

# Atomistic Theory of Elasticity for Thin Epitaxial Films

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# Atomistic Theory of Elasticity for Thin Epitaxial Films

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## Abstract

Strain has significance for both the growth characteristics and material properties of thin epitaxial films. Current methods for modeling and simulating strain in thin films are either continuum or atomistic. Continuum theories of strain are not applicable to very thin films; purely atomistic theories do not readily lend themselves to analysis and are computationally slow. In this work, a uniform approach that combines atomistic and continuum aspects of elasticity is developed and applied to epitaxial thin films. In its present form, the theory is developed for linear elasticity and for a material system in which the only defects are step edges and material interfaces. This theory is outlined for a general lattice, but an explicit version of the theory is described for a 2D cubic lattice for which the energy has 2D cubic symmetry. Force balance equations are derived for a material system with material/vacuum and material/material interfaces. Intrinsic surface stress in a material/vacuum interface is included in the theory by treating the atoms at the surface as belonging to a different material. The Keating model is found to be a special case of the present theory.

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# 1 Introduction

Strain has significance for both the growth and material properties of thin epitaxial films. During growth, strain changes the growth rate and surface morphology by changing the adatom diffusion coefficient and other energy transition barriers. For example, on a surface for which diffusion occurs through hopping, tensile strain will lower the diffusion rate; whereas, if diffusion occurs via exchange, then tensile strain should increase the diffusion rate [15, 25]. 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 [17].

Strain also affects the electronic, optical and magnetic properties of materials. For this reason, it is useful parameter in materials design, such as band-gap engineering.

Strain is induced in heteroepitaxial growth of thin films by a mismatch between the lattice constants in the substrate and those in the epilayer. For example, for Si (silicon) on Ge (germanium) the lattice mismatch is -4%; i.e., Si has a lattice constant that is 4% smaller than that of Ge.

In an epitaxial thin film, the effects of strain have a particular simplicity because of the ideal properties of the crystal structure. Grain boundaries are absent, and lattice defects, such as dislocations and stacking faults, are rare in many systems. Because of this uniformity in the crystal structure, an epitaxial thin film may be assumed to satisfy the Cauchy-Born hypothesis that the macroscopic strain is identical to the microscopic strain. In addition, the structure of an epitaxial crystal can be described by a single, uniform atomic lattice.

Previous theories for strain effects in thin films have been purely continuum or purely atomistic. The approach of Spencer, Davis and Voorhees [18, 19, 20], 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 [23, 10] 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 edge is approximated by Green's function on the step. 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.

Atomistic models for strain have been developed for thin films, including the valence force field models [8] and bond order potentials [24, 1, 14]. These models approach continuum models of elasticity in the continuum limit, so that their coefficients are related to the elastic coefficients. They are satisfactory for many purposes (and contain significantly more detail than the models proposed below), but a more unified approach to the combination of atomistic and continuum aspects of strain effects would be advantageous for both analysis and simulation of material properties and growth characteristics of thin films.

The purpose of the present paper is to develop such a unified theory for atomistic and continuum elasticity in thin films. First, we formulate a general fully nonlinear atomistic strain energy. Then under assumptions of nearest neighbor interactions and small displacements, we derive the simplest version of this theory - corresponding to a discrete quadratic strain energy on a two-dimensional cubic lattice - in order to gain qualitative understanding of strain effects in thin films. Construction of the discrete elastic energy involves specification of energy coefficients that reflect the geometry and material properties of the lattice. For simplicity, the coefficients of the strain energy and the lattice mismatch parameter are assumed to depend only on the atomic species at the endpoints of a bond for the interaction of the bond with itself, or the endpoints of a cell spanned by two bonds for the interactions of the two bonds.

Although simplified, this version is robust enough to include both atomistic and macroscopic length scales. At the macroscopic scale, the resulting theory is consistent with continuum elasticity in regions where continuum scaling is applicable. In particular, the coefficients of the strain energy can be related to the coefficients of continuum elasticity. At the microscopic scale, considerable atomistic detail can be included in our model. For exam-

ple, intrinsic surface stress, at an interface between material and vacuum, is included by simply treating the atoms at the interface as a different species. Atomistic properties of an interface between two materials can also be included by prescribing distinct elastic properties to the bounds that cross the interface.

By proper choice of the elastic coefficients the resulting atomistic elastic energy is equivalent to the energy of valence force field model. In particular, we find (see Section 7) that the Keating model is a special case of the present theory. The Keating model, however, does not attain the full set of continuum elastic coefficients, as discussed in Section 7.

The theory used here also extends the application of valence force field models to both the bulk and interfaces. Although the extension to interfaces has not been well-developed or quantitatively analyzed, we expect that it should produce results that are qualitatively correct [6]. The present work should assist in assessment of the application of valence force field models at material interfaces.

For a thin film, the principal geometric inhomogeneities are step edges (and island boundaries) on the interfaces between layers of the film and at the top interface of the film. Near a step edge on an interface, the discrete elastic equations represent an atomistic description of the effects of strain. Continuum elasticity breaks down, however, since it has a singularity at the corners in a step. The atomistic theory imposes a physically meaningful regularization of that singularity. Away from the steps, the discrete elastic equations can be thought of as a finite-difference discretization of the continuum elasticity equations.

The approach formulated here is related to the quasi-continuum theory developed by Tadmor, Ortiz, Phillips, Kaxiras and co-workers [21, 22], in that both theories combine atomistic and continuum theories. A fundamental distinction between the two methods is that the quasi-continuum method provides a framework for combining a given continuum theory and a given atomistic theory, while the present approach derives an atomistic model, under some atomistic assumptions, that is consistent with continuum theory. In addition, the quasi-continuum method has not been applied to thin film problems, and it does not use the existence of a single atomic lattice for a thin film.

Quasi-continuum theory has mainly been applied to material systems involving defects, such as dislocations or cracks, in the crystal lattice geometry.

For thin films, the “defects” are step edges, which are much simpler since they do not involve a change in the topology of the lattice. As a result, linear elasticity and a single atomic lattice are applicable to the system. Moreover, adaptive meshing, invoking a coarser mesh away from the steps, is not expected to entail new physics in our approach, but should be implemented using well-developed numerical analysis methods.

The equations of continuum elasticity are reviewed in Section 2, along with the use of a reference frame that may be nonequilibrium, as introduced in [18]. A general formulation for the atomistic strain energy and the resulting force balance equations, as well as a linearized theory, is described in Section 3. This theory is specialized to a two-dimensional cubic lattice, and its continuum limit is analyzed in Section 4. Determination of the elastic parameters for this case is described in Section 5. For a layered thin film, with step edges on the interface between different materials and on the interface between material and vacuum, the discrete elastic energy and the corresponding force balance equations are derived in Section 6, with many details deferred to the Appendices. Intrinsic surface stress is also included in this analysis. In Section 7, the elastic energy from the Keating model is found to be a special case of the present theory, and the role of inner relaxation of the lattice is discussed. Conclusions and prospects for future developments are presented in Section 8.

Partial motivation for this work has been the need for a strain model that is suitable for coupling with a growth model for an epitaxial thin film. In particular, the model developed in Section 6 has been coupled to a model for motion of steps in a related work by the authors and their co-workers [16].

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, Alexander Schindler, Geoff Simms, Jerry Tersoff, Dimitri Vvedensky and Peter Voorhees.

## 2 Continuum Elasticity

Continuum elasticity is formulated in terms of a displacement field  $\mathbf{u} = \mathbf{u}(\mathbf{x})$ , which is the difference  $\mathbf{u} = \mathbf{X}(\mathbf{x}) - \mathbf{x}$  between the equilibrium position  $\mathbf{x}$  of a material point and the perturbed position  $\mathbf{X}(\mathbf{x})$  of that point due to some elastic deformation. 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  $\mathbf{S}$  respecting the symmetry properties of the system.

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, or undeformed configuration. 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. In particular, for modeling heteroepitaxy, it is most useful to use the equilibrium configuration for the substrate as a reference configuration throughout the substrate and epilayer. This formulation was originally introduced by Spencer, Voorhees and Davis [18] in their study of morphological stability in heteroepitaxy. Following them, we introduce the lattice mismatch parameter

$$\epsilon = \frac{a - h}{h} \quad (2.2)$$

and define the (nonequilibrium) reference position  $\mathbf{x}$  and the resulting displacement vector  $\mathbf{u}$  by

$$\begin{aligned} (1 + \epsilon)\mathbf{x} &= \mathbf{x}_e \\ \mathbf{u} &= \mathbf{X} - \mathbf{x} = \mathbf{u}_e + \epsilon\mathbf{x} \end{aligned} \quad (2.3)$$

in which  $\mathbf{x}_e$  and  $\mathbf{u}_e = \mathbf{X} - \mathbf{x}_e$  are the equilibrium position and displacement vectors.

The components of the original strain tensor  $\mathbf{S}_e$  come from the matrix

$$\begin{aligned} \frac{\partial \mathbf{u}_e}{\partial \mathbf{x}_e} &= \frac{\partial \mathbf{x}}{\partial \mathbf{x}_e} \frac{\partial(\mathbf{u} - \epsilon\mathbf{x})}{\partial \mathbf{x}} \\ &= \frac{\partial \mathbf{x}}{\partial \mathbf{x}_e} \left( \frac{\partial \mathbf{u}}{\partial \mathbf{x}} - \epsilon I \right). \end{aligned} \quad (2.4)$$

in which  $I$  is the identity tensor. We omit area factor  $(\partial \mathbf{x} / \partial \mathbf{x}_e)$ , as discussed below, to obtain the redefined strain tensor  $\mathbf{S}$

$$S_{k\ell} = \frac{1}{2}(\partial_k u_\ell + \partial_\ell u_k) - \epsilon \delta_{k\ell}. \quad (2.5)$$

Our use of the parameter  $\epsilon$  in the definition of the strain is equivalent to its use in [5, 18], where it was built into the constitutive law for the stress, except for two corrections. First, in the elastic energy densities we retain a constant proportional to  $\epsilon^2$ , which does not change the solution of the elastic equations, but does affect the comparison of energy values for different material configurations, as used in [16] for motion of strained steps. Second, we modify the elastic coefficients by a factor  $(1 - \epsilon)$  as described at the end of this Section. With these two corrections, the total elastic energy is unchanged by the introduction of the reference configuration. In principle, these  $\epsilon^2$  corrections are significant for elasticity that is exactly linear. These terms are not consistent, however, with the linearization of nonlinear elasticity.

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

$$\begin{aligned} E &= \mathbf{S} : \mathbf{T} = \sum_{k,\ell} S_{k\ell} T_{k\ell} \\ \mathcal{E} &= \int_{\Omega} E d\mathbf{x} . \end{aligned} \quad (2.6)$$

For linear elasticity with cubic symmetry (i.e., invariance with respect to the transformations  $x_k \leftrightarrow x_\ell$  and  $x_k \rightarrow -x_k$ ), the stress tensor  $\mathbf{T}$  is

$$T_{k\ell} = (2\alpha - 4\beta - 2\gamma)\delta_{k\ell}S_{k\ell} + 2\gamma\delta_{k\ell}S_{mm} + 4\beta S_{k\ell}. \quad (2.7)$$

In two dimensions with cubic symmetry, the elastic energy density is

$$\begin{aligned} E &= \mathbf{S} : \mathbf{T} \\ &= 2\alpha(S_{11}^2 + S_{22}^2) + 8\beta S_{12}^2 + 4\gamma S_{11}S_{22} \\ &= 2\alpha((\partial_1 u_1)^2 + (\partial_2 u_2)^2) + 2\beta(\partial_1 u_2 + \partial_2 u_1)^2 + 4\gamma(\partial_1 u_1)(\partial_2 u_2) \\ &\quad - 4(\alpha + \gamma)\epsilon(\partial_1 u_1 + \partial_2 u_2) + 4(\alpha + \gamma)\epsilon^2. \end{aligned} \quad (2.8)$$

For linear elasticity in an isotropic material, the stress tensor  $\mathbf{T}$  is

$$T_{k\ell} = a\delta_{k\ell}S_{mm} + bS_{k\ell} \quad (2.9)$$

in which  $a = \lambda/2$  and  $b = \mu$  in which  $\lambda$  and  $\mu$  are the Lamé coefficients, which is the case of cubic symmetry with

$$\begin{aligned} \alpha &= (a + b)/2 \\ \beta &= b/4 \\ \gamma &= a/2. \end{aligned} \quad (2.10)$$



The resulting elastic energy density in 2D is

$$\begin{aligned}
E &= \mathbf{S} : \mathbf{T} \\
&= (a+b)(S_{11}^2 + S_{22}^2) + 2bS_{12}^2 + 2aS_{11}S_{22} \\
&= (a+b)((\partial_1 u_1)^2 + (\partial_2 u_2)^2) + \frac{b}{2}(\partial_1 u_2 + \partial_2 u_1)^2 + 2a(\partial_1 u_1)(\partial_2 u_2) \\
&\quad - \epsilon(4a+2b)(\partial_1 u_1 + \partial_2 u_2) + \epsilon^2(4a+2b).
\end{aligned} \tag{2.11}$$

