism $x_i=g_i(\mathbf{y})$ between the two configurations.

We now specify that the deformation $\mathbf{X}(\mathbf{x})$ defined above is the deformation from the reference configuration, and thus the displacement $\mathbf{u}(\mathbf{x})=\mathbf{X}(\mathbf{x})-\mathbf{x}$ is the displacement between the deformed position and the reference position of a particle. It follows then that $\mathbf{\Phi}(\mathbf{y})=\mathbf{X}(\mathbf{g}(\mathbf{y}))$ is the deformation from the equilibrium configuration. It is the deformation $\mathbf{\Phi}(\mathbf{y})$ that is the relevant quantity for the elastic energy. We denote the displacement from the equilibrium configuration as $\tilde{\mathbf{u}}=\mathbf{u}+\mathbf{v}$ where $\mathbf{v}=\mathbf{g}(\mathbf{y})-\mathbf{y}=\mathbf{x}-\mathbf{y}$ is the displacement from the equilibrium position to the reference position.

The deformation gradient in the reference coordinates is $\mathbf{F}=D\mathbf{X}$ and in the equilibrium coordinates is $\tilde{\mathbf{F}}=D\mathbf{\Phi}$. Strain is measured by the Cauchy–Green tensor [19] $\mathbf{C}=\mathbf{F}^{\mathrm{T}}\mathbf{F}$ in the reference coordinates and $\tilde{\mathbf{C}}=\tilde{\mathbf{F}}^{\mathrm{T}}\tilde{\mathbf{F}}$ in the equilibrium coordinates. Since $\mathbf{\Phi}=\mathbf{X}\circ\mathbf{g}$ we have by the chain rule $\tilde{\mathbf{F}}=\mathbf{F}D\mathbf{g}$ and thus

$$\tilde{\mathbf{C}}=D\mathbf{g}^{\mathrm{T}}\mathbf{C}D\mathbf{g}. \tag{2.2}$$

If we write (2.2) out in terms of displacements we have

$$\mathbf{I}+\nabla_{\mathbf{y}}\tilde{\mathbf{u}}+\nabla_{\mathbf{y}}\tilde{\mathbf{u}}^{\mathrm{T}}+\nabla_{\mathbf{y}}\tilde{\mathbf{u}}^{\mathrm{T}}\nabla_{\mathbf{y}}\tilde{\mathbf{u}}=(\mathbf{I}+\nabla_{\mathbf{y}}\mathbf{v}^{\mathrm{T}})(\mathbf{I}+\nabla_{\mathbf{x}}\mathbf{u}+\nabla_{\mathbf{x}}\mathbf{u}^{\mathrm{T}}+\nabla_{\mathbf{x}}\mathbf{u}^{\mathrm{T}}\nabla_{\mathbf{x}}\mathbf{u})(\mathbf{I}+\nabla_{\mathbf{y}}\mathbf{v}). \tag{2.3}$$

We now make the basic assumption of linear elasticity that the displacement gradients are small and thus all terms quadratic or higher in them may be neglected. If we apply this assumption to the gradients of all displacements $\mathbf{u}$, $\tilde{\mathbf{u}}$, $\mathbf{v}$ in (2.3) we find

$$\mathbf{I}+\nabla_{\mathbf{y}}\tilde{\mathbf{u}}+\nabla_{\mathbf{y}}\tilde{\mathbf{u}}^{\mathrm{T}}=\mathbf{I}+\nabla_{\mathbf{x}}\mathbf{u}+\nabla_{\mathbf{x}}\mathbf{u}^{\mathrm{T}}+\nabla_{\mathbf{y}}\mathbf{v}+\nabla_{\mathbf{y}}\mathbf{v}^{\mathrm{T}}.$$

Now let $\tilde{\mathbf{e}}=\frac{1}{2}(\nabla_{\mathbf{y}}\tilde{\mathbf{u}}+\nabla_{\mathbf{y}}\tilde{\mathbf{u}}^{\mathrm{T}})$ and $\mathbf{e}=\frac{1}{2}(\nabla_{\mathbf{x}}\mathbf{u}+\nabla_{\mathbf{x}}\mathbf{u}^{\mathrm{T}})$ be the infinitesimal strain tensors measured from the equilibrium and reference coordinates, respectively, to get

$$\mathbf{e}=\tilde{\mathbf{e}}-\tfrac{1}{2}(\nabla_{\mathbf{y}}\mathbf{v}+\nabla_{\mathbf{y}}\mathbf{v}^{\mathrm{T}}), \tag{2.4}$$

which gives the relationship between the two strain tensors valid so long as linear elasticity is valid.

A convenient notation for our purposes will be to write the displacement gradients $\nabla_{\mathbf{y}}\mathbf{v}$ as a general matrix of the form $\varepsilon\mathbf{J}=\nabla_{\mathbf{y}}\mathbf{v}$ where $\mathbf{J}$ will be some O(1) matrix, and ε is a small parameter (whose exact physical meaning we will see shortly). (2.4) then becomes

$$e_{k\ell}=\tfrac{1}{2}(\partial_k u_\ell+\partial_\ell u_k)-\varepsilon\tfrac{1}{2}(J_{k\ell}+J_{\ell k}). \tag{2.5}$$

The transformation (2.4) is in fact mathematically equivalent to the method of eigenstrains [8,9].

In this paper, we will use the form of $\varepsilon\mathbf{J}$

$$\varepsilon J=\begin{pmatrix}\varepsilon & 0\\ 0 & \varepsilon\end{pmatrix} \tag{2.6}$$

with

$$\varepsilon=\frac{a-h}{h},$$

where h is the lattice spacing of the substrate, and a will be the lattice spacing of either the film or the surface layer. We will refer to $\varepsilon\mathbf{J}$ in this case as the shift matrix. This allows the effect of either lattice mismatch at the substrate/film interface or surface stress (see the end of this section) to be included in the model, by changing the reference configuration to be one with a different lattice spacing than the equilibrium configuration. This particular choice of the shift matrix corresponds to choosing the equilibrium lattice of the substrate as the reference configuration.

For the remainder of this section, we assume for simplicity that the reference configuration is the same as the equilibrium configuration.

The elastic energy density E and total energy $\mathscr{E}$ in a domain Ω are

$$E=\frac{1}{2}\sum_{k,\ell}e_{k\ell}T_{k\ell}, \tag{2.7}$$

$$\mathscr{E}=\int_\Omega E\,\mathrm{d}\mathbf{x}. \tag{2.8}$$

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

$$E=(1/2)C_{11}(e_{11}^2+e_{22}^2)+2C_{44}e_{12}^2+C_{12}e_{11}e_{22}, \tag{2.9}$$

$$T_{kl}=2C_{44}e_{kl},\quad k\neq l,$$

$$T_{kk}=C_{11}e_{kk}+C_{12}\sum_{j\neq k}e_{jj}, \tag{2.10}$$

where C_{11}, C_{44} and C_{12} are the cubic elastic moduli.

