A VARIATIONAL MODEL FOR DISLOCATIONS AT SEMI-COHERENT INTERFACES

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ABSTRACT. We propose and analyze a simple variational model for dislocations at semi-coherent interfaces. The energy functional describes the competition between two terms: a surface energy induced by dislocations and a bulk elastic energy, spent to decrease the amount of dislocations needed to compensate the lattice misfit. We prove that, for minimizers, the former scales like the surface area of the interface, the latter like its diameter.

The proposed continuum model is built on some explicit computations done in the framework of the semi-discrete theory of dislocations. Even if we deal with finite elasticity, linearized elasticity naturally emerges in our analysis since the far field strain vanishes as the interface size increases.

CONTENTS

INTRODUCTION

Dislocations are line topological defects in the periodic structure of crystals. Their motion represents the microscopic mechanism of plastic flow, while their presence at grain boundaries decreases the energy induced by lattice misfits.

In this paper we propose and analyze a variational model describing dislocations at semi-coherent interfaces, focusing on flat two dimensional interfaces between two crystalline materials with different underlying lattice structures Λ^+ and Λ^-. Specifically, we assume that the lattice Λ^+ (lying on top of Λ^-) is a dilation with factor $\alpha > 1$ of Λ^-. We are interested in semi-coherent interfaces, corresponding to small misfits $\alpha \approx 1$.

Since in the reference configuration (where both crystals are in equilibrium) the density of the atoms of Λ^+ is lower than that of Λ^-, in the vicinity of the interface there are many atoms having the "wrong" coordination number (namely, the wrong number of nearest neighbors, see first picture in Figure 1). Such atoms form line singularities (relatively closed paths lying on the interface), which correspond to edge dislocations. The crystal can reduce the number of such dislocations through a compression strain acting on Λ^+ near the interface, at the price of storing some far field elastic energy. A deformation that coincides with $x \mapsto \alpha^{-1}x$ near the interface would provide a defect-free perfect match between the crystal lattices (see third picture in Figure 1). In fact, the true deformed configuration is the result of a balance (see middle picture in Figure 1) between the elastic energy spent to match the crystal structures and the dislocation energy spent to release the far field elastic energy, with the former scaling (for defect free configurations) like the volume of the body and the latter like the surface area of the interface.
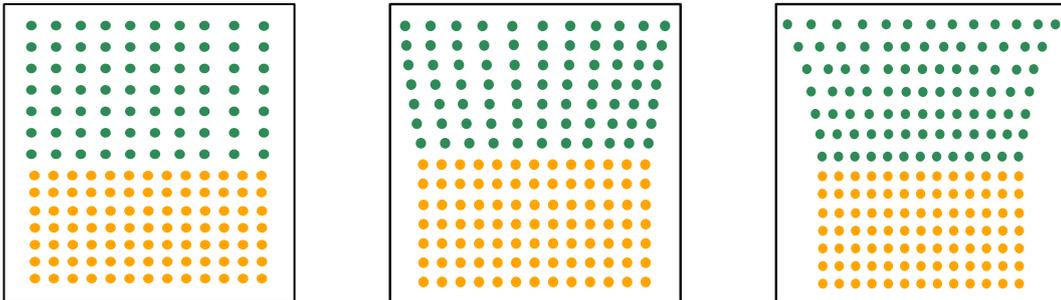

FIGURE 1. Left: A bulk stress-free configuration. Right: a defect-free configuration. Center: a schematic picture of a true energy minimizer; the density of atoms on the top and on the bottom of the interface is almost the same, giving rise to a semi-coherent interface.

This is why the common perspective of the scientific community working on this problem has been to understand which configurations of dislocations minimize the elastic stored energy, and much effort has been devoted to describe those configurations for which the dislocation energy contribution is predominant, and the far field elastic energy is negligible ([21], [11]). As a matter of fact, for large crystals, periodic patterns of edge dislocations are observed at interfaces [8].

Here, we propose a simple variational model to analyze the competition between surface and elastic energy. We show that, for large interfaces, the dislocation energy of minimizers scales like the area of the interface, while the elastic far field energy like its diameter.

The proposed model is not purely discrete; indeed it is a continuum model that stems from some heuristic considerations and some rigorous computations done in the framework of the so called semi-discrete theory of dislocations.

In single crystals, the energy induced by straight edge dislocations has a logarithmic tail, which diverges as the ratio between the crystal size and the atomic distance tends to $+\infty$. The Γ-convergence analysis for these systems as the atomic distance tends to zero has been recently done in [7], [5] showing that dipoles as well as isolated dislocations do not contribute to decrease the elastic energy, so that in single crystals only the so called *geometrically necessary dislocations* are good competitors in the energy minimization.

Quite different is the case of polycrystals treated in this paper, where dislocations contribute to decrease the elastic energy. The first rigorous variational justification of dislocation nucleation in heterostructured nanowires was obtained by Müller and Palombaro [18] in the context of nonlinear elasticity. The model proposed in [18] was later generalized to a discrete to continuum setting in [14, 15] (see also [2] for recent advancements in the microscopic setting). A variational model for misfit dislocations in elastic thin films, in connection with epitaxial growth, has been recently proposed in [9] (we refer the readers interested in the mathematical theory of epitaxy to the lecture notes [16]). Finally, a rigorous derivation of a small angle grain boundary has been obtained in the recent paper [13].

In the first part of the paper we set and analyze the problem in the semi-discrete framework, which provides the theoretical background for the proposed continuum model. In the semi-discrete model, the reference configuration of the hyperelastic body is the cylindrical region $\Omega_r := S_r \times (-hr, hr)$, where $r, h > 0$ and $S_r := [-r/2, r/2]^2$. The interface $S_r \times \{0\}$ separates the two regions of the body, $\Omega_r^- := S_r \times (-hr, 0)$ and $\Omega_r^+ := S_r \times (0, hr)$, with underlying crystal structures Λ^- and Λ^+ respectively. We will refer to Ω_r^- and Ω_r^+ as the underlayer and overlayer, respectively. We assume that the material equilibrium is the identity I in Ω_r^- (implying that the underlayer is already in equilibrium) and αI in Ω_r^+, where $\alpha > 1$ measures the misfit between the two lattice parameters. Notice that the identical deformation of Ω_r, which corresponds to a dislocation-free configuration, is not stress-free, since the overlayer is not in equilibrium. Furthermore, in order to simplify the analysis, we assume that Ω_r^- is rigid, so that only Ω_r^+ is subjected to deformations.

We assume that deformations try to minimize a stored elastic energy (in Ω_r^+), whose density is described by a nonlinear frame indifferent function $W : \mathbb{M}^{3\times3} \to [0, +\infty)$. In classical finite elasticity, W acts on deformation gradients $F := \nabla v$. In this model dislocations are introduced as line defects of the strain: more precisely, we allow the strain field F to have a non vanishing curl, concentrated on dislocation lines on the interface S_r. Therefore, the admissible strains are maps $F \in L^p(\Omega_r; \mathbb{M}^{3\times3})$ (where $1 < p < 2$ is fixed, according to the growth assumptions on W, see (4)) that satisfy

$$(1) \qquad \operatorname{curl} F = \sum_i -\mathbf{b}_i \otimes \dot{\gamma}_i \, d\mathcal{H}^1 {\llcorner} \gamma_i$$

in the sense of measures and such that $F = I$ in Ω_r^-. Here $\{\gamma_i\}$ is a finite collection of closed curves, and $\mathbf{b}_i \in \mathbb{R}^3$ denotes the *Burgers vector*, which is constant on each γ_i. The Burgers vector belongs to the set of slip directions, which is a given material property of

the crystal. We assume that the slip directions are given by $b\{z_1e_1+z_2e_2, z_1, z_2 \in \mathbb{Z}\}$, where $b > 0$ represents the lattice spacing of Λ^-, and that the dislocation curves γ_i have support on the grid $\left[\left((b\mathbb{Z} \times \mathbb{R}) \cup (\mathbb{R} \times b\mathbb{Z})\right) \cap S_r\right] \times \{0\}$. Notice that this choice is consistent with the cubic crystal structure, and that b is independent of r, i.e., independent of the size of the body.

In Section 1 we study the asymptotic behaviour of minimizers of the elastic energy functional with respect to all possible pairs of compatible (i.e., satisfying (1)) strains and dislocations, refining the analysis first done in [18]. In Proposition 1.2 we show that, as $r \to +\infty$, the elastic energy of minimizers per unit area of the interface tends to a given surface energy density E_α. As a consequence, we show that there exists a critical r^* such that, for larger size of the interface, dislocations are energetically favorable (see Theorem 1.5). The proof of these results is based on an explicit construction of an array of dislocations (see Figure 2) and of admissible fields, which is optimal in the energy scaling (see Proposition 1.6). While we could guess that the dislocation configuration is somehow optimal, the strains that we consider as energy competitors are surely not, so that our construction does not provide the sharp formula for the surface energy density E_α, which depends on the specific form of the elastic energy density W. Indeed, the main
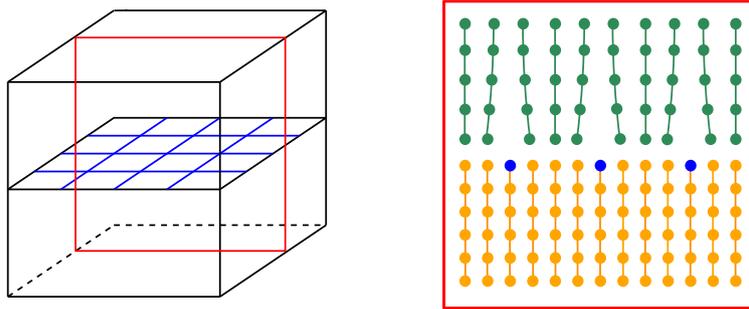

FIGURE 2. Left: The 3D crystal. Right: a 2D cross-section with the lattice structure. Red squares: The 2D slice. Green: The lattice Λ^+. Orange: The lattice Λ^-. Blue: Edge dislocations.

problem raised in this paper concerns the identification of the sharp energy density E_α and of the corresponding optimal geometries for the dislocations net. Less ambitious is the question about the optimal spacing between the dislocation lines. As already explained, by scaling arguments the optimal geometry of dislocations should release the far field elastic energy as much as possible. This consideration leads us to construct and analyze a net of dislocations with spacing $\frac{b}{\alpha-1}$. One of the main goals of this paper is to show that, for large interfaces, such density of dislocations is optimal in energy. In order to prove this fact, we propose and analyze a simplified continuous model for dislocations at semi-coherent interfaces, describing in particular heterogeneous nanowires.