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

$$\delta\mathcal{E} = 0. \tag{2.12}$$

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

$$\begin{aligned}
0 &= \partial_1 \left( \frac{\partial}{\partial u_{k,1}} E \right) + \partial_2 \left( \frac{\partial}{\partial u_{k,2}} E \right) \quad k = 1, 2 \quad \text{in } \Omega \\
0 &= n_1 \left( \frac{\partial}{\partial u_{k,1}} E \right) + n_2 \left( \frac{\partial}{\partial u_{k,2}} E \right) \quad k = 1, 2 \quad \text{on } \partial\Omega
\end{aligned}$$

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

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

these equations are equivalent to the elastic equations

$$\nabla \cdot \mathbf{T} = 0 \quad \text{in } \Omega \tag{2.13}$$

$$\mathbf{n} \cdot \mathbf{T} = 0 \quad \text{on } \partial\Omega. \tag{2.14}$$

In order that the energy is unaffected by the change from equilibrium to nonequilibrium reference coordinates, the elastic coefficients must be changed, since they are not dimensionless. Consider an idealized energy density  $E_e = \alpha_e S_e^2$  and  $E = \alpha S^2$  for the equilibrium and nonequilibrium configurations respectively. Since  $S_e = (1 + \epsilon)^{-1} S$  and  $d\mathbf{x}_e = (1 + \epsilon)^3 d\mathbf{x}$ ,

$$\begin{aligned}
\mathcal{E}_e &= \int \alpha_e S_e^2 d\mathbf{x}_e \\
&= \int \alpha_e (1 + \epsilon)^2 S^2 d\mathbf{x} \\
&= \int \alpha S^2 d\mathbf{x} \\
&= \mathcal{E}
\end{aligned} \tag{2.15}$$

if the elastic coefficients satisfy  $\alpha = (1 + \epsilon)\alpha_e$ . This should be true for each elastic coefficient; i.e.,

$$(\alpha, \beta, \gamma) = (1 + \epsilon)(\alpha_e, \beta_e, \gamma_e). \quad (2.16)$$

Note that this scaling with respect to  $\epsilon$  has been derived for three spatial dimensions, but it is also correct for two-dimensions, since in 2D the two-dimensional energy integral has units of energy per length.

### 3 Discrete Elastic Energy Model

The principal goal of this paper is to formulate a theory of elasticity that is consistent with both continuum theory and a discrete lattice model. This section describes the framework for this theory for both linear and nonlinear elasticity and for a general lattice.

#### 3.1 Nonlinear Elasticity

Let  $\nu$  be the lattice coordinate, and let  $\mathcal{L}$  denote the lattice of these coordinates (e.g.  $\mathcal{L} = \mathbb{Z}^2$  for a simple cubic lattice in 2D). Denote the atomic positions by  $\mathbf{x}_\nu$  for the reference positions and  $\mathbf{X}_\nu$  for the actual positions under deformation, for  $\nu \in \mathcal{L}$ , so that  $\mathbf{u}_\nu = \mathbf{X}_\nu - \mathbf{x}_\nu$  is the displacement vector. The strain energy depends only on the coordinates of the atoms, so that

$$\mathcal{E} = \mathcal{E}(\{\mathbf{X}_\nu\}_{\nu \in \mathcal{L}}). \quad (3.1)$$

In principle  $\mathcal{E}$  must be calculated from quantum mechanics, and represents the potential energy surface of the atomic configuration. In this section, the only assumptions on  $\mathcal{E}$  are invariance under translation and rotation, and a restriction to local interactions. Symmetry requirements due to symmetry of the underlying lattice will be imposed in the next section.

Denote a bond between sites  $\nu$  and  $\mu$  as

$$\mathbf{b} = (\nu, \mu) \quad (3.2)$$

and the bond vectors between these atoms as

$$\mathbf{r}_\mathbf{b} = \mathbf{x}_\mu - \mathbf{x}_\nu \quad (3.3)$$

$$\mathbf{R}_\mathbf{b} = \mathbf{X}_\mu - \mathbf{X}_\nu \quad (3.4)$$

in which  $\mathbf{r}_{\mathbf{b}}$  and  $\mathbf{R}_{\mathbf{b}}$  is the relative position of atom  $\mu$  to atom  $\nu$  in the reference position and in the deformed positions, respectively. Because of locality restrictions, bond vectors will only be defined between certain pairs of atoms (e.g. nearest neighbors); the set of these “active” bonds is denoted as  $\mathcal{B}$ . In addition we denote  $\mathcal{B}_{\nu}$  to be the set of bonds in  $\mathcal{B}$  having one endpoint at  $\nu$ .

The energy  $\mathcal{E}$  is translationally invariant if and only if it is only a function of the relative positions of the atoms; i.e., a function only of the bond vectors. Rotational invariance requires that  $\mathcal{E}$  is a function only of the scalar products between bond vectors. Therefore

$$\mathcal{E} = \mathcal{E}(\{\mathbf{R}_{\mathbf{b}} \cdot \mathbf{R}_{\mathbf{b}'}\}_{\mathbf{b}, \mathbf{b}' \in \mathcal{B}}). \quad (3.5)$$

$\mathcal{E}$  may be further specified by making assumptions of locality; i.e., atoms will only interact directly with their nearby neighbors. Define the interaction set  $\mathcal{I} \subset \mathcal{B} \times \mathcal{B}$  consisting of pairs of bonds  $(\mathbf{b}, \mathbf{b}')$  whose interaction contributes to the energy. Also define  $\mathcal{I}_{\mathbf{b}}$  to be the set of pairs of bonds  $(\mathbf{b}, \mathbf{b}')$  such that  $(\mathbf{b}, \mathbf{b}') \in \mathcal{I}$ .

Next, write  $\mathcal{E}$  as a cluster expansion

$$\mathcal{E} = \sum_{\mathbf{b} \in \mathcal{B}} \mathcal{E}_c(\mathbf{R}_{\mathbf{b}}, \{\mathbf{R}_{\mathbf{b}'}\}_{\mathbf{b}' \in \mathcal{I}_{\mathbf{b}}}) \quad (3.6)$$

where  $\mathcal{E}_c$  is the generic energy of a bond cluster. A bond cluster is just the collection of bonds that interact with a given bond.

The cluster energy  $\mathcal{E}_c$  may be further decomposed as a sum over  $m$ -body terms, and the size of  $m$  is restricted as an additional simplification. For example, in [7] and [2] only 2- and 3-body interactions were considered. Up to 5-body interactions were found to be necessary in Martin’s study of diamond like solids [13]. We will restrict the cluster expansion of  $\mathcal{E}_c$  to involve interactions between a bond and itself (which is a 2-body interaction) and between two bonds that share a common endpoint (which is a 3-body interaction). This is equivalent to restricting the interaction set  $\mathcal{I}_{\mathbf{b}}$  to consist of bonds  $\mathbf{b}'$  sharing an endpoint with  $\mathbf{b}$ .

Because of the restriction to interactions between bonds that share an endpoint, the total energy can be written as a sum  $\sum_{\nu} E_{\nu}$  in which  $E_{\nu}$  is the energy due to interactions between bonds that share the endpoint  $\nu$ . Moreover, since the energy is a function of inner products between bonds,

then it consists of the interactions of a bond  $\mathbf{R}$  with itself, which have the form  $I(\mathbf{R}^2)$ , and the interactions between two bonds  $\mathbf{R}$  and  $\mathbf{R}'$ , which has the form  $J = J(\mathbf{R}^2, \mathbf{R}'^2, \mathbf{R} \cdot \mathbf{R}')$ . Therefore the total energy is

$$\begin{aligned} \mathcal{E} &= \sum_{\nu} E_{\nu} \\ E_{\nu} &= \sum_{\mathbf{b} \in \mathcal{B}_{\nu}} I(\mathbf{R}_{\mathbf{b}}^2) + \sum_{(\mathbf{b}, \mathbf{b}') \in \mathcal{I} \cap \mathcal{B}_{\nu} \times \mathcal{B}_{\nu}} J(\mathbf{R}_{\mathbf{b}}^2, \mathbf{R}_{\mathbf{b}'}^2, \mathbf{R}_{\mathbf{b}} \cdot \mathbf{R}_{\mathbf{b}'}). \end{aligned} \quad (3.7)$$

### 3.2 Linear Elasticity

Now consider the approximation by linear elasticity, for which the energy is quadratic in the displacements. First define the strain components. For every pair of bonds  $(\mathbf{b}, \mathbf{b}')$  in the interaction set  $\mathcal{I}$  the strain component  $S_{\mathbf{b}, \mathbf{b}'}$  is the linearization of the inner product of the bond vectors. The bond vector  $\mathbf{R}$  consists of the reference bond vector  $\mathbf{r}$  plus the perturbed bond displacement  $\mathbf{d}$ ; i.e.  $\mathbf{R} = \mathbf{r} + \mathbf{d}$ . Therefore the linearization, in the limit of small displacement  $\mathbf{d}$ , of the inner product  $(\mathbf{R} \cdot \mathbf{R}')/2$  is

$$S_{\mathbf{b}, \mathbf{b}'} = (1/2)(\mathbf{r} \cdot \mathbf{d}' + \mathbf{r}' \cdot \mathbf{d}). \quad (3.8)$$

From translation and rotation invariance and the restriction to three body terms, as expressed in Eq. (3.7), as well as the restriction to quadratic terms, the energy density for linear elasticity thus has the form

$$E_{\nu} = \sum_{(\mathbf{b}, \mathbf{b}') \in \mathcal{I} \cap \mathcal{B}_{\nu} \times \mathcal{B}_{\nu}} \alpha_{\mathbf{b}} S_{\mathbf{b}, \mathbf{b}}^2 + \beta_{\mathbf{b}, \mathbf{b}'} S_{\mathbf{b}, \mathbf{b}'}^2 + \gamma_{\mathbf{b}, \mathbf{b}'} S_{\mathbf{b}, \mathbf{b}} S_{\mathbf{b}', \mathbf{b}'} + \eta_{\mathbf{b}, \mathbf{b}'} S_{\mathbf{b}, \mathbf{b}} S_{\mathbf{b}, \mathbf{b}'} \quad (3.9)$$

in which the energy coefficients  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\eta$  may depend on the point  $\nu$ . The corresponding stress tensor is the derivative of the energy with respect to the strain component.

## 4 Two-Dimensional Cubic Lattice and Continuum Elasticity

For a two-dimensional cubic lattice, the general theory developed in the previous section is considerably simplified. We begin by supposing there is a

single simple cubic lattice with lattice constant  $h$  filling  $\mathbb{R}^2$ , as in Figure 1. As in Section 2, the lattice provides a set of (possibly nonequilibrium) reference positions from which to measure the actual positions of the atoms in a given state of deformation.

For the atom with lattice coordinates  $(i, j)$ , the reference position  $\mathbf{x}$ , deformed position  $\mathbf{X}$  and displacement  $\mathbf{u}$  are denoted

$$\begin{aligned}\mathbf{X}(i, j) &= (X_1(i, j), X_2(i, j)) \\ \mathbf{x}(i, j) &= (x_1(i, j), x_2(i, j)) \\ \mathbf{u}(i, j) &= (u_1(i, j), u_2(i, j)) = \mathbf{X}(i, j) - \mathbf{x}(i, j).\end{aligned}\tag{4.1}$$

The lattice constant  $h$  for the reference lattice is

$$|\mathbf{x}(i+1, j) - \mathbf{x}(i, j)| = |\mathbf{x}(i, j+1) - \mathbf{x}(i, j)| = h.\tag{4.2}$$

The lattice constant for the equilibrium lattice is  $a = h(1 + \epsilon)$ .

