

## Research



**Cite this article:** Español MI, Golovaty D, Wilber JP. 2018 Discrete-to-continuum modelling of weakly interacting incommensurate two-dimensional lattices. *Proc. R. Soc. A* **474**: 20170612. <http://dx.doi.org/10.1098/rspa.2017.0612>

Received: 5 September 2017

Accepted: 22 December 2017

**Subject Areas:**

materials science, mathematical modelling

**Keywords:**

heterostructure, bilayer graphene, domain wall, moiré pattern, discrete-to-continuum modelling, Ginzburg–Landau energy

**Author for correspondence:**

Dmitry Golovaty  
e-mail: [dmitry@uakron.edu](mailto:dmitry@uakron.edu)

# Discrete-to-continuum modelling of weakly interacting incommensurate two-dimensional lattices

Malena I. Español, Dmitry Golovaty and J. Patrick Wilber

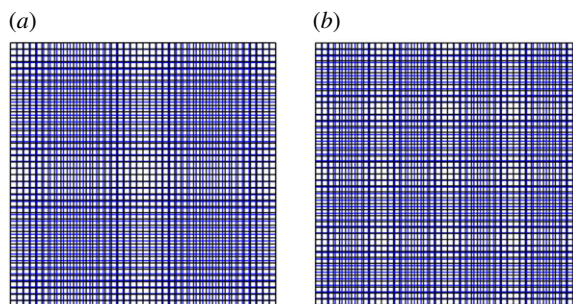
Department of Mathematics, University of Akron, Akron, OH 44325, USA

DG, 0000-0003-0696-2211

In this paper, we derive a continuum variational model for a two-dimensional deformable lattice of atoms interacting with a two-dimensional rigid lattice. The starting point is a discrete atomistic model for the two lattices which are assumed to have slightly different lattice parameters and, possibly, a small relative rotation. This is a prototypical example of a three-dimensional system consisting of a graphene sheet suspended over a substrate. We use a discrete-to-continuum procedure to obtain the continuum model which recovers both qualitatively and quantitatively the behaviour observed in the corresponding discrete model. The continuum model predicts that the deformable lattice develops a network of domain walls characterized by large shearing, stretching and bending deformation that accommodates the misalignment and/or mismatch between the deformable and rigid lattices. Two integer-valued parameters, which can be identified with the components of a Burgers vector, describe the mismatch between the lattices and determine the geometry and the details of the deformation associated with the domain walls.

## 1. Introduction

The mechanical properties of interacting layers of two-dimensional crystals are currently a topic of intense investigation. Bilayer graphene is perhaps the most notable motivation for these studies. Other motivating examples include few layer crystals of hexagonal boron nitride (h-BN), molybdenum disulfide ( $\text{MoS}_2$ ) and tungsten diselenide ( $\text{WSe}_2$ ). More generally, there is an



**Figure 1.** Moiré patterns in two parallel square lattices with slightly different lattice constants  $h_1$  and  $h_2$ . Here,  $h_1/h_2 = 0.95$  (a) and  $h_1/h_2 = 0.91$  (b). Note that the period of the moiré pattern decreases as the ratio of lattice constants decreases. (Online version in colour.)

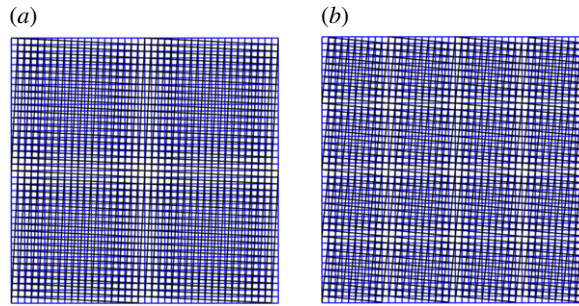
interest in modelling and simulating the mechanical properties of van der Waals heterostructures, a term that describes stacks of possibly different two-dimensional crystals [1,2]. Interest in these heterostructures is currently driven by the idea that it may be possible to engineer advanced materials with novel properties by stacking different types of individual layers in appropriate sequences.

For bilayer graphene and other interacting layers of two-dimensional crystals, the deformation of the bilayer is determined by the strong, bonded interactions between nearest neighbours on a given layer and by the weak, non-bonded interactions between nearby atoms on different layers. The weak interactions, although sufficient to hold the layers together, permit sliding and rotations between the layers. Hence if the layers have different lattice geometries or lattice parameters or if a bilayer is synthesized with local regions in different stacking arrangements, the layers may adjust by shifting or rotating locally.

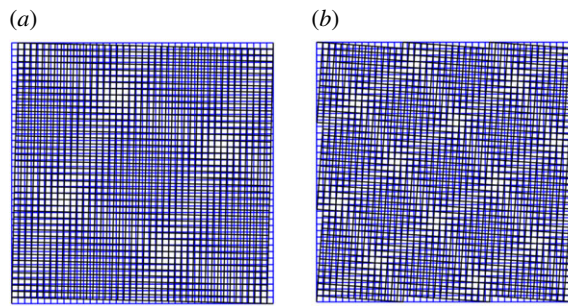
These adjustments can induce strain within each layer that can be relaxed by both in-plane and out-of-plane, atomic-scale displacements of the atoms on the layers. What typically occurs for layers with slightly mismatched lattices is that the atomic-scale displacements create relatively large commensurate regions separated by localized incommensurate regions. In the commensurate regions, the interlayer energy is minimized. In the localized incommensurate regions, or domain walls, strain may be relaxed by out-of-plane displacement. These displacements can generate interesting larger-scale pattern formation that may strongly influence the electrical, thermal and other properties of the bilayer [1,3].

One example of this pattern formation in bilayer graphene is called a relaxed moiré pattern [4,5]. When two lattices with different lattice geometries or the same geometry but different orientations are stacked, a larger periodic pattern, called a moiré pattern, emerges (figures 1–3). In this paper, we work with square lattices. Moiré patterns occur in these lattices because of spatial variations in registry that arise from slightly dissimilar lattice parameters (figure 1) and/or relative rotations (figures 2 and 3).

These moiré patterns are a strictly visual effect. However, if the atoms on one or both of the lattices are then relaxed to accommodate the mismatch between the lattices, additional patterns can occur. In [4], the authors study these relaxed moiré patterns by simulating interacting, identical graphene lattices where one lattice is slightly rotated with respect to the other. In [5], the authors report on similar simulations for a slightly rotated graphene lattice interacting with an h-BN substrate, which also has the structure of a hexagonal lattice with a slightly larger lattice constant than that of graphene. In both papers, simulations in some cases predict a two-dimensional pattern of domain walls, intersecting at so-called hot spots, exhibiting large out-of-plane displacements. The domain walls separate large, flat domains of commensurate regions.



**Figure 2.** Moiré patterns in two identical parallel, and slightly misoriented, square lattices with relative rotation of  $2.86^\circ$  (a) and  $5.71^\circ$  (b). Note that the period of the moiré pattern decreases as the relative rotation increases. (Online version in colour.)



**Figure 3.** Moiré patterns in two slightly misoriented lattices that also have slightly different lattice constants  $h_1$  and  $h_2$ . The relative rotation and the ratio of lattice constants are  $1.36^\circ$  and  $h_1/h_2 = 0.95$  (a) and  $4.08^\circ$  and  $h_1/h_2 = 0.95$  (b). (Online version in colour.)

In this paper, we present discrete-to-continuum modelling of a bilayer of two-dimensional lattices. Our goal is to develop a continuum model that can describe how mismatch and misorientation between the lattices influence the deformation of the bilayer. For simplicity, we assume that one of the lattices is rigid and that both lattices are square. Our discrete-to-continuum procedure yields a continuum energy with terms describing the elastic energy of the deformable lattice and a term for the interaction energy between the deformable and rigid lattices.

For the elastic contributions, our discrete-to-continuum procedure starts with a square lattice in which the atoms are connected by extensional, torsional and dihedral springs that model the resistance of the lattice to stretching and bending. The discrete energies of these springs are upscaled by introducing a small parameter  $\varepsilon$  defined as the ratio of the distance between the lattices to the lateral extent of the deformable lattice. Assuming that the deformed lattice is embedded in a smooth surface, we expand the parameterization of this surface and the spring energies in  $\varepsilon$ . Then, an appropriate truncation of the resulting series yields a continuum elastic energy, which is close to the energy of the classical von Föppl–Kármán shell theory [6]. Our recent work on a similar one-dimensional problem [7] indicates that this choice of truncation provides a reasonable generic approximation of the mesoscopic elastic energy.

For the interaction term, the goal of our discrete-to-continuum procedure is to develop a continuum energy that retains information about the mismatch between the lattices. At the discrete level, the lattices may be mismatched because the rigid and deformable lattices have different lattice parameters and because of a small rotation between the lattices. This mismatch is easily described locally and allows us to define an energy density that contains a continuum expression for the local mismatch.

The continuum energy that we obtain combines the elastic and weak contributions and has a Ginzburg–Landau-type structure. The minimizers of the continuum energy represent equilibrium shapes of the deformable lattice. To find these equilibrium shapes, we derive the Euler–Lagrange equations, which are then solved numerically. We present some basic comparisons between discrete simulations and the predictions of our continuum model. For slightly mismatched layers, our model predicts large commensurate regions separated by domain walls formed by localized out-of-plane ridges. The number of these domain walls is determined by the need to accommodate a certain number of extra rows of atoms on the deformable lattice. Qualitatively, our solutions exhibit a pattern of symmetrically spaced hot spots similar to the predictions of the atomistic simulations in [4].

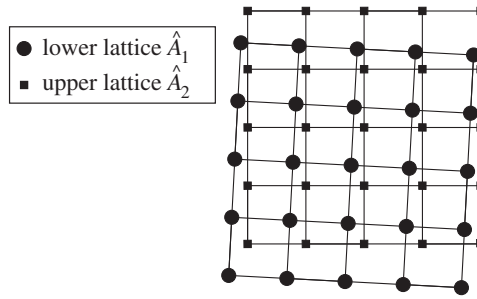
The discrete-to-continuum modelling in this paper generalizes to two dimensions the work in [7], in which a continuum theory for weakly interacting chains of atoms is derived. The atomistic model includes stretching and bending energies for strong covalent bonds between atoms in the same chain and an interaction energy between atoms in adjacent chains. The corresponding continuum energy, derived at mesoscopic scale, is of Ginzburg–Landau type, with an elastic contribution given by the Föppl–von Kármán energy. Numerical simulations demonstrate that the predictions of the continuum model are in close correspondence with predictions from atomistic simulations.

In [8,9], the authors present a multi-scale model that predicts the deformation of bilayers of graphene and bilayers of other two-dimensional materials. In their model, the total energy of the bilayer has an elastic contribution, associated with the stretching and bending of the individual layers and a misfit energy, which describes the van der Waals interactions between the two layers. The misfit energy is defined using the generalized stacking-fault energy for bilayers originally introduced in [10], which the authors developed in an earlier publication [11] from density functional theory calculations. The misfit energy is a function of the separation and registry between layers.

The authors use their model to explain the structure of deformed bilayer graphene in terms of dislocation theory. In [8], the model is applied to determine the structure and energetics of four interlayer dislocations in bilayer graphene, where the different cases are determined by the angle between the Burgers vector and the line of dislocation. In [9], the authors use the model to study deformations that result from a small rotation between the layers. The model predicts two distinct equilibrium structures, which the authors call a breathing mode and a bending mode. The latter, more stable at small rotation angles, is characterized by a twist in the dislocation structure near the dislocation nodes, at which there are also large out-of-plane displacements. The authors note that this newly discovered structure has both different symmetry and period from the classical moiré structure that is often assumed for rotated bilayer graphene.

The continuum model we develop in this paper has essential elements in common with the model presented in [8,9]. Specifically, our model contains terms for the elastic energy of the deformable layer and a term for the van der Waals interactions between the two layers. However, we derive all terms in our continuum energy by upscaling from an atomistic description of the problem. Our upscaling procedure introduces a small parameter that determines the relative size of the various contributions to the continuum energy. Hence, we gain insight into how the balance of these terms produces phenomena like relaxed moiré patterns in interacting bilayers. Furthermore, our modelling sets the stage for additional analysis to rigorously determine the relation between atomistic and continuum descriptions of the problem [12–14].

This paper is organized as follows. In §2, we formulate a discrete energy for a system of two weakly interacting square lattices. In §3, we derive the continuum elastic and interaction energies. The latter keeps track of the mismatch between the lattices. The next section includes numerical results that compare the atomistic model with the continuum model. Furthermore, in this section, we show how parameters in different ranges give rise to qualitatively different deformations. A concluding section summarizes the paper.