Although we deal with a continuum model, our approach is built on the analysis developed in the first part of this paper, and it is consistent with the discrete analysis developed in [14, 15]. In this model we work with actual gradient fields far from the interface, where the curl of the strain is now a diffuse measure, in contrast with (1). Dislocation nucleation

is taken into account by introducing a free parameter into the total energy and eventually optimizing over it. Specifically, we assume that the underlayer occupies the cylindrical region Ω_R^- (which is fixed), while the reference configuration of the overlayer is Ω_r^+, where $r = \theta R$ and $\theta \in (0, 1)$ is a free parameter in the total energy functional. The class of admissible deformation maps is defined by

$$(2) \qquad \mathcal{ADM}_{\theta,R} := \left\{ v \in W^{1,2}(\Omega_r^+; \mathbb{R}^3) : v(x) = \frac{1}{\theta} x \text{ on } S_r \right\}.$$

In this way $v(S_r) = S_R$ for all $v \in \mathcal{ADM}_{\theta,R}$, so that there is a perfect match between the two layers at the interface. In view of the analysis performed in the semi-discrete setting, the area of $S_R \setminus S_r$ divided by b can be interpreted as the total dislocation length. This suggests to introduce the plastic energy defined by

$$E_R^{pl}(\theta) := \sigma r^2 (\theta^{-2} - 1) = \sigma R^2 (1 - \theta^2).$$

Here $\sigma > 0$ is a given material constant of the crystal, which multiplied by b represents the energy cost of dislocations per unit length. In principle, σ could be derived starting from the surface energy density E_α introduced in Proposition 1.2, yielding in the limit of vanishing misfit $\sigma = \lim\limits_{\alpha \to 1} \dfrac{E_\alpha}{\alpha^2 - 1}$ (see (20)). Alternatively, assuming isotropy, σ can be expressed in terms of the Lamé moduli of the linearized elastic tensor corresponding to W and of the (unknown) chemical core energy density γ^{ch} induced by dislocations (see (22) in Section 2). The latter contribution is implicitly taken into account by the nonlinear energy density W in finite elasticity.

Based on the previous considerations, our goal is to study the total energy functional defined by

$$E_{\alpha,R}^{tot}(\theta, v) := E_{\alpha,R}^{el}(\theta, v) + E_R^{pl}(\theta) = \int_{\Omega_r^+} W(\nabla v(x)) \, dx + \sigma R^2 (1 - \theta^2),$$

for $v \in \mathcal{ADM}_{\theta,R}$. Set

$$E_{\alpha,R}^{el}(\theta) := \inf \left\{ E_{\alpha,R}^{el}(\theta, v) : v \in \mathcal{ADM}_{\theta,R} \right\}, \qquad E_{\alpha,R}^{tot}(\theta) := E_{\alpha,R}^{el}(\theta) + E_R^{pl}(\theta).$$

Notice that if $\theta = 1$, then no dislocation energy is present, i.e., $E_{\alpha,R}^{tot}(1) = E_{\alpha,R}^{el}(1)$. Instead, if $\theta = \alpha^{-1}$ no elastic energy is stored (since $v(x) := \alpha x$ is admissible and $W(\alpha I) = 0$).

The remaining and main part of the paper is devoted to the analysis of minimizers of $E_{\alpha,R}^{tot}$, as $R \to +\infty$. In Theorem 3.7 we show that the optimal θ_R tends to α^{-1} from below, corresponding to the average spacing $\frac{b}{\alpha-1}$ between the dislocation lines. In particular, the dislocation energy spent to release the bulk energy is predominant, but still $\theta_R \neq \alpha^{-1}$, so that also a far field bulk energy is present (see Figure 1).

In order to compute the optimal θ_R, we perform a Taylor expansion (through a Γ-convergence analysis) of the plastic and elastic part of the energy, proving in particular that the first scales like R^2, while the second like R. Prefactors in such energy expansions are computed, depending only on α, σ and on the fourth-order tensor obtained by linearizing W.

In conclusion, the proposed functional provides a simple prototypical variational model to describe the competition between the dislocation energy concentrated in the vicinity of the interface between materials with different crystal structures, and the far field elastic energy. This model fits into the class of free boundary problems, since the overlayer is a variable in the minimization problem, though only through a scalar parameter representing its size. Our formulation is quite specific, dealing with two lattices where one is a small dilation of the other. Therefore, it is meant to model semi-coherent interfaces between two different lattices, for example in heterostructured nanowires. Nevertheless, our approach seems flexible enough to be adapted to more general situations, to model epitaxial crystal growth (where the surface energy of the free external boundary in contact with air should be added to the energy functional), and to more general interfaces, such as grain boundaries, where the misfit in the crystal structures is due to mutual rotations between the grains instead of dilations of the lattice parameters.

1. A LINE DEFECT MODEL

1.1. **Description of the model.** We introduce a semi-discrete model for dislocations, which are described as line defects of the strain.

Let $\Omega_1 = S_1 \times (-h, h)$ be the reference configuration of a cylindrical hyperelastic body. Here $h > 0$ is a fixed height and $S_1 = \{(x_1, x_2, 0) \in \mathbb{R}^3 : |x_1|, |x_2| < 1/2\}$ is a square of side one centered at the origin, separating parts of the body with underlying crystal structures Λ^- and $\Lambda^+ := \alpha \Lambda^-$, with $\alpha > 1$. For any given $r > 0$, we will consider scaled versions of the body $\Omega_r := r\Omega_1$ and $S_r := rS_1$.

Set $\Omega_r^- := S_r \times (-hr, 0)$ and $\Omega_r^+ := S_r \times (0, hr)$. We assume that the material equilibrium is the identity I in Ω_r^- (which means that the material is already in equilibrium in Ω_r^-) and αI in Ω_r^+. We are interested in small misfits, which generate so called semi-coherent interfaces; therefore, we will deal with $\alpha \approx 1$. More specifically, we assume that the lattice distances of Λ^- and Λ^+ are commensurable, and in particular that $\alpha := 1 + 1/n$ for some given $n \in \mathbb{N}$. Moreover, in order to simplify the analysis, we assume that Ω_r^- is rigid, namely, that the admissible deformations coincide with the identical deformation in Ω_r^-.

According to the hypothesis of hyperelasticity, we assume that the crystal tries to minimize a stored elastic energy (in Ω_r^+), whose density is described by a function $W \colon \mathbb{M}^{3 \times 3} \to [0, +\infty)$. We require that W is continuous and frame indifferent, i.e.,

$$(3) \qquad W(F) = W(RF) \qquad \text{for every} \quad F \in \mathbb{M}^{3 \times 3}, R \in SO(3).$$

Moreover, there exist $p \in (1, 2)$ and constants $C_1, C_2 > 0$ such that W satisfies the following growth conditions:

$$(4) \quad C_1 \left(\operatorname{dist}^2(F, \alpha SO(3)) \wedge (|F|^p + 1) \right) \le W(F) \le C_2 \left(\operatorname{dist}^2(F, \alpha SO(3)) \wedge (|F|^p + 1) \right)$$

for every $F \in \mathbb{M}^{3 \times 3}$. Here the condition $p > 1$ prevents the formation of cracks in the body, while $p < 2$ guarantees that dislocations induce finite core energy, as explained below.

In absence of dislocations, the deformed configuration of the body can be described by a sufficiently smooth deformation $v \colon \Omega_r^+ \to \mathbb{R}^3$. The corresponding elastic energy is given
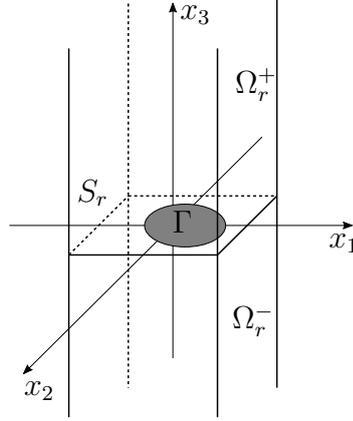
FIGURE 3. Reference configuration Ω_r .

by

$$E^{el}(v) := \int_{\Omega_r^+} W(\nabla v)\, dx. \tag{5}$$

The field ∇v is referred to as the deformation strain.

We now explain how to introduce dislocations in the present model. As in [18], dislocations are described by deformation strains whose curl is not free, but concentrated on lines lying on the interface S_r between Ω_r^- and Ω_r^+.