For linear elasticity in an isotropic material, the stress tensor **T** and the elastic energy density E are

$$E = \frac{1}{2}\lambda\left(\sum_k e_{kk}\right)^2 + \mu\sum_{k\ell}(e_{k\ell})^2, \tag{2.11}$$

$$T_{k\ell} = \lambda\delta_{k\ell}\sum_m e_{mm} + 2\mu e_{k\ell}, \tag{2.12}$$

where λ and μ 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 $\mathscr{E}$; i.e., the displacement **u** solves

$$\delta\mathscr{E} = 0, \tag{2.13}$$

where (2.13) represents the Euler equations for $\mathscr{E}$. Assuming natural boundary conditions, i.e., that there are no forces on the boundary $\partial\Omega$, the Euler equations for this variational principle are

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

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

where **n** is the normal vector with components n_k and $u_{k,\ell} = \partial_k u_\ell$. Since

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

these equations reduce to the classical Navier equations of linear elasticity:

$$\nabla \cdot \mathbf{T} = 0 \quad \text{in } \Omega, \tag{2.14}$$

$$\mathbf{n} \cdot \mathbf{T} = 0 \quad \text{on } \partial\Omega. \tag{2.15}$$

Finally, we consider the notion of surface stress, a concept which goes back to Gibbs. The surface energy per unit area, i.e., the surface tension γ, is the work required to form a unit area of surface. The surface *stress* is the work required to deform the surface. Like the bulk stress, the surface stress is in general a tensor g_{ij}, but only on the 2D surface. If A is the surface area, then γA is the surface energy, and

$$d(\gamma A) = g_{ij}\,\mathrm{d}\eta_{ij}, \tag{2.16}$$

where η_{ij} is the strain tensor of the surface. This leads immediately to

$$g_{ij} = \gamma\delta_{ij} + \frac{\partial\gamma}{\partial\eta_{ij}}. \tag{2.17}$$

At the atomic length scale, the source of surface stress is the preference the surface atoms have for a different lattice spacing than the bulk, due to their lower coordination. It is important to emphasize that in an atomistic context, (2.16) represents the resistance to changing the *excess* energy the surface atoms have over the bulk atoms. More precisely, it represents the misfit stress in the surface layer due to the different coordination and electronic environment of the surface atoms [3]. As shown below, surface stress is readily incorporated in an atomistic model simply by imposing a lattice mismatch between the surface and bulk atoms of the film.

3. The discrete model of elasticity on a 2D cubic lattice

A discrete model of elasticity is formulated in this section, for simplicity in the special case of a 2D simple cubic lattice, using a discrete elastic energy

$$\mathscr{E}[\{\mathbf{r_i}\}], \tag{3.1}$$

where $\mathscr{E}$ is a function of the atomic positions $\mathbf{r_i}$. In Appendix A, a general, nonlinear version of $\mathscr{E}$ is considered. There, laws of mechanics necessary for analysis of the force field of a step are formulated, a task which is best carried out with the full nonlinear energy. The energy here is a leading order quadratic (expanded near an energy minimum) version of that energy, agreeing with it to leading order in the displacements as shown in Appendix B. That justification for the model is left to the appendices, and the presentation here is essentially a discrete version of the continuum variational principle of (2.8), (2.13).

3.1. Finite difference notation

Denote the lattice coordinates as $\mathbf{i} = (i, j)$, and the reference position $\mathbf{x}$, deformed position $\mathbf{X}$ and displacement $\mathbf{u}$ as

$$\begin{aligned} \mathbf{X}(\mathbf{i}) &= (X_1(\mathbf{i}), X_2(\mathbf{i})), \\ \mathbf{x}(\mathbf{i}) &= (x_1(\mathbf{i}), x_2(\mathbf{i})), \\ \mathbf{u}(\mathbf{i}) &= (u_1(\mathbf{i}), u_2(\mathbf{i})) = \mathbf{X}(\mathbf{i}) - \mathbf{x}(\mathbf{i}). \end{aligned} \tag{3.2}$$

Denote the translation operators $T_k^{\pm}$and finite-difference operators $D_k^{\pm}$, D_k^0 as

$$T_k^{\pm} f(\mathbf{i}) = f(\mathbf{i} \pm \mathbf{e}_k), \tag{3.3}$$

$$\begin{aligned} D_k^{+} f(\mathbf{i}) &= h^{-1}(T_k^{+} - 1) f(\mathbf{i}), \\ D_k^{-} f(\mathbf{i}) &= h^{-1}(1 - T_k^{-}) f(\mathbf{i}), \\ D_k^{0} f(\mathbf{i}) &= (2h)^{-1}(T_k^{+} - T_k^{-}) f(\mathbf{i}), \end{aligned} \tag{3.4}$$

where $\mathbf{e}_k$ is the kth unit vector and h is the lattice spacing. Define the bond displacement $\mathbf{d}^{k\pm}$ at the point $\mathbf{i}$ as

$$\mathbf{d}^{k\pm}(\mathbf{i}) = (d_1^{k\pm}, d_2^{k\pm}) = D_k^{\pm}\mathbf{u}(\mathbf{i}) - \varepsilon \quad \mathbf{e}_k \cdot \mathbf{J}. \tag{3.5}$$

Note that $\mathbf{d}^{k\pm}$ is simply the finite difference, i.e., the discrete derivative, of the displacement $\mathbf{u}$ in the kth direction, either forwards (+) or backwards (−).

The value of ε will be the lattice mismatch, due to a shift in the choice of reference lattice, given by

$$\varepsilon = (a - h)/h, \tag{3.6}$$

where h is the equilibrium lattice constant in the substrate and a is the lattice constant of the film, surface, or whichever part of the material we are modeling. This corresponds to using the substrate for the reference lattice. ε represents in the discrete theory, what ε in (2.5) represented in the continuum theory, the size of the displacement of the reference configuration from the equilibrium configuration. The matrix $\varepsilon\mathbf{J}$ plays the role in the discrete theory of the shift matrix (2.6) of the same name, and will in fact be exactly of this form in the discrete model.

The elastic energy will be built up from discrete versions of the strain tensor that can be constructed by replacing partial derivatives by discrete derivatives:

$$\begin{aligned} e_{kk}^{\pm} &= d_k^{k\pm}, \\ e_{k\ell}^{pq} &= (d_k^{\ell q} + d_\ell^{kp})/2, \end{aligned} \tag{3.7}$$

where k and ℓ have values 1 or 2 (denoting the component number of the bond) and p and q have values ± (denoting positive or negative direction along that component). Written out explicitly, the 11 component of the discrete strain tensor is $e_{11}^{+} = D_1^{+}u_1 - \varepsilon$ and the 12 component is $e_{12}^{++} = (D_1^{+}u_2 + D_2^{+}u_1)/2$.

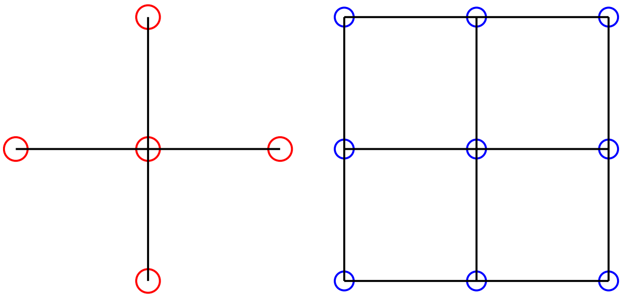

Fig. 1. Five-point stencil for energy (left) and nine-point stencil for force balance equations (right) in 2D.

3.2. The discrete elastic energy

In this section we construct a discrete elastic energy density $E(i, j)$ which may be interpreted as the energy attributed to the atom at the site (i, j). For a point (i, j) in the bulk (i.e. away from boundaries and interfaces), set

$$E = \alpha \sum_{k,p} (e^p_{kk})^2 + \sum_{k \neq \ell, p, q} \{2\beta (e^{pq}_{k\ell})^2 + \gamma e^p_{kk} e^q_{\ell\ell}\}, \tag{3.8}$$

where the discrete strains $e^{pq}_{k\ell}$ are evaluated at (i, j). In these sums, p and q have possible values $+$ and $-$, while k and ℓ have possible values 1 and 2.

This is a finite difference version of the continuum energy density, (2.8), in fact an $\mathrm{O}(h^2)$ discretization of it, with

$$(\alpha, \beta, \gamma) = (C_{11}, C_{44}, C_{12})/4. \tag{3.9}$$

Note that (3.8) is an average over the discrete strain components in different directions. Our choice of $E(i, j)$ is a quadratic function of displacement (corresponding to linear elasticity), obeys the symmetry of a cubic lattice, and has the smallest stencil possible, for both the energy density and the corresponding force balance equation. As illustrated in Fig. 1, the energy density E at a point $\mathbf{x}$ involves only the point $\mathbf{x}$ and its nearest neighbors, and the corresponding force balance equations F at a point $\mathbf{x}$ involve only the point $\mathbf{x}$ and its nearest and next-nearest neighbors.