**Figure 4.** The lattices  $\hat{A}_1$  and  $\hat{A}_2$ .

## 2. Atomistic model

Suppose that we have a discrete system that consists of two two-dimensional atomic lattices,  $\hat{A}_1$  and  $\hat{A}_2$ , stacked on top of one another. The atoms on the top lattice  $\hat{A}_2$  can move and each of these atoms interacts with its neighbours within  $\hat{A}_2$  via a given strong bond potential.  $\hat{A}_2$  describes a layer of a two-dimensional material that is nearly inextensible and has a finite resistance to bending. In equilibrium, the atoms on  $\hat{A}_2$  form a square lattice with lattice parameter  $h_2$  that occupies a square-shaped, planar domain  $D$  with sides of length  $L$  and lattice vectors parallel to the sides of  $D$ . The atoms on the bottom lattice  $\hat{A}_1$  are fixed at the nodes of another square lattice with lattice constant  $h_1$ . In this work,  $\hat{A}_1$  describes a rigid substrate. All atoms on the lower lattice are assumed to interact with all atoms on the upper lattice via an interatomic van der Waals potential. In what follows we refer to  $\hat{A}_1$  as the rigid lattice and to  $\hat{A}_2$  as the deformable lattice.

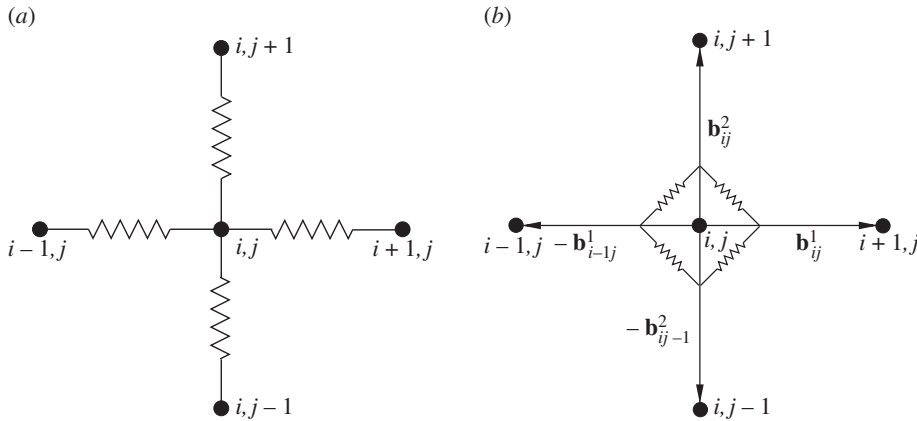
We assume that, in the reference configuration (figure 4), the lattices are flat and embedded in two parallel planes, separated by a distance  $\sigma$ . Here,  $\sigma$  is equal to the equilibrium distance between two atoms interacting via the van der Waals potential. Note that this reference configuration *may not* be in equilibrium. Suppose first that the ratio between  $\sigma$  and the equilibrium bond length  $h_1$  is large enough (for example,  $\sigma/h_1 > 3$  in the case of the Lennard-Jones potential). Then, the van der Waals interactions of an atom on  $\hat{A}_2$  with atoms on  $\hat{A}_1$  can be represented by an interaction with the plane with a uniform atomic density [15]. In equilibrium, the surfaces containing  $\hat{A}_1$  and  $\hat{A}_2$  are essentially two parallel planes. The distance between these planes should be slightly smaller than  $\sigma$ . Indeed, a given atom  $a$  on  $\hat{A}_2$  interacts not only with its closest neighbour  $b$  on  $\hat{A}_1$ , but also with the neighbours of  $b$  on  $\hat{A}_1$ . If the distance between  $a$  and  $b$  is  $\sigma$ , then the forces between  $a$  and all neighbours of  $b$  are attractive.

For smaller values of  $\sigma/h_1$ , the uniform atomic density approximation ignores possible registry effects that are significant in determining the shape of the deformable lattice  $\hat{A}_2$ . In fact, the only situation in which the two flat parallel lattices *would* correspond to an equilibrium configuration is when  $h_1 = h_2$ . In this case, all atoms on  $\hat{A}_2$  would occupy the positions above the centres of unit cells formed by the atoms on  $\hat{A}_1$  and the system would be in *global registry*. Otherwise, the local equilibrium distance depends on the lattice parameters and the relative orientation of the lattices. Hence, even though the assumed reference configuration is not stress-free, the parameter  $\sigma$  is a natural choice for the spacing between  $\hat{A}_1$  and  $\hat{A}_2$  in the reference configuration.

Here, we are concerned with the situation when the lattices  $\hat{A}_1$  and  $\hat{A}_2$  in the reference configuration have slightly different orientations and/or when  $h_1 \neq h_2$ , but  $|h_1 - h_2|/h_1 \ll 1$  (figure 4). Under these assumptions, global registry cannot be attained in a flat undeformed configuration. It follows that, in order to achieve equilibrium, the deformable lattice would have to adjust by some combination of bending and stretching.

Let the current and reference positions of the  $N_2^2$  atoms ( $N_2 := L/h_2$ ) on the deformable lattice be given by the set of vectors  $\mathbf{Q} := \{\mathbf{q}_{ij}\}_{i,j=1}^{N_2} \subset \mathbb{R}^3$  and  $\mathbf{Q}^0 := \{\mathbf{q}_{ij}^0\}_{i,j=1}^{N_2} \subset \mathbb{R}^3$ , respectively. Because the lattice is periodic, we identify  $i = N_2 + 1$  with  $i = 1$  and  $j = N_2 + 1$  with  $j = 1$ . In what follows,





**Figure 5.** The extensional (a) and torsional (b) springs connected to an atom with indices  $i, j$  in  $\hat{\mathcal{A}}_2$ . Here,  $i, j = 1, \dots, N_2$ .

we use a pair of indices separated by a comma to denote atoms on  $\hat{\mathcal{A}}_1$  and  $\hat{\mathcal{A}}_2$ , but, to avoid clutter, we omit the comma when these indices appear in subscripts.

For the rigid lattice, the current and the reference configurations are exactly the same. We denote the positions of atoms on the rigid lattice by  $\mathbf{P} := \{\mathbf{p}_{kl}\}_{k,l=-\infty}^{\infty} \subset \mathbb{R}^3$ . Note that we assume the rigid lattice is infinite in extent in order to appropriately compute the non-local van der Waals energy.

Since the system in the reference configuration consists of two parallel, planar square lattices of atoms, we select an orthonormal basis  $\{\mathbf{e}_n^m\}_{m,n=1}^2$  for each plane so that the basis vectors are parallel to the respective lattice vectors. Then

$$\mathbf{P} = \{h_1(k\mathbf{e}_1^1 + l\mathbf{e}_2^1)\}_{k,l=-\infty}^{\infty} \subset \mathbb{R}^2 \times \{0\} \quad \text{and} \quad \mathbf{Q}^0 = \{h_2(i\mathbf{e}_1^2 + j\mathbf{e}_2^2)\}_{i,j=1}^{N_2} \subset [0, L]^2 \times \{\sigma\}. \quad (2.1)$$

Here, without loss of generality, we assume that, in the reference configuration, there is an atom on the deformable lattice  $\hat{\mathcal{A}}_2$  directly above the atom  $\hat{\mathcal{A}}_1$  that lies at the origin.

For every  $i, j = 1, \dots, N_2$ , we represent the bonds between the atoms  $\mathbf{q}_{ij}$  and  $\mathbf{q}_{i+1,j}$  and the atoms  $\mathbf{q}_{ij}$  and  $\mathbf{q}_{i,j+1}$  by the vectors  $\mathbf{b}_{ij}^1 = \mathbf{q}_{i+1,j} - \mathbf{q}_{ij}$  and  $\mathbf{b}_{ij}^2 = \mathbf{q}_{i,j+1} - \mathbf{q}_{ij}$ , respectively. We assume that the total energy of the system is given by

$$E(\mathbf{Q}) := E_s(\mathbf{Q}) + E_t(\mathbf{Q}) + E_d(\mathbf{Q}) + E_w(\mathbf{Q}). \quad (2.2)$$

Here,  $E_s$  is the energy required to stretch or compress bonds between two adjacent atoms on  $\hat{\mathcal{A}}_2$ , defined by a harmonic potential

$$E_s(\mathbf{Q}) := \sum_{i,j=1}^{N_2} \frac{k_s}{2} \left[ \left( \frac{\|\mathbf{b}_{ij}^1\| - h_2}{h_2} \right)^2 + \left( \frac{\|\mathbf{b}_{ij}^2\| - h_2}{h_2} \right)^2 \right], \quad (2.3)$$

with  $k_s$  being the spring constant. The extensional springs connected to a given atom with the indices  $i, j$  are shown in figure 5a; note that due to the periodicity of the lattice only two of these springs per atom appear in the sum in (2.3).

The bending between the interatomic bonds is penalized by introducing harmonic torsional and dihedral springs between the bonds. The bending energy associated with the torsional

springs is given by

$$E_t(\mathbf{Q}) := \sum_{i,j=1}^{N_2} \frac{k_t}{2} \left[ \left( \theta(\mathbf{b}_{ij}^1, \mathbf{b}_{ij}^2) - \frac{\pi}{2} \right)^2 + \left( \theta(\mathbf{b}_{ij}^2, -\mathbf{b}_{i-1j}^1) - \frac{\pi}{2} \right)^2 + \left( \theta(-\mathbf{b}_{i-1j}^1, -\mathbf{b}_{ij-1}^2) - \frac{\pi}{2} \right)^2 + \left( \theta(-\mathbf{b}_{ij-1}^2, \mathbf{b}_{ij}^1) - \frac{\pi}{2} \right)^2 \right], \quad (2.4)$$

where  $k_t$  is the torsional spring constant and  $\theta(\mathbf{a}, \mathbf{c})$  is the angle between the vectors  $\mathbf{a}$  and  $\mathbf{c}$ . The configuration of the torsional springs associated with a given atom in  $\hat{\mathcal{A}}_2$  is shown in figure 5b. Assuming that admissible in-plane deformations of  $\hat{\mathcal{A}}_2$  are small, in the sequel we consider the expression

$$E_t(\mathbf{Q}) = \sum_{i,j=1}^{N_2} \frac{k_t}{2} \left[ \frac{(\mathbf{b}_{ij}^1 \cdot \mathbf{b}_{ij}^2)^2}{\|\mathbf{b}_{ij}^1\|^2 \|\mathbf{b}_{ij}^2\|^2} + \frac{(\mathbf{b}_{ij}^2 \cdot \mathbf{b}_{i-1j}^1)^2}{\|\mathbf{b}_{ij}^2\|^2 \|\mathbf{b}_{i-1j}^1\|^2} + \frac{(\mathbf{b}_{i-1j}^1 \cdot \mathbf{b}_{ij-1}^2)^2}{\|\mathbf{b}_{i-1j}^1\|^2 \|\mathbf{b}_{ij-1}^2\|^2} + \frac{(\mathbf{b}_{ij-1}^2 \cdot \mathbf{b}_{ij}^1)^2}{\|\mathbf{b}_{ij-1}^2\|^2 \|\mathbf{b}_{ij}^1\|^2} \right] \quad (2.5)$$

for the bending energy, which is equivalent to (2.4) to leading order.

The expressions for the extensional and torsional springs, respectively, show that the sum of the corresponding energy components is minimized when all unit cells of the lattice  $\hat{\mathcal{A}}_2$  are squares with side of length  $h_2$ . Note, however, that the lattice can be folded along the directions parallel to the sides of the domain  $D$  without incurring any energy cost. The appropriate cost can be added by incorporating dihedral springs into the lattice.