Assume for the time being that the dislocation line $\gamma \subset S_r$ is a Lipschitz, relatively closed curve in S_r. The latter condition implies that $\Omega_r \smallsetminus \gamma$ is not simply connected. Therefore, the strain is a map $F \in L^p(\Omega_r; \mathbb{M}^{3\times 3})$ that satisfies

$$\operatorname{curl} F = -\mathbf{b}_\gamma \otimes \dot{\gamma}\, d\mathcal{H}^1 \llcorner \gamma \tag{6}$$

in the sense of distributions and $F = I$ in Ω_r^-. The vector $\mathbf{b}_\gamma \in \mathbb{R}^3$ denotes the Burgers vector, which is constant on γ, and together with the dislocation line γ, uniquely characterizes the dislocation. From (6) one can deduce that in the vicinity of γ

$$|F(x)| \sim \frac{1}{\operatorname{dist}(x, \gamma)}\,, \tag{7}$$

which implies that the L^2 norm of F in a cylindrical neighborhood of γ diverges logarithmically. This is exactly why we consider energy densities W which grow slower than quadratic at infinity.

The Burgers vector belongs to the class of slip directions, which is a given material property of the crystal. As a further simplification, we assume that the slip directions are given by $b\mathbb{Z}\{e_1, e_2\}$, where $b > 0$ represents the lattice spacing of the lower crystal Ω_r^-.

If $\omega \subset \Omega_r \smallsetminus \gamma$ is a simply connected region, then (6) implies that $\operatorname{curl} F = 0$ in $\mathcal{D}'(\omega, \mathbb{M}^{3\times 3})$ and therefore there exists $v \in W^{1,p}(\omega; \mathbb{R}^3)$ such that $F = \nabla v$ a.e. in ω. Thus, any vector field F satisfying (6) is locally the gradient of a Sobolev map. In particular, if Σ is a sufficiently smooth surface having γ as its boundary, then one can

find $v \in SBV_{\text{loc}}(\Omega_r; \mathbb{R}^3)$ such that $F = \nabla v$, $v = x$ in Ω_r^- and its distributional gradient satisfies

$$Dv = \nabla v \, dx + \mathbf{b}_\gamma \otimes \nu \, d\mathcal{H}^2 \llcorner \Sigma$$

where ν is the unit normal to Σ. That is, $F = \nabla v$ is the absolutely continuous part of the distributional gradient of v. As customary (see [20]), we interpret F as the elastic part of the deformation v, so that the elastic energy induced by v is given by

$$E^{el}(v) := \int_{\Omega_r^+} W(F) \, dx.$$

From now on we will assume that the dislocation curves have support in the grid $(b\mathbb{Z} \times \mathbb{R}) \cup (\mathbb{R} \times b\mathbb{Z})$. Moreover, we will consider multiple dislocation curves. More precisely, we denote by $\mathcal{AD}$ the class of all admissible pairs $(\Gamma, \mathbf{B})$, where Γ is a finite collection of admissible closed curves $\{\gamma_i\}$, and $\mathbf{B} = \{\mathbf{b}_i\}$, $\{\mathbf{b}_i\} \in b\{z_1 e_1 + z_2 e_2 : z_1, z_2 \in \mathbb{Z}\}$, is the corresponding collection of Burgers vectors. Notice that each dislocation curve can be decomposed into "minimal components", i.e., we can always assume that $\gamma_i = \partial Q_i$, where Q_i is a square of size b with sides contained in the grid $(b\mathbb{Z} \times \mathbb{R}) \cup (\mathbb{R} \times b\mathbb{Z})$. Given an admissible pair $(\Gamma, \mathbf{B})$, we denote by $\mathbf{b} \otimes \dot{\gamma}(x)$ the field that coincides with $\mathbf{b}_i \otimes \dot{\gamma}_i(x)$ if x belongs to a single curve γ_i, and with $\mathbf{b}_i \otimes \dot{\gamma}_i(x) + \mathbf{b}_j \otimes \dot{\gamma}_j(x)$ if x belongs to two different curves γ_i and γ_j. The set of admissible deformation strains $\mathcal{AS}(\Gamma, \mathbf{B})$ associated with a given admissible dislocation $(\Gamma, \mathbf{B})$ is then defined by

$$(8) \qquad \mathcal{AS}(\Gamma, \mathbf{B}) := \left\{ F \in L^p_{\text{loc}}(\Omega_r; \mathbb{M}^{3\times 3}): F = I \text{ in } \Omega_r^-, \text{ curl } F = -\mathbf{b} \otimes \dot{\gamma} \, d\mathcal{H}^1 \llcorner \Gamma \right\},$$

where, abusing notation, we identify Γ with the union of the supports of γ_i. We define the minimal energy induced by the pair $(\Gamma, \mathbf{B})$ as

$$(9) \qquad E_{\alpha,r}(\Gamma, \mathbf{B}) := \inf \left\{ \int_{\Omega_r^+} W(F(x)) \, dx : F \in \mathcal{AS}(\Gamma, \mathbf{B}) \right\}$$

and the minimal energy induced by the lattice misfit as

$$(10) \qquad E_{\alpha,r} := \min \left\{ E_{\alpha,r}(\Gamma, \mathbf{B}) : (\Gamma, \mathbf{B}) \in \mathcal{AD} \right\}.$$

Notice that, by the growth assumptions (4) on W and by (7), the minimum problem in (10) involves only dislocations with Burgers vectors in a bounded set (and thus in a finite set), so that the existence of a minimizer is trivial. We denote by $E_{\alpha,r}(\emptyset)$ the minimal elastic energy induced by curl free strains. Notice that $E_{\alpha,r}(\Gamma, \mathbf{B}) = E_{\alpha,r}(\emptyset)$ whenever $\Gamma \cap S_r = \emptyset$.

For the sake of computational simplicity, whenever it is convenient we will assume

$$(11) \qquad \frac{r(\alpha - 1)}{2b} \in \mathbb{N}.$$

Recalling that $\alpha = 1 + \dfrac{1}{n}$, assumption (11) implies that $\dfrac{r}{2b} \in \mathbb{N}$.

1.2. **Scaling properties of the energies.** The next proposition, proved in [18, Proposition 3.2], states that the quantities defined by (9) and (10) are strictly positive.

Proposition 1.1. *For all $r > 0$ one has $E_{\alpha,r} > 0$. Moreover, $E_{\alpha,r}(\emptyset) = r^3 E_{\alpha,1}(\emptyset)$, with $E_{\alpha,1}(\emptyset) > 0$.*

Proposition 1.1 asserts that $E_{\alpha,r}(\emptyset)$ grows cubically in r. We will show that the energy (9) can grow quadratically in r by suitably introducing dislocations on S_r. In fact we will introduce dislocations on the boundary of many (of the order of $(r(\alpha - 1)/b)^2$) squares.

Proposition 1.2. *There exists $0 < E_\alpha < +\infty$ such that*

$$\tag{12} \lim_{r \to +\infty} \frac{E_{\alpha,r}}{r^2} = E_\alpha.$$

Proof. For the sake of computational simplicity, we assume that (11) holds, so that $r/2 \in b\mathbb{N}$ (see Remark 1.3 to deal with the general case). We first show that the limit exists. Let $m, n \in \mathbb{N}$ with $n > m$, and let j be the integer part of $\frac{n}{m}$, $R := nb$, $r := mb$. Then, there are j^2 disjoint squares of size r in S_R, so there are j^2 disjoint sets equivalent to Ω_r (up to horizontal translations) in Ω_R. By minimality, $E_{\alpha,r}$ is smaller than the energy stored in each of such domains, so that

$$\tag{13} \frac{E_{\alpha,r}}{r^2} \le \frac{E_{\alpha,R}}{r^2 j^2} = \frac{E_{\alpha,R}}{R^2 + q(r)},$$

where $q(r) := -\big[(\frac{R}{r} - j)^2 + 2j(\frac{R}{r} - j)\big]r^2 = o(R^2)$. Since this inequality holds true for all $r, R \in b\mathbb{N}$ with $r \le R$, we deduce that

$$\liminf_{n \to +\infty} \frac{E_{\alpha,bn}}{(bn)^2} = \limsup_{n \to +\infty} \frac{E_{\alpha,bn}}{(bn)^2} = \lim_{n \to +\infty} \frac{E_{\alpha,bn}}{(bn)^2} =: E_\alpha.$$

In order to establish that $E_\alpha > 0$, it suffices to use (13) with $r = 1$ and to recall that, by Proposition 1.2, $E_{\alpha,1} > 0$.

Next we show that $E_\alpha < +\infty$. For this purpose, we will exhibit a sequence of deformations and associated dislocations for which the energy grows at most quadratically in r. The construction uses some ideas introduced in [17] and [18]. Let $\delta := \frac{b}{(\alpha-1)} = nb$ and recall that by (11) we have $r/\delta \in \mathbb{N}$. Denote by Q_i, $i = 1, \ldots, q$, the squares of side δ with vertices in the lattice $S_r \cap \delta\mathbb{Z}^2$, and let x_i be the center of each Q_i. Since the side of S_r is r, we have that $q = (r/\delta)^2$.

We will define a deformation $v \colon \Omega_r \to \mathbb{R}^3$ such that $v = x$ in Ω_r^-, $v = \alpha x$ if $x_3 > \delta$ and the transition from x to αx is distributed into constant jumps across the squares Q_i's. In this way the energy will be concentrated in a δ-neighbourhood of the interface S_r and the contribution to the energy will come mostly from dislocations.

To this end, let C_i^1 and C_i^2 be the pyramids of base Q_i and vertices $x_i + \delta/2\, e_3$ and $x_i + \delta e_3$ respectively. Define a displacement $u \colon \Omega_r \to \mathbb{R}^3$ such that

$$u(x) = \begin{cases} (\alpha - 1)x & \text{if } x \in \Omega_r^+ \smallsetminus \cup_{i=1}^q C_i^2 \\ 0 & \text{if } x \in \Omega_r^- \, . \end{cases}$$

$$u \equiv (\alpha - 1)x_i \quad u \equiv (\alpha - 1)x_j$$
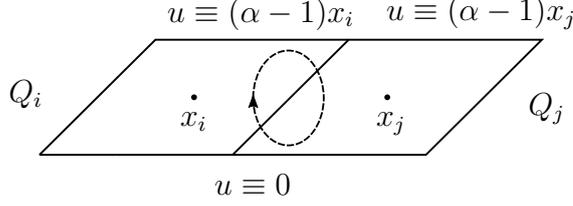
FIGURE 4. A loop winding around $\gamma_{ij} = Q_i \cap Q_j$.