Alternatively, $E(i, j)$ can be interpreted as the energy due to interactions between atoms in the material lattice. E involves both two body and three body terms, including (1) springs (i.e., harmonic potentials) between nearest neighbors (corresponding to the α terms in (3.8)), (2) bond bending terms that depend on the angle between bonds connecting $\mathbf{x}$ and two of its nearest neighbors (the β terms), and (3) springs between a point $\mathbf{x}$ and the average of two of its nearest neighbors (the γ terms); these interactions are similar to springs between next nearest neighbors. Note that the compressive terms (1) and (3) are invariant to shear, but that the bond-bending terms (2) do vary with shear. In fact, the resulting energy is positive definite. We refer the reader to the appendix of [11] for a more detailed treatment of this interpretation.

A generalization of (3.8) that we will use at interfaces, including the interface with the vacuum, is

$$E = \sum_{k,p} \alpha^p_k (e^p_{kk})^2 + \sum_{k \neq \ell, p, q} \{2\beta^{pq}_{k\ell} (e^{pq}_{k\ell})^2 + \gamma^{pq}_{k\ell} e^p_{kk} e^q_{\ell\ell}\}. \tag{3.10}$$

Consider a system involving two materials A and B. A simple choice of the elastic parameters is formulated as follows: each coefficient α^p_k, as well as the lattice mismatch parameter ε (defined as in (3.6)), corresponds to a bond between two atoms; each of the coefficients $\beta^{pq}_{k\ell}$ and $\gamma^{pq}_{k\ell}$ corresponds to the interaction of two bonds in orthogonal directions from a central point, which defines a square “cell”. For a two-point interaction between atoms of types A and B, take the coefficient α to be the average $\alpha = (\alpha^A + \alpha^B)/2$ of its values in the two materials. Similarly, for a three-point interaction, whose corresponding cell involves atoms of both types A and B, take the coefficients to averages; i.e., $\beta = (\beta^A + \beta^B)/2$ and $\gamma = (\gamma^A + \gamma^B)/2$.

Lattice sites in the vacuum are included by taking the coefficients to be 0 if a bond or cell involves a vacuum atom. Intrinsic surface stress is included at a material/vacuum interface by considering bonds between two interface sites as having different values of ε_{I}, without changing the properties of bonds between interface and bulk sites or of cells involving interface and bulk sites.

Finally, the total energy, analogous to (2.8) in the continuum case is

$$\mathscr{E} = \sum_{\mathbf{i}} E(\mathbf{i}). \tag{3.11}$$

3.3. Force balance equations

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

$$\frac{\partial \mathscr{E}}{\partial u_k(\mathbf{i})} = 0, \quad k = 1, 2 \tag{3.12}$$

for all $\mathbf{i}$. Eq. (3.12) is the discrete Euler–Lagrange equation for the functional $\mathscr{E}$ and consists of force balance laws determining the steady state position of the atom at each site. The general structure of these equations is a discrete version of a PDE, which in the bulk is simply a discretization of the classical Navier equations (2.14). Here we will introduce a notation which emphasizes this analogy. Since the energy is quadratic in $\mathbf{u}(i, j)$ and its differences, Eqs. (3.12) will be linear in $\mathbf{u}$ and its differences. The force balance equations are thus of the form

$$\mathscr{L}(i, j)\mathbf{u}(i, j) = \mathbf{F}(i, j). \tag{3.13}$$

At a bulk point (3.13) has the form

$$\mathscr{L}(i, j)\mathbf{u}(i, j) = 4\alpha D_k^+ D_k^- u_k + 4\beta \sum_{\ell \neq k} D_\ell^+ D_\ell^- u_k + 4(\gamma + \beta) \sum_{\ell \neq k} D_k^0 D_\ell^0 u_\ell = 0 \tag{3.14}$$

for $k = 1, 2$. The microscopic elastic moduli α, β, γ are equal to their interior values for the given material. Note that (3.14) is a second order accurate discretization of the continuum equation (2.14).

For a discrete model, unlike for a continuum theory, there is no fundamental difference between boundary points and interior points, other than the different form of the energy density, and the force balance equations at all points could be written in the form of (3.13). In order to make the analogy between our discrete theory and continuum theory as full as possible, we are going to distinguish between the interior points and the boundary points. To explain the idea explicitly it is helpful to exploit the linear structure of the problem. The force balance equations (3.12) constitute a discrete boundary value problem for the displacement $\mathbf{u}(i, j)$. The "boundary conditions" are simply the force balance equations at the boundary points. We may write Eq. (3.12) in the same structure as a Neumann problem for Poisson's equations, that is, a solution $\mathbf{u}(i, j)$ solves

$$\mathscr{L}\mathbf{u} = F, \tag{3.15}$$

$$\mathscr{B}\mathbf{u} = G, \tag{3.16}$$

where (3.15) stands for the interior force balance equations (3.14), and (3.16) stands for the force balance equations at all boundary points. At all points that do not have at least one boundary point in their nine point stencil, the equations will be exactly of form (3.14). We will define an interior point to be any point whose force balance equation is of this form. We will use the notation $\mathscr{L}$ exclusively for interior points. All other points, which will include surface and interface points, will be considered boundary points. Since we will not need to consider the force balance equations at the substrate–film interface, we will only deal with boundary points, and for them we will write the force balance equations as (3.16). Both $\mathscr{L}$ and $\mathscr{B}$ are linear operators, defined by the left hand sides of the force balance equation.

The next section includes the precise form of the energy $E(i, j)$, the linear operators and forces at the boundaries, $\mathscr{B}(i, j)$ and $\mathbf{G}(i, j)$ for the case of lattice mismatched heteroepitaxy with an atom sized step on the surface.

4. 2D layered material with intrinsic surface stress

Consider a 2D epitaxial thin film with parallel steps on its surface and with lattice mismatch ε_1 relative to the substrate. Set the coordinate i to be normal to the steps and j to be the growth direction. The interface between substrate and epilayer is always assumed to be horizontal ($j = 0$).

Along the interface between epilayer and vacuum, the lattice mismatch of the interface atoms (relative to the substrate) is ε_2, so that the lattice mismatch of the interface relative to the film is the difference $\delta = \varepsilon_2 - \varepsilon_1$. For simplicity the elastic coefficients α, β and γ are assumed to be uniform throughout the material system (substrate, epilayer and surface layer). Illustrations for a system consisting of substrate and epilayer are in Fig. 2 with no step and no intrinsic surface stress, Fig. 3 with intrinsic surface stress but no step, and Fig. 4 with intrinsic surface stress and a step. The lattice constant h of the substrate is chosen for the reference lattice, so that h is the nearest neighbor distance between the atoms in the lower layer in Figs. 2, 3 and 4. The corresponding shift in the strain tensor is

$$\varepsilon J = \begin{pmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_1 \end{pmatrix}, \tag{4.1}$$

where $\varepsilon = \varepsilon_1$ in the film, $\varepsilon = \varepsilon_2$ at the surface, and $\varepsilon = 0$ in the substrate.

4.1. Energy density

At an interior point, the energy density is

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

At the surface, there are nine different types of points, as illustrated in Fig. 5: the force balance equations of the nine different points in Fig. 5 each differ in either $\mathscr{B}$ or **F**; however, the form of the energy density $E(i, j)$ is the same at some points of different types. Points of type 2, 5, 8, or 9 have the energy density of a bulk point (4.2).

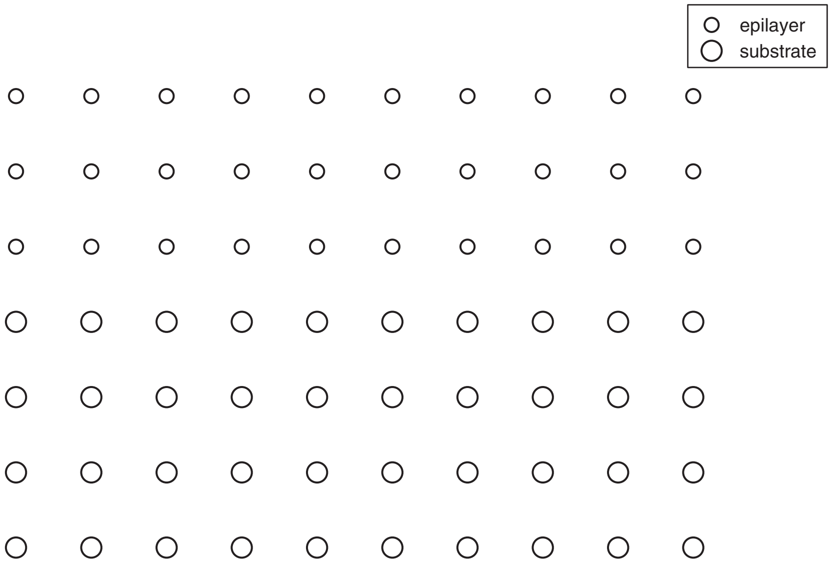

Fig. 2. Reference lattice for an epilayer on a substrate, with lattice misfit in the epilayer. The large and small circles are substrate and epilayer atoms, respectively.

