A model for dislocations in epitaxially strained elastic films[☆]

I. Fonseca[a], N. Fusco[b,*], G. Leoni[a], M. Morini[c]

[a] *Department of Mathematical Sciences, Carnegie Mellon University, Pittsburgh, PA, U.S.A.*
[b] *Dipartimento di Matematica e Applicazioni "R. Caccioppoli", Università degli Studi di Napoli "Federico II" , Napoli, Italy*
[c] *Dipartimento di Matematica, Università degli Studi di Parma , Parma, Italy*

Abstract

A variational model for epitaxially strained films accounting for the presence of dislocations is considered. Existence, regularity and some qualitative properties of solutions are addressed.
Résumé: Um modèle variationnel pour les films épitaxialement tendus tenant compte de la présence de dislocations est considéré. L'éxistence, la régularité et certaines propriétés qualitatives des solutions sont abordées.

Keywords: Epitaxially strained elastic films, misfit dislocations, free boundary problems, regularity
2000 MSC: 49J10, 49J40, 74K35, 74B05

1. Introduction

The ability to control the morphology of elastically stressed thin films is paramount in the manufacturing of microelectronics and optical devices. Due to the misfit between the film and the substrate lattice constants, the film may undergo a morphological change, known as the Asaro-Grinfeld-Tiller (AGT) instability (see [4], [30]). This is a stress relief mechanism, by which the system decreases the elastic energy by allowing non-planar morphologies when a critical thickness is achieved. Such threshold effect is usually explained as the result of two competing forms of energy: the surface energy, which favors flat configurations, and the bulk elastic energy, which in turn is decreased by wavy or corrugated configurations.

An extensive literature is devoted to the modeling and to the numerical analyis of strained epitaxial films; see for instance [26], [46], [47], [48] and the references therein.

[☆]The authors wish to acknowledge the Center for Nonlinear Analysis (NSF PIRE Grant No. OISE-0967140) where part of this work was carried out. The research of I. Fonseca was partially funded by the National Science Foundation under Grant No. DMS-1411646 and that of G. Leoni under Grants No. DMS-1412095 and DMS-1714098. The research of N. Fusco and M. Morini was partially funded by the FiDiPro project 2100002028 of the Finnish Academy of Science. The authors would like to thank Kaushik Dayal for useful conversations.

[*]Corresponding author
Email addresses: fonseca@andrew.cmu.edu (I. Fonseca), n.fusco@unina.it (N. Fusco), giovanni@andrew.cmu.edu (G. Leoni), massimiliano.morini@unipr.it (M. Morini)

Several variational models have been proposed to study epitaxial growth, both in the static case (see [5, 8, 9, 10, 11, 21, 25, 29]) as well as in the time-dependent setting (see [22, 23, 44]), starting with the free-energy approach of [31].

Experiments indicate that the nucleation of dislocations is a further mode of strain relief (in addition to the already mentioned profile buckling) for sufficiently thick films (see, for instance, [19, 26, 33, 36, 49]). Indeed, when a cusp-like morphology is formed, the resulting local stress at a surface valley has a greater energy than that produced by the nucleation of a dislocation. Once the dislocation is formed, it migrates to the film/substrate interface, and the film surface relaxes towards a planar-like morphology.

In this paper we propose a mathematical model, which takes into account the formation of misfits dislocations. We start by recalling the variational formulation studied in [10] and [21] (see also [12] and [15]) within the context of equilibrium configurations of epitaxially strained films without dislocations. As in those papers we work within the theory of linear elasticity. We consider two-dimensional configurations, corresponding to three-dimensional morphologies with planar symmetry. The reference configuration of the film is described as

$$\Omega_h := \left\{ z = (x, y) \in \mathbb{R}^2 : 0 < x < \ell,\, 0 < y < h\,(x) \right\} ,$$

where the function $h : [0, \ell] \to [0, \infty)$ represents the free-profile of the film. The vector field $u : \Omega_h \to \mathbb{R}^2$ represents the displacement of the film and

$$E\,(u) := \frac{1}{2}\left(\nabla u + \nabla^T u\right)$$

its strain. The presence of a mismatch between the lattice constants of the film and the substrate is incorporated in the model by prescribing a Dirichlet boundary condition of the form $u(x, 0) = (e_0 x, 0)$ at the interface, with $e_0 \neq 0$. This corresponds to the case of a film growing on an infinitely rigid substrate.

As customary in the physical literature, we also require the periodicity conditions $h(0) = h(\ell)$ and $\nabla u(0, y) = \nabla u(\ell, y)$. The energy associated with a dislocation-free configuration (h, u), when h is smooth, is given by

$$\mathcal{G}(h, u) := \int_{\Omega_h} \left[\mu |E(u)|^2 + \frac{\lambda}{2} (\mathrm{div} u)^2\right] dz + \gamma \mathcal{H}^1(\Gamma_h) \,,$$

where μ and λ are the Lamé coefficients of the material, γ is the surface tension on the profile of the film, Γ_h denots the graph of h, and $\mathcal{H}^1$ stands for the one-dimensional Hausdorff measure.

Equilibrium configurations corresponf to local or global minimizers of G among all admissible configurations, with prescribed volume. Notice that smooth minimizing sequences may converge to irregular configurations, with the profile h being a lower semicontinuous function of bounded variation. In particular, vertical parts and cuts may appear in the (extended) graph of h. This requires extending the definition of G to a larger class of possibly irregular reachable configurations, through a relaxation procedure. This has been done in [10] and [21] (see also [12] and [15]), and it leads to the relaxed energy:

$$\mathcal{G}(h, u) = \int_{\Omega_h} \left[\mu |E(u)|^2 + \frac{\lambda}{2} (\mathrm{div} u)^2\right] dz + \gamma \mathcal{H}^1(\Gamma_h) + 2\gamma \mathcal{H}^1(\Sigma_h) \,, \tag{1.1}$$

where Σ_h is the set of *vertical cuts* defined as

$$\Sigma_h := \{(x,y) : x \in [0,\ell),\, h(x) < y < \min\{h(x-), h(x+)\}\}\,,$$

with $h(x\pm)$ denoting the right and left limit at x. Note that the factor 2 appearing in the last term of (1) is due to the fact that in the approximation procedure vertical cuts result from the collapsing of needle-like smooth profiles into a segment whose length in the limit is counted twice.

Next we modify $\mathcal{G}$ to account for the presence of isolated misfit dislocations in the film. The mathematical modeling of dislocations has been studied by several authors; see for instance [1, 3, 6, 16, 17, 20, 27, 34, 35, 40, 45], and the references therein.

Volterra's dislocations may be viewed as topological point singularities of the field (see [41]). To be precise, given a set of points $\{z_1,\dots,z_k\} \subset \Omega_h$ and a set of vectors $\{\mathbf{b}_1,\dots,\mathbf{b}_k\} \subset \mathbb{R}^2$, a *strain field* H is compatible with a system of dislocations located at $z_1,\dots,z_k$ and having *Burgers vectors* $\mathbf{b}_1,\dots,\mathbf{b}_k$ if

$$\operatorname{curl} H = \sum_{i=1}^{k} \mathbf{b}_i \delta_{z_i}\,, \tag{1.2}$$

where δ_z denotes the Dirac delta at z. Since the elastic continuum model is not valid near the singularities, some kind of regularization is needed. A standard approach in the engineering literature (see [41]) is to remove a core $B_{r_0}(z_i)$ of radius $r_0 > 0$ around each dislocation and associate with H the (finite) elastic energy

$$\int_{\Omega_h \setminus \cup_{i=1}^k B_{r_0}(z_i)} \Big[\mu |H_{sym}|^2 + \frac{\lambda}{2}(\operatorname{tr}(H))^2\Big]\, dz\,,$$

where $H_{sym} := (H + H^T)/2$. The mathematical study of this energy can be found, e.g., in [13, 17, 28, 40].

In this paper, following [33], we consider a variant of this approach, which consists in regularizing the *dislocation measure* $\sigma := \sum_{i=1}^k \mathbf{b}_i \delta_{z_i}$ through a convolution procedure. To be precise, we replace (2) with the compatibility condition

$$\operatorname{curl} H = \sigma * \varrho_{r_0}\,, \tag{1.3}$$

where $\varrho_{r_0} := (1/r_0^2)\varrho(\cdot/r_0)$ is a convolution kernel, with ϱ a standard mollifier compactly supported in the unit ball. Here $r_0 > 0$ is a fixed constant that may be interpreted as before as the core radius. Since the set of strain fields H satisfying condition (3) and with finite energy, i.e.,

$$\int_{\Omega_h} \Big[\mu |H_{sym}|^2 + \frac{\lambda}{2}(\operatorname{tr}(H))^2\Big]\, dz < +\infty \tag{1.4}$$

is non-empty, for any given profile h and any given dislocation measure σ, the compatible strain field H minimizing the elastic energy (4) is well defined and satisfies the div-curl system

$$\begin{cases} \operatorname{curl} H = \sigma * \varrho_{r_0} \\ \mu \operatorname{div} H + (\lambda+\mu)\nabla(\operatorname{tr}(H)) = 0 \end{cases} \qquad \text{in } \Omega_h. \tag{1.5}$$

Note that the above system admits an equivalent formulation in terms of the so-called Airy stress function w associated with H through the identity

$$\nabla^2 w = \frac{1}{2}\begin{pmatrix} (2\mu+\lambda)H_{22}+\lambda H_{11} & -\mu(H_{12}+H_{21}) \\ -\mu(H_{12}+H_{21}) & (2\mu+\lambda)H_{11}+\lambda H_{22} \end{pmatrix},$$

see [24, Chapter 12]. Indeed, (5) can be rewritten as (see [33])

$$\Delta^2 w = \mathrm{curl}(\sigma * \varrho_{r_0}) \qquad \text{in } \Omega_h\,.$$

Adopting the above convolution-based regularization, the total energy associated with a profile h, a dislocation measure σ, and a strain field H, satisfying the compatibility conditions (3), is given by

$$F(h,\sigma,H) := \int_{\Omega_h} \left[\mu|H_{sym}|^2 + \frac{\lambda}{2}(\mathrm{tr}(H))^2\right] dz + \gamma\mathcal{H}^1(\Gamma_h) + 2\gamma\mathcal{H}^1(\Sigma_h)\,. \tag{1.6}$$

In Section 2 we assume that a finite number k of dislocations, with given Burgers vectors $\mathbf{B} := \{\mathbf{b}_1,\dots,\mathbf{b}_k\} \subset \mathbb{R}^2$, are already present in the film, and we address the problem of finding the optimal configuration, i.e., the profile h and the location $z_1,\dots,z_k$ of the k dislocations which minimize the total energy, under a given volume constraint $|\Omega_h| = d$. To be precise, denoting by $X(e_0;\mathbf{B})$ the set of admissible triples (h,σ,H), in Theorem 2.4 below, we prove

Theorem 1.1. *The minimization problem*

$$\min\{F(h,\sigma,H) :\ (h,\sigma,H) \in X(e_0;\mathbf{B}),\ |\Omega_h| = d\}\,. \tag{1.7}$$

admits a solution.

We then show that the equilibrium profile h obtained above satisfies the same regularity properties proved in [21] (see also [18, 25]) in the dislocation-free case. Namely,

Theorem 1.2. *Let $(\bar h,\bar\sigma,H_{\bar h,\bar\sigma}) \in X(e_0;\mathbf{B})$ be a minimizer of (7). Then $\bar h$ has at most finitely many cusp points and vertical cracks, its graph is of class C^1 away from this finite set, and of class $C^{1,\alpha}$, $\alpha \in (0,\frac{1}{2})$ away from this finite set and off the substrate.*

For a more detailed qualitative description of this regularity result we refer to Theorem 2.15 below. The overall strategy to prove this theorem is the same used in [21]. However, there are many new technical issues due to the presence of dislocations, which require new ideas. In particular, a major difficulty arises in showing that the volume constraint can be replaced by a volume penalization. In the dislocation-free case this was based on a straightforward truncation argument, which fails in the present setting because dislocations cannot be removed in this way. Indeed they act as a sort of obstacle when touching the profile, and this is overcome in Theorem 2.5, where it is shown that a delicate truncation construction is still possible without affecting the dislocations.

In Theorem 2.18 we provide analytical support to the experimental evidence that, after nucleation, dislocations lie at the bottom.

Theorem 1.3. *Assume $\mathbf{B} \neq \emptyset$, $d > 2r_0\ell$. Then there exist $\bar e > 0$ and $\bar\gamma > 0$ such that whenever $|e_0| > \bar e$, $\gamma > \bar\gamma$, and $e_0(\mathbf{b}_j\cdot\mathbf{e}_1) > 0$ for all $\mathbf{b}_j \in \mathbf{B}$, then any minimizer $(\bar h,\bar\sigma,\bar H)$ of the problem (7) has all dislocations lying at the bottom of Ω_h, in the sense that the centers z_i are of the form $z_i = (x_i, r_0)$.*

In the last part of the paper we study the nucleation of dislocations and we investigate conditions under which it is energetically favorable to create dislocations. To this purpose, we modify the energy (6) by adding a term that accounts for the energy dissipated to create dislocations. Following the physical literature (see for instance [41]), we assume that the energy cost of a new dislocation is proportional to the square of the norm of the corresponding Burgers vector. This leads to an energetic contribution $N(\sigma)$, given in (60). Therefore, our new variational problem is to

$$\text{minimize} \quad F(h,\sigma,H)+N(\sigma) \tag{1.8}$$

among all admissible configurations (h,σ,H), under a volume constraint, but without fixing the number of dislocations nor the Burgers vectors, which are allowed to be any integer multiple of certain fundamental directions in a set $\mathcal{B}^o \subset \mathbb{R}^2$.

The regularity results of Section 2 apply to the minimizers of (8). On the other hand, local and global minimizers of the minimum problem studied in Section 2 may be regarded as local minimizers of (8). Finally, in Theorem 3.5 we identify a range of parameters for which all global minimizers have nontrivial dislocation measures (see [38] for an analogous result in heterogeneous nanowires).

Theorem 1.4. *Assume that there exists* $\mathbf{b} \in \mathcal{B}^o$ *such that* $\mathbf{b}\cdot\mathbf{e}_1 \neq 0$*, and let* $d > 2r_0\ell$*. Then there exists* $\bar\gamma > 0$ *such that whenever* $|e_0| > \bar e$*, and* $\gamma > \bar\gamma$*, where* $\bar e$ *is as in Theorem 1.3, any minimizer* $(\bar h, \bar\sigma, \bar H)$ *of the problem* (8) *has nontrivial dislocations, i.e.,* $\bar\sigma \neq 0$*.*

2. Epitaxial elastic films with dislocations

2.1. Setting of the Problem

We assume that the substrate is rigid and occupies the semi-infinite strip $(0,\ell)\times(-\infty,0)$, and that the reference configuration of the elastic film is given by

$$\Omega_h := \{z=(x,y):\, 0\le x<\ell,\, 0<y<h(x)\}$$

with $h:[0,\ell]\to[0,\infty)$. The graph of h represents the *free* profile of the film and the line $y=0$ corresponds to the film/substrate interface. The space of admissible profiles is defined by

$$AP(0,\ell) := \{h:\mathbb{R}\to[0,+\infty) : h \text{ is lower semicontinuous and } \ell\text{-periodic, } \mathrm{Var}(h;0,\ell)<+\infty\}.$$

Here $\mathrm{Var}(h;0,\ell)$ denotes the *pointwise total variation* of h over the interval $(0,\ell)$, given by

$$\mathrm{Var}(h;0,\ell) := \sup\sum_{i=1}^{k}|h(x_i)-h(x_{i-1})| < +\infty,$$

where the supremum is taken over all partitions $\{x_0,x_1,\dots,x_k\}$, with $0<x_0<x_1<\cdots<x_k<\ell$, $k\in\mathbb{N}$. Since $h\in AP(0,\ell)$ is ℓ-periodic, its pointwise total variation is finite over any bounded interval of $\mathbb{R}$. Therefore, it admits right and left limits at every $x\in\mathbb{R}$ denoted by $h(x+)$ and $h(x-)$, respectively. In what follows we use the notation

$$h^+(x) := \max\{h(x+),h(x-)\}, \qquad h^-(x) := \min\{h(x+),h(x-)\}. \tag{2.1}$$

We set

$$\Omega_h^{\#} := \{(x,y) : x \in \mathbb{R},\, 0 < y < h(x)\}$$

to be the open set obtained by repeating copies of Ω_h ℓ-periodically in the x-direction. We define

$$\Gamma_h := \{(x,y) : x \in [0,\ell),\, h^-(x) \le y \le h^+(x)\}\,,$$

and *the set of vertical cracks*

$$\Sigma_h := \{(x,y) : x \in [0,\ell)\,,\, h(x) < h^-(x),\, h(x) \le y \le h^-(x)\}\,. \tag{2.2}$$

We also set

$$\widetilde{\Gamma}_h := \Gamma_h \cup \Sigma_h\,,$$

and we will use the notation

$$\Gamma_h^{\#} := \{(x,y) \in \mathbb{R}^2 :\, x \in \mathbb{R},\, h^-(x) \le y \le h^+(x)\}\,.$$

Similarly we define $\Sigma_h^{\#}$ and $\widetilde{\Gamma}_h^{\#}$.