In order to define a bond, introduce the translation operators  $T_1^+, T_1^-, T_2^+, T_2^-$  and finite-difference operators  $D_1^+, D_1^-, D_1^0, D_2^+, D_2^-, D_2^0$  as follows:

$$T_1^\pm f(i, j) = f(i \pm 1, j)\tag{4.3}$$

$$T_2^\pm f(i, j) = f(i, j \pm 1)$$

$$D_k^+ f(i, j) = h^{-1}(T_k^+ - 1)f(i, j)$$

$$D_k^- f(i, j) = h^{-1}(1 - T_k^-)f(i, j)\tag{4.4}$$

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

Define the bond vectors emanating from a point  $(i, j)$  as

$$\begin{aligned}\mathbf{R}^{1\pm}(i, j) &= \pm(\mathbf{X}(i \pm 1, j) - \mathbf{X}(i, j)) = D_1^\pm \mathbf{X}(i, j) \\ \mathbf{R}^{2\pm}(i, j) &= \pm(\mathbf{X}(i, j \pm 1) - \mathbf{X}(i, j)) = D_2^\pm \mathbf{X}(i, j).\end{aligned}\tag{4.5}$$

Define the bond displacement  $\mathbf{d}^{k\pm}$  at the point  $(i, j)$  as

$$\begin{aligned}\mathbf{d}^{1\pm}(i, j) &= (d_1^{1\pm}(i, j), d_2^{1\pm}(i, j)) = (D_1^\pm u_1(i, j) - \epsilon, D_1^\pm u_2(i, j)) \\ \mathbf{d}^{2\pm}(i, j) &= (d_1^{2\pm}(i, j), d_2^{2\pm}(i, j)) = (D_2^\pm u_1(i, j), D_2^\pm u_2(i, j) - \epsilon).\end{aligned}\tag{4.6}$$

## 4.1 Nonlinear Elasticity

At each point  $(i, j)$ , there are four 2-body interactions and six 3-body interactions. As a localization assumption, we keep only interactions between nearest neighbor bonds, i.e. between those forming an angle of 0 or  $\pi/2$ . This excludes interactions of  $\mathbf{R}^{1+}$  with  $\mathbf{R}^{1-}$  and  $\mathbf{R}^{2+}$  with  $\mathbf{R}^{2-}$ , so that there are four 3-body interactions. This is equivalent to an assumption that a particle interacts only with its neighbors and next-nearest neighbors. The energy per site in Eq. (3.7) becomes

$$E(i, j) = \sum_{i,s} I((\mathbf{R}^{is})^2) + \sum_{s_1, s_2} J((\mathbf{R}^{1s_1})^2, (\mathbf{R}^{2s_2})^2, \mathbf{R}^{1s_1} \cdot \mathbf{R}^{2s_2}) \quad (4.7)$$

where the sum is over  $i = 1, 2$  and  $s, s_1, s_2 = +, -$ .

## 4.2 Linear Elasticity

To form the energy for linear elasticity for a 2D cubic lattice, first form the strain components

$$\begin{aligned} S_{11}^+ &= D_1^+ u_1 - \epsilon \\ S_{11}^- &= D_1^- u_1 - \epsilon \\ S_{22}^+ &= D_2^+ u_2 - \epsilon \\ S_{22}^- &= D_2^- u_2 - \epsilon \\ S_{12}^{++} &= (D_1^+ u_2 + D_2^+ u_1)/2 \\ S_{12}^{+-} &= (D_1^+ u_2 + D_2^- u_1)/2 \\ S_{12}^{-+} &= (D_1^- u_2 + D_2^+ u_1)/2 \\ S_{12}^{--} &= (D_1^- u_2 + D_2^- u_1)/2. \end{aligned} \quad (4.8)$$

$E$  is a quadratic function of these 8 terms. Of the 36 possible quadratic terms in  $E$ , all but 20 are eliminated by the assumption of only nearest or next-nearest neighbor interactions. Therefore

$$\begin{aligned} E &= E(S_{11}^+, S_{11}^-, S_{22}^+, S_{22}^-, S_{12}^{++}, S_{12}^{+-}, S_{12}^{-+}, S_{12}^{--}) \\ &= \alpha_{1+}(S_{11}^+)^2 + \alpha_{2+}(S_{22}^+)^2 + \alpha_{1-}(S_{11}^-)^2 + \alpha_{2-}(S_{22}^-)^2 \\ &\quad + 2\beta_{++}(S_{12}^{++})^2 + 2\beta_{-+}(S_{12}^{-+})^2 + 2\beta_{--}(S_{12}^{--})^2 + 2\beta_{+-}(S_{12}^{+-})^2 \\ &\quad + \gamma_{++}S_{11}^+S_{22}^+ + \gamma_{+-}S_{11}^+S_{22}^- + \gamma_{-+}S_{11}^-S_{22}^+ + \gamma_{--}S_{11}^-S_{22}^- \end{aligned} \quad (4.9)$$

$$\begin{aligned}
& +\eta_{1+++}S_{11}^+S_{12}^{++} + \eta_{1++-}S_{11}^+S_{12}^{+-} + \eta_{1---}S_{11}^-S_{12}^{-+} + \eta_{1----}S_{11}^-S_{12}^{--} \\
& +\eta_{2+++}S_{22}^+S_{12}^{++} + \eta_{2+-+}S_{22}^+S_{12}^{+-} + \eta_{2-+-}S_{22}^-S_{12}^{-+} + \eta_{2----}S_{22}^-S_{12}^{--}.
\end{aligned}$$

This is the leading order approximation (for small displacement) to the non-linear energy Eq. (4.7), after the imposition of cubic symmetry.

If the energy is assumed to have 2D cubic symmetry then the coefficients are simplified as

$$\begin{aligned}
\alpha_{k\pm} &= \alpha \\
\beta_{\pm\pm} &= \beta \\
\gamma_{\pm\pm} &= \gamma \\
\eta_{\pm\pm\pm} &= 0
\end{aligned} \tag{4.10}$$

so that

$$\begin{aligned}
E &= \alpha((S_{11}^+)^2 + (S_{11}^-)^2 + (S_{22}^+)^2 + (S_{22}^-)^2) \\
&+ 2\beta((S_{12}^{++})^2 + (S_{12}^{+-})^2 + (S_{12}^{-+})^2 + (S_{12}^{--})^2) \\
&+ \gamma(S_{11}^+S_{22}^+ + S_{11}^+S_{22}^- + S_{11}^-S_{22}^+ + S_{11}^-S_{22}^-).
\end{aligned} \tag{4.11}$$

For problems in which the underlying lattice has cubic symmetry but the material geometry includes interfaces, we will relax this constraint by only keeping bond interactions that are consistent with cubic symmetry but not imposing a symmetry constraint on the strength of the interactions. The resulting energy has the form

$$\begin{aligned}
E &= \alpha_{1+}(S_{11}^+)^2 + \alpha_{2+}(S_{22}^+)^2 + \alpha_{1-}(S_{11}^-)^2 + \alpha_{2-}(S_{22}^-)^2 \\
&+ 2\beta_{++}(S_{12}^{++})^2 + 2\beta_{-+}(S_{12}^{+-})^2 + 2\beta_{--}(S_{12}^{-+})^2 + 2\beta_{+-}(S_{12}^{--})^2 \\
&+ \gamma_{++}S_{11}^+S_{22}^+ + \gamma_{+-}S_{11}^+S_{22}^- + \gamma_{-+}S_{11}^-S_{22}^+ + \gamma_{--}S_{11}^-S_{22}^-.
\end{aligned} \tag{4.12}$$

In each case, the total energy is then

$$\mathcal{E} = \sum_{i,j} E(i, j).$$

### 4.3 Force Balance Equations

The atomistic displacements  $\mathbf{u}$  are determined by minimizing the total discrete energy  $\mathcal{E}$ , resulting in the discrete variational problem

$$\delta\mathcal{E}[\mathbf{u}] = 0, \tag{4.13}$$

analogous to the corresponding variational problem in continuum elasticity. In the discrete case however, the conditions for a minimizer are expressed simply as

$$\frac{\partial \mathcal{E}}{\partial u_1(i, j)} = \frac{\partial \mathcal{E}}{\partial u_2(i, j)} = 0 \quad (4.14)$$

for all  $(i, j)$ . The conditions (4.14) are force balance laws for each of the atoms.

Since the energy is a quadratic form in the bonds, then (4.14) involves a linear combination of bonds and values of  $\epsilon$ . As defined above, the energy at a point involves only a five point stencil, as shown in Figure 2. The components of  $u(i, j)$  only appear in the energy at the 5 points  $(i, j)$ ,  $(i \pm 1, j)$ ,  $(i, j \pm 1)$ , so that the derivative of  $\frac{\partial \mathcal{E}}{\partial \mathbf{u}(i, j)}$  involves only the derivatives of  $E(i, j)$ ,  $E(i \pm 1, j)$ ,  $E(i, j \pm 1)$ . It follows that the force balance equations have a nine point stencil. Figure 2 shows the point  $(i, j)$  and the 9 point stencil centered at  $(i, j)$ . The bonds are indicated by the lines between points.

#### 4.4 The continuum limit in the bulk

According to Section 4.2, the energy density at an interior point is of the form Eq. (4.11). With this explicit form of the energy, the force balance equations (4.14), are

$$\begin{aligned} 4\alpha D_1^+ D_1^- u_1 + 4\beta D_2^+ D_2^- u_1 + 4\gamma D_1^0 D_2^0 u_2 + 4\beta D_1^0 D_2^0 u_2 &= 0 \\ 4\alpha D_2^+ D_2^- u_2 + 4\beta D_1^+ D_1^- u_2 + 4\gamma D_1^0 D_2^0 u_1 + 4\beta D_1^0 D_2^0 u_1 &= 0 \end{aligned} \quad (4.15)$$

for each point  $(i, j)$ .

The discrete elastic energy Eq. (4.11) and the force balance equations Eq. (4.15) can be interpreted as a finite difference version of the continuum elastic energy (2.8) and force balance equations Eq. (2.13). In the energy, the linear terms are replaced with centered finite difference operators, as in

$$\partial_i u_i \rightarrow D_i^0 u_i = \frac{1}{2}(D_i^+ + D_i^-)u_i \quad (4.16)$$

and the quadratic terms are discretized as

$$(\partial_i u_i)^2 \rightarrow \frac{1}{2}[(D_i^+ u_i)^2 + (D_i^- u_i)^2]$$



$$\begin{aligned}
\partial_1 u_1 \partial_2 u_2 &\rightarrow \frac{1}{4} [D_1^+ u_1 D_2^+ u_2 + D_1^+ u_1 D_2^- u_2 + D_1^- u_1 D_2^+ u_2 + D_1^- u_1 D_2^- u_2] \\
(\partial_1 u_2 + \partial_2 u_1)^2 &\rightarrow \frac{1}{4} [(D_1^+ u_2 + D_2^+ u_1)^2 + (D_1^+ u_2 + D_2^- u_1)^2 \\
&\quad + (D_1^- u_2 + D_2^+ u_1)^2 + (D_1^- u_2 + D_2^- u_1)^2].
\end{aligned}$$

By choosing the coefficients  $\alpha, \beta, \gamma$  for the discrete energy to be the same as those for the continuum energy, we see that the atomistic energy Eq. (4.11) is a finite difference version of the continuum energy Eq. (2.8). In addition, the atomistic force balance equations Eq. (4.15) are a finite difference of the continuum force balance equations Eq. (2.13); i.e., the atomistic force balance equations away from an interface are exactly a discretization of the linear continuum elastic equations

$$\operatorname{div} \mathbf{T} = 0.$$

## 5 Determination of Elastic Parameters

The goal of this section is to formulate a procedure for determination of the elastic parameters for a two-dimensional system involving a cubic lattice, multiple materials and a general geometry. This formulation can be directly encoded as an algorithm for computation of the discrete elastic energy.

### 5.1 General Formulation

In general, we assume that the elastic parameters  $\alpha, \beta, \gamma$  and  $\epsilon$  for the interaction between bonds  $\mathbf{b}$  and  $\mathbf{b}'$  depend on the type of atoms in the neighborhood of these bonds. In particular we shall assume the following:

1. The coefficient  $\alpha$  for the interaction of a bond  $\mathbf{b}$  with itself depends only on the type of material at the endpoints of  $\mathbf{b}$ .
2. The lattice mismatch parameter  $\epsilon$  for a bond  $\mathbf{b}$  depends only on the type of material at the endpoints of  $\mathbf{b}$ .
3. The coefficients  $\beta$  and  $\gamma$  for the interaction of bonds  $\mathbf{b}$  and  $\mathbf{b}'$ , which share an endpoint, depends on type of material at the four points of the square spanned by these two bonds.

These assumptions on the discrete energy model can be developed in terms of bond and cell types. The bonds and cells in the lattice can be divided into two general classes, the pure bonds and cells and the mixed bonds and cells. The pure bonds are bonds between two atoms of the same type; i.e., a bond in the bulk of either the substrate or the film. The pure cells are cells where all 4 corners of the cell are atoms of the same material; i.e., a cell entirely in the bulk of either the film or the substrate. The mixed bonds are bonds between two different kinds of atoms, and the mixed cells are those whose corners have atoms from different materials (see Figures 3 and 4).

Assumption (3), that the elastic parameters for a bond-bond interaction depend on the types of the four atoms in the corresponding cell, is a violation of the earlier assumption of only two and three particle interactions. We will continue to refer to this as a three particle interaction, however, since the dependence on the fourth point is limited, not involving its displacement. Moreover, this dependence is only invoked at a material interface, at which the energy should be different than in the bulk.