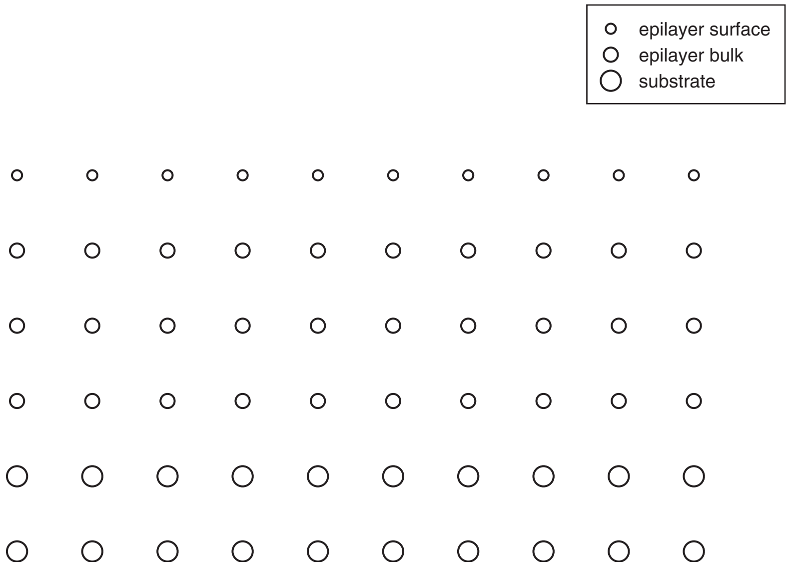

Fig. 3. Reference lattice for an epilayer on a substrate, with lattice misfit in the epilayer, and in the surface layer, representing intrinsic surface stress. The large, medium, and small circles are substrate, epilayer and surface atoms, respectively.

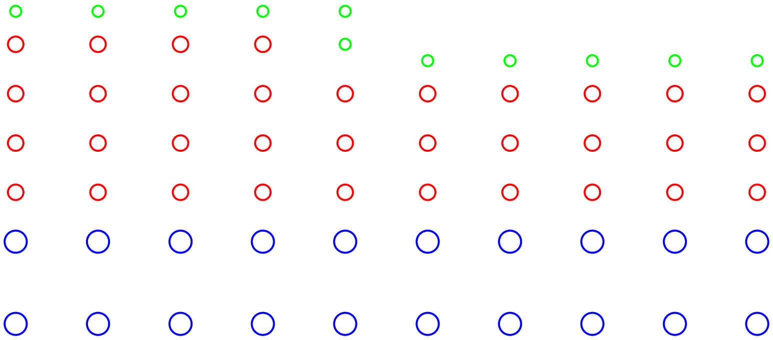

Fig. 4. Modified exact solution for an epilayer with a step on a substrate, with lattice misfit in the epilayer and intrinsic surface stress in a surface layer. The large, medium and small circles are substrate, epilayer and surface atoms, respectively. The modified exact solution for an epilayer and a step, without a surface layer, is the same with the small circles removed.

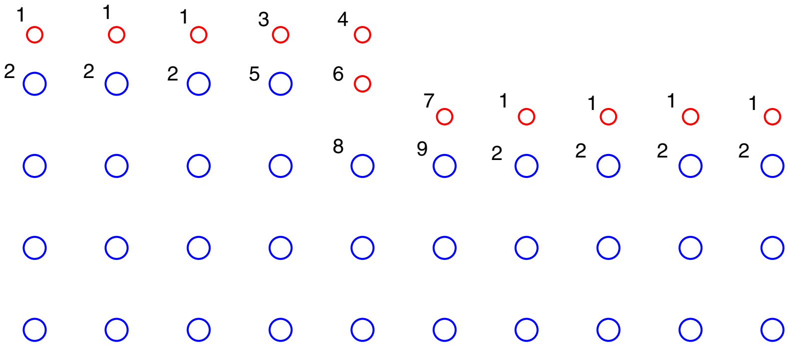

Fig. 5. Points in the reference lattice for a single material (the epilayer) with lattice misfit in the epilayer, a step on a substrate, and intrinsic surface stress in a surface layer. The numerical labels refer to types of points near the interface and step, as discussed in the text. The large and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

Consider a point (i, j) on the horizontal boundary (away from the step), which is a point of type 1, 3, or 7. The energy contribution for such a point is

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

There are also convex corners, of type 4, with energy density

$$E = \alpha[(d_1^{1-})^2 + (d_2^{2-})^2] + \frac{\beta}{2}(d_2^{1-} + d_1^{2-})^2 + \gamma d_1^{1-} d_2^{2-}, \tag{4.4}$$

and concave corner points, of type 6, with energy density

$$\begin{aligned} E = {} & \alpha[(d_1^{1+})^2 + (d_1^{1-})^2 + (d_2^{2+})^2 + (d_2^{2-})^2] + \frac{\beta}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2+})^2 \\ & + (d_2^{1-} + d_1^{2-})^2] + \gamma[d_1^{1+} d_2^{2-} + d_1^{1-} d_2^{2+} + d_1^{1-} d_2^{2-}]. \end{aligned} \tag{4.5}$$

4.2. Force balance equations

The force balance equations are the Euler–Lagrange equations, (3.12). For analysis of the Marchenko–Parshin formula, the force balance equations are needed only for the film interior and the surface. As discussed in Section 3, there are two parts to the force balance equation at a given point, the linear operator $\mathscr{L}(i, j)$ or $\mathscr{B}(i, j)$ and the force on the right hand side, $\mathbf{F}(i, j)$ or $\mathbf{G}(i, j)$.

In the film bulk, the operator $\mathscr{L}(i, j)$ is as in (3.14) and $\mathbf{F}(i, j) = 0$.

For simplicity we will refer to the boundary points by their type rather than their lattice coordinates; i.e., the boundary linear operators are $\mathscr{B}_k\mathbf{u} = (\mathscr{B}_k\mathbf{u}_1, \mathscr{B}_k\mathbf{u}_2)$, the forces as $\mathbf{G}_k = (\mathbf{G}_{k1}, \mathbf{G}_{k2})$ and the force balance equations at a point of type k are $\mathscr{B}_k\mathbf{u} = \mathbf{G}_k$.

At a horizontal edge (point types $k = 1, 3, 7$), the linear operators are

$$\mathscr{B}_k\mathbf{u}_1 = -h(4\alpha D_1^+ D_1^- u_1 + 2\gamma D_1^0 D_2^- u_2) + 4\beta D_2^- u_1 + 2\beta(1 + T_2^-) D_1^0 u_2,$$

$$\mathscr{B}_k\mathbf{u}_2 = -h(2\beta D_1^+ D_1^- u_2 + 2\beta D_1^0 D_2^- u_1) + 4\alpha D_2^- u_2 + 2\gamma(1 + T_2^-) D_1^0 u_1.$$

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 (2.15).