Observe that if $h \in AP(0,\ell)$, then

$$\|h\|_\infty \le \frac{1}{\ell}\int_0^\ell h\,dx + \mathrm{Var}(h;0,\ell) \le \frac{|\Omega_h|}{\ell} + \mathcal{H}^1(\Gamma_h)\,. \tag{2.3}$$

We work within the theory of small elastic deformations, so that

$$E(u) := \frac{1}{2}\left(\nabla u + \nabla u^T\right)$$

represents the strain, with $u : \Omega_h \to \mathbb{R}^2$ the planar displacement. The elastic energy density is

$$W(E) := \frac{1}{2}\mathbb{C}E : E = \mu|E|^2 + \frac{\lambda}{2}\big[\mathrm{tr}(E)\big]^2\,, \tag{2.4}$$

where

$$\mathbb{C}E = \begin{pmatrix} (2\mu+\lambda)E_{11} + \lambda E_{22} & 2\mu E_{12} \\ 2\mu E_{12} & (2\mu+\lambda)E_{22} + \lambda E_{11} \end{pmatrix} \tag{2.5}$$

and the *Lamé coefficients* μ and λ satisfy the ellipticity conditions

$$\mu > 0 \qquad \text{and} \qquad \mu + \lambda > 0\,. \tag{2.6}$$

Throughout this section we assume the presence of k dislocations with given Burgers vectors $\mathbf{B} := \{\mathbf{b}_1,\dots,\mathbf{b}_k\} \subset \mathbb{R}^2$ and centers $\{z_1,\dots,z_k\} \subset \Omega_h$ such that $B_{r_0}(z_i) \subset \Omega_h^{\#}$, with $r_0 \in (0,\ell/2)$ a (small) positive constant representing the *core radius* of the dislocations. With any such collection of dislocations we associate the *ℓ-periodic dislocation measure*

$$\sigma := \sum_{i=1}^k \mathbf{b}_i \delta_{z_i}^{\#}\,,$$

where, given $z \in \Omega_h$ we denote by $\delta_z^{\#}$ the ℓ-periodic extension of the Dirac delta δ_z, i.e.,

$$\delta_z^{\#} := \sum_{k\in\mathbb{Z}} \delta_{z+k\ell\mathbf{e}_1}\,.$$

To regularize σ, we fix a nonnegative radially symmetric $\varrho \in C_c^\infty(B_1(0))$, with $\int_{\mathbb{R}^2} \varrho\, dz = 1$, and we define

$$\varrho_{r_0}(z) := \frac{1}{r_0^2}\varrho\Big(\frac{z}{r_0}\Big) \quad \text{and} \quad \varrho_{r_0}^{\#} := \varrho_{r_0} * \delta_0^{\#}\,. \tag{2.7}$$

Note that $\varrho_{r_0}^{\#}$ is the ℓ-periodic extension in the x-direction of the function ϱ_{r_0}.

Given $h \in AP(0,\ell)$ we denote by $\mathcal{M}_{dis}(\Omega_h;\mathbf{B})$ the subset of the space of vector valued Radon measures $\mathcal{M}(\Omega_h^{\#};\mathbb{R}^2)$ defined by

$$\mathcal{M}_{dis}(\Omega_h;\mathbf{B}) := \Big\{\sigma \in \mathcal{M}(\Omega_h^{\#};\mathbb{R}^2) :\ \sigma = \sum_{i=1}^{k} \mathbf{b}_i \delta_{z_i}^{\#},\ z_i \in \Omega_h,\ \text{with } B_{r_0}(z_i) \subset \Omega_h^{\#}\Big\}.$$

Observe that we are not requiring that the centers of the k dislocations are all distinct, thus allowing for superpositions of different dislocations.

We recall that the curl of a function H with values in $\mathbb{M}^{2\times 2}$ is defined by

$$\operatorname{curl} H := \Big(\frac{\partial H_{12}}{\partial x} - \frac{\partial H_{11}}{\partial y}, \frac{\partial H_{22}}{\partial x} - \frac{\partial H_{21}}{\partial y}\Big).$$

The total energy functional will depend on the film profile h and on the dislocation measure $\sigma \in \mathcal{M}_{dis}(\Omega_h)$ via the associated *strain field* H satisfying the constraint $\operatorname{curl} H = \sigma * \varrho_{r_0}$, which accounts also for the interactions between the different dislocations. Moreover, the presence of a mismatch between the film and the substrate lattices is modeled by enforcing a Dirichlet boundary condition at the interface $\{y = 0\}$, namely by requiring that the tangential trace of H on the interface equals $e_0\mathbf{e}_1$, where $\mathbf{e}_1 := (1,0)$ and $e_0 \neq 0$. To be precise, we introduce the following set of admissible triples

$$\begin{aligned} X(e_0;\mathbf{B}) := \Big\{(h,\sigma,H) :\ & h \in AP(0,\ell),\ \sigma \in \mathcal{M}_{dis}(\Omega_h;\mathbf{B}),\ H \in \mathbf{H}_{\#}(\operatorname{curl};\Omega_h;\mathbb{M}^{2\times 2}) \\ & \text{such that } \operatorname{curl} H = \sigma * \varrho_{r_0} \text{ in } \Omega_h \text{ and } H[\,\mathbf{e_1}\,] = e_0\mathbf{e_1} \text{ on } \{y=0\}\Big\}, \end{aligned} \tag{2.8}$$

where we are using the fact that admissible fields H admit a tangential trace (see, e.g., Chapter 4 in [7]), and where, denoting by $H^{\#}$ the ℓ-periodic extension in the x-direction of H,

$$\begin{aligned} &\mathbf{H}_{\#}(\operatorname{curl};\Omega_h;\mathbb{M}^{2\times 2}) := \\ &\quad \{H \in L^2_{loc}(\Omega_h;\mathbb{M}^{2\times 2}) :\ \operatorname{curl} H \in L^2(\Omega_h;\mathbb{R}^2) \text{ and } \operatorname{curl} H^{\#} \in L^2_{loc}(\Omega_h^{\#};\mathbb{R}^2)\}\,. \end{aligned} \tag{2.9}$$

The total energy of the system is given by

$$F(h,\sigma,H) := \int_{\Omega_h} W(H_{sym})\, dz + \gamma\mathcal{H}^1(\Gamma_h) + 2\gamma\mathcal{H}^1(\Sigma_h) \tag{2.10}$$

for every admissible configuration $(h,\sigma,H) \in X(e_0;\mathbf{B})$, where we recall that $H_{sym} := (H + H^T)/2$ and γ is a positive constant depending on the material properties.

For every fixed profile $h \in AP(0,\ell)$ and dislocation measure σ we denote by $H_{h,\sigma}$ the unique strain field that minimizes

$$H \mapsto \int_{\Omega_h} W(H_{sym})\, dz$$

over all $H \in \mathbf{H}_{\#}(\mathrm{curl};\Omega_h;\mathbb{M}^{2\times 2})$ such that $(h,\sigma,H) \in X(e_0;\mathbf{B})$. The existence and uniqueness of $H_{h,\sigma}$ follow from the coercivity and strict convexity of the energy (18) (see (13) and (14)) and the fact that the Dirichlet condition in (16) is preserved under weak convergence in the space $\mathbf{H}_{\#}(\mathrm{curl};\Omega_h;\mathbb{M}^{2\times 2})$ (see (17)). Note that $H_{h,\sigma}$ is determined as the unique solution in $\mathbf{H}_{\#}(\mathrm{curl};\Omega_h;\mathbb{M}^{2\times 2})$ to the system

$$\begin{cases} \mathrm{curl}\, H_{h,\sigma} = \sigma * \varrho_{r_0} & \text{in } \Omega_h, \\ \mathrm{div}\, \mathbb{C}(H_{h,\sigma})_{sym} = 0 & \text{in } \Omega_h, \\ \mathbb{C}(H_{h,\sigma})_{sym}[\nu] = 0 & \text{on } \Gamma_h, \\ H_{h,\sigma}[\,\mathbf{e}_1\,] = e_0\mathbf{e}_1 & \text{on } \{y=0\}. \end{cases} \tag{2.11}$$

Note also that if $(h,\sigma,H_{h,\sigma}) \in X(e_0;\mathbf{B})$ is a (locally) minimizing configuration, with $h \in C^2_{\#}([0,\ell])$ and $h > 0$, then by considering smooth variations of h supported in the complement of the projection of $\cup_{i=1}^k \bar{B}_{r_0}(z_i)$ on the $[0,\ell]$, we obtain by standard arguments the following Euler-Lagrange equation

$$\kappa + W((H_{h,\sigma})_{sym}) = \Lambda \qquad \text{on } \overline{\Gamma_h \setminus \cup_{i=1}^k \bar{B}_{r_0}(z_i)}\,, \tag{2.12}$$

where

$$\kappa := -\left(\frac{h'}{\sqrt{1+h'^2}}\right)'$$

denotes the curvature of Γ_h and Λ is the constant Lagrange multiplier associated with the volume constraint. This motivates the following definition.

Definition 2.1. *Let $(h,\sigma,H_{h,\sigma}) \in X(e_0;\mathbf{B})$, with $h \in C^2_{\#}([0,\ell])$ and $h > 0$. We say that $(h,\sigma,H_{h,\sigma})$ is a* critical configuration *if* (19) *and* (20) *are satisfied.*

In the sequel we will use the following *canonical decomposition* of $H_{h,\sigma}$:

$$H_{h,\sigma} = e_0 Du_h + K_{h,\sigma}\,,$$

where u_h is the elastic equilibrium in Ω_h such that $u_h(x,0) = (x,0)$, that is the unique solution to the system

$$\begin{cases} \mathrm{div}\, \mathbb{C}E(u_h) = 0 & \text{in } \Omega_h, \\ \mathbb{C}E(u_h)[\,\nu\,] = 0 & \text{on } \Gamma_h, \\ u_h(x,0) = (x,0) & \text{on } \{y=0\}, \end{cases} \tag{2.13}$$

such that $(x,y) \in \Omega^{\#} \mapsto u_h(x,y) - (x,0)$ belongs to

$$LD_{\#}(\Omega_h;\mathbb{R}^2) := \Big\{ v \in L^2_{\mathrm{loc}}(\Omega_h^{\#};\mathbb{R}^2) :\, v(x,y) = v(x+\ell,y) \\ \text{for } (x,y) \in \Omega_h^{\#}\,, E(v)|_{\Omega_h} \in L^2(\Omega_h;\mathbb{R}^2) \Big\}\,,$$

and $K_{h,\sigma}$ is the unique solution in $\mathbf{H}_{\#}(\mathrm{curl};\Omega_h;\mathbb{M}^{2\times 2})$ to

$$\begin{cases} \mathrm{curl}\, K_{h,\sigma} = \sigma * \varrho_{r_0} & \text{in } \Omega_h, \\ \mathrm{div}\, \mathbb{C}(K_{h,\sigma})_{sym} = 0 & \text{in } \Omega_h, \\ \mathbb{C}(K_{h,\sigma})_{sym}[\nu] = 0 & \text{on } \Gamma_h, \\ K_{h,\sigma}[\,\mathbf{e}_1\,] = 0 & \text{on } \{y=0\}. \end{cases} \tag{2.14}$$

We set

$$v_0(x,y) := \Big(x, \frac{-\lambda y}{2\mu+\lambda}\Big) \quad \text{and} \quad W_0 := W(E(v_0))\,. \tag{2.15}$$

Observe that v_0 is the elastic equilibrium corresponding to the flat configuration and $e_0 = 1$.

2.2. Existence

We start with the following Korn-type inequality.

Lemma 2.2. *Let $\Omega \subset \mathbb{R}^2$ be a bounded open simply connected set with Lipschitz boundary and let Γ be a non-empty connected relatively open subset of $\partial\Omega$. Then, there exists a constant $C > 0$ depending only on Ω and Γ such that*

$$\|H\|_{L^2(\Omega;\mathbb{M}^{2\times 2})} \le C\big(\|H_{sym}\|_{L^2(\Omega;\mathbb{M}^{2\times 2})} + \|\operatorname{curl} H\|_{L^2(\Omega;\mathbb{R}^2)}\big) \tag{2.16}$$

for all $H \in \mathbf{H}(\operatorname{curl};\Omega;\mathbb{M}^{2\times 2})$ with tangential trace $H[\tau] = 0$ on Γ.

Proof. **Step 1.** We start by assuming that $\mathcal{H}^1(\partial\Omega\backslash\Gamma) > 0$ and, without loss of generality, that $H_{sym} \in L^2(\Omega;\mathbb{M}^{2\times 2})$. Let

$$K := \begin{pmatrix} -D_y w_1 & D_x w_1 \\ -D_y w_2 & D_x w_2 \end{pmatrix},$$

where $w = (w_1, w_2)$ is the unique solution to

$$\begin{cases} \Delta w = \operatorname{curl} H & \text{in } \Omega, \\ w = 0 & \text{on } \partial\Omega \setminus \Gamma, \\ D_\nu w = 0 & \text{on } \Gamma. \end{cases}$$

By multiplying $\Delta w_i = (\operatorname{curl} H)_i$ by w_i, $i = 1, 2$ and integrating by parts, it follows from the Poincaré inequality

$$\|K\|_{L^2(\Omega;\mathbb{M}^{2\times 2})} = \|Dw\|_{L^2(\Omega;\mathbb{M}^{2\times 2})} \le C\|\operatorname{curl} H\|_{L^2(\Omega;\mathbb{R}^2)}\,. \tag{2.17}$$

Since $\operatorname{curl}(H-K) = 0$ in Ω, by the Helmholtz decomposition theorem (see, e.g., Theorem 3.3.7 in [39]) there exists $u \in H^1(\Omega;\mathbb{R}^2)$ such that $Du = H - K$. Moreover, u is unique up to a constant. Since $(H-K)[\tau] = 0$ on Γ, we can take $u = 0$ on Γ. Using Korn's inequality (see, e.g., [43]), we have

$$\begin{aligned} \|Du\|_{L^2(\Omega;\mathbb{M}^{2\times 2})} &\le C\|E(u)\|_{L^2(\Omega;\mathbb{M}^{2\times 2})} = C\|H_{sym} - K_{sym}\|_{L^2(\Omega;\mathbb{M}^{2\times 2})} \\ &\le C\big(\|H_{sym}\|_{L^2(\Omega;\mathbb{M}^{2\times 2})} + \|\operatorname{curl} H\|_{L^2(\Omega;\mathbb{R}^2)}\big)\,, \end{aligned} \tag{2.18}$$

where in the last inequality we have used (25). By (25) and (26), we obtain (24).
Step 2. If $\mathcal{H}^1(\partial\Omega \setminus \Gamma) = 0$, then the argument is similar, and it suffices to replace the condition $w = 0$ on $\partial\Omega \setminus \Gamma$ by $\int_\Omega w\,dz = 0$. □

The next lemma provides a useful elliptic estimate for the solutions to systems of the type (22).

Lemma 2.3. *Let $h \in AP(0,\ell) \cap Lip(0,\ell)$, $h \geq c_0 > 0$, $\|h'\|_\infty \leq M$ and let $f \in L^2(0,\ell;\mathbb{R}^2)$. Then, there exists a constant $C > 0$, depending only on c_0 and M, such that if $H \in \mathbf{H}_\#(\mathrm{curl};\Omega_h;\mathbb{M}^{2\times 2})$ is the solution to*

$$\begin{cases} \mathrm{curl}\, H = f & \text{in } \Omega_h, \\ \mathrm{div}\, \mathbb{C}H_{sym} = 0 & \text{in } \Omega_h, \\ \mathbb{C}H_{sym}[\nu] = 0 & \text{on } \Gamma_h, \\ H[\,\mathbf{e}_1\,] = 0 & \text{on } \{y = 0\}, \end{cases}$$

then

$$\|H\|_{L^2(\Omega_h;\mathbb{M}^{2\times 2})} \leq C\|f\|_{L^2(0,\ell;\mathbb{R}^2)}\,. \tag{2.19}$$

Proof. Since $h \geq c_0 > 0$, the set Ω_h is connected, and since its complement is also connected, we have that Ω_h is simply connected. Hence, we can argue as in the proof of Lemma 2.2 to split $H = Du + K$, where K is defined

$$K = \begin{pmatrix} -D_y w_1 & D_x w_1 \\ -D_y w_2 & D_x w_2 \end{pmatrix}$$

with $w = (w_1, w_2)$ the unique solution to

$$\begin{cases} \Delta w = f & \text{in } \Omega_h, \\ w = 0 & \text{on } \Gamma_h, \\ D_\nu w = 0 & \text{on } \{y = 0\}. \end{cases}$$

As before we have that $\|K\|_{L^2(\Omega_h;\mathbb{M}^{2\times 2})} \leq C\|f\|_{L^2(\Omega_h;\mathbb{R}^2)}$. Note that $u \in H^1_\#(\Omega_h;\mathbb{R}^2)$ can be chosen to be identically 0 on $\{y = 0\}$ and solves

$$\begin{cases} \mathrm{div}\, \mathbb{C}E(u) = -\mathrm{div}\, \mathbb{C}K_{sym} & \text{in } \Omega_h, \\ \mathbb{C}E(u)[\nu] = -\mathbb{C}K_{sym}[\nu] & \text{on } \Gamma_h, \\ u = 0 & \text{on } \{y = 0\}. \end{cases}$$

Multiplying both sides of the equation above by u, integrating by parts, and using the fact that if $H \in \mathbb{M}^{2\times 2}$ is symmetric, then so is $\mathbb{C}H$ (see (13)), we get

$$\int_{\Omega_h} \mathbb{C}E(u) : E(u)\, dz = -\int_{\Omega_h} \mathbb{C}K_{sym} : E(u)\, dz\,.$$

Hence, also by Korn's inequality, we have

$$\|Du\|_{L^2(\Omega_h;\mathbb{M}^{2\times 2})} \leq C\|K\|_{L^2(\Omega_h;\mathbb{M}^{2\times 2})} \leq C\|f\|_{L^2(\Omega_h;\mathbb{R}^2)}\,,$$

and we conclude that (27) holds. □

Theorem 2.4. *The minimization problem*

$$\min\{F(h,\sigma,H) :\ (h,\sigma,H) \in X(e_0;\mathbf{B}),\ |\Omega_h| = d\}\,. \tag{2.20}$$

admits a solution.