A dihedral spring connects three adjacent bonds so that this spring energy is minimized when the third bond lies in the plane formed by the first two bonds (figure 6). A prototypical dihedral spring energy that satisfies this condition is given by the expression

$$e_d(\mathbf{a}, \mathbf{b}, \mathbf{c}) := \frac{k_d}{2} \cos^2 \psi = \frac{k_d}{2} \frac{((\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c})^2}{\|\mathbf{a} \times \mathbf{b}\|^2 \|\mathbf{c}\|^2},$$

where  $k_d$  is the dihedral spring constant and  $\psi$  is the dihedral angle defined as in figure 6. We assume that, for each  $i, j = 1, \dots, N_2$ , the atom  $\mathbf{q}_{ij}$  in the lattice  $\hat{\mathcal{A}}_2$  is connected to all dihedral springs shown in figure 7. Note that the actual number of dihedral springs connected to this and all other atoms is larger due to the periodicity of the lattice. The bending energy associated with the dihedral springs is then given by

$$E_d(\mathbf{Q}) := \sum_{i,j=1}^{N_2} \frac{k_d}{2} \left[ \frac{((\mathbf{b}_{i-1j}^1 \times \mathbf{b}_{ij-1}^2) \cdot \mathbf{b}_{i-1j}^2)^2}{\|\mathbf{b}_{i-1j}^1 \times \mathbf{b}_{ij-1}^2\|^2 \|\mathbf{b}_{i-1j}^2\|^2} + \frac{((\mathbf{b}_{ij}^1 \times \mathbf{b}_{ij-1}^2) \cdot \mathbf{b}_{i-1j-1}^1)^2}{\|\mathbf{b}_{ij}^1 \times \mathbf{b}_{ij-1}^2\|^2 \|\mathbf{b}_{i-1j-1}^1\|^2} + \frac{((\mathbf{b}_{ij}^1 \times \mathbf{b}_{ij}^2) \cdot \mathbf{b}_{i-1j+1}^1)^2}{\|\mathbf{b}_{ij}^1 \times \mathbf{b}_{ij}^2\|^2 \|\mathbf{b}_{i-1j+1}^1\|^2} + \frac{((\mathbf{b}_{ij}^2 \times \mathbf{b}_{i-1j}^1) \cdot \mathbf{b}_{i-1j-1}^2)^2}{\|\mathbf{b}_{ij}^2 \times \mathbf{b}_{i-1j}^1\|^2 \|\mathbf{b}_{i-1j-1}^2\|^2} \right]. \quad (2.6)$$

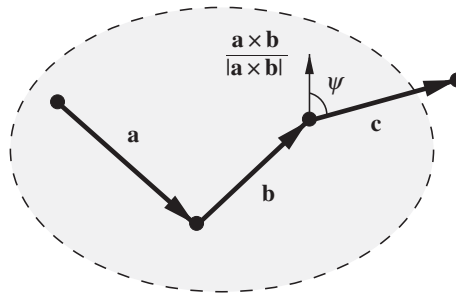
The energy of the weak van der Waals interaction between  $\hat{\mathcal{A}}_1$  and  $\hat{\mathcal{A}}_2$  is given by

$$E_w(\mathbf{Q}) = \omega \sum_{i,j=1}^{N_2} \sum_{m,n=-\infty}^{\infty} g \left( \frac{\|\mathbf{q}_{ij} - \mathbf{p}_{mn}\|}{\sigma} \right), \quad (2.7)$$

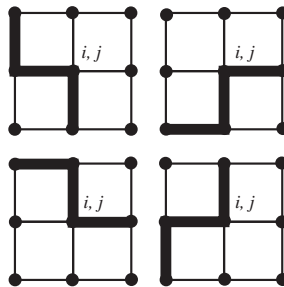
where  $g$  is a given weak pairwise interaction potential. The parameters  $\sigma$  and  $\omega$  define the equilibrium interatomic distance and the strength of the potential energy (2.7), respectively. In what follows, we assume that  $g$  is the classical Lennard-Jones 12–6 potential given by

$$g(r) = r^{-12} - 2r^{-6}. \quad (2.8)$$

Note that the inner sum in (2.7) is taken over the entire rigid lattice to properly account for weak interactions between the lattices.



**Figure 6.** A dihedral spring connecting vectors  $\mathbf{a}$ ,  $\mathbf{b}$  and  $\mathbf{c}$ . The spring energy is minimized when  $\psi = \pi/2$ .



**Figure 7.** The dihedral springs connecting atom  $i, j$  to its neighbours in  $\hat{\mathcal{A}}_2$ . Here,  $i, j = 1, \dots, N_2$ .

### 3. Continuum model

Next, we briefly describe the approach we take to derive the continuum model. We assume that the atoms of the deformable lattice  $\hat{\mathcal{A}}_2$  are embedded in a smooth surface  $\mathcal{A}_2 \subset \mathbb{R}^3$  and describe this surface parametrically in terms of the displacement field. Non-dimensionalizing the discrete problem introduces a small geometric parameter  $\varepsilon = \sigma/L$ , equal to the ratio of the equilibrium van der Waals distance to the length of the side of the domain  $D$ . Evaluating the displacements at atomic positions, substituting these into the expression (2.2) for the discrete energy, expanding the result in terms of  $\varepsilon$ , and converting the summation into integration leads to an expansion in terms of  $\varepsilon$  for the continuum energy, written as a functional of the displacement field.

We identify the leading-order terms in this expansion, up to the order at which contributions from the extensional, torsional and dihedral springs, as well the van der Waals interactions, are included. The resulting continuum energy is of Ginzburg–Landau type and contains terms of different powers in  $\varepsilon$ . The minimizers of the continuum energy typically exhibit bulk regions of registry, separated by thin walls where the gradient of the displacement field is large. Thus, within the walls, the contributions from higher-order terms generally cannot be neglected. We choose to cut off the expansion that leads to the continuum energy at the order when all components of the displacement contribute to the energy density inside the walls at leading order. Finally, in the next section, we present the results of simulations confirming that the behaviour of minimizers of the continuum energy match that of minimizers of the discrete energy.

Both the discrete and continuum non-dimensional models contain the small parameter  $\varepsilon$  and, in particular, the continuum model cannot be thought of as a limit of the discrete model as  $\varepsilon \rightarrow 0$ . Instead, we conjecture that both models converge to the same asymptotic limit as  $\varepsilon \rightarrow 0$  in the appropriate sense. The limit has to be understood within the framework of  $\Gamma$ -convergence [16] so that both energies are  $\Gamma$ -equivalent [17]. Hence, the number of terms retained in the expansion of the discrete problem in order to obtain the continuum problem should be sufficient to reproduce



the behaviour of the discrete system for a small  $\varepsilon$ . The proof of  $\Gamma$ -equivalence is a subject of a future work.

As noted above, a first step in formally deriving a continuum model is to assume that the deformed lattice  $\hat{\mathcal{A}}_2$  is embedded in a sufficiently smooth surface  $\mathcal{A}_2$ . We denote this surface in the reference configuration by  $\mathcal{A}_2^0$  and set

$$\mathcal{A}_2^0 = \{(x_1, x_2, \sigma) : x_1, x_2 \in [0, L]\}. \quad (3.1)$$

We let  $(u_1(x_1, x_2), u_2(x_1, x_2), v(x_1, x_2))$  be the displacement of the point  $(x_1, x_2, \sigma)$  on  $\mathcal{A}_2^0$ . Hence, the deformed surface  $\mathcal{A}_2$  is given by

$$\{(x_1 + u_1(x_1, x_2), x_2 + u_2(x_1, x_2), \sigma + v(x_1, x_2)) : x_1, x_2 \in [0, L]\}. \quad (3.2)$$

In particular, an atom at the point  $(x_1^{ij}, x_2^{ij}, \sigma)$  on  $\mathcal{A}_2^0$  is displaced to the point  $(x_1^{ij} + u_1(x_1^{ij}, x_2^{ij}), x_2^{ij} + u_2(x_1^{ij}, x_2^{ij}), \sigma + v(x_1^{ij}, x_2^{ij}))$ .

We assume  $\sigma \ll L$ , i.e. that the spacing between the planes is much less than the lateral extent of the system. To exploit this, we set  $\mathbf{x} = (x_1, x_2)$ ,  $\mathbf{u} = (u_1, u_2)$  and rescale as follows:

$$\boldsymbol{\chi} = \frac{\mathbf{x}}{L}, \quad \boldsymbol{\xi} = \frac{\mathbf{u}}{\varepsilon L}, \quad \eta = \frac{v}{\varepsilon L}, \quad \mathcal{E} = \frac{\varepsilon E}{\omega}. \quad (3.3)$$

This gives the non-dimensional parameters

$$\varepsilon = \frac{\sigma}{L}, \quad \delta_1 = \frac{h_1}{\sigma}, \quad \delta_2 = \frac{h_2}{\sigma}, \quad \gamma_s = \frac{k_s}{\omega \delta_2^2}, \quad \gamma_t = \frac{8k_t}{\omega \delta_2^2}, \quad \gamma_d = \frac{2k_d}{\omega}. \quad (3.4)$$

The scalings for the displacements are appropriate for small deformations considered here and eventually lead to expressions for the strains similar to those for Föppl–von Kármán theory. The constants in the definitions of  $\gamma_t$  and  $\gamma_d$  appear to simplify the expressions for the continuum elastic energy.

We obtain with a slight abuse of notation that

$$\begin{aligned} \mathcal{A}_2 &= \{(\chi_1 + \varepsilon \xi_1(\boldsymbol{\chi}), \chi_2 + \varepsilon \xi_2(\boldsymbol{\chi}), \varepsilon + \varepsilon \eta(\boldsymbol{\chi})) : \boldsymbol{\chi} \in [0, 1]^2\} \\ &= \{(\boldsymbol{\chi} + \varepsilon \boldsymbol{\xi}(\boldsymbol{\chi}), \varepsilon + \varepsilon \eta(\boldsymbol{\chi})) : \boldsymbol{\chi} \in [0, 1]^2\}. \end{aligned} \quad (3.5)$$

We assume that  $\delta_i = \mathcal{O}(1)$ ,  $i = 1, 2$ , i.e. the lattice parameters for  $\hat{\mathcal{A}}_1$  and  $\hat{\mathcal{A}}_2$  are comparable to the distance between  $\hat{\mathcal{A}}_1$  and  $\hat{\mathcal{A}}_2$  (and hence both are much smaller than the lateral extent of the system). Furthermore, in order to observe the registry effects on a macroscale, we assume that

$$\frac{\delta_2 - \delta_1}{\varepsilon \delta_2} := \alpha = \mathcal{O}(1), \quad (3.6)$$

so that the mismatch between the equilibrium lattice parameters of  $\hat{\mathcal{A}}_1$  and  $\hat{\mathcal{A}}_2$  is small.

In the rescaled coordinates, the atoms on  $\mathcal{A}_2^0$  are located at the points  $\mathbf{q}_{ij}^0 = (\boldsymbol{\chi}_{ij}, \varepsilon)$ , where  $\boldsymbol{\chi}_{ij} = \varepsilon \delta_2 (i \mathbf{e}_1^2 + j \mathbf{e}_2^2)$  for  $i, j = 1, \dots, N_2$  are obtained by dividing  $\mathbf{q}_{ij}^0$  by  $L$  in (2.1). The  $i, j$ th atom is then displaced to the point

$$\mathbf{q}_{ij} = (\boldsymbol{\chi}_{ij} + \varepsilon \boldsymbol{\xi}(\boldsymbol{\chi}_{ij}), \varepsilon + \varepsilon \eta(\boldsymbol{\chi}_{ij})), \quad (3.7)$$

for every  $i, j = 1, \dots, N_2$ . Note that here and in what follows we continue to use the notation  $\mathbf{q}_{ij}$ ,  $\mathbf{q}_{ij}^0$  and  $\mathbf{b}_{ij}^k$ , but now to denote the corresponding non-dimensional quantities.

## (a) Elastic energy contribution

Our treatment of the discrete-to-continuum limit for the elastic energy is consistent with a number of recent studies [18–22]. The principal idea is to exploit the smallness of the parameter  $\varepsilon$ . By using the Taylor expansions of  $\boldsymbol{\xi}(\boldsymbol{\chi}_{ij})$  and  $\eta(\boldsymbol{\chi}_{ij})$  in  $\varepsilon$ , each bond  $\mathbf{b}_{ij}^k$  can be written as an asymptotic series in  $\varepsilon$ . Substituting the appropriate expansions into the expressions (2.3), (2.5) and (2.6) for the extensional, torsional and dihedral energy components, respectively, and taking into account the energy rescaling in (3.3), we can redefine both energies in terms of values of  $\boldsymbol{\xi}$  and  $\eta$  at  $\boldsymbol{\chi}_{ij}$ .

where  $i, j = 1, \dots, N_2$ . We have that

$$\begin{aligned} \mathcal{E}_s[\xi, \eta] = \sum_{i,j=1}^{N_2} \frac{k_s}{2\omega} [(\xi_{1,1}^2 + \xi_{2,2}^2)\varepsilon^3 + (\delta_2(\xi_{1,1}\xi_{1,11} + \xi_{2,2}\xi_{2,22}) \\ + \eta_{,1}^2\xi_{1,1} + \eta_{,2}^2\xi_{2,2} + \xi_{1,1}\xi_{2,1}^2 + \xi_{2,2}\xi_{1,2}^2)\varepsilon^4] + \mathcal{O}(\varepsilon^5), \end{aligned} \quad (3.8)$$

while

$$\mathcal{E}_t[\xi, \eta] = \sum_{i,j=1}^{N_2} \frac{k_t}{\omega} [2(\xi_{1,2} + \xi_{2,1})^2\varepsilon^3 + 4(\xi_{1,2} + \xi_{2,1})(-\nabla\xi_1 \cdot \nabla\xi_2 + \eta_{,1}\eta_{,2})\varepsilon^4] + \mathcal{O}(\varepsilon^5) \quad (3.9)$$

and

$$\mathcal{E}_d[\xi, \eta] = \sum_{i,j=1}^{N_2} \frac{k_d\delta_z^2}{\omega} [\eta_{,11}^2 + 2\eta_{,12}^2 + \eta_{,22}^2]\varepsilon^5 + \mathcal{O}(\varepsilon^6). \quad (3.10)$$

The details of derivations that led to these expansions are given in [23].