We complete the above definition by setting $u := u_i$ in C_i^2, where u_i is the unique solution of the minimum problem

$$
(14) \quad m_{\delta,p,(\alpha-1)I} := \min \left\{ \int_{C_i^2} |\nabla v|^p \; : \; v \in W_{loc}^{1,p}(\mathbb{R}_+^3), \; v \equiv (\alpha - 1)x_i \text{ in } C_i^1, \right.
$$
$$
\left. v(x) = (\alpha - 1)x \text{ in } \mathbb{R}_+^3 \setminus C_i^2 \right\},
$$

where $\mathbb{R}_+^3 := \mathbb{R}^3 \cap \{x_3 > 0\}$. Notice that $m_{\delta,p,(\alpha-1)I}$ is independent of i and that u is well defined; indeed if Q_i and Q_j are adjacent squares, i.e.,

$$Q_j = Q_i \mp \delta e_s \qquad \text{for some} \quad s \in \{1,2\},$$

then

$$u_j(x) = u_i(x \pm \delta e_s) \mp (\alpha - 1)\delta e_s \quad \text{for every} \quad x \in Q_j \times [0, +\infty].$$

Moreover, in Proposition 1.6 we will show that $0 < m_{\delta,p,(\alpha-1)I} < +\infty$ and

$$
(15) \quad m_{\delta,p,(\alpha-1)I} = \delta^3 (\alpha - 1)^p \, m_{1,p,I} \, .
$$

Set $v = x + u$. Notice that the deformation v has constant jump equal to $(\alpha - 1)x_i$ across Q_i. Therefore, if Q_i and Q_j are adjacent and we set $\gamma_{ij} := Q_i \cap Q_j$, we have that γ_{ij} is a dislocation line with Burgers vector $\mathbf{b}_{ij} = (\alpha - 1)(x_j - x_i)$ (see Figure 5). By construction $\gamma_{i,j}$ lies in the grid $(b\mathbb{Z} \times \mathbb{R}) \cup (\mathbb{R} \times b\mathbb{Z})$. Moreover, since $\delta = b/(\alpha - 1)$, $\mathbf{b}_{ij} \in \pm b\{e_1, e_2\}$. Therefore, setting $\Gamma := \{\gamma_{ij}\}$ and $\mathbf{B} := \{\mathbf{b}_{ij}\}$, we have that $(\Gamma, \mathbf{B}) \in \mathcal{AD}$ and $\nabla v \in \mathcal{AS}(\Gamma, \mathbf{B})$.

We are left to estimate from above the elastic energy of v. Recalling that $W(\alpha I) = 0$, the growth condition (4) and (15), we get

$$
\int_{\Omega_r^+} W(\nabla v) = \sum_{i=1}^q \int_{C_i^2} W(\nabla v) \leq C \sum_{i=1}^q \int_{C_i^2} (|\nabla v|^p + 1)
$$
$$
\leq Cq \left| C_i^2 \right| + q\delta^3 (\alpha - 1)^p \, m_{1,p,I} = q\delta^3 \left(C + (\alpha - 1)^p \, m_{1,p,I} \right) .
$$

Writing $q = r^2/\delta^2$ and $\delta = b/(\alpha - 1)$ yields

$$
(16) \quad \int_{\Omega_r^+} W(\nabla v) \leq r^2 b \left[(\alpha - 1)^{p-1} \, m_{1,p,I} + (\alpha - 1)^{-1} C \right] .
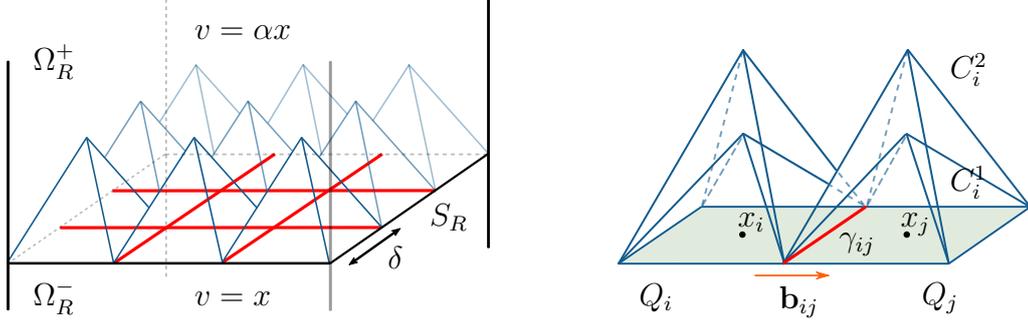$$

$\square$

FIGURE 5. The double pyramid construction.

Remark 1.3. In the case when (11) does not hold, it suffices to observe that

$$E_{\alpha,[\frac{r}{2\delta}]2\delta} \leq E_{\alpha,r} \leq E_{\alpha,[\frac{r}{2\delta}]2\delta+2\delta} \quad \text{and} \quad \lim_{r\to\infty} \frac{([\frac{r}{2\delta}]2\delta)^2}{r^2} = \lim_{r\to\infty} \frac{([\frac{r}{2\delta}]2\delta + 2\delta)^2}{r^2} = 1,$$

where $[a]$ denotes the integer part of a. The above inequalities follow from the fact that if $r_1 < r_2$, then the restriction to Ω_{r_1} of any test function for E_{α,r_2} provides a test function for E_{α,r_1}.

Remark 1.4. The proof of the asymptotic behavior of the energy described by Proposition 1.2 strongly relies on the assumption made on the admissible dislocation lines. In fact, local lower bounds of the energy can be easily obtained in a neighborhood of the dislocation lines, as long as these are sufficiently regular and well separated.

As a corollary of Propositions 1.1 and 1.2 we obtain the following theorem, asserting that nucleation of dislocations is energetically convenient for sufficiently large values of r.

Theorem 1.5. *There exists a threshold r^* such that, for every $r > r^*$,*

$$E_{\alpha,r} < E_{\alpha,r}(\emptyset).$$

1.3. **Double pyramid construction.** Fix $\delta > 0$ and let C^1 and C^2 be the pyramids with common base the square $(-\delta/2, \delta/2)^2 \times \{0\}$ and heights $\delta/2$ and δ respectively. Note that $C^1 \subset C^2$. Set $S := C^2 \cap \{\delta/2 < x_3 < \delta\}$ and $T := (C^2 \smallsetminus C^1) \cap \{0 < x_3 < \delta/2\}$. See Figure 6 for a cross section of the construction in cylindrical coordinates.
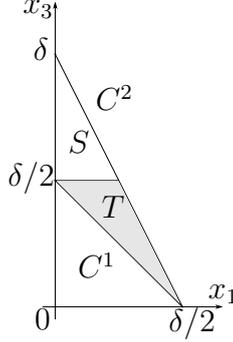
Let $A \in \mathbb{M}^{3\times 3}$ with $A \neq 0$, and consider the following minimization problem

$$(17) \quad m_{\delta,p,A} := \inf \left\{ \int_{C^2} |\nabla v|^p \, dx : v \in W_{loc}^{1,p}(\mathbb{R}^3_+), \, v \equiv 0 \text{ in } C^1, \, v \equiv Ax \text{ in } \mathbb{R}^3_+ \smallsetminus C^2 \right\},$$

where $\mathbb{R}^3_+ := \mathbb{R}^3 \cap \{x_3 > 0\}$.

Proposition 1.6. *The following facts hold true:*

   i) *For every $1 < p < 2$, there exists a minimizer of problem (17) and the minimal value $m_{1,p,A}$ is streactly positive;*
   ii) *$m_{1,2,A} = +\infty$;*
   iii) *for all positive δ and λ we have $m_{\delta,p,\lambda A} = \delta^3 \lambda^p m_{1,p,A}$.*

FIGURE 6. Section $\varphi = 0$ of the double pyramid.

Proof. Property iii) holds because if v is a competitor for $m_{\delta,p,\lambda A}$, then $\tilde{v}(x) := v(\delta x)/\lambda \delta$ is a competitor for $m_{1,p,A}$.

As far as i) is concerned, first remark that $m_{1,p,A} > 0$. Indeed, arguing by contradiction assume that $m_{1,p,A} = 0$; Then, by the direct method of the calculus of variations, we would have a minimizer v satisfying $\nabla v \equiv 0$ in C^2 and $\nabla v \equiv A$ in $\mathbb{R}^3_+ \setminus C^2$, which provides a contradiction since this is only possible when $A = 0$.

Now, we will prove that $m_{1,p,A} < +\infty$ by exhibiting an admissible deformation v with finite energy. In order to simplify the computations, we will show it in the case when C^1 and C^2 are the cones with base the disk of diameter 1 and center the origin, and heights $1/2$ and 1 respectively. The estimate in the case of two pyramids can be proved in the same way, with minor changes.