Proof. Let $\{(h_n, \sigma_n, H_n)\} \subset X(e_0; \mathbf{B})$ be a minimizing sequence. By the compactness results in [21, Proposition 2.2 and Lemma 2.5], we may assume that, up to a subsequence (not relabeled), there exists $h \in AP(0, \ell)$ such that

i) $h_n \to h$ in $L^1(0, \ell)$;

ii) $\mathbb{R}^2 \setminus \Omega^{\#}_{h_n} \to \mathbb{R}^2 \setminus \Omega^{\#}_h$ in the sense of the Hausdorff metric.

Moreover, in [10, Lemma 2.1] it is shown that

$$\mathcal{H}^1(\Gamma_h) + 2\mathcal{H}^1(\Sigma_h) \leq \liminf_n \left[\mathcal{H}^1(\Gamma_{h_n}) + 2\mathcal{H}^1(\Sigma_{h_n})\right]. \tag{2.21}$$

Setting $\sigma_n = \sum_{i=1}^k \mathbf{b}_i \delta^{\#}_{z_{i,n}}$, we can assume (up to extracting a further subsequence if needed) that $z_{i,n} \to z_i \in \overline{\Omega_h}$, with $B_{r_0}(z_i) \subset \Omega^{\#}_h$. Note that if $z_i \cdot \mathbf{e}_1 = \ell$ using the lateral periodicity we can assume that $z_i \cdot \mathbf{e}_1 = 0$, and so by (2.1) we have that $z_i \in \Omega_h$.

Set $V_n := \Omega_{h_n} \cup ((0, \ell) \times (-1, 0])$ and $V := \Omega_h \cup ((0, \ell) \times (-1, 0])$. Since $H_n[\,\mathbf{e_1}\,] = e_0 \mathbf{e_1}$ on $\{y = 0\}$, by setting $H_n := \nabla u_0$ in $(0, \ell) \times (-1, 0]$, where $u_0(x, y) := (e_0 x, 0)$, we have that $H_n \in \mathbf{H}(\mathrm{curl}; V_n; \mathbb{M}^{2\times 2})$. Note that the sets V_n are simply connected. Consider an increasing sequence of simply connected Lipschitz sets $U_j \subset V$ such that $(0, \ell) \times (-1, 0] \subset U_j$, $\partial U_j \cap \Gamma_h = \emptyset$ and $\cup_{j\in\mathbb{N}} U_j = V$. By Lemma 2.2 we have that for every j, the strain fields H_n are equibounded in $L^2(U_j; \mathbb{M}^{2\times 2})$. Note also that $\operatorname{curl} H_n = \sigma_n * \varrho_{r_0} \to \sigma * \varrho_{r_0}$ in $L^2(V; \mathbb{R}^2)$, where $\sigma := \sum_{i=1}^k \mathbf{b}_i \delta^{\#}_{z_i}$. Thus, by a diagonalization argument, we may find $H \in \mathbf{H}(\mathrm{curl}; V; \mathbb{M}^{2\times 2})$ such that $\operatorname{curl} H = \sigma * \varrho_{r_0}$, and, up to the extraction of a further subsequence (not relabeled), $H_n \rightharpoonup H$ weakly in $L^2(U_j; \mathbb{M}^{2\times 2})$ for every j. Since $H_n = \nabla u_0$ in $(0, \ell) \times (-1, 0]$, we have that $H = \nabla u_0$ in $(0, \ell) \times (-1, 0]$, and, in turn, $H[\mathbf{e}_1] = e_0 \mathbf{e}_1$ on $\{y = 0\} \cap \partial\Omega_h$. It follows that $(h, \sigma, H) \in X(e_0; \mathbf{B})$ and for every $j \in \mathbb{N}$

$$\begin{aligned}\int_{U_j \cap \Omega_h} W(H_{sym})\, dz &\leq \liminf_n \int_{U_j \cap \Omega_h} W((H_n)_{sym})\, dz \\ &\leq \liminf_n \int_{\Omega_{h_n}} W((H_n)_{sym})\, dz. \end{aligned} \tag{2.22}$$

By (29) and (30) and the arbitrariness of j we conclude that

$$F(h, \sigma, H) \leq \liminf_n F(h_n, \sigma_n, H_n).$$

Thus (h, σ, H) is a global minimizer. □

2.3. Regularity

In this subsection we establish the regularity properties of minimizers of problem (28). We shall follow the general strategy developed in [21, 25] to which we refer for all parts of the proofs that will remain unchanged.

Theorem 2.5. *Let $d \geq 2r_0\ell$ and let $(\bar{h}, \bar{\sigma}, H_{\bar{h},\bar{\sigma}})$ be a minimizing configuration for problem (28) such that $\bar{h}^-$ is not flat. There exist $\beta > 0$ depending only on $\|\bar{h} - d/\ell\|_{L^2(0,\ell)}$ and $F(\bar{h}, \bar{\sigma}, H_{\bar{h},\sigma})$, and $\Lambda > 0$ depending on μ, λ, e_0, r_0 and β, such that $(\bar{h}, \bar{\sigma}, H_{\bar{h},\bar{\sigma}})$ is also a minimizer of*

$$\min\left\{F(h, \sigma, H) + \beta \int_0^\ell |h - \bar{h}|^2\, dx + \Lambda\big||\Omega_h| - d\big| : (h, \sigma, H) \in X(e_0; \mathbf{B})\right\}. \tag{2.23}$$

Before giving the proof we need the following technical lemma.

Lemma 2.6. *For all $\varepsilon > 0$ there exists $\Lambda(\varepsilon)$ (depending also on β, μ, λ, e_0, and r_0) with the following property: For all $\Lambda \geq \Lambda(\varepsilon)$ if $(g, \tau, H_{g,\tau})$ is a minimizer of (31), with $|\Omega_g| > d$, $\tau = \sum_{i=1}^k \mathbf{b}_i \delta^{\#}_{z_i}$, and if $\Gamma' \subset \partial B_{r_0}(z_j) \cap \Gamma_g$ for some $j \in \{1, \dots, k\}$, with $z_j \cdot e_2 > r_0$, is any connected arc, then $\mathcal{H}^1(\Gamma') \leq \varepsilon$.*

Proof. In order to prove the lemma observe that in $B_{r_0}(z_j)$ we can write $H_{g,\tau} = Dv + K$, where

$$K := \begin{pmatrix} k_1 & 0 \\ k_2 & 0 \end{pmatrix},$$

with

$$k_l(x, y) := -\sum_{i=1}^k (\mathbf{b}_i \cdot \mathbf{e}_l) \int_0^y \varrho^{\#}_{r_0}(x - x_i, t - y_i)\, dt \text{ for } l = 1, 2,$$

where $\varrho^{\#}_{r_0}$ is defined in (15), and $v \in H^1_{\#}(\Omega_h; \mathbb{R}^2)$ satisfies

$$\begin{cases} \operatorname{div} \mathbb{C}E(v) = -\operatorname{div} \mathbb{C}K_{sym} & \text{in } \Omega_g, \\ \mathbb{C}E(v)[\nu] = -\mathbb{C}K_{sym}[\nu] & \text{on } \Gamma_g, \\ v = 0 & \text{on } \{y = 0\}. \end{cases}$$

Since K and Γ' are both smooth, v is smooth in $B_{r_0}(z_j) \cup \Gamma'$. Let $\Gamma'' \subset \Gamma'$ be the subarc with the center of Γ' and such that $\mathcal{H}^1(\Gamma'') = \frac{1}{2}\mathcal{H}^1(\Gamma')$. By elliptic estimates for the Lamé system (see for instance [25, Proposition 8.9]) there exists a constant $C_1 > 0$ depending only on $\mathcal{H}^1(\Gamma')$, r_0, the Lamé coefficients μ and λ, and on $F(\bar{h}, \bar{\sigma}, H_{\bar{h},\bar{\sigma}})$, such that

$$\sup_{\Gamma''} |Dv| \leq C_1 .$$

In particular, the constant $C_1 = C_1(\Gamma')$ above is uniformly bounded if $\mathcal{H}^1(\Gamma')$ is bounded away from 0. In turn, we obtain

$$\sup_{\Gamma''} |H_{g,\tau}| \leq C_1 + C_2 , \tag{2.24}$$

where the constant $C_2 > 0$ depends only on r_0.

Fix $\varphi \in C^\infty_c(I)$, $\varphi \geq 0$, where I is an open interval contained in the projection of Γ'' onto the x-axis. Since $z_j \cdot e_2 > r_0$, for $t > 0$ sufficiently small we have that $B_{r_0}(z_j - t\|\varphi\|_\infty) \subset \Omega^{\#}_{g - t\varphi}$ and so we can take as admissible competitor the triple $(g - t\varphi, \sigma_t, H_t)$, where $\tau_t := \sum_{i \neq j} \mathbf{b}_i \delta^{\#}_{z_i} + \mathbf{b}_j \delta^{\#}_{z_j - t\|\varphi\|_\infty \mathbf{e}_2}$, $H_t := H_{g,\tau} + K_t$, where

$$K_t := \begin{pmatrix} k_{t,1} & 0 \\ k_{t,2} & 0 \end{pmatrix},$$

with

$$k_{t,l}(x, y) := -\left(\int_0^y \varrho^{\#}_{r_0}(x - x_j, s - y_j - t\|\varphi\|_\infty)\, ds - \int_0^y \varrho^{\#}_{r_0}(x - x_j, s - y_j)\, ds \right) \mathbf{b}_j \cdot \mathbf{e}_l$$

for $l=1,2$. By minimality, we have

$$F(g-t\varphi,\tau_t,H_t)+\beta\int_0^\ell |g-t\varphi-\bar h|^2\,dx+\Lambda(|\Omega_{g-t\varphi}|-d)$$
$$\geq F(g,\tau,H_{g,\tau})+\beta\int_0^\ell |g-\bar h|^2\,dx+\Lambda(|\Omega_g|-d)\,.$$

By dividing both sides by $t>0$ and letting $t\to 0^+$, we obtain

$$\int_{\Omega_g}\mathbb{C}((H_{g,\tau})_{sym}):\dot K_{sym}\,dz+\int_I W((H_{g,\tau})_{sym})(x,g(x))\varphi(x)\,dx$$
$$-\gamma\int_I\frac{g'\varphi'}{\sqrt{1+g'^2}}\,dx-2\beta\int_I(g-\bar h)\varphi\,dx-\Lambda\int_I\varphi\,dx\geq 0\,,\quad (2.25)$$

where

$$\dot K_{sym}:=\begin{pmatrix}\dot k_1 & \dot k_2/2\\ \dot k_2/2 & 0\end{pmatrix},\qquad \dot k_l(x,y):=\|\varphi\|_\infty\varrho_{r_0}(z-z_j)\mathbf{b}_j\cdot\mathbf{e}_l\ \text{for } l=1,2.$$

Since $\Gamma''\subset\partial B_{r_0}(z_j)\cap\Gamma_g$, integrating by parts we get

$$-\gamma\int_I\frac{g'\varphi'}{\sqrt{1+g'^2}}\,dx\leq\frac{\gamma}{r_0}\|\varphi\|_\infty\ell\,.$$

Thus, by taking a sequence $\{\varphi_n\}$ as above converging pointwise to 1 in I, from (33) we get that there exists $C_3>0$ depending only on r_0 and the Lamé coefficients λ, μ, such that

$$\Lambda\mathcal{H}^1(\Gamma')\leq c(r_0)\Lambda\mathcal{L}^1(I)\quad (2.26)$$
$$\leq C_3\bigg(\int_{\Omega_g}|(H_{g,\tau})_{sym}|\,dz+\ell\sup_{\Gamma''}|H_{g,\tau}|^2+\frac{\gamma\ell}{r_0}+\beta\int_I|g-\bar h|\,dx\bigg)\,,$$

where we used the fact that $\mathcal{H}^1(\Gamma'')=\frac12\mathcal{H}^1(\Gamma')$. Now assume by contradiction that there exist $\Lambda_n\to+\infty$ and minimizers $(g_n,\tau_n,H_{g_n,\tau_n})$ of (31), with $|\Omega_{g_n}|>d$, $\tau_n=\sum_{i=1}^k\mathbf{b}_i\delta^\#_{z_{i,n}}$, and $\Gamma'_n\subset\Gamma_{g_n}\cap\partial B_{r_0}(z_{j,n})$ for some $j\in\{1,\dots,k\}$, with

$$\inf_n\mathcal{H}^1(\Gamma'_n)>0\,.$$

Thus, from (32) we deduce that

$$\sup_{\Gamma''_n}|H_{g_n,\tau_n}|\leq C_4\,,$$

with C_4 independent of n. Recalling (34) and observing that by mininimality

$$\sup_n\bigg(\|(H_{g_n,\tau_n})_{sym}\|_{L^2(\Omega_{g_n};\mathbb{M}^{2\times2})}+\beta\int_0^\ell|g_n-\bar h|^2\,dx\bigg)<+\infty\,,$$

we conclude that

$$\Lambda_n\mathcal{H}^1(\Gamma'_n)\leq C$$

for some constant C independent of n, which is impossible since $\Lambda_n\to+\infty$. □

Proof of Theorem 2.5. We fix β such that

$$F(\bar h,\bar\sigma,H_{\bar h,\bar\sigma})<\frac{\beta}{4}\int_0^b\Big|\bar h-\frac{d}{b}\Big|^2\,dx\,. \tag{2.27}$$

In order to prove the result we will show that any minimizing configuration $(g,\tau,H_{g,\tau})$ for (31) satisfies the volume constraint $|\Omega_g|=d$, provided that Λ is sufficiently large. We argue by contradiction and consider several cases.

Step 1. If $|\Omega_g|<d$, then define $h:=g+(d-|\Omega_g|)/\ell$ and for all $(x,y)\in\Omega_h$

$$H(x,y):=\begin{cases} e_0Dv_0(x,y) & \text{if } 0<y<\dfrac{d-|\Omega_g|}{\ell}\,,\\[2mm] H_{g,\tau}\Big(x,y-\dfrac{d-|\Omega_g|}{\ell}\Big) & \text{if } y\ge\dfrac{d-|\Omega_g|}{\ell}\,,\end{cases}$$

where v_0 is defined as in (23) and σ is the dislocation measure obtained by moving in the e_2 direction all the centers z_i, $i=1,\dots,k$ of τ by the vector $(d-|\Omega_g|)\mathbf{e}_2/\ell$. Then by (23),

$$\begin{aligned}F(h,\sigma,H)&+\beta\int_0^\ell|h-\bar h|^2\,dx+\Lambda\big||\Omega_h|-d\big|-F(g,\tau,H_{g,\tau})\\&-\beta\int_0^\ell|g-\bar h|^2\,dx-\Lambda\big||\Omega_g|-d\big|\\&=e_0^2W_0(d-|\Omega_g|)+\beta\int_0^\ell\frac{d-|\Omega_g|}{\ell}\Big(2(g-\bar h)+\frac{d-|\Omega_g|}{\ell}\Big)\,dx-\Lambda(d-|\Omega_g|)\\&\le e_0^2W_0(d-|\Omega_g|)-\Lambda(d-|\Omega_g|)\,,\end{aligned}$$

where we used the fact that $\int_0^\ell g\,dx=|\Omega_g|<d=\int_0^\ell\bar h\,dx$. By taking $\Lambda>e_0^2W_0$, we obtain a contradiction to the minimality of $(g,\tau,H_{g,\tau})$.

Step 2. If $|\Omega_g|>d$, we distinguish two cases. Let y_{max} be the maximal height of points in Γ_g and for all $i=1,\dots,k$ write $z_i=(x_i,y_i)$.