As in the discussion above, we would like to truncate these energy expansions in such a way that the limiting behaviour of the minimizers of the truncated energy is in some way close to the behaviour of minimizers of the original discrete model. Here, we impose the following three criteria on the truncated model: (i) it should be well posed mathematically; (ii) it should preserve all relevant interactions between atoms; and (iii) it should respect the standard invariance assumptions of continuum mechanics.

The first criterion limits the choice of where to terminate the expansions. For example, there could be sign constraints placed on the highest derivative terms to guarantee that the continuum variational problem has a minimum. However, for some truncations of the energy expansion, these constraints might not be satisfied and the variational problem is not solvable. Adding the additional, higher derivatives terms would typically yield a model that can be solved. The downside of this, however, is that the model quickly becomes extremely complicated.

Because we expect the minimizers of the discrete energy (2.2) to develop domain walls of characteristic width  $\varepsilon$ , we should also expect some derivatives of the minimizers to appear as powers of  $\varepsilon^{-1}$  inside the walls. Accordingly, all terms in the expansions (3.8)–(3.10) may then contribute roughly the same amount to the overall energy, making the asymptotic procedure that led to (3.8)–(3.10) invalid. Note that, as an alternative to formulating a purely continuum theory, here one might opt to use a quasi-continuum method, in which the singular regions are resolved using the original discrete formulation [19].

On the other hand, in the regions between the walls, all minimizers should have bounded derivatives and the terms with higher powers of  $\varepsilon$  in (3.8)–(3.10) should simply provide small corrections to the lower-order contributions. The situation is not unlike that arising in continuum modelling of crystalline solids, where the structural defects—such as dislocations—are described only in terms of their influence on the global strain field, without properly resolving the defect core.

Motivated by these ideas, we make the following choices when truncating  $\mathcal{E}_s$ ,  $\mathcal{E}_t$  and  $\mathcal{E}_d$ :

$$\mathcal{E}_s[\xi, \eta] \sim \sum_{i,j=1}^{N_2} \frac{k_s\varepsilon^3}{2\omega} \left[ \left( \xi_{1,1} + \frac{\varepsilon\eta_{,1}^2}{2} \right)^2 + \left( \xi_{2,2} + \frac{\varepsilon\eta_{,2}^2}{2} \right)^2 \right], \quad (3.11)$$

$$\mathcal{E}_t[\xi, \eta] \sim \sum_{i,j=1}^{N_2} \frac{8k_t\varepsilon^3}{\omega} \left[ \frac{\xi_{1,2} + \xi_{2,1}}{2} + \frac{\varepsilon}{2}\eta_{,1}\eta_{,2} \right]^2 \quad (3.12)$$

and

$$\mathcal{E}_d[\xi, \eta] \sim \sum_{i,j=1}^{N_2} \frac{k_d\delta_z^2\varepsilon^5}{\omega} [\eta_{,11}^2 + 2\eta_{,12}^2 + \eta_{,22}^2]. \quad (3.13)$$

Note that here we neglected some third-order terms in  $\varepsilon$ , in particular the terms that contain second-order derivatives in  $\xi$  or are cubic in derivatives of  $\xi$ . Further, we incorporated some quartic terms in the derivative of  $\eta$  that allow us to complete squares in (3.11) and (3.12). We conjecture that incorporating/deleting these higher-order terms from the truncated energy still gives minimizers with the structure close to that of the minimizers of the discrete energy as  $\varepsilon \rightarrow 0$ .

We now recall that  $\mathcal{A}_2^0$  has a unit area in non-dimensional coordinates and that the spacing between the atoms is equal to  $\varepsilon\delta_2 \ll 1$ . Hence, the number of atoms on  $\mathcal{A}_2^0$  is  $\sim 1/\varepsilon^2$  and therefore

$$\mathcal{E}_s[\xi, \eta] \sim \frac{\gamma_s \varepsilon}{2} \int_{[0,1]^2} \left[ \left( \xi_{1,1} + \frac{\varepsilon \eta_{1,1}^2}{2} \right)^2 + \left( \xi_{2,2} + \frac{\varepsilon \eta_{2,2}^2}{2} \right)^2 \right] d\chi =: \mathcal{F}_s^\varepsilon[\xi, \eta],$$

while

$$\mathcal{E}_t[\xi, \eta] \sim \gamma_t \varepsilon \int_{[0,1]^2} \left[ \frac{\xi_{1,2} + \xi_{2,1}}{2} + \frac{\varepsilon}{2} \eta_{1,1} \eta_{2,2} \right]^2 d\chi =: \mathcal{F}_t^\varepsilon[\xi, \eta]$$

and

$$\mathcal{E}_d[\xi, \eta] \sim \frac{\gamma_d \varepsilon^3}{2} \int_{[0,1]^2} [\eta_{1,1}^2 + 2\eta_{1,2}^2 + \eta_{2,2}^2] d\chi =: \mathcal{F}_d^\varepsilon[\xi, \eta]. \quad (3.14)$$

## (b) Van der Waals energy contribution

We now derive the continuum version of (2.7), which is the contribution to the energy from the van der Waals interactions. We shall see that the continuum version has the form

$$\mathcal{F}_w^\varepsilon[\xi, \eta] = \frac{1}{\varepsilon} \int_{[0,1]^2} G(\chi, \xi, \eta) d\chi. \quad (3.15)$$

We note that this expression is the generalized stacking-fault energy proposed by Vitek [10], which has been extensively used in the studies of dislocations and grain boundaries (see, for example, [11] and the references therein). The function  $G$  gives a continuum description of the lattice mismatch that arises from incommensurability.

We shall first focus in the inner double sum on the right-hand side of (2.7) and try to estimate the interaction of a given atom on the deformable lattice with all the atoms on the rigid lattice. We accomplish this by developing an expression for the local mismatch between the two lattices as a function of  $\chi$ ,  $\xi$  and  $\eta$ .

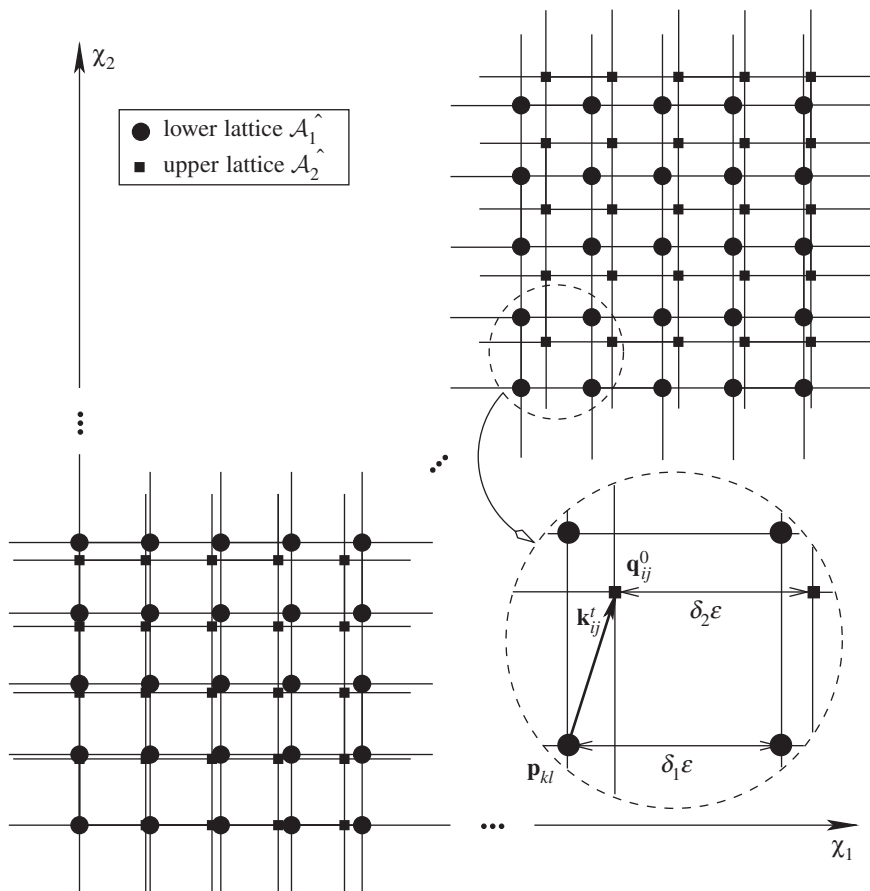
Our starting point is to pick an atom  $i, j$  on  $\hat{\mathcal{A}}_2$ . A discrete description of the total interaction energy between this atom and the atoms on the rigid lattice  $\hat{\mathcal{A}}_1$  is given by

$$\sum_{m,n=-\infty}^{\infty} g\left(\frac{d_{ij}^{mn}}{\varepsilon}\right), \quad (3.16)$$

where  $g$  is defined in (2.8) and  $d_{ij}^{mn}$  is the distance between the fixed atom  $i, j$  on  $\hat{\mathcal{A}}_2$  and the atom  $m, n$  on  $\hat{\mathcal{A}}_1$ . Note that here we could use a finite sum instead due to the fast decay of the interaction potential  $g$  with distance.

To write down an expression for  $d_{ij}^{mn}$ , we let  $\mathbf{k}_{ij}$  denote the local horizontal mismatch between the atomic lattices  $\hat{\mathcal{A}}_1$  and  $\hat{\mathcal{A}}_2$  in the *reference* configuration, as measured at the atom  $i, j$  on  $\hat{\mathcal{A}}_2$ . To determine  $\mathbf{k}_{ij}$ , we project the point  $\mathbf{q}_{ij}^0$  onto the plane of the rigid lattice  $\hat{\mathcal{A}}_1$ . The projection falls inside one of the unit cells of  $\hat{\mathcal{A}}_1$ . Let  $k, l$  be the indices of the lower left atom of this unit cell. We define  $\mathbf{k}_{ij}$  to be a vector connecting the atom  $k, l$  on  $\hat{\mathcal{A}}_1$  to the projection of  $\mathbf{q}_{ij}^0$  onto the plane of  $\hat{\mathcal{A}}_1$  (figures 8 and 9).