At a convex corner ($k = 4$), the operators are

$$\mathscr{B}_4\mathbf{u}_1 = 4\alpha D_1^- u_1 + 2\beta D_2^- u_1 + \gamma(1 + T_1^-) D_2^- u_2 + \beta(1 + T_2^-) D_1^- u_2,$$

$$\mathscr{B}_4\mathbf{u}_2 = 4\alpha D_2^- u_2 + 2\beta D_1^- u_2 + \gamma(1 + T_2^-) D_1^- u_1 + \beta(1 + T_1^-) D_2^- u_1.$$

At a concave corner ($k = 6$), the operators are

$$\begin{aligned} \mathscr{B}_6\mathbf{u}_1 = {} & -4h\alpha D_1^+ D_1^- u_1 - 2h\beta D_2^+ D_2^- u_1 + 2\beta D_2^- u_1 + \gamma(D_2^+ u_2 - T_1^+ D_2^- u_2 + 2T_1^- D_2^0 u_2) \\ & + \beta(D_1^+ u_2 - T_2^+ D_1^- u_2 + 2T_2^- D_1^0 u_2), \end{aligned}$$

$$\begin{aligned} \mathscr{B}_6\mathbf{u}_2 = {} & -4h\alpha D_2^+ D_2^- u_2 - 2h\beta D_1^+ D_1^- u_2 + 2\beta D_1^- u_2 + \gamma(D_1^+ u_1 - T_2^+ D_1^- u_1 + 2T_2^- D_1^0 u_1) \\ & + \beta(D_2^+ u_1 - T_1^+ D_2^- u_1 + 2T_1^- D_2^0 u_1). \end{aligned}$$

We note that at the convex and concave corner points, the force balance equations are *not* discretizations of (2.15) for any choice of a normal vector. They are purely atomistic conditions. At points of type $k = 2, 5, 8$ or 9, the operators are

$$\mathscr{B}_k\mathbf{u}_1 = -h(4\alpha D_1^+ D_1^- u_1 + 4\beta D_2^+ D_2^- u_1 + 4(\gamma + \beta) D_1^0 D_2^0 u_2),$$

$$\mathscr{B}_k\mathbf{u}_2 = -h(4\alpha D_2^+ D_2^- u_2 + 4\beta D_1^+ D_1^- u_2 + 4(\gamma + \beta) D_1^0 D_2^0 u_1).$$

The corresponding forces are

$$
\begin{aligned}
&\mathbf{G}_1 = \mathbf{G}_7 = (0, 2\gamma\varepsilon_2 + (2\gamma + 4\alpha)\varepsilon_1),\\
&\mathbf{G}_2 = 2\mathbf{G}_8 = \mathbf{G}_9 = (0, 2\gamma\delta),\\
&\mathbf{G}_3 = \mathbf{G}_1 + (\gamma\delta, 0),\\
&\mathbf{G}_4 = ((4\alpha + \gamma)\varepsilon_2 + \gamma\varepsilon_1, (4\alpha + \gamma)\varepsilon_2 + \gamma\varepsilon_1),\\
&\mathbf{G}_5 = \mathbf{G}_2 + (\gamma\delta, 0),\\
&\mathbf{G}_6 = (\gamma(\varepsilon_1 + \varepsilon_2) + 4\alpha\delta, 2\gamma\varepsilon_1 + 4\alpha\delta),
\end{aligned}
\tag{4.6}
$$

where $\delta = (\varepsilon_1 - \varepsilon_2)$.

5. Force field at a step

In this section 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 and exact solutions

As explained in Section 4 we choose diagonal shift matrices $\varepsilon_k J = \mathrm{diag}(\varepsilon_k, \varepsilon_k)$ with $\varepsilon_1 = (a - h)/h$ in the film, and $\varepsilon_2 = (a_S - h)/h$ at the surface layer, where a_S is the preferred lattice spacing of the surface atoms, representing intrinsic surface stress (see Section 2). This choice corresponds to a reference lattice with the lattice spacing of the substrate throughout the material. At the atomistic level, this means that zero displacement corresponds to a homogeneous strain such that the lattice constant has changed from its equilibrium value a to a new value h throughout the material.

Using the half space reference lattice we will define two exact solutions to our discrete boundary value problem, one without, and one including, surface stress. The first is really a special case of the second but it is helpful in understanding the meaning of the solutions to consider it separately.

The first solution $\mathbf{u}^{\mathbf{P}}$ is defined as

$$\mathbf{u}^{\mathbf{P}}(i, j) = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{for } j \leqslant 0 \tag{5.1}$$

in the substrate and

$$\mathbf{u}^{\mathbf{P}}(i, j) = \begin{pmatrix} 0 \\ j(\rho_1 + 1)\varepsilon_1 h \end{pmatrix} \quad \text{for } 1 \leqslant j \leqslant N \tag{5.2}$$

in the film. Here, ρ_1, given by

$$\rho_1 = \gamma/\alpha, \tag{5.3}$$

is the Poisson ratio of the film. For the solution $\mathbf{u}^{\mathbf{P}}$, the horizontal spacing of the atoms is that of the substrate lattice; while the vertical displacement compensates for the lattice mismatch in the film.

In the case with surface stress, let points $j \leqslant 0$ be the substrate, $1 \leqslant j \leqslant N$ be all but the top layer of the film, and $j = N + 1$ the surface layer. The solution $\mathbf{u}^{\mathbf{SP}}$ equals $\mathbf{u}^{\mathbf{P}}$ for $j \leqslant N$, that is, (5.1) in the substrate and (5.2) in the film. Finally, at the surface layer

$$\mathbf{u}^{\mathbf{SP}}(i, N + 1) = \begin{pmatrix} 0 \\ (N(\rho_1 + 1)\varepsilon_1 + (\rho_2 + 1)\varepsilon_1)h \end{pmatrix} \quad \text{for } 1 \leqslant j \leqslant N, \tag{5.4}$$

where ρ_2 is the “effective” Poisson ratio in the top layer, given by

$$\rho_2 = \frac{\gamma(\varepsilon_1 + \varepsilon_2)}{2\alpha\varepsilon_1}. \tag{5.5}$$

It is easily verified that both $\mathbf{u}^{\mathbf{P}}$ and $\mathbf{u}^{\mathbf{SP}}$ are exact solutions of the boundary value problem (3.15), (3.16) for a half space, satisfying both the interior and boundary equations. In particular, there are no remaining unbalanced forces at any point.

5.2. *The force at a step*

The Poisson ratio solutions $\mathbf{u}^{\mathbf{P}}$ and $\mathbf{u}^{\mathbf{SP}}$ give the exact solution of the discrete traction problem for a mismatched substrate–film half space. In this section we define the force of a step as the effective traction imposed at the surface when the system is held in one of these two solutions, and a step is introduced.

With a step, the Poisson ratio solutions need to be altered, to accommodate the changed geometry. For both solutions, we make the simplest extension, taking $j = N$ as the surface layer on the lower terrace $i \geqslant 1$ and $j = N + 1$ as the surface layer on the top terrace $i \leqslant 0$. The modified versions of $\mathbf{u}^{\mathbf{SP}}$ is illustrated in Fig. 4. The modified version of $\mathbf{u}^{\mathbf{P}}$ is obtained by omitting the smallest circles in this figure.

Since the boundary value problem (3.15), (3.16) is linear, the principle of superposition says that

$$F = \bar{\mathbf{F}} + \tilde{\mathbf{F}}, \tag{5.6}$$

$$G = \bar{\mathbf{G}} + \tilde{\mathbf{G}}, \tag{5.7}$$

$$\mathbf{u} = \bar{\mathbf{u}} + \tilde{\mathbf{u}}, \tag{5.8}$$

where

$$\mathscr{L}\bar{\mathbf{u}} = \bar{\mathbf{F}}, \quad \mathscr{B}\bar{\mathbf{u}} = \bar{\mathbf{G}}, \tag{5.9}$$

$$\mathscr{L}\tilde{\mathbf{u}} = \tilde{\mathbf{F}}, \quad \mathscr{B}\tilde{\mathbf{u}} = \tilde{\mathbf{G}}. \tag{5.10}$$

Let $\bar{\mathbf{u}}$ be either of the Poisson ratio solutions, so that $\tilde{\mathbf{u}} = \mathbf{u} - \mathbf{u}^{\mathbf{P}}$ or $\tilde{\mathbf{u}} = \mathbf{u} - \mathbf{u}^{\mathbf{SP}}$.