Case 1. If $y_i<y_{max}-r_0$ for all $i=1,\dots,k$, we truncate g in such a way that, denoting by h the resulting function, we still have $B_{r_0}(z_i)\subset\Omega_h^\#$ for all i and $|\Omega_h|\ge d$. Since $h\le g$, we can estimate

$$\begin{aligned}F(h,\tau,H_{g,\tau})&+\beta\int_0^\ell|h-\bar h|^2\,dx+\Lambda\big(|\Omega_h|-d\big)-F(g,\tau,H_{g,\tau})\\&-\beta\int_0^\ell|g-\bar h|^2\,dx-\Lambda\big(|\Omega_g|-d\big)\\&\le\beta\int_0^\ell(g-h)(2\bar h-h-g)\,dx-\Lambda\int_0^\ell(g-h)\,dx\\&\le\big(2\beta\|\bar h\|_\infty-\Lambda\big)\int_0^\ell(g-h)\,dx\le(2\beta C_0-\Lambda)\int_0^\ell(g-h)\,dx<0\,,\end{aligned}$$

provided $\Lambda>2\beta C_0$, which would contradict the minimality of $(\bar h,\bar\sigma,\bar H)$. Note that the constant C_0 bounding $\|\bar h\|_\infty$ from above only depends on $F(\bar h,\bar\sigma,H_{\bar h,\bar\sigma})$ (see (11)).

Case 2. Assume now that there exists j such that $y_j = y_{max} - r_0$. We claim that for every $i \in \{1, \dots, k\}$ the intersection $\Gamma_g \cap \partial B_{r_0}(z_i)$ is either empty or a (possibly degenerate) connected arc. Indeed, if this were not true for some $i \in \{1, \dots, k\}$, we could find two points w_1, $w_2 \in \Gamma_g \cap \partial B_{r_0}(z_i)$ such that the graph of g is detached from $\partial B_{r_0}(z_i)$ above the arc $\widehat{w_1 w_2}$ connecting w_1 and w_2 on $\partial B_{r_0}(z_i)$. Denote by D the region bounded by $\widehat{w_1 w_2}$ and the arc on Γ_g connecting the two points. Fix a point w in the interior of $\widehat{w_1 w_2}$ and consider the tangent to $\partial B_{r_0}(z_i)$ at w. Moving this tangent outward in the direction $w - z_i$, we cut out a region $D' \subset D$ bounded by this line and Γ_g such that $|D'| \le |\Omega_g| - d$. Note that by doing so we get a new profile $\hat{g}$ such that $\mathcal{H}^1(\Gamma_{\hat{g}}) < \mathcal{H}^1(\Gamma_g)$ and, in turn,

$$F(\hat{g}, \tau, H_{g,\tau}) < F(g, \tau, H_{g,\tau})\,. \tag{2.28}$$

Therefore, arguing as in the previous step, we contradict the minimality of $(g, \tau, H_{g,\tau})$, provided that Λ is chosen as before. Thus, the claim holds.

Set

$$J := \{j \in \{1, \dots, k\} : y_j = y_{max} - r_0\}\,.$$

Since $y_{max}\ell \ge |\Omega_g| > d \ge 2r_0\ell$, we have that $y_{max} - 2r_0 =: \delta > 0$. Hence, $y_j = r_0 + \delta$ for every $j \in J$. Let

$$0 < \varepsilon < \min\{\delta, \ell\}/k\,. \tag{2.29}$$

Let $\Lambda_\varepsilon > 0$ be so large that

$$\frac{1}{\Lambda} F(\bar{h}, \bar{\sigma}, H_{\bar{h},\bar{\sigma}}) < \varepsilon \tag{2.30}$$

for all $\Lambda > \Lambda_\varepsilon$. Fix $j \in J$ and assume that $0 < x_j < \ell$ (the cases $x_j = 0$ and $x_j = \ell$ are similar). By the previous claim, the set $\Gamma_g \cap \partial B_{r_0}(z_j)$ is a (possibly degenerate) connected arc Γ_j of left endpoint p_j and right endpoint q_j.

Since $y_j \ge r_0 + \delta$, we may apply Lemma 2.6 to conclude that, choosing a possibly larger Λ_ε, then $\mathcal{H}^1(\Gamma_j) < \varepsilon$. Let $\Pi_2 : \mathbb{R}^2 \to \mathbb{R}$ be the projection onto the y-axis. Then $\mathcal{L}^1(\Pi_2(\Gamma_j) \le \mathcal{H}^1(\Gamma_j) < \varepsilon$. Hence,

$$q_j \cdot e_2 \ge y_{max} - \varepsilon = 2r_0 + \delta - \varepsilon\,. \tag{2.31}$$

If q_j belongs to $\Gamma_g \cap \partial B_{r_0}(z_{j_1})$ for some $j_1 \ne j$, then by (37) and (39),

$$y_{j_1} = (z_{j_1} - q_j) \cdot e_2 + q_j \cdot e_2 \ge -r_0 + 2r_0 + \delta - \varepsilon = r_0 + \delta - \varepsilon$$

Let q_{j_1} be the right endpoint of the (possibly degenerate) connected arc $\Gamma_g \cap \partial B_{r_0}(z_{j_1})$. Since $y_{j_1} > r_0$ by Lemma 2.6 and (39) we obtain as before that the arc Γ_{j_1} of endpoints q_j and q_{j_1} has length less than ε and that $q_{j_1} \cdot e_2 \ge 2r_0 + \delta - 2\varepsilon$. If q_{j_1} belongs to $\Gamma_g \cap \partial B_{r_0}(z_{j_2})$ for some $j_2 \ne j_1$, we continue this process, otherwise we stop and repeat a similar procedure for the left endpoint p_j. Let J_j be the set of the indices $i \in \{1, \dots, k\}$ corresponding to balls selected in this procedure. Note that by construction $y_i > r_0$ for every $i \in J_j$, and so

$$\sum_{j \in J} \sum_{i \in J_j} \mathcal{L}^1(\Pi_2(\Gamma_g \cap \partial B_{r_0}(z_i))) \le \sum_{j \in J} \sum_{i \in J_j} \mathcal{H}^1(\Gamma_g \cap \partial B_{r_0}(z_i)) \le k\varepsilon\,.$$

Since the union of all the arcs $\Gamma_g \cap \partial B_{r_0}(z_i)$ is connected and Γ_j is one of them this implies that

$$y_{max} - k\varepsilon \le g(x) \le y_{max} \tag{2.32}$$

for all $x \in (0,\ell)$ such that $(x, g(x)) \in \Gamma_g \cap \partial B_{r_0}(z_i)$ for some $i \in J_j$.
Let $\Pi_1 : \mathbb{R}^2 \to \mathbb{R}$ be the projection onto the x-axis. Since

$$\sum_{j\in J}\sum_{i\in J_j} \mathcal{L}^1(\Pi_1(\Gamma_g \cap \partial B_{r_0}(z_i))) \le \sum_{j\in J}\sum_{i\in J_j} \mathcal{H}^1(\Gamma_g \cap \partial B_{r_0}(z_i)) \le k\varepsilon < \ell\,,$$

the open set $U := (0,\ell) \setminus \cup_{j\in J}\cup_{i\in J_j} \Pi_1(\Gamma_g \cap \partial B_{r_0}(z_i))$ is nonempty.
Case 2a. Assume that there exists a connected component I_i of U and $s < t \in I_i$ such that $\Gamma_g \cap (s,t)\times\mathbb{R}$ lies strictly above the segment γ connecting $(s, g^-(s))$ with $(t, g^-(t))$. Let ν be the unit vector orthogonal to γ and pointing upward. Moving γ in the direction of ν, we can choose $\eta > 0$ so that the region D bounded by the segment $\gamma + \eta\nu$ and $\Gamma_g \cap (s,t)\times\mathbb{R}$ satisfies $|D| \le |\Omega_g| - d$ and $D \cap \cup_{i=1}^k B_{r_0}(z_i) = \emptyset$. Then, arguing as in the proof of (36) we get a contradiction provided that Λ is chosen as before.
Case 2b. For every connected component I_i of the set U we have that g^- is a convex function in the interval I_i. In this case we claim that there exists a constant $c > 0$ independent of g such that

$$y_{max} - c\varepsilon \le g(x) \le y_{max} \quad \text{for all } x \in (0,\ell)\,. \tag{2.33}$$

In view of (40) it suffices to prove (41) in each I_i. Fix I_i and let a_i be its left endpoint. Then the point $(a_i, g(a_i))$ belongs to one of the balls $B_{r_0}(z_l)$ for some $j \in J$ and $l \in J_j$. Let θ_i be the angle that the oriented segment of endpoints z_l and $(a_i, g(a_i))$ forms with the x-axis. By (40), we have that $\theta_i \ge \frac{\pi}{4}$ for ε sufficiently small. Since g is a convex function in the interval I_i, it lies above the line

$$t \mapsto (a_i, g(a_i)) + t\left(1, -\frac{\cos\theta_i}{\sin\theta_i}\right)$$

tangent to the ball $\partial B_{r_0}(z_l)$ at $(a_i, g(a_i))$. Since $\mathcal{H}^1(\Gamma_g \cap \partial B_{r_0}(z_l)) \le \varepsilon$, we have that $\cos\theta_i \le \cos(\pi/2 - \varepsilon/r_0) = \sin(\varepsilon/r_0) \le \varepsilon/r_0$. Hence, for $t > 0$,

$$g(a_i) - t\frac{\cos\theta_i}{\sin\theta_i} \ge g(a_i) - \frac{t\sqrt{2}}{r_0}\varepsilon \ge y_{max} - k\varepsilon - \frac{\ell\sqrt{2}}{r_0}\varepsilon\,,$$

where in the last inequality we used (40). This proves that (41) holds. By (31) we have

$$F(g,\tau,H_{g,\tau}) + \beta\int_0^b |g-\bar h|^2\,dx + \Lambda\big||\Omega_g| - d\big| \le F(\bar h,\bar\sigma,H_{\bar h,\bar\sigma})$$

and so by (38), $\big||\Omega_g| - d\big| < \varepsilon$. In turn, by (41),

$$d \le y_{max}\ell \le d + (1 + c\ell)\varepsilon\,,$$

which, again by (41), yields

$$-c\varepsilon \le g(x) - \frac{d}{\ell} \le (1 + c\ell)\varepsilon/\ell \tag{2.34}$$

for all $x \in (0,\ell)$. It follows that $\|g - d/\ell\|_2 \le c\varepsilon$ for a possibly larger constant c still independent of g. Hence, using the minimality of $(g,\tau,H_{g,\tau})$ and (35), we obtain

$$\begin{aligned}\|\bar h - d/\ell\|_2 &\le \|\bar h - g\|_2 + \|g - d/\ell\|_2 \le \sqrt{\frac{1}{\beta}F(\bar h,\bar\sigma,H_{\bar h,\bar\sigma})} + \|g - d/\ell\|_2\\ &< \frac{1}{2}\|\bar h - d/\ell\|_2 + c\varepsilon\,,\end{aligned}$$

which is a contradiction if we choose ε small enough. □

Next we show that volume constrained minimizing configurations are also a unilateral minimizers of a simpler penalized problem.

Theorem 2.7. *Let $d > 0$ and let $(\bar h, \bar\sigma, H_{\bar h,\bar\sigma})$ be a minimizing configuration for problem (28). Fix $\Lambda > e_0^2 W_0$. Then $(\bar h, \bar\sigma, H_{\bar h,\bar\sigma})$ is a minimizer of*

$$\min\Big\{ F(h,\sigma,H) + \Lambda\big(d - |\Omega_h|\big) : (h,\sigma,H) \in X(e_0;\mathbf{B}),\, |\Omega_h| \le d \Big\}. \tag{2.35}$$

Proof. The proof is similar to the one of Step 1 of the proof of Theorem 2.5, with $\beta = 0$. □

The next lemma is proved in [25, Lemma 6.5] and will be used to prove the interior ball condition stated in Lemma 2.9 below.

Lemma 2.8. *Let $k \in AP(0,\ell)$ be nonnegative, let $B_\varrho(z_0)$ be a ball such that $B_\varrho(z_0) \subset \{(x,y) : x \in (0,\ell)$ and $y < k(x)\}$, and let $z_1 = (x_1,y_1)$ and $z_2 = (x_2,y_2)$ be points in $\partial B_\varrho(z_0) \cap (\Gamma_k \cup \Sigma_k)$. Let γ be the shortest arc on $\partial B_\varrho(z_0)$ connecting z_1 and z_2 (any of the two possible arcs if z_1 and z_2 are antipodal) and let γ' be the arc on $\Gamma_k \cup \Sigma_k$ connecting z_1 and z_2. Then*

$$\mathcal{H}^1(\gamma') - \mathcal{H}^1(\gamma) \ge \frac{1}{\varrho}|D|\,,$$

where D is the region enclosed by $\gamma \cup \gamma'$.

Lemma 2.9. *Let $\Lambda > 0$ and let $(g,\tau,H_{g,\tau}) \in X(e_0;\mathbf{B})$ be a minimizing configuration for the problem (43). If $\varrho < \min\{1/\Lambda, r_0\}$, then for all $z \in \Gamma_g \cup \Sigma_g$ there exists a ball $B_\varrho(z_0) \subset \Omega_g^\# \cup \big(\mathbb{R}\times(-\infty,0]\big)$ such that $\partial B_\varrho(z_0) \cap (\Gamma_g \cup \Sigma_g) = \{z\}$.*

Proof. Fix $\varrho < \min\{r_0, 1/\Lambda\}$. We argue by contradiction and assume that there exists $B_\varrho(z_0) \subset \Omega_g^\# \cup \big(\mathbb{R}\times(-\infty,0]\big)$ touching $\widetilde\Gamma_g = \Gamma_g \cup \Sigma_g$ in at least two points $w_1 = (s_1,t_1)$, $w_2 = (s_2,t_2) \in S_\varrho^+(z_0)$, where $S_\varrho^+(z_0)$ denotes the upper half of $\partial B_{r_0}(z_0)$. Consider the region D bounded by the arc γ on $S_\varrho^+(z_0)$ connecting w_1 and w_2 and $\widetilde\Gamma_g$. Since $\varrho < r_0$, necessarily $D \cap \cup_{i=1}^k B_{r_0}(z_i) = \emptyset$. Hence we may modify g by replacing it with the function $\tilde g$ which coincides with g in $[0,\ell)\setminus(s_1,s_2)$ and whose graph on (s_1,s_2) is given by γ. Denote by γ' the arc on $\widetilde\Gamma_g$ connecting w_1 and w_2. Then we have

$$F(\tilde g, v) + \Lambda\big(d - |\Omega_{\tilde g}|\big) - F(g,v) - \Lambda\big(d - |\Omega_g|\big) \le \mathcal{H}^1(\gamma) - \mathcal{H}^1(\gamma') + \Lambda|D| < 0\,,$$

where the last inequality is a consequence of Lemma 2.8 and the fact that $\varrho < 1/\Lambda$. This contradicts the minimality of $(g,\tau,H_{g,\tau})$. The conclusion of the lemma follows arguing as in [14, Lemma 2] or [21, Proposition 3.3, Step 2]. □

Theorem 2.5 will be used to study the regularity of those profiles for which the function h^- defined in (9) is not flat. Note the assumption that h^- is flat does not exclude a priori the presence of vertical cuts (see (10)). This possibility is ruled out by the next result.

Theorem 2.10. *Let $(\bar{h}, \bar{\sigma}, H_{\bar{h},\bar{\sigma}})$ be a minimizing configuration of problem* (28) *such that $\bar{h}^-$ is constant. Then $\Sigma_{\bar{h}} = \emptyset$.*

Proof. By Theorem 2.7 and Lemma 2.9 we deduce that $\Omega^{\#}_{\bar{h}} \cup \big(\mathbb{R} \times (-\infty, 0]\big)$ satisfies an interior ball condition with $\varrho < \min\{r_0, 1/(e_0^2 W_0)\}$. If $\Sigma_{\bar{h}}$ were nonempty, then each vertical cut would meet the (horizontal) graph of $\bar{h}^-$ perpendicularly, but this would prevent the existence of an interior sphere at the corner. Hence, $\Sigma_{\bar{h}} = \emptyset$ and the proof is complete. □

We now recall some regularity estimates, based on the theory developed by Grisvard ([32]), proved in [21] for solutions of the Lamé system in planar domains with a corner.

Let Ω be a bounded open set in $\mathbb{R}^2$ whose boundary can be decomposed in three curves

$$\partial\Omega = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3,$$

where Γ_1 and Γ_2 are two segments meeting at the origin with an (internal) angle $\omega \in (\pi, 2\pi)$ and Γ_3 is a smooth curve joining the two remaining endpoints of Γ_1 and Γ_2 in a smooth way and not passing through the origin. We shall refer to such an open set as a *regular domain with corner angle* ω.

The next result is a particular case of [32, Théorème I].