To compute the local horizontal mismatch between the lattices in the *current* configuration, we recall that  $\varepsilon \xi(\varepsilon\delta_2 i, \varepsilon\delta_2 j)$  is the projection of the displacement vector for the atom  $i, j$  onto the plane



**Figure 8.** The reference configuration of the system of two square lattices  $\hat{\mathcal{A}}_1$  and  $\hat{\mathcal{A}}_2$  in non-dimensional coordinates. The rigid lattice occupies an entire plane, while the deformable lattice is defined over the domain  $[0, 1]^2 \subset \mathbb{R}^2$ . Only two patches of the lattice structure are shown: near and away from the origin. The lattice parameters  $\delta_1$  of  $\hat{\mathcal{A}}_1$  and  $\delta_2$  of  $\hat{\mathcal{A}}_2$  are slightly different.

of  $\hat{\mathcal{A}}_2$  in the reference configuration. It follows that the local horizontal mismatch in the current configuration is

$$\mathbf{k}_{ij} + \varepsilon \xi(\varepsilon \delta_2 i, \varepsilon \delta_2 j). \quad (3.17)$$

It is now clear that

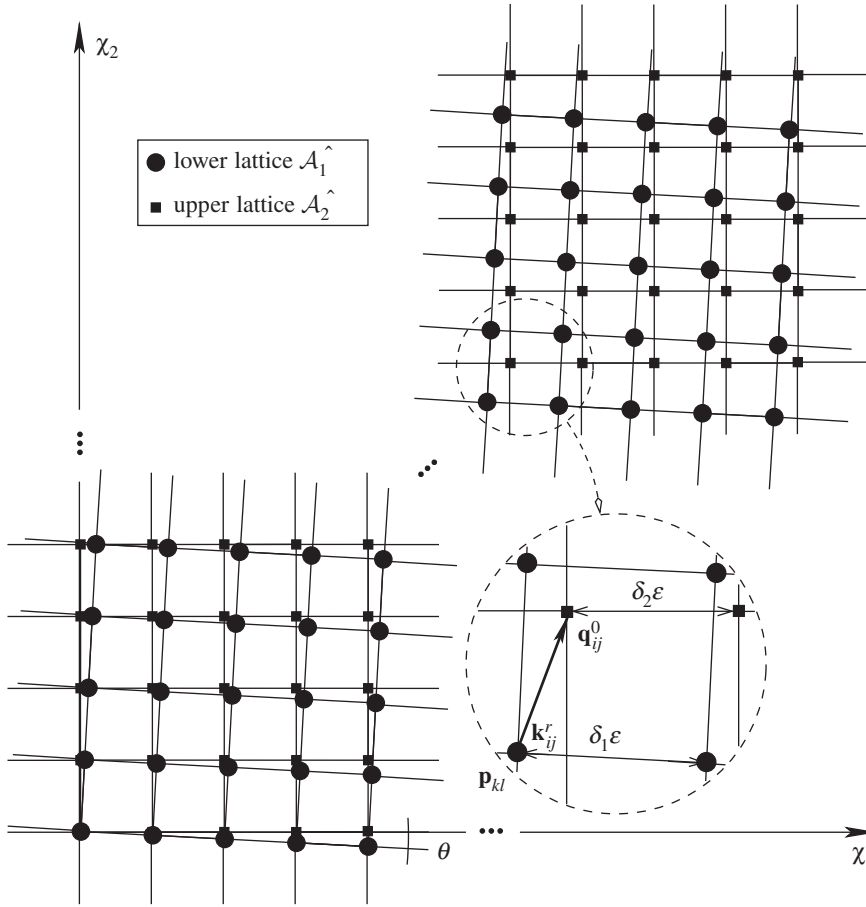
$$d_{ij}^{mn} = (\|\varepsilon \delta_1(k-m)\mathbf{e}_1^1 + \varepsilon \delta_1(l-n)\mathbf{e}_2^1 + \mathbf{k}_{ij} + \varepsilon \xi(\varepsilon \delta_2 i, \varepsilon \delta_2 j)\|^2 + (\varepsilon + \varepsilon \eta(\varepsilon \delta_2 i, \varepsilon \delta_2 j))^2)^{1/2}, \quad (3.18)$$

where  $\varepsilon \delta_1(k-m)\mathbf{e}_1^1 + \varepsilon \delta_1(l-n)\mathbf{e}_2^1$  is the position of the atom  $k, l$  on  $\hat{\mathcal{A}}_1$  with respect to the atom  $m, n$  on the same lattice. The expression  $\varepsilon + \varepsilon \eta(\varepsilon \delta_2 i, \varepsilon \delta_2 j)$  gives the vertical distance between the lattices at the atom  $i, j$  on  $\hat{\mathcal{A}}_2$ .

Recall that we postulated in (3.6) that the relative mismatch between the lattice parameters  $\alpha \varepsilon$  is small. Assuming, in addition, that the angle  $\theta$  of misorientation between two lattices is small, i.e.

$$\Theta := \frac{\theta}{\varepsilon} = O(1), \quad (3.19)$$

we can linearize  $\mathbf{k}_{ij}$  in  $\varepsilon$  so that the relative contributions to  $\mathbf{k}_{ij}$  from mismatch and misorientation can be computed separately and then added together. Consequently, we consider two possible choices for the reference configuration.



**Figure 9.** The reference configurations of the system of two square lattices  $\hat{\mathcal{A}}_1$  and  $\hat{\mathcal{A}}_2$  in non-dimensional coordinates. The rigid lattice occupies an entire plane, while the deformable lattice is defined over the domain  $[0, 1]^2 \subset \mathbb{R}^2$ . Only two patches of the lattice structure are shown: near and away from the origin. The lattice orientations of  $\hat{\mathcal{A}}_1$  and  $\hat{\mathcal{A}}_2$  differ by a small angle  $\theta$ .

*Case I.*  $\hat{\mathcal{A}}_1$  and  $\hat{\mathcal{A}}_2$  have the same orientation, but different lattice parameters. The corresponding reference configuration is shown in figure 8. Because of our assumption that an atom on  $\hat{\mathcal{A}}_2$  at the origin lies directly above an atom on  $\hat{\mathcal{A}}_1$ , we have that

$$\begin{aligned} \mathbf{k}_{ij}^t &= (\text{mod}(i\varepsilon\delta_2, \varepsilon\delta_1), \text{mod}(j\varepsilon\delta_2, \varepsilon\delta_1)) \\ &= (\delta_2 - \delta_1)(i\varepsilon, j\varepsilon) - \varepsilon\delta_1(i_1, j_1) = \varepsilon\alpha(i\varepsilon\delta_2, j\varepsilon\delta_2) - (i_1\varepsilon\delta_1, j_1\varepsilon\delta_1), \end{aligned} \quad (3.20)$$

where  $\alpha$  is as defined in (3.6) and  $i_1, j_1 \in \mathbb{N}$ . Because

$$(i\varepsilon\delta_2, j\varepsilon\delta_2) = \chi_{ij}, \quad (3.21)$$

the continuum approximation of  $\mathbf{k}_{ij}^t$  is

$$\mathbf{k}_{ij}^t = \varepsilon\alpha\chi_{ij} - (i_1\varepsilon\delta_1, j_1\varepsilon\delta_1). \quad (3.22)$$

*Case II.*  $\hat{\mathcal{A}}_1$  and  $\hat{\mathcal{A}}_2$  have different orientations, but the same lattice parameter. The corresponding reference configuration is shown in figure 9. From the figure and since  $\delta_1 = \delta_2$ ,

$$\begin{aligned} \mathbf{k}_{ij}^r &= \varepsilon\delta_1(i\mathbf{e}_1^2 + j\mathbf{e}_2^2) - \varepsilon\delta_1(k\mathbf{e}_1^1 + l\mathbf{e}_2^1) \\ &= \varepsilon\delta_1(i(\mathbf{e}_1^2 - \mathbf{e}_1^1) + j(\mathbf{e}_2^2 - \mathbf{e}_2^1)) + \varepsilon\delta_1(i_2\mathbf{e}_1^1 + j_2\mathbf{e}_2^1), \end{aligned} \quad (3.23)$$

where  $i_2 = i - k$  and  $j_2 = j - l$ . The lattice  $\hat{\mathcal{A}}_1$  is rotated with respect to  $\hat{\mathcal{A}}_2$  by the angle  $\theta$  with the corresponding rotation matrix

$$R(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} = \begin{pmatrix} \cos \varepsilon \Theta & -\sin \varepsilon \Theta \\ \sin \varepsilon \Theta & \cos \varepsilon \Theta \end{pmatrix} \sim \begin{pmatrix} 1 & -\varepsilon \Theta \\ \varepsilon \Theta & 1 \end{pmatrix}$$

with respect to the basis  $\{\mathbf{e}_1^2, \mathbf{e}_2^2\}$ , where we took into account (3.19). It follows that

$$\mathbf{e}_1^2 - \mathbf{e}_1^1 = \mathbf{e}_1^2 - R(\theta) \mathbf{e}_1^2 \sim -\varepsilon \Theta \mathbf{e}_2^2$$

and

$$\mathbf{e}_2^2 - \mathbf{e}_2^1 = \mathbf{e}_2^2 - R(\theta) \mathbf{e}_2^2 \sim \varepsilon \Theta \mathbf{e}_1^2.$$

Inserting these expressions into (3.23) and using (3.21), we find that the continuum approximation for  $\mathbf{k}_{ij}^r$  is

$$\mathbf{k}_{ij}^r \sim \varepsilon \Theta \chi_{ij}^\perp + \varepsilon \delta_1 (i_2 \mathbf{e}_1^1 + j_2 \mathbf{e}_2^1), \quad (3.24)$$

where  $\chi^\perp = (\chi_2, -\chi_1)$ .

We conclude that a continuum approximation of  $\mathbf{k}_{ij}$  is

$$\mathbf{k}_{ij} \sim \mathbf{k}_{ij}^t + \mathbf{k}_{ij}^r = \varepsilon \alpha \chi_{ij} + \varepsilon \Theta \chi_{ij}^\perp + (\hat{i} \varepsilon \delta_1, \hat{j} \varepsilon \delta_1), \quad (3.25)$$

where  $\hat{i} = i_2 - i_1$  and  $\hat{j} = j_2 - j_1$ .

Substituting the expression for  $\mathbf{k}_{ij}$  into (3.18) we obtain

$$\begin{aligned} \frac{d_{ij}^{mn}}{\varepsilon} &\sim (\|\delta_1((k-m+\hat{i})\mathbf{e}_1^1 + (l-n+\hat{j})\mathbf{e}_2^1) + \alpha \chi_{ij} + \Theta \chi_{ij}^\perp + \xi(\chi_{ij})\|^2 + (1 + \eta(\chi_{ij}))^2)^{1/2} \\ &\sim (\|\delta_2((k-m+\hat{i})\mathbf{e}_1^2 + (l-n+\hat{j})\mathbf{e}_2^2) + \alpha \chi_{ij} + \Theta \chi_{ij}^\perp + \xi(\chi_{ij})\|^2 + (1 + \eta(\chi_{ij}))^2)^{1/2}, \end{aligned}$$

for finite  $m, n \in \mathbb{Z}$  because the basis of  $\hat{\mathcal{A}}_1$  is a small perturbation of the basis of  $\hat{\mathcal{A}}_2$  due to smallness of  $\theta$ . Returning to (3.16), we see that the function  $G$  that gives a continuum description of the van der Waals energy arising from the local lattice mismatch is defined by

$$G(\chi, \xi(\chi), \eta(\chi)) := \mathcal{G}(\alpha \chi + \Theta \chi^\perp + \xi(\chi), \eta(\chi)), \quad (3.26)$$

where

$$\mathcal{G}(\mathbf{p}, t) := \sum_{m,n=-\infty}^{\infty} g\left(\sqrt{\|\delta_2 m \mathbf{e}_1^2 + \delta_2 n \mathbf{e}_2^2 + \mathbf{p}\|^2 + (1+t)^2}\right), \quad (3.27)$$

for every  $\mathbf{p} \in \mathbb{R}^2$  and  $t > -1$ . With a slight abuse of notation, here we changed the indices  $m \rightarrow k-m+\hat{i}$  and  $n \rightarrow k-n+\hat{j}$ , respectively. Note that the infinite sum in (3.27) converges due to the rapid decay of  $g$ .

Finally, the non-dimensional version of (2.7) takes the form

$$\begin{aligned} \mathcal{E}_w(\mathbf{Q}) &= \varepsilon \sum_{i,j=1}^{N_2} \sum_{m,n=-\infty}^{\infty} g(\|\mathbf{q}_{ij} - \mathbf{p}_{mn}\|) \sim \frac{1}{\varepsilon} \sum_{i,j=1}^{N_2} G(\chi, \xi, \eta) \varepsilon^2 \\ &\sim \frac{1}{\varepsilon} \int_{[0,1]^2} G(\chi, \xi, \eta) d\chi =: \mathcal{F}_w^\varepsilon[\xi, \eta], \end{aligned} \quad (3.28)$$

thus establishing (3.15).



### (c) Continuum energy

Putting together all the contributions, the system is described by the following continuum energy functional:

$$\begin{aligned} \mathcal{F}^\varepsilon[\xi, \eta] := & \frac{\varepsilon}{2} \int_{[0,1]^2} f \left( D(\nabla \xi) + \frac{\varepsilon}{2} \nabla \eta \otimes \nabla \eta \right) d\mathbf{x} \\ & + \frac{\gamma_d \varepsilon^3}{2} \int_{[0,1]^2} |\nabla \nabla \eta|^2 d\mathbf{x} + \frac{1}{\varepsilon} \int_{[0,1]^2} G(\mathbf{x}, \xi, \eta) d\mathbf{x}. \end{aligned} \quad (3.29)$$

Here,  $D(A) = (A + A^T)/2$  is the symmetric part of  $A$  for any  $A \in M^{2 \times 2}$  and

$$f(M) = \gamma_s(m_{11}^2 + m_{22}^2) + 2\gamma_t m_{12}^2,$$

for any  $M = \begin{pmatrix} m_{11} & m_{12} \\ m_{12} & m_{22} \end{pmatrix} \in M_{\text{sym}}^{2 \times 2}$ .