## 5.2 Multiple Materials and a Vacuum

Consider a system consisting of two materials, 1 (e.g., the substrate) and 2 (e.g., the epilayer), as well as a vacuum region. It is convenient to extend the reference lattice into the vacuum and label the points there as type V. The two materials have their own set of elastic parameters  $\alpha^\ell, \beta^\ell, \gamma^\ell, \epsilon^\ell$ , for  $\ell = 1, 2$ . In addition, the interface between type 1 and type 2 atoms may have a different set of elastic parameters  $\alpha^3, \beta^3, \gamma^3, \epsilon^3$ .

As a simple realization of the model assume the following:

4. For pure bonds and cells of type  $\ell$  (for  $\ell = 1, 2$ ), the elastic parameters are  $\alpha^\ell, \beta^\ell, \gamma^\ell, \epsilon^\ell$ .
5. For a mixed bond or cell containing both materials 1 and 2, the elastic parameters are  $\alpha^3, \beta^3, \gamma^3, \epsilon^3$ .
6. For a mixed bond or cell containing a vacuum point, the elastic coefficients are  $\alpha = \beta = \gamma = 0$ .

A consequence of Assumptions (3) and (5) is that the energy and force balance equations are identical at all points on an edge away from corners.

In particular the edge point next to a corner has the same energy and force balance formulas as points that are further from the corner. This property is not true for alternative formulations of the energy at an interface and is the motivation for these specific Assumptions.

For example, suppose that the elastic parameters for the interaction of two  $\mathbf{b}$  and  $\mathbf{b}'$  with a common endpoint is determined only by the types of the three endpoint atoms, rather than the four atoms of the corresponding cell as in Assumption (3). Then the force balance equation at an edge point adjacent to a corner is different from that at other edge points.

### 5.3 Intrinsic Surface Stress

At a material/vacuum interface the coordination number of the bonds between surface atoms is different than it is in the bulk. This changes the forces between the surface atoms, as well as between surface atoms and their neighbors in the bulk, which is referred to as intrinsic surface stress. For a material of type 1, we will model the intrinsic surface stress by considering the atoms at the vacuum interface to be of a different type 2. In particular, we assume there to be elastic parameters  $\alpha^2, \beta^2, \gamma^2, \epsilon^2$  for the interface atoms, and elastic parameters  $\alpha^3, \beta^3, \gamma^3, \epsilon^3$  for the bonds between the interface atoms and the bulk. The elastic parameters for this system are then determined as in Assumptions (4)-(6).

This procedure could be generalized in a number of ways. For example, a system consisting two materials and a vacuum with intrinsic surface stress at the material/vacuum interfaces will have two types of surface atoms and cells involving atoms of more than 2 types.

## 6 Discrete Layered Material: Interface of Material and Vacuum without Intrinsic Surface Stress

We consider an epitaxial thin film on substrate with a lattice mismatch between substrate and film, as in Figure 5. Denote the lattice constant in the substrate as  $h_s$  and in the film as  $h_f$ . To provide a uniform description of the atomistic strain, we choose to use a single lattice with space  $h = h_s$ , so

that the lattice mismatch  $\epsilon$  is  $\epsilon_s = 0$  in the substrate and  $\epsilon_f = (h_f - h_s)/h_s$  in the film.

Assumptions (4)-(6) of Section 5 are sufficient for complete determination of the atomistic strain energy for this system. Force balance equations can then be derived as in Section 4.3. In this Section and in the Appendices, we consider three specific cases: The first is the interface of a material with a vacuum with no intrinsic stress on the surface. Explicit expressions for energy and force balance at each point are presented in the next subsection. Second is the interface between two materials with an interfacial region that is distinct from either of the bulk materials, which is presented in Appendix A. Third is the interface with the vacuum again, but with intrinsic stress on the surface, which is presented in Appendix B. The first and third cases are special cases of the second.

The simplest geometry is that of a material with an interface onto a vacuum. For simplicity, we treat the vacuum as consisting of “empty” points and all other points as identical. Assumptions (4) - (6) of Section 5 prescribe the form of the energy at all points in this system. The goal of this section is to derive explicit expressions for the energy density and the force balance equations for this system.

## 6.1 Edge points

First we consider a horizontal edge point  $(i, j)$ . We only consider the case where it is the upper edge of the material. Figure 6 shows that 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 the assumption 7, the energy contribution for a horizontal edge point is

$$\begin{aligned}
 E &= \alpha[(d_1^{1+})^2 + (d_1^{1-})^2 + (d_2^{2-})^2] \\
 &+ \frac{\beta}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2-})^2] \\
 &+ \gamma[d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2-}].
 \end{aligned} \tag{6.1}$$

Similar considerations lead to the energy contribution from a vertical edge point. The stencil of a right vertical edge point is just that of Figure 6 turned

sideways and the energy contribution, analogous to (6.1) is

$$\begin{aligned}
E &= \alpha[(d_1^{1-})^2 + (d_2^{2+})^2 + (d_2^{2-})^2] \\
&+ \frac{\beta}{2}[(d_2^{1-} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2-})^2] \\
&+ \gamma[d_1^{1-}d_2^{2+} + d_1^{1-}d_2^{2-}].
\end{aligned} \tag{6.2}$$

Note that (6.1) (or (6.2)) can be obtained from the general energy (4.11) by discarding any finite difference terms in (4.11) that correspond to bonds that are outside the material at a horizontal boundary point (or vertical boundary point, respectively). This is not equivalent to discretizing the energy (2.8) at edges simply by using one-sided differences where centered differences do not exist, and in the continuum limit, these energy contributions will not converge to (2.8).

## 6.2 Corner points

The two types of corners are convex corners, as illustrated in Figure 7, and concave corners, illustrated in Figure 8. For  $(i, j)$  a convex corner point, with 9 point stencil as in Figure 7, we have the energy

$$\begin{aligned}
E &= \alpha[(d_1^{1-})^2 + (d_2^{2-})^2] \\
&+ \frac{\beta}{2}(d_2^{1-} + d_1^{2-})^2 \\
&+ \gamma d_1^{1-}d_2^{2-}.
\end{aligned} \tag{6.3}$$

As in the case of the edge energies, this energy can be obtained from the full energy (4.11) by discarding all terms that involve bonds that are outside the material.

Finally we consider the concave corner, whose 9 point stencil is shown in Figure 8. Since all 4 bonds from  $(i, j)$  exist in the material, then the full set of  $\alpha$  and  $\beta$  coefficients are present. The  $++$  cell at  $(i, j)$  is an empty space cell, however, so that  $\gamma_{++}(i, j) = 0$ . The resulting energy for a concave corner is

$$\begin{aligned}
E &= \alpha[(d_1^{1+})^2 + (d_1^{1-})^2 + (d_2^{2+})^2 + (d_2^{2-})^2] \\
&+ \frac{\beta}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2-})^2] \\
&+ \gamma[d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2+} + d_1^{1-}d_2^{2-}].
\end{aligned} \tag{6.4}$$

### 6.3 Force balance equations and the Continuum Limit

Here the force balance equations, which come from the energy minimization conditions Eq. (4.14), are reported.

In the bulk in either material 1 or 2, the elastic energy is given by (4.11) and the continuum limit is identical to the continuum elasticity equations in either material.

At a horizontal edge, say at the top of the film, our equations are

$$0 = -h(4\alpha D_1^+ D_1^- u_1 + 2\gamma D_1^0 D_2^- u_2) + 4\beta D_2^- u_1 + 2\beta(1 + T_2^-) D_1^0 u_2 \quad (6.5)$$

$$4(\alpha + \gamma)\epsilon = -h(2\beta D_1^+ D_1^- u_2 + 2\beta D_1^0 D_2^- u_1) + 4\alpha D_2^- u_2 + 2\gamma(1 + T_2^-) D_1^0 u_1. \quad (6.6)$$

At a vertical edge, we have the similar equations:

$$4(\alpha + \gamma)\epsilon = 4\alpha D_1^- u_1 - 2h\beta D_2^+ D_2^- u_1 - 2h\beta D_1^- D_2^0 u_2 + 2\gamma(1 + T_1^-) D_2^0 u_2 \quad (6.7)$$

$$0 = -4h\alpha D_2^+ D_2^- u_2 - 2h\gamma D_1^- D_2^0 u_1 + 4\beta D_1^- u_2 + 2\beta(1 + T_1^-) D_2^0 u_1. \quad (6.8)$$

The lattice parameter  $h$  arises as these equations are a mixture of 1st and second order terms. The leading order part of these equations is a discretization of the usual vanishing normal stress at:

$$\hat{\mathbf{n}} \cdot \mathbf{T}|_{\text{boundary}} = 0.$$

Next we derive the force balance equations at corners. At a convex corner, as shown in Figure 7, the equations are

$$(4\alpha + 2\gamma)\epsilon = 4\alpha D_1^- u_1 + 2\beta D_2^- u_1 + \gamma(1 + T_1^-) D_2^- u_2 + \beta(1 + T_2^-) D_1^- u_2 \quad (6.9)$$

$$(4\alpha + 2\gamma)\epsilon = 4\alpha D_2^- u_2 + 2\beta D_1^- u_2 + \gamma(1 + T_2^-) D_1^- u_1 + \beta(1 + T_1^-) D_2^- u_1. \quad (6.10)$$

For a concave corner, the equations are

$$2\gamma\epsilon = -4h\alpha D_1^+ D_1^- u_1 - 2h\beta D_2^+ D_2^- u_1 + 2\beta D_2^- u_1$$

$$\begin{aligned}
& +\gamma(D_2^+u_2 - T_1^+D_2^-u_2 + 2T_1^-D_2^0u_2) \\
& +\beta(D_1^+u_2 - T_2^+D_1^-u_2 + 2T_2^-D_1^0u_2)
\end{aligned} \tag{6.11}$$

$$\begin{aligned}
2\gamma\epsilon = & -4h\alpha D_2^+D_2^-u_2 - 2h\beta D_1^+D_1^-u_2 + 2\beta D_1^-u_2 \\
& +\gamma(D_1^+u_1 - T_2^+D_1^-u_1 + 2T_2^-D_1^0u_1) \\
& +\beta(D_2^+u_1 - T_1^+D_2^-u_1 + 2T_1^-D_2^0u_1).
\end{aligned} \tag{6.12}$$

The force balance equations at a corner do *not* admit interpretations as  $\mathbf{n} \cdot \mathbf{T} = 0$ , for any vector  $\mathbf{n}$ . The formal continuum limit of the right hand side of Eq. (6.9) for the convex corner and Eq. (6.11) for the concave corner are  $4\alpha u_{1,1} + 2\beta(u_{1,2} + u_{2,1}) + 2\gamma u_{2,2}$  and  $2\beta(u_{1,2} + u_{2,1}) + \gamma u_{2,2}$  respectively. These differ from the components of  $\mathbf{T}$  because the numerical coefficients of  $\alpha$  and  $\gamma$  are equal in  $\mathbf{T}$ . Equations Eq. (6.10) and Eq. (6.12) contain similar discrepancies.

The equations Eq. (6.5) - Eq. (6.12) must be appropriately modified if the local geometry is a rotation of the geometry analyzed above, for example if the material is above the horizontal boundary or to the right of the vertical boundary, or if the corner point faces in a direction other than the upper right.

With this modification, the four sets of force balance equations Eq. (6.5) - Eq. (6.12) are complete. On a horizontal (or vertical) segment of the interface, the force balance equations Eq. (6.5)-Eq. (6.6) (or Eq. (6.7)-Eq. (6.8), respectively) hold at every point, including points that are adjacent to corners. Similarly, equations Eq. (6.9)-Eq. (6.10) (or Eq. (6.11)-Eq. (6.12)) hold at every convex (or concave, respectively) corner point, including adjacent corner points as in a step.

As described in 5.2, the force balance equations Eq. (6.5)-Eq. (6.6) (or Eq. (6.7)-Eq. (6.8)) would not hold at edge points adjacent to a corner if the elastic parameters were determined differently than in Assumptions (3) and (6). If the elastic parameters for a bond-bond interaction were determined only by the types of the three endpoint atoms, then at an corner the interaction between the bonds forming the corner would be kept in the energy. Since this involves an interaction between the two edge points adjacent to the corner (one on a vertical edge, the other on a horizontal edge), it implies a change in the force balance equations at those two points.