Theorem 2.11. *Let $\Omega \subset \mathbb{R}^2$ be a regular domain with corner angle $\omega \in (\pi, 2\pi)$ and let $w \in H^1(\Omega; \mathbb{R}^2)$ be a weak solution of the Neumann problem*

$$\begin{cases} \operatorname{div} \mathbb{C}E(w) = f & \text{in } \Omega, \\ \mathbb{C}E(w)[\nu] = g & \text{on } \partial\Omega, \end{cases} \tag{2.36}$$

where $f \in L^p\big(\Omega; \mathbb{R}^2\big)$ and $g \in W^{1-1/p,p}(\partial\Omega \setminus \{0\}; \mathbb{R}^2)$, $p \in (1, 2)$. Then, there exist numbers c_α, c'_α such that w may be decomposed as

$$w = w_{\rm reg} + \sum_\alpha c_\alpha \mathcal{S}_\alpha + \sum_\alpha c'_\alpha \frac{\partial}{\partial\alpha}\mathcal{S}_\alpha,$$

where $w_{reg} \in W^{2,p}(\Omega; \mathbb{R}^2)$ and in the first sum α ranges among all complex numbers with $\operatorname{Re}\alpha \in \left(0, \frac{2(p-1)}{p}\right)$ which are solutions of the equation

$$\sin^2 \alpha\omega = \alpha^2 \sin^2 \omega, \tag{2.37}$$

and in the second sum α ranges only among solutions with multiplicity two of (45) *in the same strip. Moreover, the functions $\mathcal{S}_\alpha$ are independent of f and in polar coordinates*

$$\mathcal{S}_\alpha(r, \theta) = r^\alpha g_\alpha(\theta)\ ,$$

for some smooth function g_α. The above decomposition holds provided that (45) *has no solutions with real part equal to $\frac{2(p-1)}{p}$.*

Though this result gives no information about the roots of equation (45), it is clear that the solutions contained in the strip $0 < \operatorname{Re}\alpha < 1$ are bounded. Hence, by analyticity, they are finitely many. A more precise information is provided by the following result, proved in [42, Theorem 2.2].

Theorem 2.12. *If $\omega \in (0, 2\pi)$, then equation (45) has no roots in the strip $0 < \operatorname{Re}\alpha \leq \frac{1}{2}$.*

We will use the two previous results to get an a priori estimate for the solutions to (44). We recall that an *infinitesimal rigid motion* is an affine displacement of the form $a + Ax$, where A is a skew symmetric 2×2 matrix and a is a constant vector.

Proposition 2.13. *Let Ω be as in Theorem 2.11. There exist $p \in (4/3, 2)$ and $C > 0$ such that if $f \in L^p(\Omega; \mathbb{R}^2)$, $g \in W^{1-1/p,p}(\partial\Omega \setminus \{0\}; \mathbb{R}^2)$ and $w \in W^{1,2}(\Omega; \mathbb{R}^2)$ is a weak solution to problem (44), then*

$$\|w\|_{W^{2,p}(\Omega;\mathbb{R}^2)} \leq C\big(\|w\|_{L^p(\Omega;\mathbb{R}^2)} + \|f\|_{L^p(\Omega;\mathbb{R}^2)} + \|g\|_{W^{1-1/p,p}(\partial\Omega\setminus\{0\};\mathbb{R}^2)}\big)\,. \tag{2.38}$$

Proof. As observed above, the strip $0 < \operatorname{Re}\alpha < 1$ contains only finitely many solutions to equation (45). Hence, by Theorem 2.12 there exists $\varepsilon > 0$ such that all solutions are contained in the strip $\frac{1}{2} + \varepsilon < \operatorname{Re}\alpha < 1$. Therefore, if we choose $p > 4/3$ such that $2 - \frac{2}{p} < \frac{1}{2} + \varepsilon$, from Theorem 2.11 we get that any weak solution to (44), with $f \in L^p(\Omega; \mathbb{R}^2)$ and $g \in W^{1-1/p,p}(\partial\Omega \setminus \{0\}; \mathbb{R}^2)$ is in $W^{2,p}(\Omega; \mathbb{R}^2)$.

To prove (46), set $V := W^{2,p}(\Omega; \mathbb{R}^2)/\sim$, where for every $u, v \in W^{2,p}(\Omega; \mathbb{R}^2)$, we have set $u \sim v$ if and only if $u - v$ is an infinitesimal rigid motion. We define a norm in V setting

$$\|[u]\|_V := \|E(u)\|_{L^p(\Omega;\mathbb{R}^2)} + \|\nabla^2 u\|_{L^p(\Omega)}$$

for every equivalence class $[u]$, with $u \in W^{2,p}(\Omega; \mathbb{R}^2)$. Note that this definition is well posed, since if $u \sim v$, then $E(u) = E(v)$ and $\nabla^2 u = \nabla^2 v$. Note also that in view of Korn's inequality, V is a Banach space.

Consider now the operator $L : V \to L^p(\Omega; \mathbb{R}^2) \times W^{1-1/p,p}(\partial\Omega \setminus \{0\}; \mathbb{R}^2)$ defined for any $[u] \in V$ as

$$L[u] := (\operatorname{div} \mathbb{C}E(u), \mathbb{C}E(u)[\nu])\,.$$

By the first part of the proof we have that L is a linear, continuous, and invertible operator between two Banach spaces. Therefore, the conclusion follows from the open mapping theorem. □

Proposition 2.14. *Let Ω be a regular domain with corner $\omega \in (\pi, 2\pi)$ and let $u \in H^1(\Omega; \mathbb{R}^2)$ be a weak solution to the Neumann problem*

$$\begin{cases} \operatorname{div} \mathbb{C}E(w) = f & \text{in } \Omega, \\ \mathbb{C}E(w)[\nu] = g & \text{on } \Gamma_1 \cup \Gamma_2, \end{cases}$$

with $f \in L^p(\Omega; \mathbb{R}^2)$ and $g \in W^{1-1/p,p}((\Gamma_1 \cup \Gamma_2) \setminus \{0\}; \mathbb{R}^2)$. Then, there exist $\bar{r} > 0$, with $\overline{B}_{\bar{r}}(0) \cap \Gamma_3 = \emptyset$, $C > 0$, and $\alpha > 1/2$, depending only on λ, μ, ω, $\|f\|_{L^p(\Omega;\mathbb{R}^2)}$ and $\|g\|_{W^{1-1/p,p}((\Gamma_1\cup\Gamma_2)\setminus\{0\};\mathbb{R}^2)}$, such that for all $r \in (0, \bar{r})$,

$$\int_{B_r(0)\cap\Omega} |\nabla w|^2\, dz \leq C r^{2\alpha} \int_\Omega \big(1 + |w|^2 + |\nabla w|^2\big)\, dz\,. \tag{2.39}$$

Proof. Set $B_{\hat{r}} := B_{\hat{r}}(0)$ and fix $\hat{r} > 0$ such that $B_{\hat{r}} \cap \Gamma_3 = \emptyset$ and $\partial B_{\hat{r}} \cap \Gamma_1 \cup \Gamma_2 \neq \emptyset$, and $0 < \bar{r} < \hat{r}$. Let $\varphi \in C_c^\infty(B_{\hat{r}})$ be such that $\varphi \equiv 1$ on $B_{\bar{r}}$. From the equation satisfied by

$w\varphi$ and from (46) we get

$$\begin{aligned}\|w\varphi\|_{W^{2,p}(\Omega;\mathbb{R}^2)} &\le C\big(\|w\|_{W^{1,p}(\Omega;\mathbb{R}^2)} + \|f\|_{L^p(\Omega;\mathbb{R}^2)} \\ &\qquad + \|g\|_{W^{1-1/p,p}((\Gamma_1\cup\Gamma_2)\setminus\{0\};\mathbb{R}^2)} + \|w\|_{W^{1-1/p,p}(\partial\Omega\setminus\{0\};\mathbb{R}^2)}\big) \\ &\le C\big(\|w\|_{W^{1,p}(\Omega;\mathbb{R}^2)} + \|f\|_{L^p(\Omega;\mathbb{R}^2)} + \|g\|_{W^{1-1/p,p}((\Gamma_1\cup\Gamma_2)\setminus\{0\};\mathbb{R}^2)}\big)\end{aligned}$$

for some $\frac{4}{3} < p < 2$ and some $C > 0$ depending only on λ, μ and ω. Thus, if $0 < r < \bar r$, using the Sobolev imbedding theorem we have

$$\begin{aligned}\int_{B_r\cap\Omega} |\nabla w|^2\,dz &\le c\bigg(\int_{B_r\cap\Omega} |\nabla(w\varphi)|^{\frac{2p}{2-p}}\,dz\bigg)^{\frac{2-p}{p}} r^{\frac{4(p-1)}{p}} \le cr^{\frac{4(p-1)}{p}}\|w\varphi\|^2_{W^{2,p}(\Omega;\mathbb{R}^2)} \\ &\le cr^{\frac{4(p-1)}{p}}\big(1+\|w\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\big)^2 \le cr^{2\alpha}\int_\Omega \big(1+|w|^2+|\nabla w|^2\big)\,dz\,,\end{aligned}$$

where $\alpha := 2(p-1)/p$ is strictly greater than $1/2$ since $p > 4/3$. □

For $g \in AP(0,\ell)$ we denote the set of *cusp points* by

$$\Sigma_{g,c} := \{(x, g(x)) : x \in [0,\ell)\,, g^-(x) = g(x)\,,\ \text{and } g'_+(x) = -g'_-(x) = +\infty\}\,,$$

where g^- is defined in (9), while g'_+ and g'_- denote the right and left derivatives, respectively.

As usual, the set $\Sigma^\#_{g,c}$ is obtained by replacing $[0,\ell)$ by $\mathbb{R}$ in the previous formula and coincides with the ℓ-periodic extension of $\Sigma_{g,c}$.

Theorem 2.15 (Regularity)**.** *Let $(\bar h, \bar\sigma, H_{\bar h,\bar\sigma}) \in X(e_0;\mathbf{B})$ be a minimizer of (28), with $\bar\sigma = \sum_{i=1}^k \mathbf{b}_i\delta^\#_{z_i}$. Then:*

(i) $\bar h$ has at most finitely many cusp points and vertical cracks $[0,\ell)$, i.e.,

$$\operatorname{card}\big(\{x\in[0,\ell) : (x,y)\in\Sigma_{\bar h}\cup\Sigma_{\bar h,c} \text{ for some } y\ge 0\}\big) < +\infty\,;$$

(ii) the curve $\Gamma^\#_{\bar h}$ is of class C^1 away from $\Sigma^\#_{\bar h}\cup\Sigma^\#_{\bar h,c}$ and

$$\lim_{x\to x_0^\pm} \bar h'(x) = \pm\infty \qquad \text{for every } x_0 \text{ s.t. } (x_0,\bar h(x_0))\in\Sigma^\#_{\bar h}\cup\Sigma^\#_{\bar h,c};$$

(iii) $\Gamma^\#_{\bar h}\cap\{y>0\}$ is of class $C^{1,\alpha}$ away from $\Sigma^\#_{\bar h}\cup\Sigma^\#_{\bar h,c}$ for all $\alpha\in(0,1/2)$;

(iv) setting

$$A := \{(x,y)\in\mathbb{R}^2 : \bar h(x) > 0,\ \bar h \text{ continuous at } x\}\,,$$

$\Gamma^\#_{\bar h}$ is analytic in $A\setminus\cup_{i=1}^k\cup_{m\in\mathbb{Z}}\overline{B}_{r_0}(z_i+m\ell\mathbf{e}_1)$.

The proof of the regularity theorem is based upon the strategy introduced in [21] (see also [25]). We only outline the main steps, by highlighting the changes needed in the present situation and referring the reader to the aforementioned papers for the details.

Proof of Theorem 2.15. We start by observing that we may assume that $\bar{h}^-$ is not constant, since otherwise the conclusion follows from Theorem 2.10. Note also the if $d < 2r_0\ell$, then necessarily $\mathbf{B} = \emptyset$, and thus the result follows from [18, Theorem 2.5] (see also [25, Theorem 2.7]). Therefore, from now on we shall assume that $d \geq 2r_0\ell$ and $\bar{h}^-$ is not constant.

Step 1. (Lipschitz partial regularity) From Theorem 2.7 and Lemma 2.9 we have that $\widetilde{\Gamma}_{\bar{h}}$ satisfies an interior ball condition with radius $\varrho < \min\{1/(e_0^2 W_0), r_0\}$. By applying [14, Lemma 3] we get that $\widetilde{\Gamma}_{\bar{h}}$ has the following properties: For any $z_0 \in \widetilde{\Gamma}_{\bar{h}}$ there exist an orthonormal basis $\mathbf{i}, \mathbf{j} \in \mathbb{R}^2$ and a rectangle

$$Q := \{z_0 + s\mathbf{i} + t\mathbf{j} : -a' < s < a',\, -b' < t < b'\},$$

with $a',\, b' > 0$, such that $\Omega_{\bar{h}} \cap Q$ has one of the following two representations:
(j) There exists a Lipschitz function $f : (-a', a') \to (-b', b')$ such that $f(0) = 0$ and

$$\Omega_{\bar{h}} \cap Q = \{z_0 + s\mathbf{i} + t\mathbf{j} : -a' < s < a',\, -b' < t < f(s)\} \cap ((0,\ell) \times \mathbb{R}).$$

Moreover, the function f admits at every point left and right derivatives, which are left and right continuous, respectively.
(jj) There exist two Lipschitz functions $f_1,\ f_2 : [0, a') \to (-b', b')$ such that $f_i(0) = (f_i)'_+(0) = 0$ for $i = 1,\, 2$, $f_1 \leq f_2$, and

$$\Omega_{\bar{h}} \cap Q = \{z_0 + s\mathbf{i} + t\mathbf{j} : 0 < s < a',\, -b' < t < f_1(s) \text{ or } f_2(s) < t < b'\}.$$

Moreover, the functions $f_1,\, f_2$ admit at every point left and right derivatives, which are left and right continuous, respectively. Note that (j) and (jj) imply statement (i) of the theorem and the fact that

$$\lim_{x \to x_0^{\pm}} \bar{h}'_{\pm}(x) = \pm\infty \qquad \text{for every } x_0 \text{ s.t. } (x_0, \bar{h}(x_0)) \in \Sigma_{\bar{h}} \cup \Sigma_{\bar{h},c}.$$

Step 2. (C^1-regularity) From property (j) of Step 1 we have that the curve $\Gamma_{\bar{h}}$ is locally Lipschitz in $[0,\ell) \times \mathbb{R}$ away from finitely many singularities of cusp or cut type. Moreover, outside the singular set, $\Gamma_{\bar{h}}$ admits left and right tangent, which are left and right continuous respectively. Therefore, to prove statement (ii) it is enough to show that left and right tangents coincide at every point $z_0 \notin \Sigma_{\bar{h}} \cup \Sigma_{\bar{h},c}$.

Assume by contradiction that this does not happen for some $z_0 = (x_0, y_0) \notin \Sigma_{\bar{h}} \cup \Sigma_{\bar{h},c}$. If $y_0 = 0$, then by interior ball condition we can say that there are no dislocation balls in a neighborhood $B_r(z_0)$ of z_0 and thus $H_{\bar{h},\bar{\sigma}}$ in such a neighborhood is a gradient Dv, with v satisfying

$$\begin{cases} \operatorname{div} \mathbb{C}E(v) = 0 & \text{in } \Omega_{\bar{h}} \cap B_r(z_0), \\ \mathbb{C}E(v)[\nu] = 0 & \text{on } \Gamma_{\bar{h}} \cap B_r(z_0), \\ v(x,0) = e_0(x,0) & \text{on } \{y = 0\} \cap B_r(z_0). \end{cases}$$

We may therefore apply the argument used in [18, Theorem 4.9 and Proposition 5.1] to obtain a contradiction.

Assume now that $y_0 > 0$. In this case we decompose $H_{\bar{h},\bar{\sigma}} = Dv + K$, where

$$K := \begin{pmatrix} k_1 & 0 \\ k_2 & 0 \end{pmatrix},$$

with

$$k_l(x,y) := -\sum_{i=1}^{k} (\mathbf{b}_i \cdot \mathbf{e}_l) \int_0^y \varrho_{r_0}(x - x_i, t - y_i)\, dt \text{ for } l = 1, 2,$$

and v satisfies

$$\begin{cases} \operatorname{div} \mathbb{C}E(v) = -\operatorname{div} \mathbb{C}K_{sym} & \text{in } \Omega_{\bar h}, \\ \mathbb{C}E(v)[\nu] = -\mathbb{C}K_{sym}[\nu] & \text{on } \Gamma_{\bar h}. \end{cases}$$

Using (47) in place of [21, Equation (3.52)] and arguing as in [21, Theorem 3.13], we can prove that there exist $C > 0$, a radius $\bar r > 0$, and $\alpha \in (\frac{1}{2}, 1)$ such that

$$\int_{B_r(z_0) \cap \Omega^{\#}_{\bar h}} |\nabla v|^2\, dz \le C r^{2\alpha} \qquad \text{for all } r \le \bar r.$$

In turn, since K is smooth this implies that for a possibly larger constant

$$\int_{B_r(z_0) \cap \Omega^{\#}_{\bar h}} |H_{\bar h, \bar\sigma}|^2\, dz \le C r^{2\alpha} \qquad \text{for all } r \le \bar r.$$

Moreover, by Theorem 2.5 there exist Λ, $\beta > 0$ such that $(\bar h, \bar\sigma, H_{\bar h, \bar\sigma})$ is a minimizer of

$$\min\left\{ F(h,\sigma,H) + \beta \int_0^\ell |h - \bar h|^2\, dx + \Lambda \big| |\Omega_h| - d \big| : (h,\sigma,H) \in X(e_0; \mathbf{B}) \right\}. \tag{2.40}$$

To fix the ideas let us assume that $z_0 = (x_0, \bar h(x_0))$ does not belong to a vertical segment of $\Gamma_{\bar h}$; i.e., $\bar h$ is continuous at x_0. The other case can be dealt with similarly.