Introduce the cylindrical coordinates $x_1 = \rho \cos \varphi$, $x_2 = \rho \sin \varphi$ and $x_3 = z$, with $\rho > 0$ and $\varphi \in [0, 2\pi)$. Set $v := 0$ in C^1 and $v(x) := Ax$ in $\mathbb{R}^3_+ \setminus C^2$. First we extend v to S. To this end, for all $\bar{\varphi} \in [0, 2\pi)$ we define v in the triangle $S_{\bar{\varphi}} := S \cap \{\varphi = \bar{\varphi}\}$ by linear interpolation of the values of v at the three vertices of $S_{\bar{\varphi}}$. Notice that v is Lipschitz continuous in S. Next, we extend v to $T := C^2 \setminus (S \cup C^1)$. For this purpose, for all $\bar{\varphi} \in [0, 2\pi)$ and $\bar{z} \in (0, \frac{1}{2})$ consider the segment $L_{\bar{\varphi}, \bar{z}} := T \cap \{\varphi = \bar{\varphi}\} \cap \{z = \bar{z}\}$, and define v on $L_{\bar{\varphi}, \bar{z}}$ by linear interpolation of the values of v on the two extreme points of $L_{\bar{\varphi}, \bar{z}}$.

We will now estimate the L^p norm of ∇v in C^2. Since v is piecewise Lipschitz in $C^2 \setminus T$, we only have to compute the energy in T. By construction we have that

$$(18) \qquad |\nabla v(x, y, z)| \leq \frac{c}{z} \qquad \text{for all } (x, y, z) \in T,$$

where c are suitable positive constant depending only on A. A straightforward computation yields $m_{1,p,A} \leq C(p, A)$ with the constant C depending only on A and p, and diverging as $p \to 2^-$. By the direct method of the calculus of variations we easily deduce i).

Finally, let us prove ii), i.e., that $m_{1,2,A} = +\infty$. For every admissible function v and all $0 < \varepsilon < 1/2$, by Jensen's inequality we have

$$\int_{T \cap \{\varepsilon < z < \frac{1}{2}\}} |\nabla v|^2 \, dx \geq \int_{T \cap \{\varepsilon < z < \frac{1}{2}\}} \left|\frac{\partial v}{\partial \rho}\right|^2 dx \geq c \int_\varepsilon^{\frac{1}{2}} \frac{1}{s} \left(\int_{T \cap \{z = s\}} \frac{\partial v}{\partial \rho} \, d\rho\right)^2 ds \geq c \log \frac{1}{\varepsilon}.$$

Taking the limit $\varepsilon \to 0$ yields $\int_{C^2} |\nabla v|^2 = +\infty$. $\square$

2. Some considerations on the proposed model

In this section we discuss some features and limits of the semi-discrete model presented in Section 1, in connection with modeling epitaxial growth, heterostructured nanowires and grain boundaries. Such limits of the theory will be overcome in the continuous model discussed an analyzed in details in the next section. In this respect, the semi-discrete model is somehow meant as a theoretical background to derive material constants, and in particular the energy per unit dislocation length and interface area, that will be involved in the continuous model discussed in Section 3.

In the construction illustrated in the proof of Proposition 1.2, $v(S_r)$ is the union of disjoint squares of size δ, separated by strips of width b; dislocation lines lie in the middle of such strips (see Fig. 8). Note that some lines of atoms (in the deformed configuration) fall out of S_r (see Figure 7), suggesting that the chosen reference configuration is not convenient to describe heterostructured nanowires, or epitaxial growth.

FIGURE 7.   A 2D discrete cross section of the crystal, deformed according to the construction made in the proof of Proposition 1.2.

In fact, this is not the physical configuration we are interested in modeling and analyzing. In order to prevent unphysical configurations like in Figure 7, where some lines of atoms fall out of S_r, in the next section we will rather modify our point of view: We will deal with a reference configuration $\Omega_{R,r} := \Omega_R^- \cup S_r \cup \Omega_r^+$ with $r := \theta R$ for some $0 < \theta < 1$ (see Figure 9), enforcing that $v(S_r) = S_R$, thus describing a perfect match between the two parts of the crystal as in Figure 1. The new parameter θ represents the ratio between the size of S_r and that of its deformed counterpart $v(S_r)$. Optimization over θ corresponds to "getting rid" of unnecessary atoms at the interface and will yield (see (54)) $\theta \approx \alpha^{-1}$ in the limit $R \to \infty$.

In this context it is quite natural to measure the dislocation length in the deformed configuration $v(\Omega_r^+)$. In the construction made in the proof of Proposition 1.2, the number of dislocation straight-lines is of the order $\frac{2r}{\delta}$, where $\delta = \frac{b}{\alpha-1}$. Mimicking the same construction in the new reference configuration $\Omega_{R,r}$, in order to enforce $v(S_r) = S_R$, now we have to choose $\delta = \frac{b}{\theta^{-1}-1}$. The total length L of dislocations (in the deformed configuration) is then of the order $L = \frac{2r^2}{b}(\theta^{-2} - \theta^{-1})$. The above formula can be obtained alternatively

as follows. Let $\tilde{L}$ be the total length of dislocations in the reference configuration. Then, $b\tilde{L}$ coincides with the total variation of μ, the curl of the deformation strain, which is a measure concentrated on S_r. By a direct computation the total variation $|\mu|(S_r)$ is given by $r^2 2\left(\theta^{-1} - 1\right)$. Therefore,

$$L = \theta^{-1}\tilde{L} = \frac{\theta^{-1}}{b}r^2 2\left(\theta^{-1} - 1\right) = \frac{2r^2}{b}(\theta^{-2} - \theta^{-1}).$$

We are interested in small misfits $\theta^{-1} \approx 1$. Therefore, $(\theta^{-2} - \theta^{-1}) \approx \frac{1}{2}(\theta^{-2} - 1)$, so that the total length of dislocations is of the order

$$L = \frac{1}{b}r^2(\theta^{-2} - 1) = \frac{1}{b} \text{ Area Gap},$$

where Area Gap, in a continuous modeling of the crystal, represents the difference between the area of the base of the deformed configuration $v(\Omega_r^+) = S_R$ of Ω_r^+, and the area of the base of the reference configuration, namely the area of S_r (see Figure 8 and Figure 9).
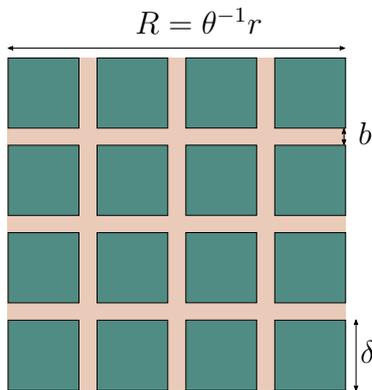

FIGURE 8. The deformed configuration $v(S_r)$. The total dislocation length is given, in first approximation, by the area of the region in lighter color divided by b.

We do not claim that our constructions are optimal in energy. Nevertheless, we believe that, as $r, R \to \infty$, the optimal configuration of dislocations exhibit some periodicity. As a matter of fact, in Proposition 1.2 we have proved that

$$(19) \qquad E_{\alpha,r} \approx r^2 E_\alpha = \sigma_{\alpha,\theta} \text{ Area Gap} \qquad \text{as } r \to +\infty,$$

for

$$\sigma_{\alpha,\theta} := \frac{E_\alpha}{\theta^{-2} - 1}.$$

In view of the considerations above, this reflects that the energy is proportional to the total dislocation length. In particular, as $r \to \infty$ and $\alpha \to 1^+$, we expect that $E_{\alpha,r}$ be minimized by a periodic configuration of more and more dilute and well separated dislocations. Taking this into account, we expect that

$$(20) \qquad \lim_{\alpha \to 1^+} \frac{E_\alpha}{\alpha^2 - 1} = \lim_{\alpha \to 1^+} \sigma_{\alpha,\alpha^{-1}} =: \sigma,$$

for some $0 < \sigma < \infty$, where $b\sigma$ represents the self energy of a single dislocation line per unit length.

Let us compare the nonlinear energy induced by dislocations with the solid framework of linearized elasticity. It is well known that the energy per unit (edge dislocation) length in a single crystal of size r is given by $b^2 \frac{\mu}{4\pi(1-\nu)} \ln(\frac{r}{b})$ (see, e.g., [12, 19]), where μ is the shear modulus and ν is the Poisson's ratio. Based on the heuristic observation that the periodicity of the lattice is restored on lines at the interface which are equidistant from two consecutive edge dislocations, one could exploit this formula, with r replaced by the average distance $\delta = \frac{b}{\alpha-1}$ between dislocations. Moreover, due to the fact that Ω_R^- is rigid, the stress and the corresponding energy are concentrated on half disks around each dislocation (in fact, half cylinders around the dislocation lines). A purely dimensional argument yields that the resulting strain is twice the one induced by the dislocations in a purely elastic single crystal; the corresponding elastic energy density, being quadratic, should be multiplied by 4, but it is concentrated on half domain (the half cylinders). The resulting energy is then twice the energy induced by the dislocations in a purely elastic crystal. These heuristic arguments lead us to consider the following energy per unit dislocation length:

$$(21) \qquad \gamma^{lin} := b^2 \frac{\mu}{2\pi(1-\nu)} \ln\left(\frac{1}{\alpha-1}\right).$$

To such energy, a chemical core energy γ^{ch} per unit dislocation length should be added. Notice that this contribution is already present in our nonlinear formulation, and it is stored in the region where $|\nabla v|$ is large, and the energy density $W(\nabla v)$ behaves like $|\nabla v|^p$. We deduce that, for small misfits,

$$(\gamma^{lin} + \gamma^{ch})\frac{1}{b} \text{ Area Gap } \approx E_{\alpha,r} \approx \sigma \text{ Area Gap},$$

which yields the following expression for σ:

$$(22) \qquad \sigma = b\frac{\mu}{2\pi(1-\nu)} \ln\left(\frac{1}{\alpha-1}\right) + \frac{1}{b}\gamma^{ch}.$$

Finally, we notice that $\sigma(\alpha^2 - 1)$ is noting but the energy per unit surface area, so that the total energy is given by

$$E_{\alpha,r} \approx r^2(\alpha^2 - 1)\left(b\frac{\mu}{2\pi(1-\nu)} \ln\left(\frac{1}{\alpha-1}\right) + \frac{1}{b}\gamma^{ch}\right).$$

3. A SIMPLIFIED CONTINUOUS MODEL FOR DISLOCATIONS

Based on the analysis and the considerations on the semi-discrete model discussed in Section 2, here we want to propose a simplified and more realistic model for dislocations at interfaces. Instead of working with SBV functions with piece-wise constant jumps on the interface, we allow only for regular jumps but we introduce a penalization to the elastic energy, which represents the dislocation energy.