## 7 Atomistic Considerations

### 7.1 The Keating Model

The elastic energy per atom  $E_\nu^K$  for the Keating model [8] and  $E_\nu^L$  for the linearized Keating model are

$$E_\nu^K = \sum_{\mathbf{b} \in \mathcal{B}_\nu} \alpha^K \mathbf{R}_{\mathbf{b}}^2 + \sum_{\mathbf{b} \in \mathcal{B}_\nu} \sum_{\mathbf{b}' \in \mathcal{I}_{\mathbf{b}} \cap \mathcal{B}_\nu} \beta^K (\mathbf{R}_{\mathbf{b}} \cdot \mathbf{R}_{\mathbf{b}'})^2 \quad (7.1)$$

$$E_\nu^L = \sum_{\mathbf{b} \in \mathcal{B}_\nu} \alpha^K S_{\mathbf{b}, \mathbf{b}}^2 + \sum_{\mathbf{b} \in \mathcal{B}_\nu} \sum_{\mathbf{b}' \in \mathcal{I}_{\mathbf{b}} \cap \mathcal{B}_\nu} \beta^K S_{\mathbf{b}, \mathbf{b}'}^2. \quad (7.2)$$

These are specific examples of the general nonlinear and linearized energies - Eq. (3.7) and Eq. (3.9) - derived in Section 3. In particular, for the case of a 2D cubic lattice, the energy for the linearized Keating model is equivalent to our discrete energy density Eq. (4.11) with  $\gamma = 0$ .

The appeal of the Keating model is that its energy is easily understood, but it does not correspond to the full continuum elastic theory, and it is not clear how to extend this model at interfaces. Our atomistic model, on the other hand, is consistent with the full range of continuum elasticity, and it extends to systems with material interfaces.

### 7.2 Inner Relaxation

In models which lack inversion symmetry (cubic lattices do not) after one imposes the Cauchy-Born hypothesis on the lattice as a method for relating the microscopic and macroscopic strain, there is an additional relaxation that can take place to minimize the energy further. This extra displacement is not seen at the macroscopic level, where one only has the macroscopic displacement. Extension of the present theory to other lattices is straightforward. In particular, the inner relaxation that is required for lattices that lack inversion symmetry is handled directly by our model. Since we work directly with the atomic configuration, then for a properly formulated atomistic model, the inner relaxation will occur automatically when the elastic energy is minimized. In addition, the relation between the continuum elastic coefficients and the atomistic coefficients must include the effects of the inner relaxation, as discussed in [12, 13, 3, 4].



This is, in fact, one of the major differences between our method and the quasi-continuum method. In the quasi-continuum method [21, 22] one works at the continuum level, not the atomistic one, minimizing a certain Dirichlet integral like quantity. It is only when a numerical value of the energy in a region is actually needed that the method switches to an atomistic one, and some kind of atomistic energy is used to compute the total energy of the system. In order to do this an artificial lattice is used to compute the energy if it was in the state of the macroscopic deformation. There is no real physical lattice, and consequently, the macroscopic strain must be imposed on the artificial lattice. The way this is done is through the Cauchy-Born hypothesis. Thus, in the quasicontinuum method, it is essential to take inner elasticity into account, when it is present. In our method, since we always work with the physical lattice, we automatically carry out the inner relaxation.

## 8 Conclusions and Future Directions

This paper describes a new theory for elastic strain models at the atomistic level. In this approach, the atomistic strain energy is required to be consistent with macroscopic elasticity and with the symmetries of the crystal lattice. Further requirements on the extent of elastic interactions have been imposed for simplicity, but these could readily be relaxed if needed. As we have seen in Section 7, our energy is consistent with (but more general than) the well-known Keating model for atomistic strain. Moreover, the explicit correspondence between continuum elasticity and atomistics in our approach provides a route for enhancing our computational model to accommodate more complicated and realistic atomistic features.

For the special case of a simple cubic lattice in 2D, an explicit form of the elastic energy has been derived in the presence of material and vacuum interfaces, including intrinsic surface stress at the interface with a vacuum. Although real materials are not two-dimensional or simple cubic, this example is presented as the simplest context for investigation of the effects of atomistic strain. For example, the force balance equations at a corner on a material interface are readily available and compact enough to be comprehensible. We believe that this simple geometry will correctly capture many qualitative properties, such as intrinsic surface stress and the elastic interac-

tion of steps.

The theory presented here can be generalized in several directions. First, an explicit form of the elastic energy is easily derived for 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. For numerical solution with more complex geometries, we expect to work directly with the elastic energy, rather than deriving force balance equations. Explicit force balance equations are useful in providing insight into the nature of the discrete equations and their relation to the continuum equations. On the other hand, the force balance equations are more difficult to derive and write out than the energy. For numerical purposes, it is sufficient to evaluate the energy, since the coefficients of the linear force balance equations can be exactly computed by finite differences of values of the energy.

Second, the theory formulated here is well suited for computation. Numerical determination of the strain field can be effected either by solving the force balance equations or by minimization of the elastic energy. 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 straightforward; i.e., it is a numerical analysis problem that does not require additional physics.

Third, the detailed linear atomistic strain model for a cubic lattice can be generalized to a nonlinear model. The Keating model, whose linearization is contained within the present theory, is a natural starting point. A nonlinear strain model is necessary for extension of this theory to include lattice defects such as dislocations; it may also have significance at steps where the strain energy is larger than in the bulk.

Our motivation for developing this theory is to use it for simulation of strain effects in epitaxial growth. In a companion paper [16] 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, aimed at simulation of quantum dot growth as well as other problems, are currently underway.

## A Interface between Two Materials with an Interfacial Region

Consider an interface between 2 materials; i.e., an epilayer on a substrate as in Figure 11. Call the substrate the type 1 material, and the film the type 2 material. The only new local geometries are those at the interface between the type 1 and type 2 materials. The 9 point stencil of any point that is not an interfacial point will have only points of the same type, and so its energy contribution will be one of the ones of the previous sections. In this section we will consider all the interfacial points that require new treatment, and find the energy and force balance equations at these points.

We will classify the bonds as type 1, type 2 or type 3 as follows: A type 1 bond is one between two type 1 atoms, a type 2 bond is one between two type 2 atoms, and a type 3 bond is a bond between a type 1 atom and a type 2 atom, (see Figure 9). We classify a cell of type 1, 2, or 3, according to its corner points. A cell is of type 1 or 2 if all 4 corners are type 1 or 2 atoms. But if it is a mixture of points, it is a type 3 cell (see Figure 10). We will regard the interfacial region between the type 1 and type 2 materials, as a 3rd material with its own elastic constants.

So if  $d^{js}(i, j)$  is a bond of type  $\ell$ , then

$$\alpha_{js}(i, j) = \alpha^\ell \tag{A.1}$$

and if  $d^{1s_1}$  and  $d^{2s_2}$  border a cell of type  $\ell$  then

$$\begin{aligned} \beta_{s_1, s_2}(i, j) &= \beta^\ell \\ \gamma_{s_1 s_2}(i, j) &= \gamma^\ell. \end{aligned} \tag{A.2}$$

Additionally, we determine the lattice mismatch parameters  $\epsilon_1, \epsilon_2, \epsilon_3$  according to the bond type.

The elastic energy density is different from the energy density in the interior at the following points: Straight horizontal interfaces, straight vertical interfaces, and corners in the interfaces, which can be reentrant into either the substrate or the film. The energy density at these points will be derived below. In addition, the force balance equations are different from the equations in the interior at the off-diagonal points at an interfacial corner. The force balance equations are also different at adjacent corners, as occur in a

step (of 1 unit cell height). In fact the 9 point stencils at these points are different from the stencils for the regular (isolated) convex corner points or edge points.

## A.1 Edge Points

At a horizontal interface, there is a type 1 point  $(i, j)$  and its type 2 neighbor  $(i, j + 1)$ . The energy at the type 1 point  $(i, j)$  is

$$\begin{aligned}
E &= \alpha^1[(d_1^{1+})^2 + (d_1^{1-})^2 + (d_2^{2-})^2] + \alpha^3(d_2^{2+})^2 \\
&+ \frac{\beta^1}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2+})^2] \\
&+ \frac{\beta^3}{2}[(d_2^{1+} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2-})^2] \\
&+ \gamma^3(d_1^{1+}d_2^{2+} + d_1^{1-}d_2^{2+}) + \gamma^1(d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2-})
\end{aligned} \tag{A.3}$$

and at the type 2 point  $(i, j + 1)$  it is

$$\begin{aligned}
E &= \alpha^2[(d_1^{1+})^2 + (d_1^{1-})^2 + (d_2^{2+})^2] + \alpha^3(d_2^{2-})^2 \\
&+ \frac{\beta^2}{2}[(d_2^{1+} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2+})^2] \\
&+ \frac{\beta^3}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2-})^2] \\
&+ \gamma^2(d_1^{1+}d_2^{2+} + d_1^{1-}d_2^{2+}) + \gamma^3(d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2-}).
\end{aligned} \tag{A.4}$$

At a vertical interface there is a type 1 point  $(i, j)$  and its type 2 neighbor at  $(i + 1, j)$ . The energy at the type 1 point  $(i, j)$  is

$$\begin{aligned}
E &= \alpha^1[(d_1^{1-})^2 + (d_2^{2+})^2 + (d_2^{2-})^2] + \alpha^3(d_1^{1+})^2 \\
&+ \frac{\beta^1}{2}[(d_2^{1-} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2-})^2] \\
&+ \frac{\beta^3}{2}[(d_2^{1+} + d_1^{2+})^2 + (d_2^{1+} + d_1^{2-})^2] \\
&+ \gamma^3(d_1^{1+}d_2^{2+} + d_1^{1+}d_2^{2-}) + \gamma^1(d_1^{1-}d_2^{2+} + d_1^{1-}d_2^{2-})
\end{aligned} \tag{A.5}$$

and at the type 2 point  $(i + 1, j)$  it is

$$E = \alpha^2[(d_1^{1+})^2 + (d_2^{2+})^2 + (d_2^{2-})^2] + \alpha^3(d_1^{1-})^2$$

$$\begin{aligned}
& + \frac{\beta^2}{2}[(d_2^{1+} + d_1^{2+})^2 + (d_2^{1+} + d_1^{2-})^2] \\
& + \frac{\beta^3}{2}[(d_2^{1-} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2-})^2] \\
& + \gamma^2(d_1^{1+}d_2^{2+} + d_1^{1+}d_2^{2-}) + \gamma^3(d_1^{1-}d_2^{2+} + d_1^{1-}d_2^{2-}).
\end{aligned} \tag{A.6}$$

## A.2 Corner Points

There are two different corner configurations to consider. The corner could be reentrant into the type 2 material, so this would be convex in type 1 and concave in type 2, or it could be reentrant into type 1, so it is concave in type 1 and convex in type 2. For each configuration, we need an energy contribution from both the type 1 and the type 2 corner points. For the corner reentrant into the type 2 material, the energy at the type 1 point  $(i, j)$  is

$$\begin{aligned}
E & = \alpha^1[(d_1^{1-})^2 + (d_2^{2-})^2] + \alpha^3[(d_1^{1+})^2 + (d_2^{2+})^2] \\
& + \frac{\beta^3}{2}[(d_2^{1+} + d_1^{2+})^2 + (d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2+})^2] + \frac{\beta^1}{2}(d_2^{1-} + d_1^{2-})^2 \\
& + \gamma^3(d_1^{1+}d_2^{2+} + d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2+}) + \gamma^1d_1^{1-}d_2^{2-}
\end{aligned} \tag{A.7}$$

and at the type 2 point  $(i + 1, j + 1)$  it is

$$\begin{aligned}
E & = \alpha^2[(d_1^{1+})^2 + (d_2^{2+})^2 + (d_2^{2-})^2 + (d_1^{1-})^2] \\
& + \frac{\beta^2}{2}[(d_2^{1+} + d_1^{2+})^2 + (d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2+})^2] + \frac{\beta^3}{2}(d_2^{1-} + d_1^{2-})^2 \\
& + \gamma^2(d_1^{1+}d_2^{2+} + d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2+}) + \gamma^3d_1^{1-}d_2^{2-}.
\end{aligned} \tag{A.8}$$

For the corner reentrant into the type 1 the energy at the type 1 point  $(i, j)$  is

$$\begin{aligned}
E & = \alpha^1[(d_1^{1+})^2 + (d_1^{1-})^2 + (d_2^{2+})^2 + (d_2^{2-})^2] \\
& + \frac{\beta^1}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2-})^2] + \frac{\beta^3}{2}(d_2^{1+} + d_1^{2+})^2 \\
& + \gamma^1(d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2+} + d_1^{1-}d_2^{2-}) + \gamma^3d_1^{1+}d_2^{2+}
\end{aligned} \tag{A.9}$$

and at the type 2 point  $(i + 1, j + 1)$  it is

$$E = \alpha^2[(d_1^{1+})^2 + (d_2^{2+})^2] + \alpha^3[(d_1^{1-})^2 + (d_2^{2-})^2]$$

$$\begin{aligned}
& + \frac{\beta^3}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2-})^2] + \frac{\beta^2}{2}(d_2^{1+} + d_1^{2+})^2 \\
& + \gamma^3(d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2+} + d_1^{1-}d_2^{2-}) + \gamma^2d_1^{1+}d_2^{2+}. \tag{A.10}
\end{aligned}$$

### A.3 Force Balance Equations

As mentioned above, force balance equations will be presented for straight interfaces (both horizontal and vertical) and for corners (reentrant into material 1 or material 2). In addition, new force balance equations are presented for the interface points that are adjacent to a reentrant corner point.