Note that the elastic contribution to the energy (3.29) is like that of the Föppl–von Kármán theory. The corresponding variational problem is of Ginzburg–Landau type, where the minimizers are determined via a competition between the elastic energy and the potential energy, which has multiple wells associated with the low-energy commensurate regions. The system is forced to reside in these wells, with the sharp transition between the wells being smoothed out due to the penalty imposed by the elastic energy. Consequently, we expect the minimizers of (3.29) to develop walls of characteristic width  $\varepsilon$ .

Now let  $\mathbf{b}_1(\nabla \xi, \nabla \eta)$  and  $\mathbf{b}_2(\nabla \xi, \nabla \eta)$  denote the columns of the matrix  $D(\nabla \xi) + \frac{\varepsilon}{2} \nabla \eta \otimes \nabla \eta$ . The Euler–Lagrange equations for the functional  $\mathcal{F}^\varepsilon$  are

$$\left. \begin{aligned} -\varepsilon \operatorname{div}[K_1 \mathbf{b}_1(\nabla \xi, \nabla \eta)] + \frac{1}{\varepsilon} G_{\xi_1}(\mathbf{x}, \xi, \eta) &= 0, \\ -\varepsilon \operatorname{div}[K_2 \mathbf{b}_2(\nabla \xi, \nabla \eta)] + \frac{1}{\varepsilon} G_{\xi_2}(\mathbf{x}, \xi, \eta) &= 0 \end{aligned} \right\} \quad (3.30)$$

and

$$\varepsilon^3 \gamma_d \Delta^2 \eta - \varepsilon^2 \operatorname{div}(K_1 \mathbf{b}_1(\nabla \xi, \nabla \eta) \cdot \nabla \eta, K_2 \mathbf{b}_2(\nabla \xi, \nabla \eta) \cdot \nabla \eta) + \frac{1}{\varepsilon} G_\eta(\mathbf{x}, \xi, \eta) = 0.$$

Here, the first two equations describe the force balance in the plane of the deformable lattice, while the last equation is the vertical force balance. The anisotropy matrices  $K_1$  and  $K_2$  are given by

$$K_1 = \begin{pmatrix} \gamma_s & 0 \\ 0 & \gamma_t \end{pmatrix} \quad \text{and} \quad K_2 = \begin{pmatrix} \gamma_t & 0 \\ 0 & \gamma_s \end{pmatrix}. \quad (3.31)$$

## 4. Numerical results

In this section, we numerically solve the system of Euler–Lagrange equations (3.30) subject to periodic boundary conditions to explore the behaviour of minimizers of the continuum model.

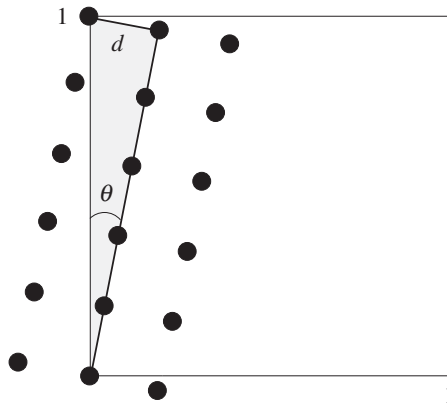
### (a) Periodic boundary conditions

First, we identify the constraints on the dimensionless parameters of the problem guaranteeing that the rotated rigid lattice  $\hat{A}_1$  coincides with its periodic extension to the exterior of the unit square  $[0, 1]^2$ . As suggested by figure 10, a sufficient condition for periodicity is that each corner of  $[0, 1]^2$  is occupied by an atom of the rotated lattice. Using the shaded triangle in figure 10, we conclude for the case shown that

$$n := \frac{\cos \theta}{d} \in \mathbb{N} \quad \text{and} \quad \sin \theta = d, \quad (4.1)$$

where  $n + 1$  is the number of atomic rows that intersect each side of the square  $[0, 1]^2$ .

In fact, the second equation in (4.1) can be generalized via the following analogy. By rolling the square in figure 10 into a tube with the axis parallel to, for example, the horizontal side of the square, we obtain a tube with a lattice of atoms that can be placed on a helix. Following the



**Figure 10.** Rotated lattice with periodic boundary conditions on  $[0, 1]^2$ . A sufficient condition for periodicity is that each corner of  $[0, 1]^2$  is occupied by an atom of the rotated lattice.

helix around the tube for a single rotation corresponds to advancing by one unit of length along the axis of the tube. We can say, for example, that the resulting helical structure has *chirality* 1. Then, if this structure consisted of  $k$  parallel equidistant helices with the axes that coincide with the axis of the tube, the chirality of the structure would have been equal to  $k$ . Unwrapping the structure of any chirality back onto the unit square would still produce a square lattice that can be periodically extended to the exterior of the square. It is not difficult to observe that the set of equations (4.1) can thus be written in a more general form,

$$n := \frac{\cos \theta}{d} \in \mathbb{N} \quad \text{and} \quad \sin \theta = kd, \quad k \in \mathbb{N}, \quad (4.2)$$

to incorporate lattices of any chirality. Note that, if the chirality  $k$  is equal to 0, then the lattice vectors are parallel to the sides of the square.

Based on (4.2), we use the following procedure to generate the parameters for the rigid lattice  $\hat{\mathcal{A}}_1$ . Recall that we denoted the number of atomic rows for the deformable lattice  $\hat{\mathcal{A}}_2$  in  $[0, 1]^2$  by  $N_2$ , so that

$$\varepsilon \delta_2 N_2 = 1. \quad (4.3)$$

After selecting two small integers  $m \in \mathbb{Z}$  and  $k \in \mathbb{N}$ , we set

$$N_1 = N_2 - m, \quad (4.4)$$

and find the angle  $\theta$  from

$$\theta = \text{atan} \left( \frac{k}{N_1} \right) \quad (4.5)$$

and the lattice constant for  $\hat{\mathcal{A}}_1$  from

$$\delta_1 = \frac{1}{\varepsilon \sqrt{N_1^2 + k^2}}. \quad (4.6)$$

Both of these expressions follow trivially from (4.2) by setting  $n = N_1$  and using that  $d = \varepsilon \delta_1$  for  $\hat{\mathcal{A}}_1$ .

The parameters  $\delta_1$ ,  $N_1$  and  $\theta$  as given by (4.4)–(4.6) are used in discrete simulations below. We are now in a position to determine the parameters  $\alpha$  and  $\Theta$  for the corresponding continuum

simulations. Indeed, from (3.19) we have that

$$\Theta = \frac{\theta}{\varepsilon} = \frac{1}{\varepsilon} \operatorname{atan} \left( \frac{k}{N_1} \right) = \frac{1}{\varepsilon} \operatorname{atan} \left( \frac{\varepsilon k \delta_2}{\varepsilon \delta_2 (N_2 - m)} \right) = \frac{1}{\varepsilon} \operatorname{atan} \left( \frac{\varepsilon k \delta_2}{1 - \varepsilon \delta_2 m} \right) \sim \delta_2 k, \quad (4.7)$$

using (4.3)–(4.5), and that  $\varepsilon \delta_2 N_2 = 1$ . Further,

$$\begin{aligned} \frac{\delta_2 - \delta_1}{\delta_2} &= 1 - \frac{1}{\varepsilon \delta_2 \sqrt{N_1^2 + k^2}} = 1 - \frac{1}{\varepsilon \delta_2 \sqrt{(N_2 - m)^2 + k^2}} \\ &= 1 - \frac{1}{\sqrt{(1 - \varepsilon \delta_2 m)^2 + \varepsilon^2 \delta_2^2 k^2}} \sim -\varepsilon \delta_2 m, \end{aligned} \quad (4.8)$$

by (4.3), (4.4) and (4.6). It follows from (4.8) that the parameter  $\alpha$ , defined in (3.6), is given by

$$\alpha \sim -\delta_2 m. \quad (4.9)$$

For convenience, in what follows we refer to the parameter  $m$ , which measures the difference between the number of rows of atoms in the two lattices, as the *disparity*. Note that one can think of  $m$  and  $k$  as the components of a Burgers vector  $\beta := (m, k)$  and interpret a wall in a system of two lattices as an edge and a screw dislocation when  $\beta := (m, 0)$  and  $\beta := (0, k)$ , respectively [9].

## (b) Comparison between the discrete and continuum simulations

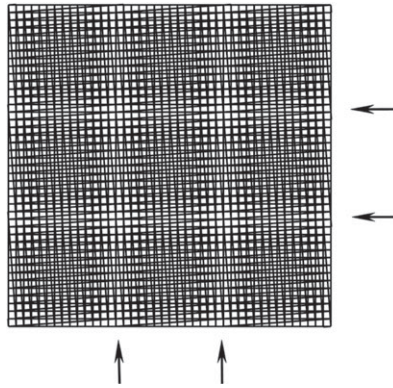
For the numerical simulations below, we used COMSOL [24] to solve the system of partial differential equations (3.30) of the continuum model and LAMMPS [25] to minimize the discrete energy (2.2). For the continuum simulations, we used the dissipation-dominated (gradient flow) dynamics to drive the energy of the system towards a (possibly local) minimum. The same task was accomplished for the discrete system of atoms by performing molecular dynamics simulations at a sufficiently low temperature. Both sets of simulations were conducted assuming periodic boundary conditions in the plane of the rigid lattice with period 1 in the  $\chi_1$ - and  $\chi_2$ -directions. For the initial conditions, we assumed that the deformable lattice is parallel to and at a distance  $\varepsilon$  from the rigid lattice in non-dimensional coordinates. We set  $\delta_2 = 1$  and chose  $m = 0$ ,  $k = 3$  and  $\varepsilon = 0.0238$  to generate a periodic system using the equations in the previous section. The resulting lattices have the same lattice constants but they are slightly rotated with respect to each other.

This periodic system has the moiré pattern depicted in figure 11, where the brighter regions indicated by arrows correspond to the least optimal registry from the point of view of the weak interaction. Indeed, this interaction prefers an atom of the deformable lattice to lie above the midpoint of a unit cell of the rigid lattice. One expects that, if the deformable lattice is allowed to relax, the darker regions would slightly rotate to increase the relative area of optimal registry. This should incur large elastic costs in the lighter regions of suboptimal registry, either by in-plane shear and/or by out-of-plane displacement.

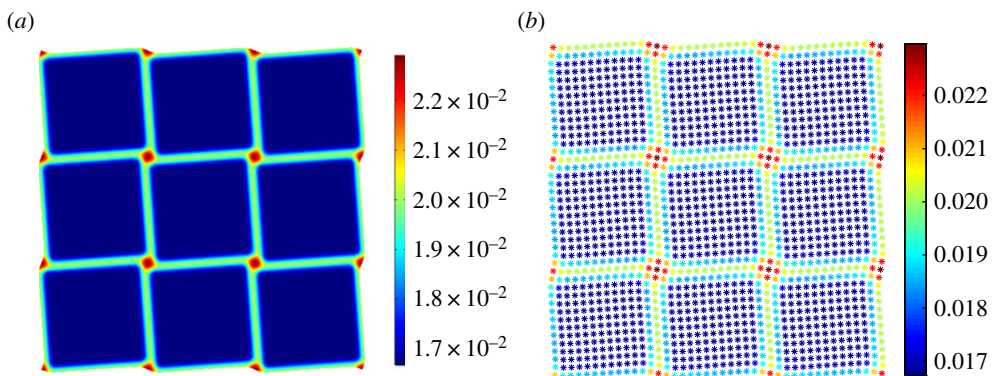
We picked  $\gamma_s = 12$ ,  $\gamma_t = 16$  and  $\gamma_d = 0.1$  for the elastic constants and determined the spring constants of the discrete model from (3.4) assuming that  $\omega = 1$ . The results of the corresponding discrete and continuum simulations are shown in figure 12.