The meaning of the decomposition is clearest in the case without intrinsic surface stress. Then $\tilde{\mathbf{u}} = \mathbf{u} - \mathbf{u}^{\mathbf{P}}$ is the additional displacement that the step induces relative to the Poisson ratio configuration of the film in the absence of a step. The force $\tilde{\mathbf{G}}$ is the effective traction that induces this extra displacement; i.e., it is the effective force at a step.

Similarly, in the case with surface stress, $\tilde{\mathbf{u}} = \mathbf{u} - \mathbf{u}^{\mathbf{SP}}$ is the additional displacement that the step induces relative to the Poisson ratio configuration of the film. Although $\mathbf{u}^{\mathbf{SP}}$ is not the displacement for a flat surface, it does have the correct values far from the step. Therefore it is a valid displacement field from which to measure the effect of the step, and the resulting force field $\tilde{\mathbf{G}}$ can be defined as the effective force due to the step.

As a consistency check, suppose that $\mathbf{u}^{\mathbf{0}}$ is a different reference displacement field with the same values as $\mathbf{u}^{\mathbf{SP}}$ away from the step. As discussed below, the monopole and dipole at the step are determined by the monopole and dipole in the far field. This implies that the difference in reference fields $\mathbf{u}^{\mathbf{0}} - \mathbf{u}^{\mathbf{SP}}$ does not induce a monopole and dipole. So calculation of the monopole and dipole using $\tilde{\mathbf{u}} = \mathbf{u} - \mathbf{u}^{\mathbf{0}}$ would give the same values as for $\tilde{\mathbf{u}} = \mathbf{u} - \mathbf{u}^{\mathbf{SP}}$.

To summarize: in either the case without or with surface stress we take $\bar{\mathbf{u}} = \mathbf{u}^{\mathbf{P}}$ or $\mathbf{u}^{\mathbf{SP}}$, respectively, and define the force of the step as

$$\begin{aligned}\mathscr{F} &= \tilde{\mathbf{G}}\\ &= \mathbf{G} - \mathscr{B}\bar{\mathbf{u}}.\end{aligned} \tag{5.11}$$

Since the forces $\mathbf{G}$ and the boundary operators $\mathscr{B}$ are given exactly in Section 4.2, formula (5.11) gives an explicit formula, from which the force of the step is computed in the next subsection.

5.3. *Monopole and dipole moment*

Our choices for the exact solutions $\mathbf{u}^{\mathbf{P}}$ and $\mathbf{u}^{\mathbf{SP}}$ ensure that $\mathscr{F}_1 = \mathscr{F}_2 = \mathbf{0}$, since they are solutions of the half space problem. The remaining forces are

$$\mathscr{F}_{\mathbf{3}} = \mathscr{F}_{\mathbf{5}} = (\gamma\delta, 0),$$

$$\mathscr{F}_{\mathbf{4}} = (4\alpha\varepsilon_2 - \gamma\delta - (\gamma^2/\alpha)(\varepsilon_1 + \varepsilon_2), -\gamma(\varepsilon_1 + \varepsilon_2) - 4\alpha\delta),$$

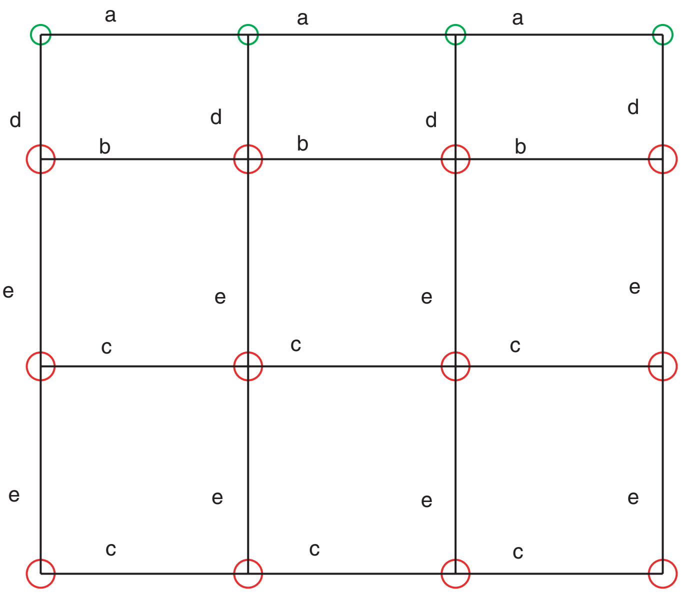

Fig. 6. Bonds in the lattice for a single material (the epilayer) with lattice misfit in the epilayer, and intrinsic surface stress in a surface layer. Bonds "a", "b" and "c" are horizontal; bonds "d" and "e" are vertical. The large and small circles are bulk and interface atoms, respectively, in the epilayer.

$$\mathscr{F}_{\mathbf{6}} = ((4\alpha - \gamma)\delta - (\gamma^2/2\alpha)(3\varepsilon_1 + \varepsilon_2) + \beta\gamma\delta/2\alpha,\ (4\alpha - 2\gamma)\delta + 2\gamma\varepsilon_1 - \beta\gamma\delta/\alpha),$$

$$\mathscr{F}_{\mathbf{7}} = ((\beta - \gamma)\gamma\delta/2\alpha,\ \beta\gamma\delta/\alpha),$$

$$\mathscr{F}_{\mathbf{8}} = (-(\gamma + \beta)\gamma\delta/2\alpha,\ \gamma\delta),$$

$$\mathscr{F}_{\mathbf{9}} = (-(\gamma + \beta)\gamma\delta/2\alpha,\ 0). \tag{5.12}$$

Two multipole coefficients of the resulting force field have macroscopic significance. Because of balance of forces and torques (a proof of which is given in Appendix A), the monopole term **M** and torque component D of the dipole for the microscopic force field are the same as those for the macroscopic force field.

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

$$\mathbf{M} = h(4(\alpha^2 - \gamma^2)\alpha^{-1}\varepsilon_1, 0). \tag{5.13}$$

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

$$D = h(4\alpha(\varepsilon_1 - \varepsilon_2) - (\gamma^2/\alpha)(4\varepsilon_1 - 2\varepsilon_2)). \tag{5.14}$$

Now use the notion of force developed in Appendix A to calculate the surface stress. Label the bonds as in Fig. 6, and drop a vertical line through the lattice. Surface stress is the force that the atoms on one side of the line exert on the atoms on the other. Moreover, it is only the tangential component of this force (the normal component vanishes at the flat surface). So, from the results of the Appendix, it is enough to compute

$$\frac{\partial \mathscr{E}}{\partial \Delta x}, \tag{5.15}$$

where Δx is the horizontal distance between the two portions of material. Referring to Fig. 6, define the force at each level a,b,c as

$$T^v = \frac{\partial \mathscr{E}}{\partial \Delta x}(i,\ j_v), \tag{5.16}$$

where j_v denotes the value of j at the level $v = a$, b, or c. These can be calculated as

$$\begin{aligned} T^a &= 4\alpha\varepsilon_2 - 2\gamma\rho_2(\varepsilon_1 + \varepsilon_2), \\ T^b &= 4\alpha\varepsilon_1 - 2\gamma(\rho_1\varepsilon_1 + \rho_2(\varepsilon_1 + \varepsilon_2)), \\ T^c &= 4\alpha\varepsilon_1 - 4\gamma\rho_1\varepsilon_1. \end{aligned} \tag{5.17}$$

Note that T^c is the bulk stress that lies between two atoms across a horizontal bond at any level in the film below the surface; while T^a and T^b are distinct from this bulk stress.

As explained in Section 2, surface stress in our atomistic context is the gradient of the *excess* energy at the surface with respect to the positions of the surface atoms [3]. It is necessary to subtract off the stress in the bulk from stress at the surface to compute the true surface stress. Accordingly, the surface stress is

$$\begin{aligned} g &= T^a + T^b - 2T^c \\ &= -4\alpha(\varepsilon_1 - \varepsilon_2) - 4\gamma\rho_2(\varepsilon_1 + \varepsilon_2) + 6\gamma\rho_1\varepsilon_1 \\ &= -4\alpha(\varepsilon_1 - \varepsilon_2) + (\gamma^2/\alpha)(4\varepsilon_1 - 2\varepsilon_2). \end{aligned} \tag{5.18}$$

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.