For points at a straight horizontal edge, there are new equations for the type 1 point  $(i, j)$  and the type 2 point  $(i, j + 1)$ . The force balance equations at the type 1 point  $(i, j)$  are

$$\begin{aligned}
0 & = -4h\alpha^1 D_1^+ D_1^- u_1 + 4\beta^1 D_2^- u_1 - 4\beta^3 D_2^+ u_1 \\
& \quad - 2h\gamma^1 D_1^0 D_2^- u_2 - 2h\gamma^3 D_1^0 D_2^+ u_2 \\
& \quad + 2\beta^1(1 + T_2^-) D_1^0 u_2 - 2\beta^3(1 + T_2^+) D_1^0 u_2 \tag{A.11} \\
-4\alpha^3 \epsilon_3 & + (4\gamma^1 - 2\gamma^3 + 4\alpha^1) \epsilon_1 - 2\gamma^3 \epsilon_2
\end{aligned}$$

$$\begin{aligned}
& = 4\alpha^1 D_2^- u_2 - 4\alpha^3 D_2^+ u_2 - 2h(\beta^1 + \beta^3) D_1^+ D_1^- u_2 \\
& \quad - 2h\beta^1 D_1^0 D_2^- u_1 - 2h\beta^3 D_1^0 D_2^+ u_1 \\
& \quad + 2\gamma^1(1 + T_2^-) D_1^0 u_1 - 2\gamma^3(1 + T_2^+) D_1^0 u_1. \tag{A.12}
\end{aligned}$$

The force balance equations at the type 2 point  $(i, j + 1)$  are

$$\begin{aligned}
0 & = -4h\alpha^2 D_1^+ D_1^- u_1 + 4\beta^3 D_2^- u_1 - 4\beta^2 D_2^+ u_1 \\
& \quad - 2h\gamma^3 D_1^0 D_2^- u_2 - 2h\gamma^2 D_1^0 D_2^+ u_2 \\
& \quad + 2\beta^3(1 + T_2^-) D_1^0 u_2 - 2\beta^2(1 + T_2^+) D_1^0 u_2 \tag{A.13} \\
2\gamma^3 \epsilon_1 & + (2\gamma^3 - 4\gamma^2 - 4\alpha^2) \epsilon_2 + 4\alpha^3 \epsilon_3
\end{aligned}$$

$$\begin{aligned}
& = 4\alpha^3 D_2^- u_2 - 4\alpha^2 D_2^+ u_2 - 2h(\beta^2 + \beta^3) D_1^+ D_1^- u_2 \\
& \quad - 2h\beta^3 D_1^0 D_2^- u_1 - 2h\beta^2 D_1^0 D_2^+ u_1 \\
& \quad + 2\gamma^3(1 + T_2^-) D_1^0 u_1 - 2\gamma^2(1 + T_2^+) D_1^0 u_1. \tag{A.14}
\end{aligned}$$

For a vertical boundary we have, analogously, a type 1 point  $(i, j)$  and immediately to its right a type 2 point  $(i + 1, j)$ . The force balance equations at the type 1 point  $(i, j)$  are

$$-2\gamma^3 \epsilon_2 + (4\gamma^1 - 2\gamma^3 + 4\alpha^1) \epsilon_1 - 4\alpha^3 \epsilon_3$$

$$\begin{aligned}
&= 4\alpha^1 D_1^- u_1 - 4\alpha^3 D_1^+ u_1 - 2h(\beta^1 + \beta^3) D_2^+ D_2^- u_1 \\
&\quad - 2h\beta^1 D_2^0 D_1^- u_2 - 2h\beta^3 D_2^0 D_1^+ u_2 \\
&\quad + 2\gamma^1(1 + T_1^-) D_2^0 u_2 - 2\gamma^3(1 + T_1^+) D_2^0 u_2 \tag{A.15}
\end{aligned}$$

$$\begin{aligned}
0 &= -4h\alpha^1 D_2^+ D_2^- u_2 + 4\beta^1 D_1^- u_2 - 4\beta^3 D_1^+ u_2 \\
&\quad - 2h\gamma^1 D_2^0 D_1^- u_1 - 2h\gamma^3 D_2^0 D_1^+ u_1 \\
&\quad + 2\beta^1(1 + T_1^-) D_2^0 u_1 - 2\beta^3(1 + T_1^+) D_2^0 u_1. \tag{A.16}
\end{aligned}$$

The force balance equations at the type 2 point  $(i + 1, j)$  are

$$\begin{aligned}
2\gamma^3 \epsilon_1 &+ (2\gamma^3 - 4\gamma^2 - 4\alpha^2) \epsilon_2 + 4\alpha^3 \epsilon_3 \\
&= +4\alpha^3 D_1^- u_1 - 4\alpha^2 D_1^+ u_1 - 2h(\beta^2 + \beta^3) D_2^+ D_2^- u_1 \\
&\quad - 2h\beta^3 D_2^0 D_1^- u_2 - 2h\beta^2 D_2^0 D_1^+ u_2 \\
&\quad + 2\gamma^3(1 + T_1^-) D_2^0 u_2 - 2\gamma^2(1 + T_1^+) D_2^0 u_2 \tag{A.17}
\end{aligned}$$

$$\begin{aligned}
0 &= -4h\alpha^2 D_2^+ D_2^- u_2 + 4\beta^3 D_1^- u_2 - 4\beta^2 D_1^+ u_2 \\
&\quad - 2h\gamma^3 D_2^0 D_1^- u_1 - 2h\beta^2 D_2^0 D_1^+ u_1 \\
&\quad + 2\beta^3(1 + T_1^-) D_2^0 u_1 - 2\gamma^2(1 + T_1^+) D_2^0 u_1. \tag{A.18}
\end{aligned}$$

At a corner, there are new force balance equations at the four vertices of the cell at the corner, the points  $(i, j)$ ,  $(i + 1, j)$ ,  $(i, j + 1)$ ,  $(i + 1, j + 1)$ . The difference from the force balance on the edges is because that the stencil is different at these four points. For the corner points  $(i, j)$  and  $(i + 1, j + 1)$  we get fully new equations, and we present those now. The force balance equations at the type 1 point,  $(i, j)$  are

$$\begin{aligned}
-2\gamma^3 \epsilon_2 &+ (4\alpha^1 + 2\gamma^1 - \gamma^3) \epsilon_1 + (\gamma^3 - 4\alpha^3) \epsilon_3 \\
&= 4\alpha^1 D_1^- u_1 - 4\alpha^3 D_1^+ u_1 + 2(\beta^1 + \beta^3) D_2^- u_1 - 4\beta^3 D_2^+ u_1 \\
&\quad + \gamma^1(1 + T_1^-) D_2^- u_2 + \beta^1(1 + T_2^-) D_1^- u_2 \\
&\quad + \gamma^3(-D_2^- u_2 + T_1^- D_2^+ u_2 - 2T_1^+ D_2^0 u_2) \\
&\quad + \beta^3(-D_1^- u_2 + T_2^- D_1^+ u_2 - 2T_2^+ D_1^0 u_2) \tag{A.19}
\end{aligned}$$

$$\begin{aligned}
-2\gamma^3 \epsilon_2 &+ (4\alpha^1 + 2\gamma^1 - \gamma^3) \epsilon_1 + (\gamma^3 - 4\alpha^3) \epsilon_3 \\
&= 4\alpha^1 D_2^- u_2 - 4\alpha^3 D_2^+ u_2 + 2(\beta^1 + \beta^3) D_1^- u_2 - 4\beta^3 D_1^+ u_2 \\
&\quad + \gamma^1(1 + T_2^-) D_1^- u_1 + \beta^1(1 + T_1^-) D_2^- u_1 \\
&\quad + \gamma^3(-D_1^- u_1 + T_2^- D_1^+ u_1 - 2T_2^+ D_1^0 u_1) \\
&\quad + \beta^3(-D_2^- u_1 + T_1^- D_2^+ u_1 - 2T_1^+ D_2^0 u_1). \tag{A.20}
\end{aligned}$$

The force balance equations at the type 2 point  $(i + 1, j + 1)$  are

$$\begin{aligned}
\gamma^3 \epsilon_3 &+ (\gamma^3 - 2\gamma^2) \epsilon_2 \\
&= -4h\alpha^2 D_1^+ D_1^- u_1 - 2h\beta^2 D_2^+ D_2^- u_1 + 2\beta^3 D_2^- u_1 - 2\beta^2 D_2^+ u_1 \\
&\quad + \gamma^3 (1 + T_1^-) D_2^- u_2 + \beta^3 (1 + T_2^-) D_1^- u_2 \\
&\quad + \gamma^2 (-D_2^- u_2 + T_1^- D_2^+ u_2 - T_1^+ 2D_2^0 u_2) \\
&\quad + \beta^2 (-D_1^- u_2 + T_2^- D_1^+ u_2 - 2T_2^+ D_1^0 u_2) \tag{A.21}
\end{aligned}$$

$$\begin{aligned}
\gamma^3 \epsilon_3 &+ (\gamma^3 - 2\gamma^2) \epsilon_2 \\
&= -4h\alpha^2 D_2^+ D_2^- u_2 - 2h\beta^2 D_1^+ D_1^- u_2 + 2\beta^3 D_1^- u_2 - 2\beta^2 D_1^+ u_2 \\
&\quad + \gamma^3 (1 + T_2^-) D_1^- u_1 + \beta^3 (1 + T_1^-) D_2^- u_1 \\
&\quad + \gamma^2 (-D_1^- u_1 + T_2^- D_1^+ u_1 - 2T_2^+ D_1^0 u_1) \\
&\quad + \beta^2 (-D_2^- u_1 + T_1^- D_2^+ u_1 - 2T_1^+ D_2^0 u_1). \tag{A.22}
\end{aligned}$$

The stencils for  $(i+1, j)$  and  $(i, j+1)$  only differ from those for normal edge points considered above by one of the bonds at the stencil edge. However, the relevant bond and cell types are exactly the same as before. So the coefficients in the elastic equations for these points are the same as for normal type 2 edge points, and consequently, the left hand sides of the elastic equations will be the same; i.e., at  $(i + 1, j)$  and  $(i, j + 1)$  the left hand sides are identical to equations (A.17-A.18) and (A.13-A.14) respectively. What does change is the right hand side (RHS) of the equations involving the lattice mismatch parameters. Thus, for the two off diagonal points, we will only show the right hand sides. The right hand side of the force balance equations at the point  $(i + 1, j)$  are

$$\text{RHS(A.17)} = \gamma^3 \epsilon_1 + (2\gamma^3 - 4\gamma^2 - 4\alpha^2) \epsilon_2 + (4\alpha^3 + \gamma_3) \epsilon_3 \tag{A.23}$$

$$\text{RHS(A.18)} = \gamma^3 \epsilon_3 - \gamma^3 \epsilon_2. \tag{A.24}$$

At the point  $(i, j + 1)$  the right hand sides are

$$\text{RHS(A.13)} = \gamma^3 \epsilon_3 - \gamma^3 \epsilon_2 \tag{A.25}$$

$$\text{RHS(A.14)} = \gamma^3 \epsilon_1 + (2\gamma^3 - 4\gamma^2 - 4\alpha^2) \epsilon_2 + (4\alpha^3 + \gamma^3) \epsilon_3. \tag{A.26}$$

Now we present the analogous equations for the corner reentrant into the type 1 material. Again, we will present the full equations for the corner



points  $(i, j)$  and  $(i + 1, j + 1)$ . The force balance equations at the point  $(i, j)$  are

$$\begin{aligned}
-\gamma^3 \epsilon_3 &+ (2\gamma^1 - \gamma^3) \epsilon_1 \\
&= -4h\alpha^1 D_1^+ D_1^- u_1 - 2h\beta^1 D_2^+ D_2^- u_1 + 2\beta^1 D_2^- u_1 - 2\beta^3 D_2^+ u_1 \\
&\quad -\gamma^3(1 + T_1^+) D_2^+ u_2 - \beta^3(1 + T_2^+) D_1^+ u_2 \\
&\quad +\gamma^1(D_2^+ u_2 - T_1^+ D_2^- u_2 + 2T_1^- D_2^0 u_2) \\
&\quad +\beta^1(D_1^+ u_2 - T_2^+ D_1^- u_2 + 2T_2^- D_1^0 u_2)
\end{aligned} \tag{A.27}$$

$$\begin{aligned}
-\gamma^3 \epsilon_3 &+ (2\gamma^1 - \gamma^3) \epsilon_1 \\
&= -4h\alpha^1 D_2^+ D_2^- u_2 - 2h\beta^1 D_1^+ D_1^- u_2 + 2\beta^1 D_1^- u_2 - 2\beta^3 D_1^+ u_2 \\
&\quad -\gamma^3(1 + T_2^+) D_1^+ u_1 - \beta^3(1 + T_1^+) D_2^+ u_1 \\
&\quad +\gamma^1(D_1^+ u_1 - T_2^+ D_1^- u_1 + 2T_2^- D_1^0 u_1) \\
&\quad +\beta^1(D_2^+ u_1 - T_1^+ D_2^- u_1 + 2T_1^- D_2^0 u_1).
\end{aligned} \tag{A.28}$$