The displacement field and the shear deformation observed in continuum simulations closely correspond to those determined for the discrete model. We observe that in both simulations the deformable lattice relaxes by generating six shear bands per period—three in the horizontal and three in the vertical directions, respectively. The shear bands coincide with the bright regions of the moiré pattern in figure 11, where the number of the bright regions is determined by the chirality  $k$ . The square-shaped regions of the deformable lattice between the shear bands rotate so that their orientations coincide with that of the rigid lattice. We refer to the shear bands as *domain walls* separating the regions of optimal lattice registry.

Further inspection of figure 12 shows that the domain walls also exhibit significant out-of-plane displacements that reach their maximum values at ‘hot spots’—the points of intersection between



**Figure 11.** Moiré pattern for  $m = 0$ ,  $k = 3$  and  $\varepsilon = 0.0238$ . The bands along which the van der Waals energy density is the highest for the given initial spacing are indicated by arrows.



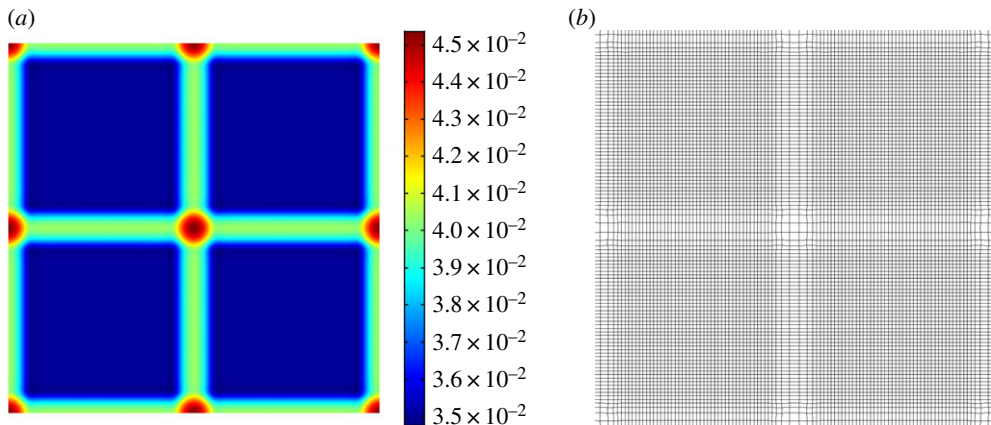
**Figure 12.** Continuum (a) and discrete (b) simulation results corresponding to the moiré pattern in figure 11. (Online version in colour.)

the walls. The minimum value of the displacement in figure 12 corresponds to the equilibrium distance between an atom of the deformable lattice and the rigid lattice when this atom is positioned directly above the middle of a unit cell of the rigid lattice. In turn, the maximum value of the displacement corresponds to an atom at the equilibrium distance from the rigid lattice while positioned directly above an atom of that lattice. The displacements are maximized at hot spots, where the registry between the lattices is the least favourable from the point of view of weak interactions, while they are minimized in the square-shaped regions of the optimal registry.

### (c) Pattern formation in continuum simulations

In this section, we study pattern formation in the deformable lattice by solving the governing system (3.30) for several combinations of geometric parameters of the model. In the remainder of this section, each simulation is described by two figures. The first figure represents the deformed configuration with colour scale indicating the local distance from the deformable to the rigid lattice. The second figure shows the deformation of a uniform grid drawn on the deformable lattice in the reference state, projected onto the  $\chi_1\chi_2$ -plane. Note that all lengths scale with  $\varepsilon$  and, in particular, the equilibrium distances depend on  $\varepsilon$ .

Suppose first that  $\varepsilon = 0.05$ ,  $\gamma_s = 1$ ,  $\gamma_t = 1$ ,  $\gamma_d = 0.1$ ,  $m = -2$  and  $k = 0$ . Since  $k = 0$ , both the deformable and the rigid lattices have exactly the same orientation. At the same time, their lattice parameters are different so that the rigid lattice has exactly two extra vertical rows and two extra horizontal rows of atoms per period. The shape of the relaxed deformable lattice is shown in



**Figure 13.** Continuum simulations for  $\varepsilon = 0.05$ ,  $\gamma_s = 1$ ,  $\gamma_t = 1$ ,  $\gamma_d = 0.1$ ,  $m = -2$  and  $k = 0$ . Deformed configuration with the colour indicating the local distance from the deformable to the rigid lattice (a) and the projection of the deformed uniform grid onto the  $\chi_1\chi_2$ -plane (b). (Online version in colour.)

figure 13. The deformable lattice relaxes by contraction in the bulk to compensate for the extra rows of atoms on the rigid lattice. The bulk contraction enlarges the regions of registry, but leads to expansion in misregistered regions. Recall that, in equilibrium, the atoms of the deformable lattice are further from the substrate when they are out of registry than when they are in registry. Therefore, the rows of atoms in the misregistered regions are also pushed further away from the substrate to form the sets of two horizontal and two vertical walls within each period. Each wall accommodates exactly one extra row of atoms on the rigid lattice.

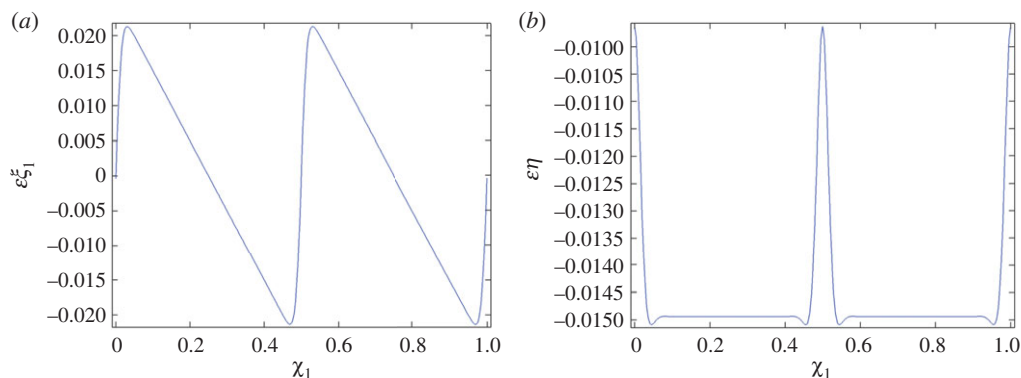
Note that, when  $m > 0$ , the situation is partly reversed: the deformable lattice now has more rows than the rigid lattice, hence it slightly expands in the bulk and contracts in the misregistered regions. However, the rows of atoms in the misregistered regions are again pushed away from the substrate generating the walls such that each accommodates exactly one extra row of atoms on the deformable lattice. Generally, a wall formed by bulk compression (when  $m < 0$ ) is wider than a wall formed by bulk expansion (when  $m > 0$ ). Because the structure of the network of walls is primarily dictated by the underlying moiré pattern, rather than the width of the walls, in what follows we show results for  $m < 0$ .

The corresponding non-dimensional displacement components  $\varepsilon\xi_1$  and  $\varepsilon\eta$  are shown in figure 14 as functions of  $\chi_1$  while holding  $\chi_2 = 0.25$  fixed. These graphs are very similar to what is observed for an analogous one-dimensional system considered in [7]. In particular, the small dips next to the cross-section of a wall in figure 14b result from the presence of the bending stiffness term and the linear stiffness of the van der Waals interaction near equilibrium. A macroscopic version of this effect is well known for elastic beams on a liquid [26].

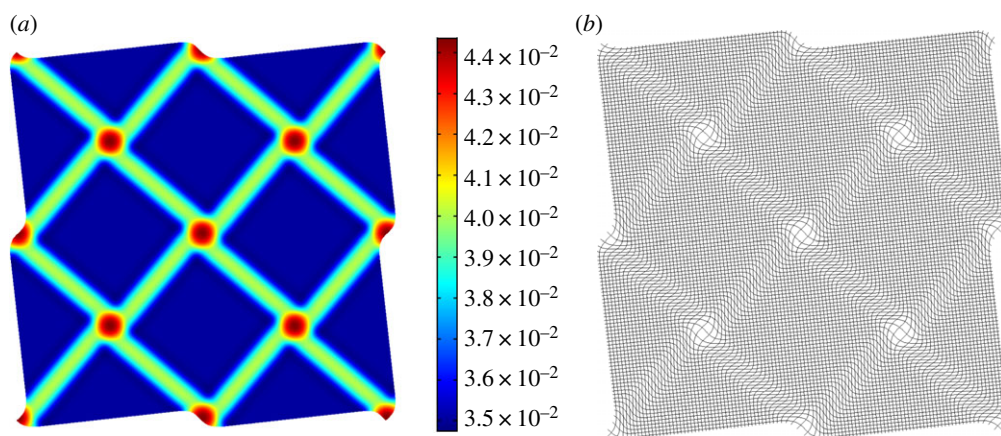
We now explore the influence of the chirality  $k$  and the disparity  $m$  on the pattern of walls that form in the deformable lattice when both  $k$  and  $m$  are not equal to zero. Examining figures 15–17, we observe that the number of walls that intersect each side of the square domain is given by the chirality  $k$ . There are two sets of parallel walls. For example, in figure 15, the set of walls running from southeast to northwest corresponds to a stretch in the horizontal direction and a shear in the vertical direction. Conversely, the other set corresponds to a stretch in the vertical direction and a shear in the horizontal direction. Proceeding along any vertical line intersecting the square domain, one encounters exactly  $|m|$  walls characterized by stretch in the vertical direction. Since the deformable lattice has  $|m|$  fewer rows of atoms than the rigid lattice, each wall serves to accommodate exactly one extra row of the rigid lattice. A similar statement applies along any horizontal line. Note also that out-of-plane deflection occurs along all walls.

Finally, increasing  $\varepsilon$  results in a larger angle of rotation between the rigid and deformable lattices that requires larger shear deformation to accommodate the weak interactions (figure 18).

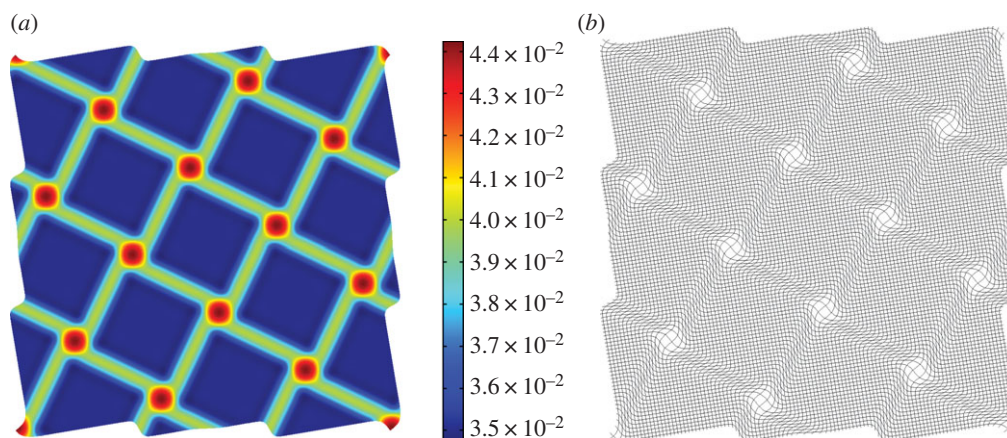




**Figure 14.** Continuum simulations for  $\varepsilon = 0.05$ ,  $\gamma_s = 1$ ,  $\gamma_t = 1$ ,  $\gamma_d = 0.1$ ,  $m = -2$  and  $k = 0$ . The dependence of  $\varepsilon\xi_1$  (a) and  $\varepsilon\eta$  (b) on  $\chi_1$  when  $\chi_2 = 0.25$ . (Online version in colour.)

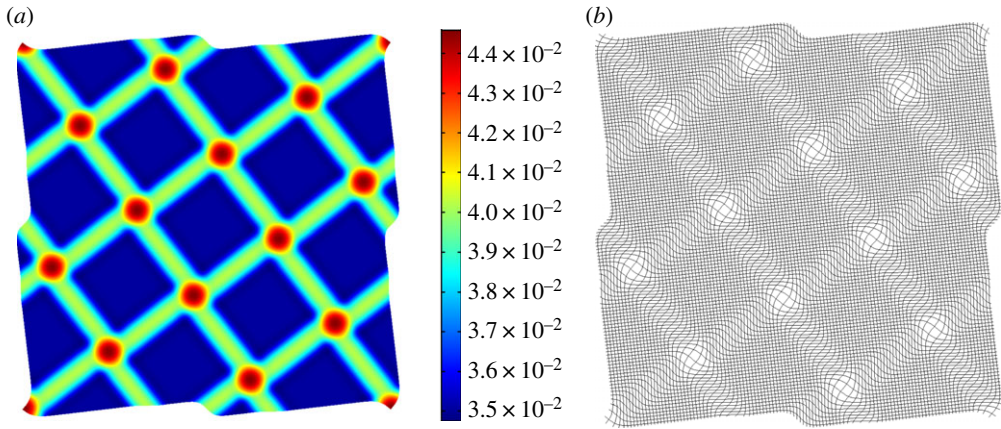


**Figure 15.** Continuum simulations for  $\varepsilon = 0.05$ ,  $\gamma_s = 1$ ,  $\gamma_t = 1$ ,  $\gamma_d = 0.1$ ,  $m = -2$  and  $k = 2$ . Deformed configuration with the colour indicating the local distance from the deformable to the rigid lattice (a) and the projection of the deformed uniform grid onto the  $\chi_1\chi_2$ -plane (b). (Online version in colour.)