3.1. **The simplified energy functional.** Fix $\alpha > 1$, $R > 0$, $\theta \in [\alpha^{-1}, 1]$ and set $r := \theta R$. Let $\Omega_R^- := S_R \times (-hR, 0)$, where $S_R \subset \mathbb{R}^2$ is the square of side length R centered at the origin and $h > 0$ a fixed height. Define now the reference configuration (see Figure 9),

$$\Omega_{R,r} := \Omega_R^- \cup S_r \cup \Omega_r^+.$$

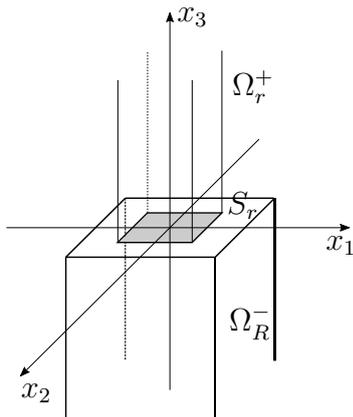As in Section 1 we will suppose that Ω_R^- is rigid and that Ω_r^+ is in equilibrium with αI.

FIGURE 9. Reference configuration $\Omega_{R,r}$.

We assume that there exists an energy density $W \colon \mathbb{M}^{3\times 3} \to [0, +\infty)$ that is continuous, C^2 in a neighborhood of $\alpha SO(3)$ and frame indifferent (see (3)). Furthermore we suppose that

$$(23) \qquad\qquad\qquad\qquad W(\alpha I) = 0$$

and that for every $F \in \mathbb{M}^{3\times 3}$

$$(24) \qquad\qquad\qquad C_1 \operatorname{dist}^2(F, \alpha SO(3)) \le W(F)$$

for some constant $C_1 > 0$. Here we assume that W grows more than quadratically, since the energy density describes now only the bulk elastic energy stored in the crystal, i.e., the strain is actually curl-free, while the core dislocation energy is taken into account by an additional plastic term, defined in (26) below. In fact one could also consider weaker growth conditions away from the well (see [1]); however we will stick to (24) for simplicity. The class of admissible deformation maps is defined by

$$(25) \qquad \mathcal{ADM}_{\theta,R} := \left\{ v \in W^{1,2}(\Omega_r^+; \mathbb{R}^3) : v(x) = \frac{1}{\theta} x \text{ on } S_r \right\}.$$

In this way $v(S_r) = S_R$ for all $v \in \mathcal{ADM}_{\theta,R}$. A deformation $v \in \mathcal{ADM}_{\theta,R}$ stores an elastic energy

$$E_{\alpha,R}^{el}(\theta, v) := \int_{\Omega_r^+} W(\nabla v(x)) \, dx \, .$$

To this energy we add a dislocation energy $E_R^{pl}(\theta)$ proportional to the area of $S_R \setminus S_r$, representing the total dislocation length,

$$(26) \qquad E_R^{pl}(\theta) := \sigma r^2(\theta^{-2} - 1) = \sigma R^2(1 - \theta^2).$$

Here $\sigma > 0$ is a given constant, which in our model is a material property of the crystal, representing (multiplied by b) the energy cost of dislocations per unit length. In principle, σ could be derived starting from the semi-discrete model discussed in Section 1. Assuming isotropic linearized elasticity, a possible choice is to set σ according to (20) (where the Lamé coefficients are obtained from W by linearization), so that $b\sigma$ represents the energy induced by a single dislocation line per unit length. We are thus led to study the energy functional

$$E_{\alpha,R}^{tot}(\theta, v) := E_{\alpha,R}^{el}(\theta, v) + E_R^{pl}(\theta) = \int_{\Omega_r^+} W(\nabla v(x))\, dx + \sigma R^2(1 - \theta^2).$$

We further define

$$(27) \qquad E_{\alpha,R}^{el}(\theta) := \inf \left\{ E_{\alpha,R}^{el}(\theta, v) : v \in \mathcal{ADM}_{\theta,R} \right\}, \qquad E_{\alpha,R}^{tot}(\theta) := E_{\alpha,R}^{el}(\theta) + E_R^{pl}(\theta).$$

As explained in the Introduction, the case $\theta = 1$ corresponds to a dislocation free configuration, i.e., $E_{\alpha,R}^{tot}(1) = E_{\alpha,R}^{el}(1)$. Instead, if $\theta = \alpha^{-1}$ no elastic energy is stored, since $v(x) := \alpha x$ is admissible and $W(\alpha I) = 0$. In order to simplify notation we set $E_\alpha^{el}(\theta) := E_{\alpha,\frac{1}{\theta}}^{el}(\theta)$, which corresponds to the minimum energy in the unit cylinder, i.e., with $r = 1$.

Proposition 3.1. *The elastic energy $E_{\alpha,R}^{el}(\theta)$ satisfies:*

  i) $E_{\alpha,R}^{el}(\theta) = R^3\theta^3 E_\alpha^{el}(\theta)$;
  ii) $E_\alpha^{el}(\theta) > 0$ *if and only if $\theta > \alpha^{-1}$.*

Proof. Property i) follows by noticing that if v is in $\mathcal{ADM}_{\theta,R}$, then $\tilde{v}(x) := v(R\theta x)/R\theta$ is in $\mathcal{ADM}_{\theta,\frac{1}{\theta}}$. For the second property, we have to prove that $E_\alpha^{el}(\theta) = 0$ if and only if $\theta = \alpha^{-1}$. We already pointed out that $E_\alpha^{el}(\alpha^{-1}) = 0$. Suppose that $E_\alpha^{el}(\theta) = 0$. Then there exists a sequence $v_n \in H^1(\Omega_1^+; \mathbb{R}^3)$ such that $v_n|_{S_1} = \theta^{-1} x$ and

$$(28) \qquad \int_{\Omega_1^+} W(\nabla v_n)\, dx \to 0 \quad \text{as } n \to \infty.$$

The Rigidity Theorem 3.3, the growth assumption (24) and the compactness of $SO(3)$ in combination with (28) imply that there exists a fixed rotation $\mathcal{R} \in SO(3)$ such that (up to subsequences)

$$\int_{\Omega_1^+} |\nabla v_n - \alpha\mathcal{R}|^2\, dx \to 0 \quad \text{as } n \to \infty.$$

Setting $\zeta_n := (1/|\Omega_1^+|) \int_{\Omega_1^+} (v_n(x) - \alpha\mathcal{R}x)$, from the Poincaré inequality and the trace theorem we deduce that

$$(29) \qquad \int_{S_1} |v_n - \alpha\mathcal{R}x - \zeta_n|^2\, dx \to 0 \quad \text{as } n \to \infty.$$

Since $v_n = \theta^{-1}x$ on S_1, (29) yields

$$(30) \qquad (\theta^{-1}I - \alpha\mathcal{R})x - \zeta_n \to 0 \quad \text{in } L^2(S_1)\,,$$

which implies $\zeta_n \to 0$, $\mathcal{R} = I$ and $\theta = \alpha^{-1}$. $\qquad\qquad\square$

In analogy with Theorem 1.5, we find that for R sufficiently large, configurations with dislocations are energetically preferred.

Theorem 3.2. *There exists a threshold R^* such that, for every $R > R^*$*

$$(31) \qquad \inf_{\theta \in [\alpha^{-1}, 1)} E_{\alpha,R}^{tot}(\theta) < E_{\alpha,R}^{tot}(1) = E_{\alpha,R}^{el}(1)\,.$$

Proof. The left hand side of (31) can grow at most quadratically in R, indeed

$$\inf_{\theta \in [\alpha^{-1}, 1)} E_{\alpha,R}^{tot}(\theta) \le E_{\alpha,R}^{tot}(\alpha^{-1}) = \sigma R^2 \left(1 - \frac{1}{\alpha^2}\right)\,.$$

In contrast, by Proposition 3.1, the right hand side $E_{\alpha,R}^{tot}(1)$ grows cubically in R. $\qquad\square$

The minimal energy induced by the lattice misfit is given by

$$(32) \qquad E_{\alpha,R}^{tot} := \inf_{\theta \in [\alpha^{-1}, 1]} E_{\alpha,R}^{tot}(\theta)\,.$$

One can show that $E_{\alpha,R}^{tot}(\cdot)$ is continuous, so that the infimum is in fact a minimum. Our goal is to study the asymptotic behavior of $E_{\alpha,R}^{tot}$ as $R \to \infty$. In Theorem 3.7 we will write $E_{\alpha,R}^{tot}$ as an expansion in powers of R.

3.2. **An overview of the Rigidity Estimate and Linearization.** We recall the Rigidity Estimate from [10]. In this section, $U \subset \mathbb{R}^3$ will be a Lipschitz bounded domain.