Observe that by a standard extension argument we may define v in a fixed neighborhood of z_0 in such a way that, denoting by $\tilde v$ the resulting function, for all $0 < r \le \bar r$ we have

$$\int_{B_r(z_0)} |\nabla \tilde v|^2\, dz \le c(L) \int_{B_r(z_0) \cap \Omega_{\bar h}} |\nabla v|^2\, dz\,,$$

where the constant $c(L)$ depends only on the Lipschitz constant L of the function $\bar h$. Finally set $H := D\tilde v + K$ and observe that

$$\int_{B_r(z_0)} |H|^2\, dz \le C r^{2\alpha} \qquad \text{for all } r \le \bar r. \tag{2.41}$$

For $r > 0$ (sufficiently small) we denote

$$x'_r := \max\{x \in (0,\ell) :\ x \le x_0 \text{ and there exists } y \text{ such that } (x,y) \in \Gamma_{\bar h} \cap \partial B_r(z_0)\}\,,$$

$$x''_r := \min\{x \in (0,\ell) :\ x \ge x_0, \text{ and there exists } y \text{ such that } (x,y) \in \Gamma_{\bar h} \cap \partial B_r(z_0)\}\,,$$

and we let $(x'_r, \bar h(x'_r))$ and $(x''_r, \bar h(x''_r))$ be the corresponding points on $\Gamma_{\bar h} \cap \partial B_r(z_0)$. Construct h_r as the greatest lower semicontinuous function coinciding with $\bar h$ outside $[x'_r, x''_r]$ and with the affine function

$$x \mapsto \bar h(x'_r) + \frac{\bar h(x''_r) - \bar h(x'_r)}{x''_r - x'_r}(x - x'_r)$$

in (x_r', x_r''). For $r > 0$ sufficiently small $(h_r, \bar\sigma, H)$ is admissible for the penalized minimization problem (48) . Hence,

$$F(\bar h, \bar\sigma, H_{\bar h,\bar\sigma}) \le F(h_r, \bar\sigma, H) + \beta \int_0^b |h_r - \bar h|^2\, dx + \Lambda \big| |\Omega_{h_r}| - d \big| .$$

Since $h_r = \bar h$ outside $[x_r', x_r'']$ and $H = H_{\bar h,\bar\sigma}$ outside $B_r(z_0)$, using (49), we get

$$\begin{aligned} \int_{x_r'}^{x_r''} \sqrt{1 + (\bar h')^2}\, dx &\le \int_{x_r'}^{x_r''} \sqrt{1 + (h_r')^2}\, dx + C \int_{B_r(z_0)} |H|^2\, dz + Cr^2 \\ &\le \int_{x_r'}^{x_r''} \sqrt{1 + (h_r')^2}\, dx + Cr^{2\alpha} \end{aligned} \tag{2.42}$$

for r small enough. On the other hand, since the right and the left derivatives $\bar h'_+$ and $\bar h'_-$ exist and are continuous in a neighborhood of x_0, it can be checked that (see [21, Proof of Theorem 3.14])

$$\int_{x_r'}^{x_r''} \sqrt{1 + (\bar h')^2}\, dx - \int_{x_r'}^{x_r''} \sqrt{1 + (h_r')^2}\, dx \ge C_0 r$$

for r sufficiently small, where $C_0 > 0$ depends only on the angle at the corner point z_0. Since $2\alpha > 1$ this contradict (50).

Step 3. ($C^{1,\alpha}$-regularity) Fix an open subarc $\Gamma \subset \Gamma_{\bar h} \setminus (\Sigma_{\bar h} \cup \Sigma_{\bar h,c})$ not intersecting $\{y = 0\}$. As in Step 2, we consider only the case in which Γ does not contain vertical parts, the other case being analogous. Let I be the projection of Γ onto the x-axis. By taking Γ smaller, if needed, we may assume that $I \times (0, \infty)$ intersects at most one ball $B_{r_0}(z_j)$, $j = 1, \dots, k$ and, by Step 2, that $\bar h \in C^1(\bar I)$. Fix $J \subset\subset I$ and consider the decomposition of $H_{\bar h,\bar\sigma}$ introduced in Step 2. For any $\alpha \in (0,1)$ there exist C, $\bar r > 0$ such that if $z_0 = (x_0, \bar h(x_0))$, $x_0 \in J$, then

$$\int_{B_r(z_0) \cap \Omega^{\#}_{\bar h}} |\nabla v|^2\, dz \le Cr^{2\alpha} \qquad \text{for all } r \le \bar r\,.$$

Such a decay estimate can be established exactly as in [21, Theorem 3.16]. Note that both C and $\bar r$ are uniform with respect to $x_0 \in J$. Arguing as in the previous step, we may extend $H_{\bar h,\bar\sigma}$ to $B_{\bar r}(z_0)$ in such a way that the resulting strain field H satisfies

$$\int_{B_r(z_0)} |H|^2\, dz \le Cr^{2\alpha} \qquad \text{for all } r \le \bar r, \tag{2.43}$$

for a possibly larger constant C still independent of z_0. Fix $r < \bar r$ and consider the affine function s connecting z_0 and $(x_0 + r, \bar h(x_0 + r))$. If the graph of s over the interval $(x_0, x_0 + r)$ does not intersect any of the balls $B_{r_0}(z_j)$, $j = 1, \dots, k$, we can proceed as in [25, Step 5 of the proof of Theorem 6.9]. Thus assume that the graph of s over the interval $(x_0, x_0 + r)$ intersects a ball $B_{r_0}(z_j)$. Note that by construction of I there can only be one such ball. Define h_r as

$$h_r(x) := \begin{cases} \bar h(x) & x \in [0, \ell) \setminus (x_0, x_0 + r), \\ \max\{f_j(x), s(x)\} & x \in [x_0, x_0 + r], \end{cases}$$

where $f_j(x) := y_j + \sqrt{r_0^2 - (x - x_j)^2}$. Note that $(h_r, \bar\sigma, H)$ is admissible for problem (48). Then using the minimality of $(\bar h, \bar\sigma, H_{\bar h,\bar s})$, the decay estimate (51), and arguing as in Step 2 we obtain

$$\int_{x_0}^{x_0+r} \sqrt{1+(\bar h')^2}\,dx \le Cr^{2\alpha} + \int_{x_0}^{x_0+r} \sqrt{1+(h_r')^2}\,dx\,,$$

for some constant C independent of $x_0 \in J$. This inequality can be equivalently written as

$$\begin{aligned}
&\int_{x_0}^{x_0+r} \sqrt{1+(\bar h')^2}\,dx - \sqrt{(\bar h(x_0+r)-\bar h(x_0))^2 + r^2} \\
&\qquad \le Cr^{2\alpha} + \int_{x_0}^{x_0+r} \Big(\sqrt{1+(h_r')^2} - \sqrt{1+(s')^2}\Big)\,dx \\
&\qquad = Cr^{2\alpha} + \int_{(x_0,x_0+r)\cap\{f_j>s\}} \Big(\sqrt{1+(f_j')^2} - \sqrt{1+(s')^2}\Big)\,dx \\
&\qquad = Cr^{2\alpha} + \int_{(x_0,x_0+r)\cap\{f_j>s\}} \Big(\sqrt{1+(f_j')^2} - \sqrt{1+(f_j'(\bar x))^2}\Big)\,dx \le C'r^{2\alpha}\,. \qquad (2.44)
\end{aligned}$$

Note that in the second equality we used the fact that since $\bar h \ge f_j$ and the graph of s joins two points of the graph of $\bar h$, it must intersect the graph of f_j twice. Hence, by the mean value theorem we may find $\bar x \in (x_0, x_0+r)\cap\{f_j > s\}$ such that $f_j'(\bar x) = s'(\bar x)$. In the last inequality we used the fact that f_j' is Lipschitz. On the other hand, using the inequality

$$\sqrt{1+b^2} - \sqrt{1+a^2} \ge \frac{a(b-a)}{\sqrt{1+a^2}} + \frac{(b-a)^2}{2(1+\max\{a^2,b^2\})^{3/2}}$$

with $a := \fint_{x_0}^{x_0+r} \bar h'\,dx$ and $b := \bar h'(x)$, and integrating the result in (x_0, x_0+r), we get

$$\begin{aligned}
&\frac{1}{2(1+M^2)^{3/2}} \fint_{x_0}^{x_0+r} \Big(\bar h'(x) - \fint_{x_0}^{x_0+r} \bar h'\,ds\Big)^2\,dx \\
&\qquad \le \frac1r \int_{x_0}^{x_0+r} \sqrt{1+\bar h'^2}\,dx - \frac1r \sqrt{(\bar h(x_0+r)-\bar h(x_0))^2 + r^2} \le C'r^{2\alpha-1}\,,
\end{aligned}$$

where M is the Lipschitz constant of $\bar h$ in I and we used (52). In particular,

$$\fint_{x_0}^{x_0+r} \Big|\bar h'(x) - \fint_{x_0}^{x_0+r} \bar h'\,ds\Big|\,dx \le C''r^{\alpha-\frac12}\,.$$

A similar inequality holds also in the interval $(x_0 - r, x_0)$. Hence, by the arbitrariness of $x_0 \in J$ and [2, Theorem 7.51] we conclude that $\bar h \in C^{1,\alpha-\frac12}(J)$ for all $\alpha \in (1/2, 1)$, as claimed. This concludes the proof of statement (iii) of the theorem.

Step 4. To prove the analytic regularity, observe that in $A \setminus \cup_{i=1}^k \cup_{m\in\mathbb{Z}} \overline{B}_{r_0}(z_i)$ we can perform variations of the profile $\bar h$ to prove that (20) holds in the weak sense. Thus, in particular, the curvature κ is of class $C^{0,\alpha}$ in $A \setminus \cup_{i=1}^k \cup_{m\in\mathbb{Z}} \overline{B}_{r_0}(z_i)$ for all $\alpha \in (0, \frac12)$. A standard bootstrap argument implies the C^∞-regularity. Analyticity then follows from Theorem 4.9 and the remarks at the end of Section 4.2 in [37]. □

2.4. Dislocations accumulate at the bottom

In this subsection we consider nearly flat profiles h. We will show that if e_0 is sufficiently large and (h, σ, H) is any admissible configuration in $X(e_0; \mathbf{B})$, then, by moving the dislocations centers of σ in the direction $-\mathbf{e_2}$, the elastic energy decreases. This is made precise by the following proposition.

Proposition 2.16. *Given $d > 2r_0\ell$ and $\alpha \in (0,1)$, there exist $\overline{e} > 0$ and $\delta > 0$ such that if $e_0(\mathbf{b}_i \cdot \mathbf{e}_1) > 0$ for all $\mathbf{b}_i \in \mathbf{B}$, $i = 1, \dots, k$ and $|e_0| > \overline{e}$, then for every $(h, \sigma, H_{h,\sigma}) \in X(e_0; \mathbf{B})$, with $\|h - d/\ell\|_{C^{1,\alpha}_{\#}(0,\ell)} \le \delta$ and $\sigma = \sum_{i=1}^k \mathbf{b}_i \delta^{\#}_{z_i}$, with $z_j \cdot \mathbf{e}_2 > 0$ for some $j \in \{1, \dots, k\}$, we have*

$$\int_{\Omega_h} W((H_{h,\sigma_s})_{sym})\, dz < \int_{\Omega_h} W((H_{h,\sigma})_{sym})\, dz$$

for all $s > 0$ sufficiently small, where $\sigma_s := \sum_{i=1, i\neq j}^k \mathbf{b}_i \delta^{\#}_{z_i} + \mathbf{b}_j \delta^{\#}_{z_j - s\mathbf{e_2}}$. In particular, if $(h, \sigma, H_{h,\sigma})$ is a minimizer of (28), then all dislocations lie at the bottom of Ω_h, that is all the centers z_i are of the form $z_i = (x_i, r_0)$.

Proof. Assume, without loss of generality, that $e_0 > 0$. It is enough to show that for e_0 sufficiently large and δ small

$$\frac{d}{ds} F(h, \sigma_s, H_{h,\sigma_s})\Big|_{s=0} > 0\,, \tag{2.45}$$

where $(h, \sigma, H_{h,\sigma}) \in X(e_0; \mathbf{B})$ is as in the statement. For simplicity set

$$H_s := H_{h,\sigma_s} \qquad \text{and} \qquad H := H_0 = H_{h,\sigma}\,.$$

and recall that, by (19), H_s is the unique periodic solution to the following system

$$\begin{cases} \operatorname{curl} H_s = \displaystyle\sum_{i=1, i\neq j}^k \mathbf{b}_i \varrho^{\#}_{r_0}(\cdot - z_i) + \mathbf{b}_j \varrho^{\#}_{r_0}(\cdot - z_j - s\mathbf{e_2}) & \text{in } \Omega_h, \\ \operatorname{div} \mathbb{C}(H_s)_{sym} = 0 & \text{in } \Omega_h, \\ \mathbb{C}(H_s)_{sym}[\nu] = 0 & \text{on } \Gamma_h, \\ H_s[\,\mathbf{e}_1\,] = e_0 \mathbf{e}_1 & \text{on } \{y = 0\}. \end{cases}$$

Then the derivative in (53) reduces to

$$\frac{d}{ds}\left(\frac{1}{2}\int_{\Omega_h} \mathbb{C}(H_s)_{sym} : (H_s)_{sym}\, dz\right)\Big|_{s=0} = \int_{\Omega_h} \mathbb{C}H_{sym} : \dot{H}_{sym}\, dz\,, \tag{2.46}$$

where $\dot{H} = \frac{d}{ds} H_{s|_{s=0}}$ is determined as the unique periodic solution to

$$\begin{cases} \operatorname{curl} \dot{H} = -\mathbf{b}_j D_y \varrho^{\#}_{r_0}(\cdot - z_j) & \text{in } \Omega_h, \\ \operatorname{div} \mathbb{C}\dot{H}_{sym} = 0 & \text{in } \Omega_h, \\ \mathbb{C}\dot{H}_{sym}[\nu] = 0 & \text{on } \Gamma_h, \\ \dot{H}[\,\mathbf{e}_1\,] = 0 & \text{on } \{y = 0\}. \end{cases} \tag{2.47}$$

We now consider the canonical decomposition $H = e_0 Du_h + K_{h,\sigma}$, where u_h and $K_{h,\sigma}$ are defined as in (21) and (22), respectively. Moreover, we decompose also $\dot{H}$ as $\dot{H} = Dv + K$, where

$$K := \begin{pmatrix} -D_{yy}w_1 & D_{xy}w_1 \\ -D_{yy}w_2 & D_{xy}w_2 \end{pmatrix} \tag{2.48}$$

with $w = (w_1, w_2)$ the unique solution in $H^1_{\#}(\Omega_h;\mathbb{R}^2)$ to

$$\begin{cases} \Delta w = -\mathbf{b}_j \varrho_{r_0}(\cdot - z_j) & \text{in } \Omega_h, \\ w = 0 & \text{on } \Gamma_h, \\ w = 0 & \text{on } \{y = 0\}. \end{cases}$$

We note that since $D_{xx}w = 0$ and $\varrho_{r_0}((x,0) - z_j) = 0$ on $\{y = 0\}$ (the last condition comes from the fact that $B_{r_0}(z_j) \subset \Omega_h$), from the equation satisfied by w we deduce that $D_{yy}w = 0$ on $\{y = 0\}$, which in turn implies that $K[\,\mathbf{e}_1\,] = -Dv[\,\mathbf{e}_1\,] = 0$. Thus, v can be chosen to be identically zero on $\{y = 0\}$. Then, by (21) we have

$$\begin{aligned} &\int_{\Omega_h} \mathbb{C}H_{sym} : \dot{H}_{sym}\,dz = e_0 \int_{\Omega_h} \mathbb{C}E(u_h) : \dot{H}_{sym}\,dz + \int_{\Omega_h} \mathbb{C}(K_{h,\sigma})_{sym} : \dot{H}_{sym}\,dz \\ &= e_0 \int_{\Omega_h} \mathbb{C}E(u_h) : E(v)\,dz + e_0 \int_{\Omega_h} \mathbb{C}E(u_h) : K_{sym}\,dz + \int_{\Omega_h} \mathbb{C}(K_{h,\sigma})_{sym} : \dot{H}_{sym}\,dz \\ &= e_0 \int_{\Omega_h} \mathbb{C}E(u_h) : K_{sym}\,dz + \int_{\Omega_h} \mathbb{C}(K_{h,\sigma})_{sym} : \dot{H}_{sym}\,dz \\ &= e_0 \int_{\Omega_h} \mathbb{C}E(v_0) : K_{sym}\,dz + e_0 \int_{\Omega_h} \big(\mathbb{C}E(u_h) - \mathbb{C}E(v_0)\big) : K_{sym}\,dz \\ &\quad + \int_{\Omega_h} \mathbb{C}(K_{h,\sigma})_{sym} : \dot{H}_{sym}\,dz. \end{aligned} \tag{2.49}$$