The force balance equations at the point  $(i + 1, j + 1)$  are

$$\begin{aligned}
2\gamma^3 \epsilon_1 &+ (\gamma^3 - 2\gamma^2 - 4\alpha^2) \epsilon_2 + (4\alpha^3 - \gamma^3) \epsilon_3 \\
&= 4\alpha^3 D_1^- u_1 - 4\alpha^2 D_1^+ u_1 + 4\beta^3 D_2^- u_1 - 2(\beta^2 + \beta^3) D_2^+ u_1 \\
&\quad -\gamma^2(1 + T_1^+) D_2^+ u_2 - \beta^2(1 + T_2^+) D_1^+ u_2 \\
&\quad +\gamma^3(D_2^+ u_2 - T_1^+ D_2^- u_2 + 2T_1^- D_2^0 u_2) \\
&\quad +\beta^3(D_1^+ u_2 - T_2^+ D_1^- u_2 + 2T_2^- D_1^0 u_2)
\end{aligned} \tag{A.29}$$

$$\begin{aligned}
2\gamma^3 \epsilon_1 &+ (\gamma^3 - 2\gamma^2 - 4\alpha^2) \epsilon_2 + (4\alpha^3 - \gamma^3) \epsilon_3 \\
&= 4\alpha^3 D_2^- u_2 - 4\alpha^2 D_2^+ u_2 + 4\beta^3 D_1^- u_2 - 2(\beta^2 + \beta^3) D_1^+ u_2 \\
&\quad -\gamma^2(1 + T_2^+) D_1^+ u_1 - \beta^2(1 + T_1^+) D_2^+ u_1 \\
&\quad +\gamma^3(D_1^+ u_1 - T_2^+ D_1^- u_1 + 2T_2^- D_1^0 u_1) \\
&\quad +\beta^3(D_2^+ u_1 - T_1^+ D_2^- u_1 + 2T_1^- D_2^0 u_1).
\end{aligned} \tag{A.30}$$

Similar to the previous case, the off diagonal points will have their right hand sides altered from the case of type 1 edge points. The right hand side of the force balance equations at the point  $(i + 1, j)$  are

$$\text{RHS(A.11)} = \gamma_3 \epsilon_1 - \gamma_3 \epsilon_3 \tag{A.31}$$

$$\text{RHS(A.12)} = -(\gamma^3 + 4\alpha^3) \epsilon_3 + (4\gamma^1 - 2\gamma^3 + 4\alpha^1) \epsilon_1 - \gamma^3 \epsilon_2. \tag{A.32}$$

The right hand side of the force balance equations at the point  $(i, j + 1)$  are

$$\text{RHS(A.15)} = -\gamma^3\epsilon_2 + (4\gamma^1 - 2\gamma^3 + 4\alpha^1)\epsilon_1 - (\gamma^3 + 4\alpha^3)\epsilon_3 \quad (\text{A.33})$$

$$\text{RHS(A.15)} = \gamma^3\epsilon_2 - \gamma^3\epsilon_3. \quad (\text{A.34})$$

In addition to the force balance equations presented above, new force balance laws are needed if there are adjacent corners. For example, at a step, the point at the convex corner of the step differs from the usual convex corner point in that the  $(i+1, j-1)$  atom is a material 1 point, not a material 2 point as for the convex corner considered already. As for the off diagonal corner points, this will not change the coefficient types in the equations for this point, but, because of the change of the bond types, it will change the coefficients of the lattice mismatch parameter. Thus, the coefficients of the  $u$  derivatives will be the same as the normal convex corner point equations, but the right hand sides will change slightly.

The case of two consecutive steps is similar.

## B Interface of Material and Vacuum with Intrinsic Surface Stress

We will now reconsider an interface between a material (of type 1) and a vacuum as in Figure 12. Because of the change in coordination number for the atoms at the top of the material, their displacement is significantly different from the atoms in the interior of the material. This change in displacement leads to an intrinsic surface stress. We will develop a model for intrinsic surface stress by taking the atoms at the top to be of a different material type 2; i.e., the atom at  $(i, j)$  is a type 2 atom if there is vacuum at any of its nearest neighbors or next nearest neighbors.

We will consider the 4 geometries treated in Section 6, the horizontal and vertical edges, and the convex and concave corners. The energy and force balance equations at atoms in the interior of the material are the same as Eq. (4.11), Eq. (4.15) for the bulk material. The energy at atoms that are one atom removed from the vacuum interface, i.e., those that have a type 2 atom as a nearest neighbor or next nearest neighbor, are the same as for the type 1 boundary atoms in the material interface problem. The energy for atoms in the type 2 layer are the same as for the type 2 boundary atoms in the

material interface problem, except that terms involving bonds that extend into the vacuum are omitted. Thus, the only atoms with new energies and new force balance equations are the surface atoms.

For completeness, we write out the energy at points on the boundary of the material and for points that are a single atom away from the top boundary.

## B.1 Edge Points

For straight horizontal boundaries there is the type 1 point  $(i, j)$  and its type 2 neighbor at  $(i, j + 1)$ . The energy at the type 1 point  $(i, j)$  is the same as in Eq. (A.3), and at the type 2 point  $(i, j + 1)$  it is

$$\begin{aligned}
E &= \alpha^2[(d_1^{1+})^2 + (d_1^{1-})^2] + \alpha^3(d_2^{2-})^2 \\
&+ \frac{\beta^3}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2-})^2] \\
&+ \gamma^3(d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2-}).
\end{aligned} \tag{B.35}$$

For straight vertical boundaries there is the type 1 point  $(i, j)$  and its type 2 neighbor at  $(i + 1, j)$ . The energy at the type 1 point  $(i, j)$  is same as in Eq. (A.5), and at the type 2 point  $(i + 1, j)$  it is

$$\begin{aligned}
E &= \alpha^2[(d_2^{2+})^2 + (d_2^{2-})^2] + \alpha^3(d_1^{1-})^2 \\
&+ \frac{\beta^3}{2}[(d_2^{1-} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2-})^2] \\
&+ \gamma^3(d_1^{1-}d_2^{2+} + d_1^{1-}d_2^{2-}).
\end{aligned} \tag{B.36}$$

## B.2 Corner Points

As for the vacuum interface, we need to consider the convex and concave corners.

For the convex corner, type 1 point  $(i, j)$  is the same as in Eq. (A.7), and at the type 2 point  $(i + 1, j + 1)$  it is

$$\begin{aligned}
E &= \alpha^2[(d_1^{1-})^2 + (d_2^{2-})^2] + \frac{\beta^3}{2}(d_2^{1-} + d_1^{2-})^2 \\
&+ \gamma^3d_1^{1-}d_2^{2-}.
\end{aligned} \tag{B.37}$$

For the concave corner, the energy at the type 1 point  $(i, j)$  is the same as in Eq. (A.9), and at the type 2 point  $(i + 1, j + 1)$  it is

$$\begin{aligned}
E &= \alpha^2[(d_1^{1+})^2 + (d_2^{2+})^2] + \alpha^3[(d_1^{1-})^2 + (d_2^{2-})^2] \\
&+ \frac{\beta^3}{2}[(d_2^{1+} + d_1^{2-})^2 + (d_2^{1-} + d_1^{2+})^2 + (d_2^{1-} + d_1^{2-})^2] \\
&+ \gamma^3(d_1^{1+}d_2^{2-} + d_1^{1-}d_2^{2+} + d_1^{1-}d_2^{2-}).
\end{aligned} \tag{B.38}$$

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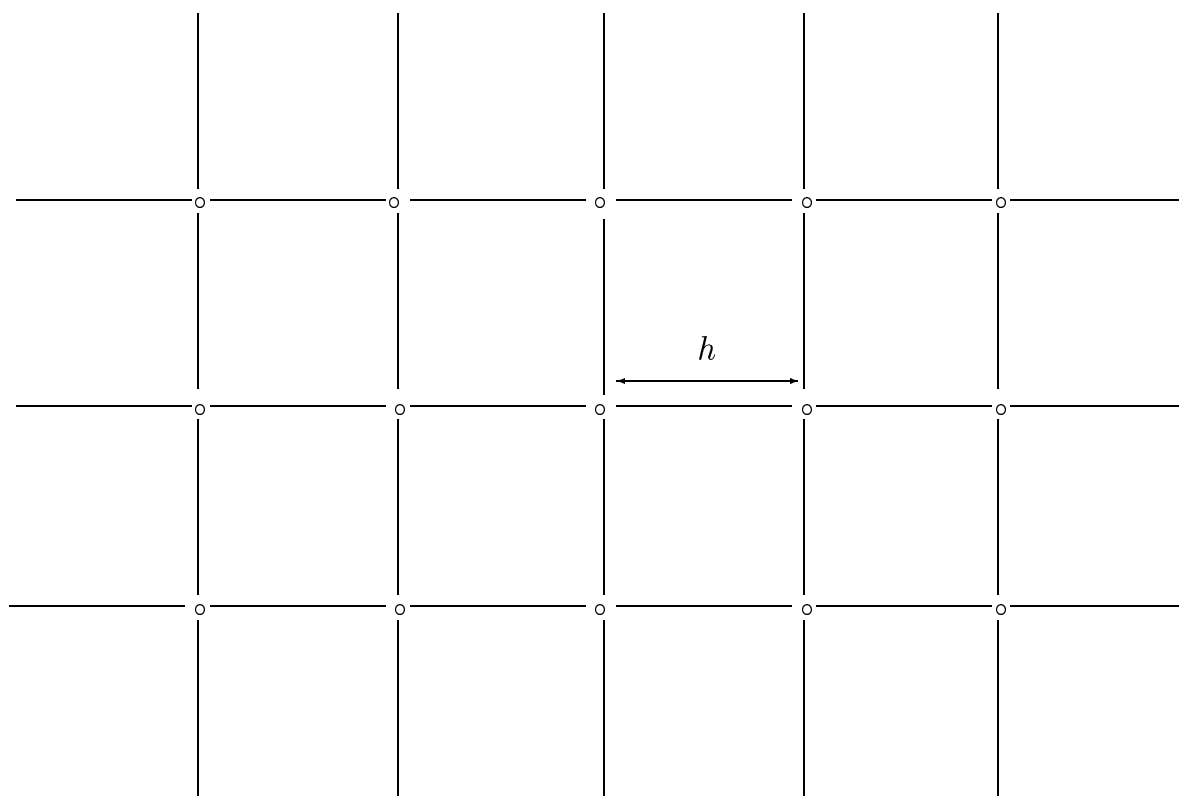


Figure 1: 2d simple cubic lattice with lattice constant  $h$ .

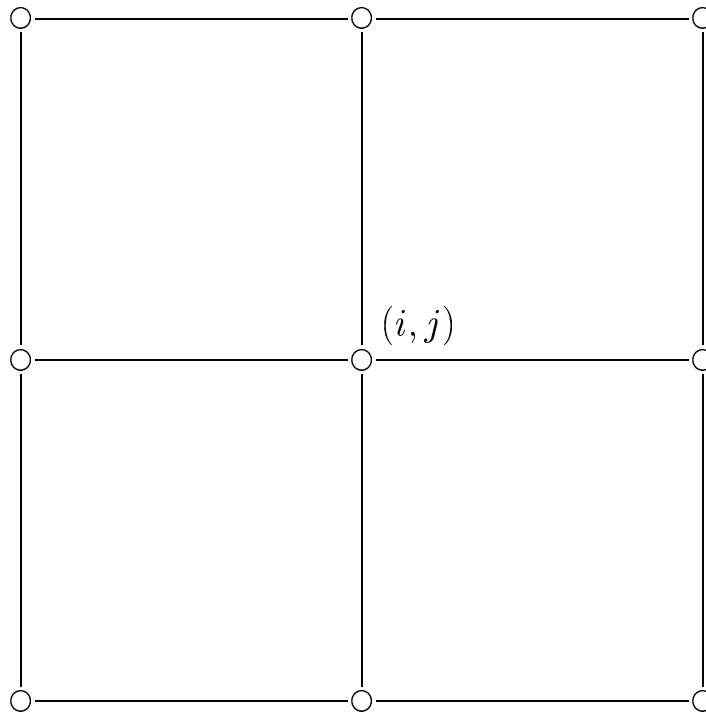


Figure 2: 9 point stencil for the force balance equations in the bulk of a material; local energy is based on a 5 point stencil.

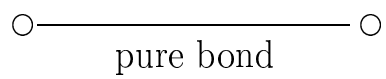


Figure 3: Examples of pure and mixed type bonds.