Comparison of Eqs. (5.14) with (5.18) shows

$$D = -hg \tag{5.19}$$

for elastic surface stress g. For making comparisons of the monopole and dipole with the Marchenko–Parshin results (1.2) and (1.3), we consider the case that they considered, and that is the case of no lattice mismatch between film and substrate. This corresponds to setting $\varepsilon_1 = 0$ in these formulas. In this case, monopole (5.13) vanishes, the substrate lattice spacing h is the same as the film lattice spacing, and therefore the step height, and we find complete agreement between our results (5.13), (5.19) and the results of Marchenko and Parshin.

Note that in addition to confirming the Marchenko–Parshin formula Eq. (5.19) our theory includes the case $\varepsilon_1 \neq 0$ in which there is lattice misfit. In this case, the resulting monopole term does not vanish, so that the formula for the moment is dependent on the choice of center point for the dipole.

The force distribution Eq. (5.11) 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, formulas (5.13), (5.14), (5.18) and (5.19) for force monopole, dipole moment, elastic surface stress and the relation between them are somewhat insensitive to the elastic model. For example, a direct calculation shows that these formulas are not changed by the addition of any terms proportional to $e_{11}^{+}e_{11}^{-}$ and $(e_{12}^{++})^2$ at the concave corner.

Our confirmation of Eqs. (5.19) is in contrast to the results of Shilkrot and Srolovitz [12]. 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. (5.19). The difference between our result and that of [12] could be due to the difference in the elastic model or it could be due to the difficulty in going from a multipole expansion to displacements that was found by [6].

We conclude by addressing the issue of the exact relationship between our result and that of Marchenko and Parshin. For a certain class of microscopic models, we have shown that the monopole and dipole terms of a step agree with those of Marchenko and Parshin's continuum formulas (1.1). We next argue that the meaning of (1.1) is nothing more than these two moments.

The appendices of this paper contain a proof that the basic conservation laws of continuum mechanics for force and torque hold in our discrete setting. It follows that the monopole and dipole moments of the force $\mathscr{F}$ are preserved in the far field. So our theory agrees with Marchenko and Parshin in the far field up to the dipole term. We appeal then to Saint–Venant's principle, which says that two different tractions give rise to the same displacement in the far field if they are "statically equivalent", i.e., if they have the same force and moment [13, p. 90]. In conclusion, our demonstration that the effective traction of the step in our model is statically equivalent to (1.1) validates the result (1.1). Moreover, the Marchenko–Parshin theory leaves the horizontal component unspecified. Note, however, that there is not yet, to our knowledge, a version of Saint–Venant's principle that has been rigorously proven for lattices. For a current review of Saint–Venant's principle, see [4,5].

6. Conclusions and future directions

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 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.

Although the connection between a lattice statics model and finite difference equations for the continuum elastic energy has been discussed before (e.g. [2,18]), the finite difference formulation for the force balance equations Eq. (3.14) along with the boundary conditions of Section 4.2 appears to be new and is well suited for computation.

We have used this lattice statics model for simulation of strain effects in epitaxial growth. In a companion paper [11] with several collaborators, we have performed numerical simulation of step interactions on a 2D, 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.

Appendix A. Conservation laws of classical mechanics

To justify both the conservation laws (balance of momentum and torque) as well as the definition of the force exerted by one part of the body on another part, we will consider the mechanics of particles with potentials of the type used commonly in materials science. The potentials considered here are different from the ones normally considered in Newtonian mechanics, because of the presence of 3-body (and possibly higher) interactions. The use of such interactions implies that not all forces will be central forces, and we cannot expect Newton's third law to hold. In fact, with 3-body terms in the energy, it no longer even makes sense to define the force that one particle exerts on another. Nevertheless, we may formulate the laws of mechanics in the Lagrangian framework. As in the case of modern continuum mechanics it is best to formulate mechanics dynamically, even if one is only interested in statics. Accordingly, we suppose we have N particles at positions $\{\mathbf{r}_i(t)\}_{i=1}^N$ at time t. They interact through the potential $U(\{\mathbf{r_i}\})$. We suppose U can be decomposed as a sum of 2 and 3 body interactions:

$$U(\{\mathbf{r}_i\}) = \sum_{i,j} V(\mathbf{r}_i, \mathbf{r}_j) + \sum_{i,j,k} W(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k), \tag{A.1}$$

where the sums are taken over all pairs and triplets of particles. The Lagrangian is

$$L = \frac{1}{2} \sum_{i=1}^{N} \dot{\mathbf{r}}_i \cdot \dot{\mathbf{r}}_i - U(\{\mathbf{r}_i\}) \tag{A.2}$$

and the equations of motion are

$$\ddot{\mathbf{r}}_i = \nabla_{\mathbf{r}_i} U(\{\mathbf{r}_i\}) \tag{A.3}$$

(we assume all particles are identical, and thus set their common mass equal to 1).

A basic assumption is that the potential energy (A.1) is translationally and rotationally invariant. Translational invariance is equivalent to the assumption that the interactions V and W only depend on displacements between the particles, the "bond vectors" $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. The assumption of rotational invariance is then equivalent to the dependence of V and W being only through the scalar products $\mathbf{r}_{ij} \cdot \mathbf{r}_{k\ell}$. As a result, Lagrangian (A.2) is itself rotationally and translationally invariant. We may thus appeal to Noether's theorem [1] and conclude that the total momentum and total angular momentum of any finite system of particles are conserved.

Now consider the equation of motion (A.3). We define the force on the jth particle as

$$\mathbf{F}_j = \nabla_{\mathbf{r}_j} U(\{\mathbf{r}_i\}). \tag{A.4}$$

Suppose we form a block, $\mathscr{B}$ out of K particles, relabeling if necessary, so they are the first K particles with positions $\{\mathbf{r}_i\}_{i=1}^K$. We may define the total momentum of this block as

$$\mathbf{P} = \sum_{i=1}^{K} \dot{\mathbf{r}}_i \tag{A.5}$$

and the total angular momentum

$$\mathbf{A} = \sum_{i=1}^{K} \mathbf{r}_i \times \dot{\mathbf{r}}_i. \tag{A.6}$$

The equations of motion then imply

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{P} = \mathbf{F} = \sum_{i=1}^{K} \mathbf{F}_i, \tag{A.7}$$

where **F** is the total force acting on the cluster. Furthermore, we may define the total moment acting on the cluster as

$$\mathbf{M} = \sum_{i=1}^{K} \mathbf{r}_i \times \mathbf{F}_i, \tag{A.8}$$

and then, by the usual classical computation, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{A} = \mathbf{M}. \tag{A.9}$$

Laws (A.7) and (A.9) are the usual momentum and angular momentum laws. They are analogous to the corresponding laws in modern continuum mechanics, as explicated in [19], and should pass to them in the continuum limit. Our goal is to use them in an analogous way in our atomistic context.

We will now consider the static case which is our primary interest. We will use the special structure of energy (A.1) to decompose the forces acting on $\mathscr{B}$ into internal and external forces. We will write

$$\mathscr{E} = \mathscr{E}_{\mathscr{B}} + \mathscr{E}_{/\mathscr{B}}, \tag{A.10}$$

where $\mathscr{E}_{\mathscr{B}}$ is the sum over 2 and 3 body interactions only involving particles in $\mathscr{B}$ and $\mathscr{E}_{/\mathscr{B}}$ is the sum over all remaining interactions. In correspondence with (A.10) the total force and moment can be decomposed as

$$\mathbf{F} = \mathbf{F}_{\mathscr{B}} + \mathbf{F}_{/\mathscr{B}},$$

$$\mathbf{M} = \mathbf{M}_{\mathscr{B}} + \mathbf{M}_{/\mathscr{B}},$$

where

$$\mathbf{F}_{\mathscr{B}} = \sum_{i=1}^{K} \nabla_{\mathbf{r}_i} \mathscr{E}_{\mathscr{B}}.$$

The force $F_{\mathscr{B}}$ is the internal force of the block $\mathscr{B}$. It is the force $\mathscr{B}$ exerts on itself.