By [22, Lemma 6.10] for every $\varepsilon > 0$ there exists $\delta > 0$ such that $\|u_h - v_0\|_{C^{1,\alpha}_{\#}(\Omega_h;\mathbb{R}^2)} \le \varepsilon$, where v_0 is defined in (23). Hence,

$$\int_{\Omega_h} \big|\big(\mathbb{C}E(u_h) - \mathbb{C}E(v_0)\big) : K_{sym}\big|\,dz \le C\varepsilon \tag{2.50}$$

for some positive constant C independent of e_0. Observe now that, using (13), (23), (55), and (56), we have

$$\begin{aligned} \int_{\Omega_h} \mathbb{C}E(v_0) : K_{sym}\,dz &= -\frac{4\mu(\mu+\lambda)}{2\mu+\lambda} \int_{\Omega_h} D_{yy}w_1\,dz \\ &= -\frac{4\mu(\mu+\lambda)}{2\mu+\lambda}\left[\int_{\Omega_h} \Delta w_1\,dz - \int_{\Gamma_h} D_x w_1 (\nu \cdot \mathbf{e}_1)\,d\mathcal{H}^1(z)\right] \\ &\ge \frac{4\mu(\mu+\lambda)}{2\mu+\lambda}\left[(\mathbf{b}_j \cdot \mathbf{e}_1)\int_{\Omega_h} \varrho_{r_0}(z - z_j)\,dz - \ell \|Dw_1\|_{L^\infty(\Omega_h;\mathbb{R}^2)} \|h - d/\ell\|_{C^{1,\alpha}_{\#}(0,\ell)}\right], \end{aligned}$$

where the second equality is due to the fact that $D_x w_1$ is ℓ-periodic in the x-direction. From the above inequality, recalling (54), (57), (58), and the assumption on h we get

$$\frac{d}{ds}F(h,\sigma_s,H_{h,\sigma_s})\Big|_{s=0} > e_0\left[\frac{4\mu(\mu+\lambda)}{2\mu+\lambda}(\mathbf{b}_j\cdot\mathbf{e}_1)\int_{\Omega_h}\varrho_{r_0}(z-z_j)\,dz - C(\varepsilon+\delta)\right] + \int_{\Omega_h}\mathbb{C}(K_{h,\sigma})_{sym}:\dot{H}_{sym}\,dz\,,$$

for a possibly larger constant C depending on the L^∞ bounds on Dw_1, hence on the $C^{1,\alpha}$ norm of h. Claim (53) follows by taking ε small enough and e_0 large enough. Indeed, by Lemma 2.3, (22), and (55),

$$\left|\int_{\Omega_h}\mathbb{C}(K_{h,\sigma})_{sym}:\dot{H}_{sym}\,dz\right| \le C|\mathbf{b_j}|\|D_y\varrho_0\|_{L^2(\mathbb{R}^2)}\|\sigma * \varrho^{\#}_{r_0}\|_{L^2(\Omega_h;\mathbb{R}^2)}\,,$$

where C is a constant depending only on the Lipschitz constant of h. □

Remark 2.17. *It can be shown that when $|e_0|$ is sufficiently large dislocations with Burgers vectors* $\mathbf{b}$ *satisfying*

$$e_0(\mathbf{b}\cdot\mathbf{e}_1) > 0$$

are energetically favorable compared to dislocations having the same centers but opposite Burgers vectors, see Corollary 3.4.

In the next theorem we show that for suitable choices of the parameters global minimizers must have all the dislocations lying on the film/substrate interface.

Theorem 2.18. *Assume $\mathbf{B}\neq\emptyset$, fix $d > 2r_0\ell$ and let $|e_0| > \bar{e}$, where $\bar{e}$ is as in Proposition 2.16. Assume also $e_0(\mathbf{b}_j\cdot\mathbf{e}_1) > 0$ for all $\mathbf{b}_j\in\mathbf{B}$. Then there exists $\bar{\gamma}$ such that if $\gamma > \bar{\gamma}$ any global minimizer $(\bar{h},\bar{\sigma},\bar{H})$ of the problem (28) has all dislocations lying at the bottom of Ω_h, i.e., $\bar{\sigma} = \sum_{i=1}^k \mathbf{b}_i\delta^{\#}_{z_i}$, where all the centers z_i are of the form $z_i = (x_i, r_0)$.*

Proof. It is enough to show that given $\gamma_n\to+\infty$ and corresponding global minimizers $(h_n,\sigma_n,H_{h_n,\sigma_n})\in X(e_0;\mathbf{B})$ of (28) with γ_n in place of γ, then for n sufficiently large the dislocation measures σ_n have all the centers lying at the bottom. Note that $(h_n,\sigma_n,H_{h_n,\sigma_n})$ is a global minimizers of

$$\min\left\{G_n(h,\sigma,H):\,(h,\sigma,H)\in X(e_0;\mathbf{B}),\,|\Omega_h| = d\right\},$$

where G_n is the rescaled functional

$$G_n(h,\sigma,H) := \frac{1}{\gamma_n}\int_{\Omega_h}W(H_{sym})\,dz + \mathcal{H}^1(\Gamma_h) + 2\mathcal{H}^1(\Sigma_h)\,.$$

Step 1. (Uniform convergence to the flat configuration) By the compactness result in [21, Proposition 2.2 and Lemma 2.5] and the semicontinuity proved in [10, Lemma 2.1], there exist $h\in AP(0,\ell)$ and a subsequence (not relabeled) such that $h_n\to h$ in $L^1(0,\ell)$ and

$$\mathcal{H}^1(\Gamma_h) + 2\mathcal{H}^1(\Sigma_h) \le \liminf_n\left(\mathcal{H}^1(\Gamma_{h_n}) + 2\mathcal{H}^1(\Sigma_{h_n})\right).$$

Thus, if we consider any $g \in AP(0,\ell)$ such that $|\Omega_g| = d$ and (σ, H) such that $(g,\sigma,H) \in X(e_0;\mathbf{B})$,

$$\begin{aligned}\mathcal{H}^1(\Gamma_h) + 2\mathcal{H}^1(\Sigma_h) &\le \liminf_n \big(\mathcal{H}^1(\Gamma_{h_n}) + 2\mathcal{H}^1(\Sigma_{h_n}\big) \\ &\le \liminf_n G_n(h_n,\sigma_n,H_{h_n,\sigma_n}) \\ &\le \liminf_n G_n(g,\sigma,H) = \mathcal{H}^1(\Gamma_g) + 2\mathcal{H}^1(\Sigma_g)\,.\end{aligned}$$

Therefore h minimizes

$$g \mapsto \mathcal{H}^1(\Gamma_g) + 2\mathcal{H}^1(\Sigma_g)$$

among all functions in $AP(0,\ell)$ such that $|\Omega_g| = d$. Hence h is the flat profile $h \equiv d/\ell$. Note that from the above chain of inequalities, taking $g = d/\ell$, we have in particular that

$$\ell = \mathcal{H}^1(\Gamma_{d/\ell}) = \lim_n \big(\mathcal{H}^1(\Gamma_{h_n}) + 2\mathcal{H}^1(\Sigma_{h_n})\big)\,.$$

Up to a subsequence we may assume that $\{\Gamma_{h_n} \cup \Sigma_{h_n}\}$ converge in the Hausdorff metric to some compact connected set K. By the compactness result [21, Proposition 2.2], we have that, up to a subsequence (not relabeled), $\mathbb{R}^2 \setminus \Omega_n^{\#} \to \mathbb{R}^2 \setminus (\mathbb{R} \times (0, d/\ell))$ in the Hausdorff metric. From this convergence it follows (see the proof of [21, Lemma 2.5]) that $\Gamma_{d/\ell} \subset K$. Hence, by Gołąb's theorem and observing that $\mathcal{H}^1(\overline{\Gamma_{h_n} \cup \Sigma_{h_n}}) = \mathcal{H}^1(\Gamma_{h_n} \cup \Sigma_{h_n})$, we have

$$\mathcal{H}^1(\Gamma_{d/\ell}) \le \mathcal{H}^1(K) \le \lim_{n\to\infty} \mathcal{H}^1(\Gamma_{h_n} \cup \Sigma_{h_n}) = \mathcal{H}^1(\Gamma_{d/\ell})\,.$$

Therefore, $\mathcal{H}^1(K \setminus \Gamma_{d/\ell}) = 0$. Since K is the Hausdorff limit of graphs, for all $x \in [0,\ell]$ the section $K \cap (\{x\} \times \mathbb{R})$ is connected. Hence, $K = \overline{\Gamma}_{d/\ell}$. From this equality and the definition of Hausdorff convergence, we get that $\sup_{[0,\ell]} |h_n - d/\ell| \to 0$ as $n \to \infty$.

Step 2. (Penalization) We now show that there exists Λ sufficiently large and independent of n such that every minimizer of

$$\min\big\{G_n(h,\sigma,H) + \Lambda||\Omega_h| - d| : (h,\sigma,H) \in X(e_0;\mathbf{B})\big\} \tag{2.51}$$

satisfies the volume constraint associated with d. We argue by contradiction and assume that there are sequences $\{\Lambda_m\}$ with $\Lambda_m \to \infty$ and $\{n_m\}$, and minimizers $(g_m, \tau_m, H_{g_m,\tau_m})$ in $X(e_0;\mathbf{B})$ of (59) with $n = n_m$ such that $|\Omega_{g_m}| \neq d$. Arguing as in Step 1 of the proof of Theorem 2.5, one can show that for n large enough $|\Omega_{g_n}| > d$. We can now proceed as in Step 2 of the same proof to show that either we can cut out a small region from Ω_{g_m}, thus strictly reducing the total energy and contradicting the minimality, or we can show that $g_m \to d/b$ uniformly (see (42)) and for every m there exist a dislocation ball $B_{r_0}(z_m)$ touching Γ_{g_m} at a point of maximum height. In particular, up to a subsequence (not relabeled), $\tau_m \rightharpoonup \tau$ with $\tau = \sum_{i=1}^k \mathbf{b}_i \delta_{z_i}^{\#}$ such that we have $z_j = (x_j, d/\ell - r_0)$ for some $j \in \{1,\dots,k\}$; i.e., the corresponding ball $B_{r_0}(z_j)$ is tangent to $\Gamma_{d/\ell}$. Note also that $H_{g_m,\tau_m} \rightharpoonup \bar{H}$ in $L^2_{loc}(\Omega_{d/\ell};\mathbb{M}^{2\times 2})$ with $\operatorname{curl} \bar{H} = \tau * \varrho_{r_0}$ and that $\bar{H}[\,\mathbf{e}_1\,] = e_0\mathbf{e}_1$. This can be shown arguing as in the proof of Theorem 2.4. Observe now that given $\eta \in (0, d/\ell)$, $\sigma \in \mathcal{M}_{dis}(\Omega_{d/\ell-\eta};\mathbf{B})$ and $H \in \mathbf{H}_{\#}(\operatorname{curl};\Omega_{d/\ell+\eta};\mathbb{M}^{2\times 2})$ such that $\operatorname{curl} H = \sigma * \varrho_0$ in $\Omega_{d/\ell+\eta}$ and $H[\,\mathbf{e}_1\,] = e_0\mathbf{e}_1$, since $g_m \to d/b$ uniformly, we have that $g_m(x) \le d/\ell + \eta$ for

all $x \in (0,\ell)$ and all m sufficiently large. Hence, by the minimality of $(g_m, \tau_m, H_{g_m,\tau_m})$ and lower semicontinuity we have

$$\begin{aligned}\int_{\Omega_{d/\ell}} W(\bar{H}_{sym})\,dz &\le \liminf_m \int_{\Omega_{g_m}} W((H_{g_m,\tau_m})_{sym})\,dz \\ &\le \liminf_m \int_{\Omega_{g_m}} W(H_{sym})\,dz = \int_{\Omega_{d/\ell}} W(H_{sym})\,dz\,.\end{aligned}$$

Since $d > 2r_0\ell$, by the arbitrariness of η, σ and H we conclude that $\bar{H} = H_{d/\ell,\tau}$ and $(\tau, H_{d/b,\tau})$ is a solution of

$$\min\Big\{\int_{\Omega_{d/\ell}} W(H_{sym})\,dz :\ H \in \mathbf{H}_{\#}(\mathrm{curl};\Omega_{d/\ell};\mathbb{M}^{2\times 2}),\\ \sigma \in \mathcal{M}_{dis}(\Omega_{d/\ell};\mathbf{B}) \text{ such that } (d/\ell,\sigma,H) \in X(e_0;\mathbf{B})\Big\},$$

which contradicts Proposition 2.16, since $|e_0| > \bar{e}$ and there is at least one dislocation which is not lying on the bottom.

Step 3. (C^1-convergence) By Step 2 and Lemma 2.9, we deduce that $\Omega^{\#}_{h_n}$ satisfies a uniform interior ball condition with any radius $\varrho < \min\{1/\Lambda, r_0\}$ and thus independent of n. This property, together with the uniform convergence proved in Step 1, implies that for n large $\Sigma_{h_n} \cup \Sigma_{h_n,c} = \emptyset$. This can be shown arguing as in Step 2 of the proof of [25, Theorem 6.9]. In turn, by Theorem 2.15, we deduce that for n sufficiently large $\Gamma^{\#}_{g_n}$ is of class $C^{1,\alpha}$ for all $\alpha \in (0,1/2)$. We now show that in fact $h_n \to d/\ell$ in $C^1_{\#}([0,\ell])$.

To this aim, fix $\varrho < \min\{1/\Lambda, r_0\}$. By Step 1 we have $a_n := \sup_{x\in[0,\ell)} |h_n(x) - d/\ell| \to 0$. Take now $z = (x, h_n(x))$ and the corresponding ball $B_\varrho(z_0) \subset \Omega^{\#}_{h_n} \cup (\mathbb{R}\times(-\infty,0])$ touching Γ_{h_n} at z. If $h_n(x) = d/\ell - a_n$ then $h_n'(x) = 0$ since $h_n \ge d/\ell - a_n$. Otherwise, let us set $\Gamma_n := \partial B_\varrho(z_0) \cap \{(x,y) : y \ge d/\ell - a_n\}$. Since $a_n \to 0$ we have $\mathcal{H}^1(\Gamma_n) \to 0$. Therefore, since $z \in \Gamma_n$, the slope of the tangent to $\partial B_\varrho(z_0)$ at z is bounded by a small constant $\omega(\mathcal{H}^1(\Gamma_n))$, where ω is a continuity modulus such that $\omega(0+) = 0$. This shows that $h_n' \to 0$ uniformly in $[0,\ell]$ as claimed.