Theorem 3.3 (Rigidity Estimate, [10]). *There exists a constant $C > 0$ depending only on the domain U such that the following holds: For every $v \in H^1(U; \mathbb{R}^3)$ there exists a constant rotation $R \in SO(3)$ such that*

$$(33) \qquad \int_U |\nabla v(x) - R|^2\, dx \le C \int_U \text{dist}^2(\nabla v(x); SO(3))\, dx\,.$$

In order to compute the Taylor expansion of $E_{\alpha,R}^{tot}$ defined in (32), we will linearize the elastic energy as in [6]. Therefore, following [6], we will make further assumptions on W. First, notice that by minimality the equilibrium αI is stress free, i.e.,

$$(34) \qquad \partial_F W(\alpha I) = 0\,.$$

By frame indifference there exists a function $V \colon \mathbb{M}_{sym}^{3\times3} \to [0, +\infty]$, such that

$$(35) \qquad W(F) = V\left(\frac{1}{2}\left(F^T F - \alpha^2 I\right)\right) \qquad \text{for every} \quad F \in \mathbb{M}_+^{3\times3}\,.$$

Here $\mathbb{M}_{sym}^{3\times3}$ is the set of 3×3 symmetric matrices, $\mathbb{M}_+^{3\times3}$ is the subset of matrices with positive determinant and F^T is the transpose matrix of F.

The regularity assumptions on W (see Subsection 3.1) imply that $V(E)$ is of class C^2 in a neighbourhood of $E = 0$. From (23), (34) and (35) it follows that $V(0) = 0$ and $\partial_E V(0) = 0$. Moreover, by (24), there exist $\gamma, \delta > 0$ such that

$$\partial_E^2 V(E)[T, T] \geq \gamma |T|^2 \quad \text{if } |E| < \delta \text{ and } T \in \mathbb{M}_{sym}^{3\times 3}.$$

By Taylor expansion we find

$$(36) \qquad\qquad V(E) = \frac{1}{2}\partial_E^2 V(0)[E, E] + o(|E|^2)\,.$$

Let $v \in W^{1,\infty}(U; \mathbb{R}^3)$ with $\nabla v \in \mathbb{M}_+^{3\times 3}$, and write $v = \alpha x + \varepsilon u$. Then from (35) it follows

$$W(\nabla v) = V\left(\alpha\varepsilon e(u) + \frac{\varepsilon^2}{2}C(u)\right),$$

where $e(u) := (\nabla u + \nabla u^T)/2$ and $C(u) := \nabla u^T \nabla u$. By (36) we get

$$(37) \qquad\qquad W(\nabla v) = \frac{\varepsilon^2}{2}A[e(u), e(u)] + o(\varepsilon^2)$$

where $A := \alpha^2 \partial_E^2 V(0)$ is the stress tensor. Notice that (37) is uniform in x, since ∇v is bounded. In particular

$$\lim_{\varepsilon \to 0}\frac{1}{\varepsilon^2}\int_U W(\alpha I + \varepsilon\nabla u)\, dx = \frac{1}{2}\int_U A[e(u), e(u)]\, dx\,.$$

In [6] it is proved that the above convergence holds also for minimizers. Specifically, let $\Sigma \subset \partial U$ be closed and such that $\mathcal{H}^2(\Sigma) > 0$. Introduce the space

$$H_{x,\Sigma}^1(U; \mathbb{R}^3) := \left\{u \in H^1(U; \mathbb{R}^3) : u(x) = x \text{ on } \Sigma\right\}$$

and, for $u \in H_{x,\Sigma}^1(U; \mathbb{R}^3)$, define the functionals

$$G_\varepsilon(u) := \frac{1}{\varepsilon^2}\int_U W(\alpha I + \varepsilon\nabla u)\, dx \qquad \text{and} \qquad G(u) := \frac{1}{2}\int_U A[e(u), e(u)]\, dx.$$

We can now recall [6, Theorem 2.1]:

Theorem 3.4 (Linearization). *If $\{u_\varepsilon\} \subset H_{x,\Sigma}^1(U; \mathbb{R}^3)$ is a minimizing sequence, i.e.,*

$$\inf_{H_{x,\Sigma}^1(U;\mathbb{R}^3)} G_\varepsilon = G_\varepsilon(u_\varepsilon) + o(1)$$

then u_ε converges weakly to the unique solution u_0 of

$$\min_{H_{x,\Sigma}^1(U;\mathbb{R}^3)} G\,.$$

Moreover we have

$$(38) \qquad\qquad \inf_{H_{x,\Sigma}^1(U;\mathbb{R}^3)} G_\varepsilon \to \min_{H_{x,\Sigma}^1(U;\mathbb{R}^3)} G \quad as \quad \varepsilon \to 0\,.$$

3.3. **Taylor expansion of the energy.** We can now carry on our analysis. We say that $\theta_R \in [\alpha^{-1}, 1]$ is a minimizing sequence for the energy $E_{\alpha,R}^{tot}$ defined in (32) if

$$E_{\alpha,R}^{tot} = E_{\alpha,R}^{tot}(\theta_R) + o(1)$$

where $o(1) \to 0$ as $R \to +\infty$.

Proposition 3.5. *Let θ_R be a minimizing sequence for $E_{\alpha,R}^{tot}$. Then*

  i) $E_\alpha^{el}(\theta_R) \to 0$ *as $R \to +\infty$;*
  ii) $\theta_R \to \alpha^{-1}$ *as $R \to +\infty$.*

Proof. By Proposition 3.1 we have (for R large enough)

$$R^3 \theta_R^3 E_\alpha^{el}(\theta_R) = E_{\alpha,R}^{el}(\theta_R) \leq E_{\alpha,R}^{tot}(\theta_R) \leq E_{\alpha,R}^{tot}(\alpha^{-1}) + 1 = \sigma R^2 \left(1 - \frac{1}{\alpha^2}\right) + 1,$$

which proves i), since $\theta_R \geq \alpha^{-1} > 0$.

Let us now prove ii). From i) we know that there exists a sequence $\{v_R\}$ in $H^1(\Omega_1^+; \mathbb{R}^3)$ such that $v_R = \theta_R^{-1} x$ on S_1 and

$$(39) \qquad \int_{\Omega_1^+} W(\nabla v_R) \, dx \to 0 \quad \text{as} \quad R \to +\infty.$$

Since $v_R = \theta_R^{-1} x$ on S_1, the proof is concluded once we show that $v_R \to \alpha x$ in $H^1(\Omega_1^+; \mathbb{R}^3)$. This can be shown following the lines of the proof of Proposition 3.1; the details are left to the reader. $\qquad\qquad\square$

If $v \in H^1(\Omega_1^+; \mathbb{R}^3)$ is such that $v = \theta^{-1} x$ on S_1, then we write

$$v = \alpha x + \left(\frac{1}{\theta} - \alpha\right) u$$

where $u \in H^1(\Omega_1^+; \mathbb{R}^3)$ is such that $u = x$ on S_1. If we set $\Sigma = S_1$ we can apply Theorem 3.4 to the functional $E_\alpha^{el}(\theta)$ to obtain the following Corollary.

Corollary 3.6. *If $\theta \to \alpha^{-1}$ then*

$$(40) \qquad\qquad \frac{1}{(\theta^{-1} - \alpha)^2} E_\alpha^{el}(\theta) \longrightarrow C^{el},$$

where

$$C^{el} := \min \left\{ \frac{1}{2} \int_{\Omega_1^+} A[e(u), e(u)] \, dx \, : \, u \in H^1(\Omega_1^+; \mathbb{R}^3), \, u = x \text{ on } S_1 \right\}.$$

From Proposition 3.5 we know that if $\{\theta_R\}$ is a minimizing sequence, than $\theta_R \to \alpha^{-1}$. We can then linearize the elastic energy along the sequence θ_R:

$$E_{\alpha,R}^{el}(\theta_R) = R^3 \theta_R^3 E_\alpha^{el}(\theta_R) = R^3 \theta_R^3 (\theta_R^{-1} - \alpha)^2 \frac{1}{(\theta_R^{-1} - \alpha)^2} E_\alpha^{el}(\theta_R)$$

$$\stackrel{(40)}{=} R^3 \theta_R^3 (\theta_R^{-1} - \alpha)^2 (C^{el} + \varepsilon_R) = k_R^{el} R^3 \theta_R (\alpha \theta_R - 1)^2,$$

where $\varepsilon_R \to 0$ as $R \to +\infty$ and $k_R^{el} := C^{el} + \varepsilon_R$. Since (by Korn's inequality) $C^{el} > 0$, $k_R^{el} > 0$ for R sufficiently large (and in fact for all R). We are thus led to define the family of polynomials

$$P_{k,R}^{tot}(\theta) := P_{k,R}^{el}(\theta) + E_R^{pl}(\theta), \tag{41}$$

where $k, R > 0$ are positive parameters and $P_{k,R}^{el}(\theta) := kR^3\theta(\alpha\theta - 1)^2$. In this way we can write

$$E_{\alpha,R}^{tot}(\theta_R) = P_{k_R^{el},R}^{tot}(\theta_R). \tag{42}$$

By optimizing $P_{k,R}^{tot}$ with respect to θ, we deduce the asymptotic behavior of $E_{\alpha,R}^{tot}$. Set

$$\mathcal{E}^{el}(R) := \frac{\sigma^2}{\alpha^3 C^{el}} R \qquad \text{and} \qquad \mathcal{E}^{pl}(R) := \sigma R^2 \left(1 - \frac{1}{\alpha^2}\right) - 2\frac{\sigma^2}{\alpha^3 C^{el}} R.$$