We claim that

$$\mathbf{F}_{\mathscr{B}} = \mathbf{M}_{\mathscr{B}} = 0$$

for any static configuration of the system. For any such configuration, consider the purely internal energy, $\mathscr{E}_{\mathscr{B}}$, of the block $\mathscr{B}$. Suppose the particles of $\mathscr{B}$ are governed solely by the internal energy $\mathscr{E}_{\mathscr{B}}$ with the static positions $\{\mathbf{r}_i\}_{i=1}^K$ as initial conditions. Under Lagrange's equations (A.3) the particles will evolve in time $\mathbf{r}_i(t)$ since the positions in the static configuration will not in general be an equilibrium one for the internal potential $\mathscr{E}_{\mathscr{B}}$. The energy $\mathscr{E}_{\mathscr{B}}$ is itself rotationally and translationally invariant, so we may apply Noether's theorem to this system, and conclude that its own momentum and angular momentum must be conserved. But by laws (A.7) and (A.9), we must therefore have $\mathbf{F}_{\mathscr{B}} = 0$ and $\mathbf{M}_{\mathscr{B}} = 0$ at all times, in particular at the initial time, when $\mathscr{B}$ is in its static configuration.

We have therefore shown that the internal force and torque with which any portion of the material acts on itself with is 0. Thus the total force and moment acting on $\mathscr{B}$ are the external force and moment $\mathbf{F}_{/\mathscr{B}}$ and $\mathbf{M}_{/\mathscr{B}}$. In the static configuration the total force and torque must vanish, and therefore we have proved:

In any static equilibrium configuration, the external force and torque acting on some portion of the material must vanish.

We will use this principle the same way it is used in continuum mechanics. The total force and torque applied to some portion of the material by the material external to it must vanish.

These arguments cannot be applied directly to the energies used in the body of this paper, because they are not themselves rotationally invariant. Rather, they are the leading order terms in the Taylor expansion of a rotationally invariant energy. In Appendix B we will justify the extension of these laws to the discrete elastic energy $\mathscr{E}$ that we have used in this paper.

Appendix B. The elastic energy as a quadratic approximation to a nonlinear energy

Here we will show that the discrete elastic energy $\mathscr{E}$ used in this paper, built up from the energy densities (3.8) and (3.10), is the leading order quadratic approximation to the nonlinear energy of Appendix A. Besides proving that the force balance laws derived there will hold for the elastic energy, this will also provide a microscopic justification for our theory. This procedure is well known in the theory of lattice statics and dynamics and is sometimes called the method of homogeneous transformations. Basic references on this subject are [2,9].

By Appendix A the potential energy U is the sum of 2 and 3 body terms which themselves depend only on the particle coordinates through the inner products of the bond vectors. Here, it is most convenient to recall the notation of Section 3 and use lattice coordinates $\mathbf{i} = (i, j)$ to enumerate the particles, using $\mathbf{x(i)}$ to denote the position of the particle whose lattice site is $\mathbf{i}$. The bond vector between the particles at sites $\mathbf{i}$ and $\mathbf{j}$ is

$$\mathbf{r}_{\mathbf{i},\mathbf{j}} = \mathbf{x}(\mathbf{j}) - \mathbf{x}(\mathbf{i}). \tag{B.11}$$

The equilibrium bond vector will be denoted by

$$\mathbf{R}_{\mathbf{i},\mathbf{j}} = \mathbf{X}(\mathbf{j}) - \mathbf{X}(\mathbf{i}). \tag{B.12}$$

For simplicity we will assume the reference lattice, is the equilibrium lattice, so $\varepsilon = 0$.

In our case, we may restrict the interactions to nearest neighbor interactions on a simple cubic lattice. This means only two types of inner products will appear,

$$|\mathbf{r}_{\mathbf{i},\mathbf{i}\pm\mathbf{e_k}}|^2,$$

the squared length of a nearest neighbor bond, and

$$\mathbf{r}_{\mathbf{i},\mathbf{i}\pm\mathbf{e_k}} \cdot \mathbf{r}_{\mathbf{ii}\pm\mathbf{e_m}},$$

the dot product between two adjacent bonds sharing the vertex point $\mathbf{i}$. We will expand the energy U in small deviations of the inner products from their equilibrium values. From (B.11) and (B.12) we have

$$\mathbf{r}_{\mathbf{i},\mathbf{i}\pm\mathbf{e_k}} = \mathbf{R}_{\mathbf{i},\mathbf{i}\pm\mathbf{e_k}} \pm (\mathbf{u}(\mathbf{i} \pm \mathbf{e_k}) - \mathbf{u}(\mathbf{i})) = \mathbf{R}_{\mathbf{i},\mathbf{i}\pm\mathbf{e_k}} + \mathbf{d}^{\mathbf{k}\pm},$$

using the bond displacement vectors from (3.5). Since $\mathbf{R}_{\mathbf{i},\mathbf{i}\pm\mathbf{e_k}} = \pm\mathbf{e_k}$, we may write

$$\mathbf{r}_{\mathbf{i},\mathbf{i}\pm\mathbf{e_k}} = \pm\mathbf{e_k} + \mathbf{d}^{\mathbf{k}\pm}.$$

Now we substitute into the inner products. For simplicity we will only consider the inner products $|\mathbf{r}_{\mathbf{i},\mathbf{i}+\mathbf{e_1}}|^\mathbf{2}$ and $\mathbf{r}_{\mathbf{i},\mathbf{i}+\mathbf{e_1}} \cdot \mathbf{r}_{\mathbf{i},\mathbf{i}+\mathbf{e_2}}$.

$$|\mathbf{r}_{\mathbf{i},\mathbf{i}+\mathbf{e_1}}|^\mathbf{2} = (\mathbf{e}_1 + \mathbf{d}^{1+}) \cdot (e_1 + \mathbf{d}^{1+}) = |\mathbf{e}_1|^2 + 2\mathbf{e}_1 \cdot \mathbf{d}^{1+} + |\mathbf{d}^{1+}|^2 = h^2 + 2hd_1^{1+} + \mathrm{O}(d^2),$$

using the fact that the lattice spacing is h, the substrate lattice constant, and

$$\mathbf{r}_{\mathbf{i},\mathbf{i}+\mathbf{e}_1} \cdot \mathbf{r}_{\mathbf{i},\mathbf{i}+\mathbf{e}_2} + (\mathbf{e}_1 + \mathbf{d}^{1+}) \cdot (\mathbf{e}_2 + \mathbf{d}^{2+}) + \mathbf{e}_1 \cdot \mathbf{e}_2 + \mathbf{e}_1 \cdot \mathbf{d}^{2+} + \mathbf{e}_1 \cdot \mathbf{d}^{2+} + \mathbf{d}^{1+} \cdot \mathbf{d}^{2+} + h(d_1^{2+} + d_2^{1+}) + \mathrm{O}(d^2),$$

where $\mathrm{O}(d^2)$ denotes terms quadratic in the bond displacement.

Assuming that having all atoms in their reference position is a locally minimizing configuration of U, we may expand about this minimum in deviations of the inner products from their equilibrium values. The leading order quadratic terms will be terms of the form

$$C(d_k^{k\pm})^2 \tag{B.13}$$

and

$$C(d_1^{2\pm} + d_2^{1\pm})^2. \tag{B.14}$$

It is clear from inspecting the various versions of the elastic energy density E, either in forms (3.8) and (3.10), after substituting the discrete strain components, or any of the explicit expressions for E in Section 4.1, that the elastic energy $\mathscr{E}$ will be exactly a sum of terms of forms (B.13) and (B.14). This is seen most explicitly in the expressions for E in Section 4.2.

What this amounts to is that the elastic energy $\mathscr{E}$ is exactly of the form of the leading order quadratic approximation to the nonlinear potential energy U expanded about a minimum. In other words, we may write

$$U = \mathscr{E} + \mathrm{O}(d^3).$$

The force balance laws stated in the proposition in Appendix A must hold for any value of the bond displacement from equilibrium, and so by this asymptotic expansion, they must also hold for the discrete elastic energy $\mathscr{E}$.

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