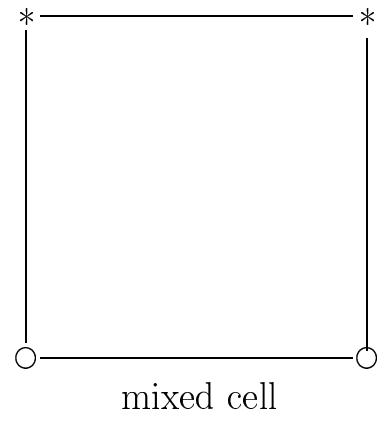
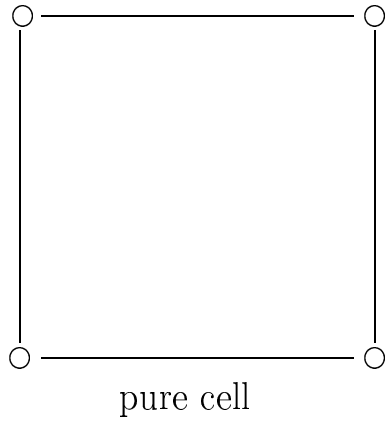


Figure 4: Examples of pure and mixed type cells.

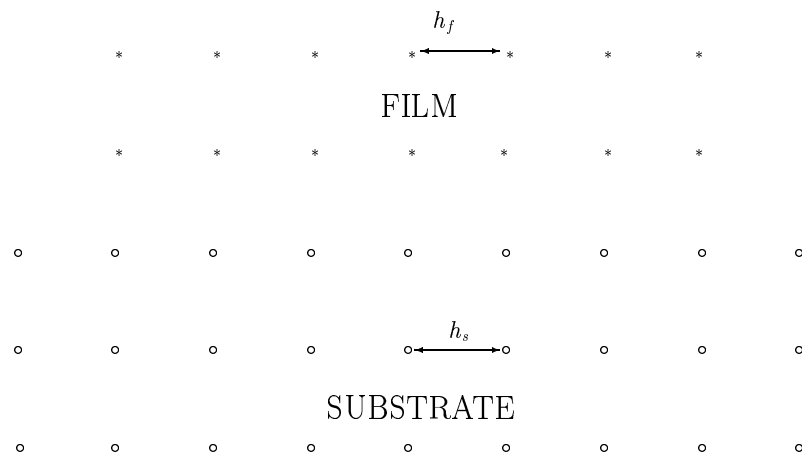


Figure 5: Thin film on a substrate. The points  $\circ$  are the substrate and  $\star$  are the film.

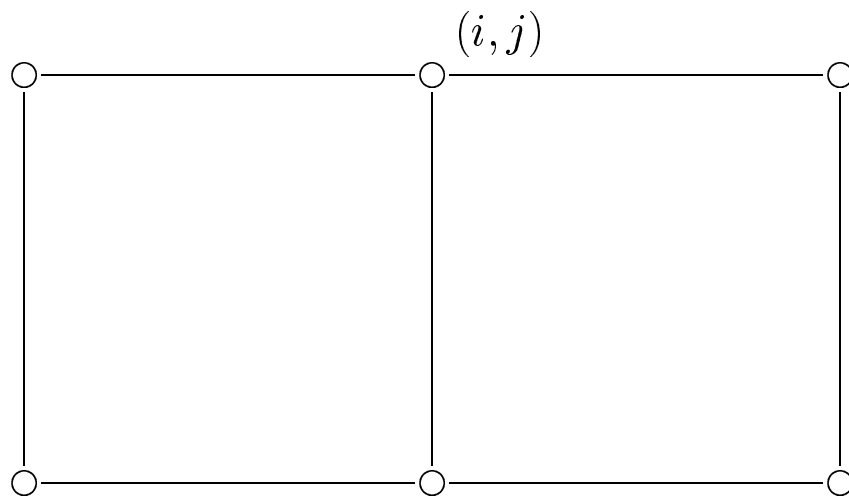


Figure 6: The reduced stencil for a horizontal edge point.

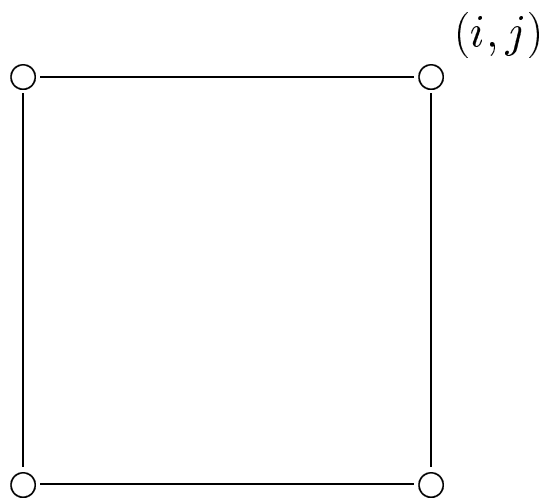


Figure 7: The reduced stencil for a convex corner.

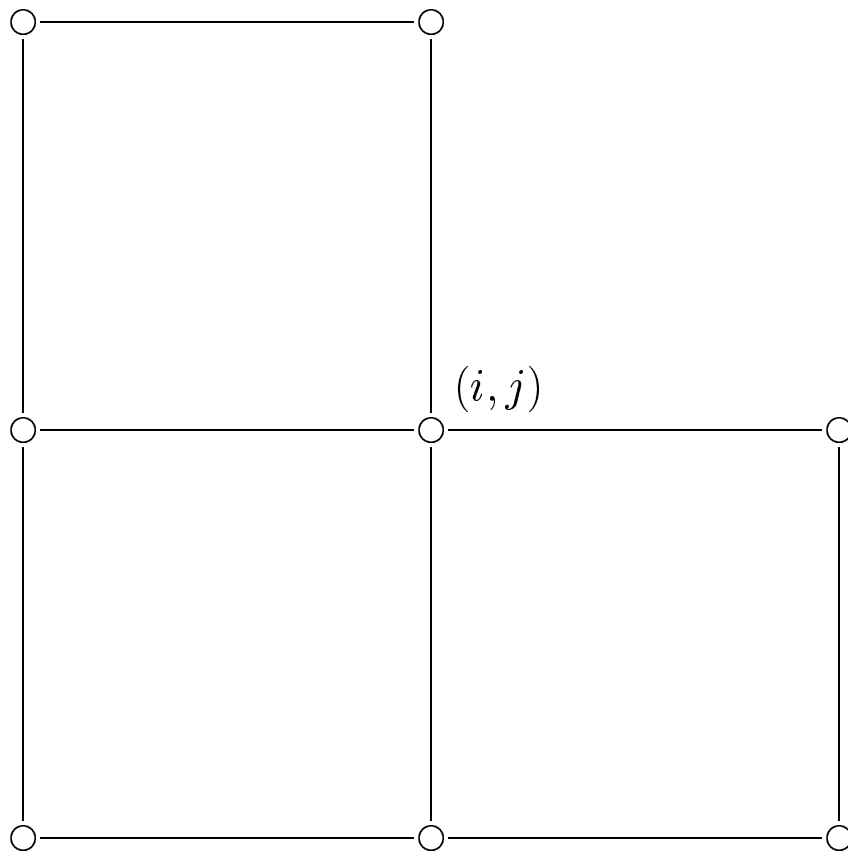


Figure 8: The reduced stencil for a concave corner.

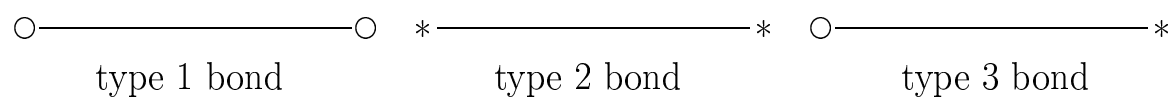


Figure 9: Examples of type 1, 2 and 3 bonds.

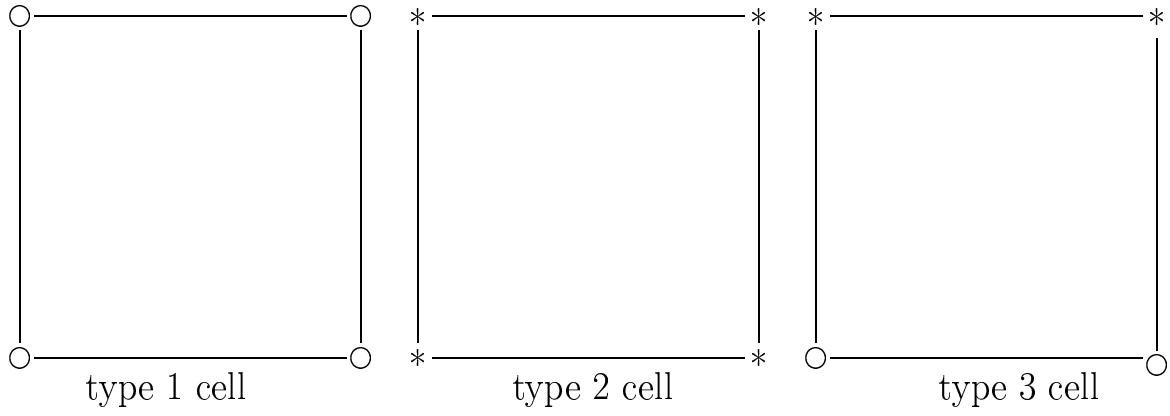


Figure 10: Examples of type 1, 2 and 3 cells.

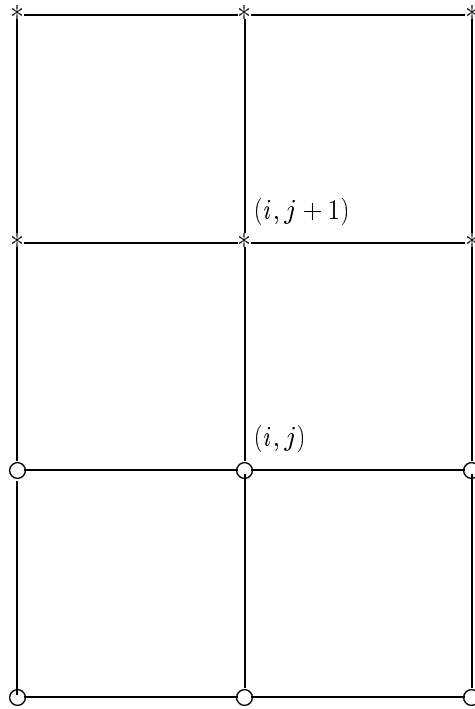


Figure 11: Horizontal interface between two materials.  $(i, j)$  is a type 1 point, and  $(i, j + 1)$  is a type 2 point. The horizontal bonds from  $(i, j)$  are type 1 bonds, and the horizontal bonds from  $(i, j + 1)$  are type 2 bonds. The vertical bond from  $(i, j)$  to  $(i, j + 1)$  is a type 3 bond, and the cells between  $j$  and  $j + 1$  are type 3 cells.



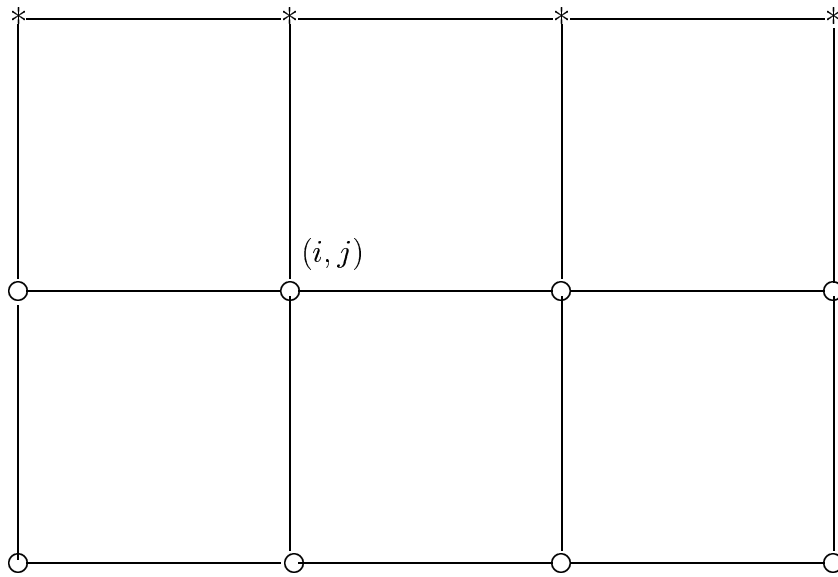


Figure 12: Horizontal edge with intrinsic surface stress. The horizontal bonds from  $(i, j)$  are type 1 bonds, and the horizontal bonds from  $(i, j + 1)$  are type 2 bonds. The vertical bond from  $(i, j)$  to  $(i, j + 1)$  is a type 3 bond, and the cells between  $j$  and  $j + 1$  are type 3 cells.