Theorem 3.7. *Let θ_R be a minimizing sequence for $E_{\alpha,R}^{tot}$. We have*

$$\theta_R = \frac{1}{\alpha}\left(1 + \frac{\sigma}{\alpha C^{el}}\frac{1}{R} + o\left(\frac{1}{R}\right)\right), \tag{43}$$

where $\frac{o(t)}{t} \to 0$ as $t \to 0$. Moreover,

$$E_{\alpha,R}^{el}(\theta_R) = \mathcal{E}^{el}(R) + o(R), \quad E_R^{pl}(\theta_R) = \mathcal{E}^{pl}(R) + o(R), \tag{44}$$

where $\frac{o(R)}{R} \to 0$ as $R \to +\infty$. In particular, we have

$$E_{\alpha,R}^{tot} = \mathcal{E}^{el}(R) + \mathcal{E}^{pl}(R) + o(R).$$

Proof. First we show that for every $k > 0$ and R large enough there exists a unique minimizer $\theta_{k,R}$ of $P_{k,R}^{tot}$ in $[\alpha^{-1}, 1]$, with $\theta_{k,R} \to \alpha^{-1}$ as $R \to +\infty$. To this purpose, we compute the derivative of $P_{k,R}^{tot}$ with respect to θ

$$(P_{k,R}^{tot})'(\theta) = R^2\left\{(3\alpha^2 kR)\theta^2 - 2(2\alpha kR + \sigma)\theta + kR\right\}.$$

One can check that it vanishes at

$$\theta_{\pm}(R) = \frac{1}{3\alpha}\left\{2 + \frac{c}{R} \pm f(R)\right\}, \tag{45}$$

where

$$f(R) := \sqrt{1 + \frac{4c}{R} + \frac{c^2}{R^2}} \qquad \text{and} \qquad c := \frac{\sigma}{\alpha k}. \tag{46}$$

Since $f(R) > 1$ we have $\theta_+(R) > \alpha^{-1}$. Moreover, $f(R) \to 1$, and thus $\theta_+(R) \to \alpha^{-1}$, as $R \to +\infty$. Hence $\theta_+(R) \in [\alpha^{-1}, 1]$ for R large enough. Also note that $\theta_-(R) < \alpha^{-1}$ for R sufficiently large. The second derivative is given by

$$(P_{k,R}^{tot})''(\theta) = R^2\left\{(6\alpha^2 kR)\theta - 2(2\alpha kR + \sigma)\right\},$$

which can be checked to be nonnegative at $\theta_+(R)$

$$(P_{k,R}^{tot})''(\theta_+(R)) = 2\alpha kR^3 f(R) \geq 0.$$

This proves that $\theta_{k,R} := \theta_+(R)$ is the unique minimizer of $P_{k,R}^{tot}$ in $[\alpha^{-1}, 1]$, for R sufficiently large. Moreover from (45) we conclude that $\theta_{k,R} \to \alpha^{-1}$ as $R \to +\infty$.

Evaluating $P^{el}_{k,R}$ and E^{pl}_R at $\theta = \theta_{k,R}$ we find

$$(47) \quad P^{el}_{k,R}(\theta_{k,R}) = \frac{2}{27\alpha^4 k^2}\{2\sigma^3 + 2\alpha k\sigma^2(3 + f(R))R +$$
$$\left(2\alpha^2 k^2 \sigma f\right) R^2 + \alpha^3 k^3(1 - f(R))R^3\},$$

$$(48) \qquad\qquad E^{pl}_R(\theta_{k,R}) = \sigma R^2(1 - \theta^2_{k,R}).$$

In order to show (43) and (44) we perform a Taylor expansion in (46) and (45). Using $\sqrt{1 + x} = 1 + x/2 - x^2/8 + x^3/16 + o(x^3)$ we compute

$$(49) \qquad f(R) = 1 + 2\left(\frac{\sigma}{\alpha k}\right)\frac{1}{R} - \frac{3}{2}\left(\frac{\sigma^2}{\alpha^2 k^2}\right)\frac{1}{R^2} + 3\left(\frac{\sigma^3}{\alpha^3 k^3}\right)\frac{1}{R^3} + o\left(\frac{1}{R^3}\right).$$

Plugging (49) into (45) and recalling that $k^{el}_R \to C^{el}$ as $R \to +\infty$, we deduce (43).

Using (49) we can expand the terms in (47) to get

$$(50) \qquad\qquad 2\alpha k\sigma^2(3 + f(R))R = (8\alpha k\sigma^2)R + 4\sigma^3 + o(R)$$

$$(51) \qquad\qquad \left(2\alpha^2 k^2 \sigma f\right) R^2 = (2\alpha^2 k^2 \sigma)R^2 + (4\alpha k\sigma^2)R - 3\sigma^3 + o(R)$$

$$(52) \qquad \alpha^3 k^3(1 - f(R))R^3 = -(2\alpha^2 k^2 \sigma)R^2 + \frac{3}{2}(\alpha k\sigma^2)R - 3\sigma^3 + o(R)$$

Recalling that $k^{el}_R \to C^{el}$ as $R \to +\infty$, plugging (50)-(52) into (47) yields the first equation in (44). Next we compute

$$(53) \qquad\qquad \theta^2_{k,R} = \frac{1}{9\alpha^2}\left\{5 + 4f(R) + 2c(4 + f(R))\frac{1}{R} + \frac{2c}{R^2}\right\}.$$

Plugging (49) into (53) gives

$$(54) \qquad\qquad \theta^2_{k,R} = \frac{1}{\alpha^2}\left\{1 + \frac{2c}{R} + o\left(\frac{1}{R^3}\right)\right\}.$$

The second relation in (44) follows by inserting (54) into (48), using again $k^{el}_R \to C^{el}$ as $R \to +\infty$.

$\square$

Remark 3.8. The analysis developed in this section can be applied to different crystal configurations. For instance, consider two concentric wires N_{int} and N_{ext}. Specifically, the external wire can be represented by $(S_{2R} \setminus S_R) \times (0, hR)$ and the internal by $S_{\theta R} \times (0, hR)$ with $\theta \in [\alpha^{-1}, 1]$. Here $h > 0$ is a fixed height and αI is the equilibrium of N_{int}, with $\alpha > 1$. The external wire is already in equilibrium. The admissible deformations of N_{int} are maps $v: N_{\text{int}} \to \mathbb{R}^3$ such that $v = \theta^{-1}x$ on the lateral boundary of N_{int}, so that it matches the internal lateral boundary of N_{ext}. The total energy is given by the sum of an elastic term and a plastic term, the latter proportional to the reference surface mismatch between the lateral boundaries of the nanowires:

$$(55) \qquad\qquad E^{tot}(v, \theta) = \int W(\nabla v)\, dx + \sigma hR^2(1 - \theta).$$

If $\theta = 1$ the two wires coincide and the energy is entirely elastic. If $\theta = \alpha^{-1}$ then the elastic energy has minimum zero and E^{tot} is purely dislocation energy. If $\theta \in (\alpha^{-1}, 1)$ then none of the two contributions is zero and we are in a mixed case. For such physical system we can carry on the same analysis as before, up to very minor changes.

4. CONCLUSIONS AND PERSPECTIVES

In this paper we have proposed a simple continuous model for dislocations at semi-coherent interfaces. Our analysis seems flexible enough to describe different interfaces and crystalline configurations. Here we discuss the main achievements of this paper, possible extensions to other physical systems, and future perspectives.

In the first part of the paper we have analyzed a line tension model for dislocations at semi-coherent interfaces, in the context of nonlinear elasticity. Within this model, we have shown that there exists a critical size of the crystal such that dislocations become energetically more favorable than purely elastic deformations. More precisely, we have shown that the energy induced by dislocations scales like the surface area of the interface, while the purely elastic energy scales like the volume of the crystal. This is compatible with the experimental observation that dislocations form periodic networks at the interface. In fact, the proof of Proposition 1.2 is based on the fact that, if a net of dislocations is optimal on an interface S_r of size r, than cutting and pasting such a geometry on S_{4r} one constructs a good periodic energy competitor for a larger interface. A more challenging question is whether the optimal geometry of dislocations is periodic in the microscopic scale b. Although we have not given a rigorous proof of this fact, we have shown an explicit construction of a periodic array of dislocations spaced at distance $\frac{b}{\alpha - 1}$, that is optimal in the scaling of the energy.

Then, we have proposed a simpler and more specific continuous model for dislocations, describing, to some extent, dislocations at grain boundaries, in heterostructured wires and in epitaxial crystal growth. In such a model the area of the reference configuration of the overlayer is a free parameter, while in the deformed configuration there is a perfect match between the underlayer and the overlayer.

The variational formulation is very basic, depending only on three parameters: the diameter of the underlayer, the misfit between the lattice parameters, and the free boundary, described by a single parameter: the area gap between the reference underlayer and overlayer, tuning the amount of dislocations at the interface.

The proposed variational model is rich enough to describe the size effects already discussed, and allows us to refine the analysis of the energy minimizers. Indeed, we have show that, in the limit $R \to +\infty$, the surface energy induced by dislocations is predominant (scaling like R^2), while the volume elastic energy represents a lower order term (scaling like R). Since the elastic energy is vanishing, we can perform a linearization: The asymptotic behaviour of the total energy functional is explicit, depending only on the material parameters in the energy functional, and on the linearized elastic tensor. The only unknown parameter in our formulation is σ, which roughly speaking (multiplied by b) represents the energy per unit dislocation length (while $\sigma(\alpha^2 - 1)$ represents the energy per unit area of the interface). We have proposed some explicit formula for σ,

depending only on the elastic tensor and on a core energy parameter γ^{ch}, describing the core (chemical) energy per unit dislocation length (see (22)).

Summarizing, this paper proposes a basic variational model describing the competition between the plastic energy spent at interfaces, and the corresponding release of bulk energy. In this variational formulation, the size of the interface of the overlayer is a free parameter. In this respect, our model fits into the class of so called free boundary problems.

The proposed energy is built upon some heuristic arguments, supported by formal mathematical derivations based on the semi-discrete theory of dislocations.

While the paper focuses on a specific configuration, the method seems flexible to be extended to several crystalline structures and to different physical contexts, such as grain boundaries, where the misfit between the crystal lattices are described by rotations rather than dilations (see [13]), and epitaxial growth, where the total energy should be completed by adding the surface energy induced by the exterior boundary of the overlayer (see [16]).

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