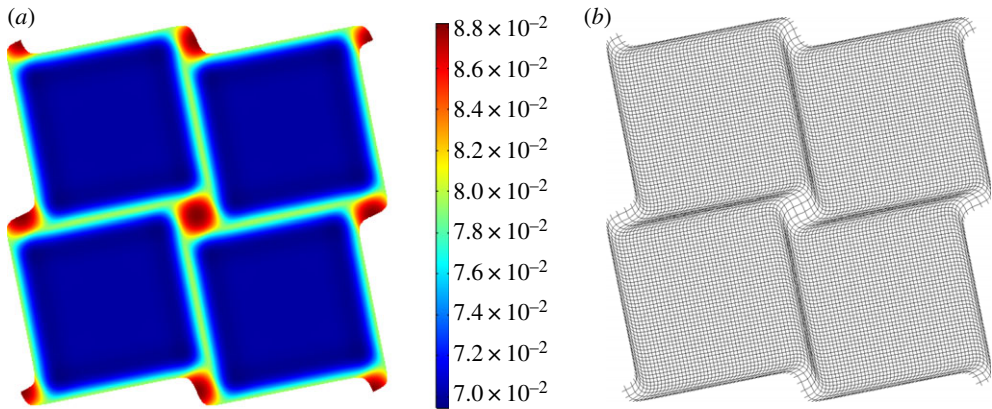


**Figure 16.** Continuum simulations for  $\varepsilon = 0.05$ ,  $\gamma_s = 1$ ,  $\gamma_t = 1$ ,  $\gamma_d = 0.1$ ,  $m = -2$  and  $k = 3$ . Deformed configuration with the colour indicating the local distance from the deformable to the rigid lattice (a) and the projection of the deformed uniform grid onto the  $\chi_1\chi_2$ -plane (b). (Online version in colour.)





**Figure 17.** Continuum simulations for  $\varepsilon = 0.05$ ,  $\gamma_s = 1$ ,  $\gamma_t = 1$ ,  $\gamma_d = 0.1$ ,  $m = -3$  and  $k = 2$ . Deformed configuration with the colour indicating the local distance from the deformable to the rigid lattice (a) and the projection of the deformed uniform grid onto the  $\chi_1\chi_2$ -plane (b). (Online version in colour.)



**Figure 18.** Continuum simulations for  $\varepsilon = 0.1$ ,  $\gamma_s = 1$ ,  $\gamma_t = 1$ ,  $\gamma_d = 0.1$ ,  $m = 0$  and  $k = 2$ . Deformed configuration with the colour indicating the local distance from the deformable to the rigid lattice (a) and the projection of the deformed uniform grid onto the  $\chi_1\chi_2$ -plane (b). (Online version in colour.)

Note that, even though  $\varepsilon$  is relatively large in figure 18, the walls are relatively narrow because of shearing [27].

## 5. Conclusion

This work generalizes to two dimensions our previous results for weakly interacting Frenkel–Kontorova chains [7]. We have applied an upscaling procedure to develop a mesoscopic continuum model of a deformable two-dimensional lattice of atoms interacting with a rigid substrate. We began with a system of atoms connected by harmonic extensional, torsional and dihedral springs so that in equilibrium this system forms a square lattice. This lattice is assumed to weakly interact with another rigid square lattice via a van der Waals potential. The upscaling procedure yields a continuum energy with terms describing the elastic energy of the deformable lattice and a term for the interaction energy between the deformable and rigid lattices. Although a continuum description, the weak interaction energy retains discrete information about mismatch between the lattices.

The numerical simulations were performed assuming periodic boundary conditions in the plane of the deformable lattice in the reference configuration. Simulations for a typical combination of geometric and material parameters demonstrate that the predictions of the mesoscopic model are in close correspondence with the configuration obtained via a discrete molecular dynamics approach. Similar to [8], we found that the deformable lattice develops a network of walls characterized by large shearing, stretching and bending deformation that accommodate the misalignment and/or mismatch between the deformable and rigid lattices. We identified two integer-valued parameters describing the mismatch between the lattices. These parameters determine the geometry and the detail of deformation associated with the walls. At the intersection of the walls, we find ‘hot spots’ characterized by large out-of-plane deformation [5].

Although the modelling presented here deals with square lattices, our approach is not limited to this choice of a system. Indeed, our procedure admits a straightforward generalization to any lattice type or atomic interactions. The periodic boundary conditions were imposed for simplicity and other boundary conditions can be considered. The model can also be extended in a standard way to include external body forces.

An interesting mathematical problem that arises from our upscaling procedure is to justify the number of terms that we retained in the asymptotic expansion of the elastic energy in  $\varepsilon$  in order to produce the continuum model. As discussed in §3a, the terms we neglected influence the behaviour of the solution inside the walls, where the deformation gradient is large. Our conjecture, confirmed by comparison with discrete simulations, is that the influence of the neglected terms on the network of walls, and, by extension, on the solution in the commensurate regions, is small. Indeed, our continuum model itself can be thought of as a truncation of an expansion of a continuum energy in terms of the same small parameter  $\varepsilon$ . We expect that both the discrete and the continuum models approach in some appropriate sense the same ‘limiting’ model as  $\varepsilon$  tends to zero. The exact framework and rigorous study of this convergence is a subject of future work.

Continuum modelling that retains discrete registry effects is important for both solving computational problems more quickly and allowing theoretical insight into mesoscopic pattern formation of bilayer graphene and two-dimensional heterostructures. Further, continuum modelling may facilitate the study of the influence of atomic relaxation of slightly mismatched heterostructures on the electronic properties of the system [4].

**Data accessibility.** This article has no additional data.

**Authors' contributions.** All authors conceived of the work, participated in all aspects of the study and drafted the manuscript. All authors approved the final version of the manuscript.

**Competing interests.** We declare we have no competing interests.

**Funding.** This work was supported by the National Science Foundation grant no. DMS-1615952.

## References

1. Geim AK, Grigorieva IV. 2013 Van der Waals heterostructures. *Nature* **499**, 419–425. (doi:10.1038/nature12385)
2. Novoselov K, Mishchenko A, Carvalho A, Neto AC. 2016 2D materials and van der Waals heterostructures. *Science* **353**, aac9439. (doi:10.1126/science.aac9439)
3. Symalla F, Shallcross S, Beljakov I, Fink K, Wenzel W, Meded V. 2015 Band-gap engineering with a twist: formation of intercalant superlattices in twisted graphene bilayers. *Phys. Rev. B* **91**, 205412. (doi:10.1103/PhysRevB.91.205412)
4. van Wijk MM, Schuring A, Katsnelson MI, Fasolino A. 2015 Relaxation of moiré patterns for slightly misaligned identical lattices: graphene on graphite. *2D Mater.* **2**, 034010. (doi:10.1088/2053-1583/2/3/034010)
5. van Wijk MM, Schuring A, Katsnelson MI, Fasolino A. 2014 Moiré patterns as a probe of interplanar interactions for graphene on h-BN. *Phys. Rev. Lett.* **113**, 135504. (doi:10.1103/PhysRevLett.113.135504)

6. Davidovitch B, Schroll RD, Cerda E. 2012 Nonperturbative model for wrinkling in highly bendable sheets. *Phys. Rev. E* **85**, 066115. (doi:10.1103/PhysRevE.85.066115)
7. Español MI, Golovaty D, Wilber JP. 2017 A discrete-to-continuum model of weakly interacting incommensurate chains. *Phys. Rev. E* **96**, 033003.
8. Dai S, Xiang Y, Srolovitz DJ. 2016 Structure and energetics of interlayer dislocations in bilayer graphene. *Phys. Rev. B* **93**, 085410. (doi:10.1103/PhysRevB.93.085410)
9. Dai S, Xiang Y, Srolovitz DJ. 2016 Twisted bilayer graphene: moiré with a twist. *Nano Lett.* **16**, 5923–5927. (doi:10.1021/acs.nanolett.6b02870)
10. Vitek V. 1968 Intrinsic stacking faults in body-centred cubic crystals. *Philos. Mag.: J. Theor. Exp. Appl. Phys.* **18**, 773–786. (doi:10.1080/14786436808227500)
11. Zhou S, Han J, Dai S, Sun J, Srolovitz DJ. 2015 Van der Waals bilayer energetics: generalized stacking-fault energy of graphene, boron nitride, and graphene/boron nitride bilayers. *Phys. Rev. B* **92**, 155438. (doi:10.1103/PhysRevB.92.155438)
12. Braides A, Solci M, Vitali E. 2007 A derivation of linear elastic energies from pair-interaction atomistic systems. *Netw. Heterogeneous Media* **2**, 551. (doi:10.3934/nhm.2007.2.551)
13. Braides A. 2014 Discrete-to-continuum variational methods for lattice systems. In *Proc. Int. Congress of Mathematicians, Seoul, Republic of Korea, 13–21 August 2014*, pp. 997–1015. Seoul, Republic of Korea: Kyung Moon SA Co. Ltd.
14. Luo T, Ming P, Xiang Y. 2017 From atomistic model to the Peierls–Nabarro model with  $\gamma$ -surface. (<http://arxiv.org/abs/1706.03145>)
15. Wilber JP, Clemons CB, Young GW, Buldum A, Quinn DD. 2007 Continuum and atomistic modeling of interacting graphene layers. *Phys. Rev. B* **75**, 045418. (doi:10.1103/PhysRevB.75.045418)
16. Braides A. 2002 *Gamma-convergence for beginners*, vol. 22. Oxford, UK: Clarendon Press.
17. Braides A, Truskinovsky L. 2008 Asymptotic expansions by  $\Gamma$ -convergence. *Contin. Mech. Thermodyn.* **20**, 21–62. (doi:10.1007/s00161-008-0072-2)
18. Le Dret H, Raoult A. 2017 Hexagonal lattices with three-point interactions. *J. Math. Pures Appl.* **108**, 613–632.
19. Blanc X, Le Bris C, Lions PL. 2007 Atomistic to continuum limits for computational materials science. *ESAIM: Math. Model. Numer. Anal.* **41**, 391–426. (doi:10.1051/m2an:2007018)
20. Meunier N, Pantz O, Raoult A. 2012 Elastic limit of square lattices with three-point interactions. *Math. Models Methods Appl. Sci.* **22**, 1250032. (doi:10.1142/S0218202512500327)
21. Schmidt B. 2008 On the passage from atomic to continuum theory for thin films. *Arch. Ration. Mech. Anal.* **190**, 1–55. (doi:10.1007/s00205-008-0138-0)
22. Blanc X, Le Bris C, Lions PL. 2002 From molecular models to continuum mechanics. *Arch. Ration. Mech. Anal.* **164**, 341–381. (doi:10.1007/s00205-002-0218-5)
23. Español MI, Golovaty D, Wilber JP. 2017 A discrete-to-continuum model of weakly interacting incommensurate two-dimensional lattices. (<http://arxiv.org/abs/1708.00974>)
24. COMSOL. *Multiphysics® v. 5.3*. Stockholm, Sweden: COMSOL AB. See <http://www.comsol.com/>.
25. Plimpton S. 1995 Fast parallel algorithms for short-range molecular dynamics. *J. Comput. Phys.* **117**, 1–19. See <http://lammps.sandia.gov>.
26. Wagner TJW, Vella D. 2011 Floating carpets and the delamination of elastic sheets. *Phys. Rev. Lett.* **107**, 044301. (doi:10.1103/PhysRevLett.107.044301)
27. Alden JS, Tsen AW, Huang PY, Hovden R, Brown L, Park J, Muller DA, McEuen PL. 2013 Strain solitons and topological defects in bilayer graphene. *Proc. Natl Acad. Sci. USA* **110**, 11 256–11 260. (doi:10.1073/pnas.1309394110)