Step 4. ($C^{1,\alpha}$-convergence and conclusion) Write $\sigma_n = \sum_{i=1}^k \mathbf{b}_i \delta^{\#}_{z_{i,n}}$, $z_{i,n} = (x_{i,n}, y_{i,n})$. We now decompose $H_{h_n,\sigma_n} = Dv_n + K_n$, where

$$K_n := \begin{pmatrix} k_{1,n} & 0 \\ k_{2,n} & 0 \end{pmatrix},$$

with

$$k_{l,n}(x,y) := -\sum_{i=1}^k (\mathbf{b}_i \cdot \mathbf{e}_l) \int_0^y \varrho_{r_0}(x - x_{i,n}, t - y_{i,n})\,dt\,,\ \text{for } l = 1,2,$$

and v_n satisfies

$$\begin{cases} \operatorname{div} \mathbb{C}E(v_n) = -\operatorname{div} \mathbb{C}(K_n)_{sym} & \text{in } \Omega_{h_n}, \\ \mathbb{C}E(v_n)[\nu] = -\mathbb{C}(K_n)_{sym}[\nu] & \text{on } \Gamma_{h_n}. \end{cases}$$

Since $h_n' \to 0$ uniformly, we can argue as in [25, Theorem 6.10] to prove that for every $\beta \in (\frac{1}{2}, 1)$ there exist $C > 0$ and a radius $\bar{r} > 0$, both independent of n, such that for all

$z_0 \in \Gamma_{h_n}$ and for all $r \le \bar r$,

$$\int_{B_r(z_0)\cap\Omega^{\#}_{h_n}} |\nabla v_n|^2\,dz \le Cr^{2\beta}$$

for n large enough. In turn, since K_n is smooth this implies that for a possibly larger constant $C>0$ (still independent of n)

$$\int_{B_r(z_0)\cap\Omega^{\#}_{h_n}} |H_{h_n,\sigma_n}|^2\,dz \le Cr^{2\alpha}$$

for all $z_0 \in \Gamma_{h_n}$, for all $r \le \bar r$, and for n large enough. From this estimate, arguing exactly as in Step 3 of Theorem 2.15, we deduce that there exists a constant $C>0$ such that for all n sufficiently large

$$\fint_{x_0}^{x_0+r} \Big|\bar h_n'(x) - \fint_{x_0}^{x_0+r} h_n'\,ds\Big|\,dx \le Cr^{\beta-\frac12}$$

for all $x \in [0,\ell)$ and $r<\bar r$. By [2, Theorem 7.51], this implies that $\|h_n\|_{C^{1,\beta-\frac12}_{\#}([0,\ell])}$ is uniformly bounded for n sufficiently large. By the arbitrariness of $\beta \in (\frac12,1)$, we have shown that $h_n \to d/\ell$ in $C^{1,\alpha}_{\#}([0,\ell])$ for all $\alpha \in (0,\frac12)$. Recalling the choice of $\bar e$, the conclusion of the theorem follows from Proposition 2.16. □

3. The nucleation energy

In this section we will address the nucleation of dislocations. Fix a finite set $\mathcal{B}^o$ of fundamentals Burgers vectors, which are linearly independent with respect to integer linear combinations; i.e., if $\mathbf{b}^o_1,\dots,\mathbf{b}^o_N$ are distinct elements of $\mathcal{B}^o$ such that $\sum_{i=1}^N n_i\mathbf{b}^o_i = 0$, with $n_i\in\mathbb{Z}$, then $n_1=\cdots=n_N=0$. Define

$$\mathcal{B} := \Big\{\sum_{i=1}^N m_i\mathbf{b}^o_i :\ m_i\in\mathbb{Z},\ \mathbf{b}^o_i\in\mathcal{B}^o,\ , N\in\mathbb{N}\Big\}.$$

For every $\mathbf{b}\in\mathcal{B}$ we set

$$\|\mathbf{b}\|^2_{\mathcal{B}^o} := \sum_{i=1}^N |m_i||\mathbf{b}^o_i|^2\,,$$

where the coefficients m_i are such that $\mathbf{b}=\sum_{i=1}^N m_i\mathbf{b}^o_i$.

Given $h\in AP(0,\ell)$, we now define the admissible dislocation measures in $\Omega^{\#}_h$, by setting

$$\mathcal{M}_{dis}(\Omega_h) := \Big\{\sigma\in\mathcal{M}(\Omega^{\#}_h;\mathbb{R}^2) :\ \sigma=\sum_{i=1}^k \mathbf{b}_i\delta^{\#}_{z_i},\ \mathbf{b}_i\in\mathcal{B},\ z_i\in\Omega_h,\ \text{with } B_{r_0}(z_i)\subset\Omega^{\#}_h,\ k\in\mathbb{N}\Big\}.$$

If $\sigma = \sum_{i=1}^k \mathbf{b}_i \delta^{\#}_{z_i} \in \mathcal{M}_{dis}(\Omega_h)$, where the z_i's are all distinct, then the corresponding nucleation energy will be defined as

$$N(\sigma) := c_o \sum_{i=1}^k \|\mathbf{b}_i\|^2_{\mathcal{B}^o}\,, \tag{3.1}$$

for some (material) constant $c_o > 0$.

3.1. The minimization problem

For any fixed mismatch strain $e_0 \neq 0$ we introduce the space of admissible configurations

$$X_{e_0} := \Big\{(h,\sigma,H) :\, h \in AP(0,\ell),\, \sigma \in \mathcal{M}_{dis}(\Omega_h),\, H \in \mathbf{H}_{\#}(\mathrm{curl};\Omega_h;\mathbb{M}^{2\times 2}) \\ \text{such that } \mathrm{curl}\, H = \sigma * \varrho_{r_0} \text{ and } H[\,\mathbf{e}_1\,] = e_0\mathbf{e}_1\Big\}\,,$$

In this section we shall discuss the minimization problem

$$\min\big\{F(h,\sigma,H) + N(\sigma) :\, (h,\sigma,H) \in X_{e_0},\, |\Omega_h| = d\big\}\,, \tag{3.2}$$

where F is defined as in (18) and $d > 0$ is the given total mass. We start by observing that the minimization problem has a solution.

Theorem 3.1. *The minimization problem* (61) *admits a solution.*

Proof. Let $\{(h_n,\sigma_n,H_n)\} \subset X_{e_0}$ be a minimizing sequence. Since $\sup_n N(\sigma_n) < \infty$ and $\min\{\|\mathbf{b}\|_{\mathcal{B}^o} :\, \mathbf{b} \in \mathcal{B}\setminus\{0\}\} > 0$, we have that the number k_n of centers of the dislocation measures $\sigma_n = \sum_{i=1}^{k_n} \mathbf{b}_{i,n}\delta^{\#}_{z_{i,n}}$ is uniformly bounded and $\sup_{i,n}\|\mathbf{b}_{i,n}\|_{\mathcal{B}^o} < +\infty$. Moreover, arguing as in the proof of Theorem 2.4 we have, up to a subsequence, that

i) $h_n \to h$ in $L^1(0,\ell)$;

ii) $\mathbb{R}^2\setminus\Omega^{\#}_{h_n} \to \mathbb{R}^2\setminus\Omega^{\#}_h$ in the sense of the Hausdorff metric,

for some $h \in AP(0,\ell)$. Therefore, up to extracting a further subsequence (not relabeled), if needed, we can assume that there exists $k \in \mathbb{N}$ such that $\sigma_n = \sum_{i=1}^k \mathbf{b}_{i,n}\delta^{\#}_{z_{i,n}}$, where $\mathbf{b}_{i,n} \to \mathbf{b}_i \in \mathcal{B}$ and $z_{i,n} \to z_i \in \Omega_h$, with $B_{r_0}(z_i) \subset \Omega^{\#}_h$. Setting $\sigma = \sum_{i=1}^k \mathbf{b}_i\delta^{\#}_{z_i}$ and observing that

$$N(\sigma) \le \liminf_n N(\sigma_n)\,,$$

we may now conclude arguing exactly as in the proof of Theorem 2.4. □

Remark 3.2 (Regularity)**.** *Let $(\bar h,\bar\sigma,H_{\bar h,\sigma}) \in X_{e_0}$ be a minimizer of problem* (61)*. Writing $\bar\sigma = \sum_{i=1}^k \mathbf{b}_i\delta^{\#}_{z_i}$, with $z_i \neq z_j$ if $i \neq j$, set $\mathbf{B} := \{\mathbf{b}_1,\dots,\mathbf{b}_k\}$. Observe that $(\bar h,\bar\sigma,H_{\bar h,\bar\sigma}) \in X(e_0;\mathbf{B})$ is also a minimizer of* (28)*. Therefore the regularity Theorem 2.15 applies.*

3.2. Existence of configurations with non trivial dislocations

We start by fixing a profile h and considering a minimizer $(\sigma, H_{h,\sigma})$ of the corresponding energy, i.e., $(h, \sigma, H_{h,\sigma}) \in X_{e_0}$ and

$$\int_{\Omega_h} W((H_{h,\sigma})_{sym})\,dz + N(\sigma) \\ = \min\left\{\int_{\Omega_h} W(H_{sym})\,dz + N(\tau) : (\tau, H) \text{ s.t. } (h, \tau, H) \in X_{e_0}\right\}. \quad (3.3)$$

We want to show that if e_0 is large enough and h is nearly flat, then any minimal configuration $(\sigma, H_{h,\sigma})$ has a nontrivial dislocation measure σ and its total variation blows up as $|e_0| \to \infty$.

Proposition 3.3. *Assume that $\mathcal{B}^o$ contains a vector $\mathbf{b}$ such that $\mathbf{b} \cdot \mathbf{e}_1 \neq 0$. For every $d > 2r_0 b$, $M \geq 0$, and $\alpha \in (0,1)$ there exist $\overline{e} > 0$ and $\delta > 0$ such that if $|e_0| > \overline{e}$, $h \in AP(0,\ell)$ and $\|h - d/\ell\|_{C^{1,\alpha}_{\#}(0,\ell)} \leq \delta$, then for every minimizer $(\sigma, H_{h,\sigma})$ of (62), the dislocation measure σ is nontrivial and the total variation $|\sigma|(\Omega_h) > M$.*

Proof. We only treat the case $e_0 > 0$. Assume that $|\sigma|(\Omega_h) \leq M$. We want to show that if e_0 is large enough, this leads to a contradiction. Fix $z_0 = (x_0, y_0) \in \Omega_h$ and consider the dislocation $\overline{\sigma} := \sigma + \mathbf{b}\delta^{\#}_{z_0} \in \mathcal{M}_{dis}(\Omega_h)$ for some $\mathbf{b} \in \mathcal{B}$ such that $\mathbf{b} \cdot \mathbf{e}_1 > 0$. Such a vector exists by our assumption on $\mathcal{B}^o$.

We consider the canonical decomposition of $H_{h,\sigma}$, i.e, $H_{h,\sigma} = e_0 Du_h + K_{h,\sigma}$, where $K_{h,\sigma}$ is the unique ℓ-periodic solution to the system

$$\begin{cases} \operatorname{curl} K_{h,\sigma} = \sigma * \varrho_{r_0} & \text{in } \Omega_h, \\ \operatorname{div} \mathbb{C}(K_{h,\sigma})_{sym} = 0 & \text{in } \Omega_h, \\ \mathbb{C}(K_{h,\sigma})_{sym}[\nu] = 0 & \text{on } \Gamma_h, \\ K_{h,\sigma}[\,\mathbf{e}_1\,] = 0 & \text{on } \{y = 0\}, \end{cases}$$

and u_h is the elastic equilibrium in Ω_h satisfying $u_h(x,0) = (x,0)$. Observe that by [22, Lemma 6.10] for every $\varepsilon > 0$ there exists $\delta > 0$ such that

$$\|h - d/\ell\|_{C^{1,\alpha}_{\#}(0,\ell)} \leq \delta \Longrightarrow \|u_h - v_0\|_{C^{1,\alpha}_{\#}(\Omega_h)} \leq \varepsilon\,, \quad (3.4)$$

where v_0 is defined in (23). Write $\mathbf{b} = (b_1, b_2)$ and consider the strain field $e_0 Du_h + K_{h,\sigma} + K$, where

$$K := \begin{pmatrix} k_1 & 0 \\ k_2 & 0 \end{pmatrix}, \qquad \text{with } k_i(x,y) := -b_i \int_0^y \varrho_{r_0}(x - x_0, t - y_0)\,dt\,, \text{ for } i = 1,2.$$

Note that by construction $\operatorname{curl} K = \mathbf{b}\,\delta^{\#}_{z_0} * \varrho_{r_0}$ and $K[\,\mathbf{e}_1\,] = 0$ on $\{y = 0\}$.

A simple calculation shows that

$$\begin{aligned}
&\int_{\Omega_h} W((H_{h,\sigma})_{sym} + K_{sym})\,dz - \int_{\Omega_h} W((H_{h,\sigma})_{sym})\,dz\\
&= \int_{\Omega_h} W(K_{sym})\,dz + \int_{\Omega_h} \mathbb{C}(H_{h,\sigma})_{sym} : K_{sym}\,dz\\
&= \int_{\Omega_h} W(K_{sym})\,dz + \int_{\Omega_h} \mathbb{C}(K_{h,\sigma})_{sym} : K_{sym}\,dz + e_0 \int_{\Omega_h} \mathbb{C}E(u_h) : K_{sym}\,dz\\
&= \int_{\Omega_h} W(K_{sym})\,dz + \int_{\Omega_h} \mathbb{C}(K_{h,\sigma})_{sym} : K_{sym}\,dz + e_0 \int_{\Omega_h} \mathbb{C}E(v_0) : K_{sym}\,dz\\
&\quad + e_0 \int_{\Omega_h} \big(\mathbb{C}E(u_h) - \mathbb{C}E(v_0)\big) : K_{sym}\,dz.
\end{aligned}$$

Observe that $\|\sigma * \varrho_{r_0}\|_{L^2(\Omega_h;\mathbb{R}^2)} \le C$, where $C = C(M)$ is a constant depending only on M. Therefore, Lemma 2.3 implies that

$$\|K_{h,\sigma}\|_{L^2(\Omega_h;\mathbb{M}^{2\times 2})} \le C\|\sigma * \varrho_{r_0}\|_{L^2(\Omega_h;\mathbb{R}^2)} \le C(M)\,.$$

Moreover, we clearly have

$$N(\overline{\sigma}) - N(\sigma) \le C\,,$$

for a possibly different constant depending on $\mathbf{b}$. Thus, since $\mathbf{b}\cdot\mathbf{e}_1 > 0$ we have

$$\int_{\Omega_h} \mathbb{C}E(v_0) : K_{sym}\,dz = \frac{4\mu(\mu+\lambda)}{2\mu+\lambda}\int_{\Omega_h} k_1\,dz < 0\,.$$

Hence, also by (63), we conclude that there exist two positive constants c_1 and c_2 (depending only on d, M, $\mathbf{b}$, and the Lamé coefficients) such that

$$\begin{aligned}
&\int_{\Omega_h} W((H_{h,\sigma})_{sym} + K_{sym})\,dz) + N(\bar\sigma) - \int_{\Omega_h} W((H_{h,\sigma})_{sym})\,dz - N(\sigma)\\
&\qquad \le c_1 + e_0\frac{4\mu(\mu+\lambda)}{2\mu+\lambda}\int_{\Omega_h} k_1\,dz + c_2 e_0\|u_h - v_0\|_{C^{1,\alpha}_{\#}(\Omega_h)}\\
&\qquad < c_1 + e_0\left(\frac{4\mu(\mu+\lambda)}{2\mu+\lambda}\int_{\Omega_h} k_1\,dz + c_2\varepsilon\right) < 0
\end{aligned}$$

provided that ε is sufficiently small and e_0 is sufficiently large. This contradicts the minimality of $(\sigma, H_{h,\sigma})$. □

Corollary 3.4. *For every $d > 0$, $M > 0$, and $\alpha \in (0,1)$ there exist $\overline{e} > 0$ and $\delta > 0$ such that if $|e_0| > \overline{e}$, $h \in AP(0,\ell)$ and $\|h - d/\ell\|_{C^{1,\alpha}_{\#}(0,\ell)} \le \delta$ and $\sigma = \sum_{i=1}^k \mathbf{b}_i\delta^{\#}_{z_i} \in \mathcal{M}_{dis}(\Omega_h)$ with $|\sigma|(\Omega_h) \le M$, $e_0(\mathbf{b}_j\cdot\mathbf{e}_1) < 0$ for $j \in J \subset \{1,\dots,k\}$, $J \neq \emptyset$, then*

$$\int_{\Omega_h} W((H_{h,\sigma})_{sym})\,dz > \int_{\Omega_h} W((H_{h,\tilde\sigma})_{sym})\,dz\,,$$

where

$$\tilde\sigma = \sum_{i\notin J} \mathbf{b}_i\delta^{\#}_{z_i} - \sum_{i\in J} \mathbf{b}_i\delta^{\#}_{z_i}\,.$$

Proof. It is enough to show that the energy strictly decreases whenever we replace $\mathbf{b}_j$, with $j \in J$, by $-\mathbf{b}_j$. Indeed, set $\bar{\sigma} := \sigma - 2\mathbf{b}_j \delta^{\#}_{z_j}$. Arguing exactly as in Proposition 3.3, we have that for $|e_0|$ sufficiently large

$$\int_{\Omega_h} W((H_{h,\bar{\sigma}})_{sym})\,dz - \int_{\Omega_h} W((H_{h,\sigma})_{sym})\,dz \\ \leq \int_{\Omega_h} W((H_{h,\sigma}+K)_{sym})\,dz - \int_{\Omega_h} W((H_{h,\sigma})_{sym})\,dz < 0\,,$$

where

$$K := \begin{pmatrix} k_1 & 0 \\ k_2 & 0 \end{pmatrix}, \qquad \text{with } k_i(x,y) := -2(\mathbf{b}_j \cdot \mathbf{e}_i) \int_0^y \varrho_{r_0}(x - x_0, t - y_0)\,dt\,, \text{ for } i = 1, 2.$$

□

As an application of Proposition 3.3 and of the theory developed in [25], we show that for suitable values of e_0 and γ the global minimizers display a nontrivial dislocation part.

Theorem 3.5 (Minimizers with dislocations)**.** *Assume that $\mathcal{B}^o$ contains a vector $\mathbf{b}$ such that $\mathbf{b} \cdot \mathbf{e}_1 \neq 0$, fix $d > 2r_0\ell$ and let $|e_0| > \bar{e}$, where $\bar{e}$ is as in Proposition 3.3. Then there exists $\bar{\gamma}$ such that if $\gamma > \bar{\gamma}$, then any global minimizer $(\bar{h}, \bar{\sigma}, \bar{H})$ of the problem (61) has nontrivial dislocations, i.e., $\bar{\sigma} \neq 0$.*

Proof. Assume without loss of generality that $e_0 > \bar{e}$ and assume by contradiction that there exists a sequence $\gamma_n \to +\infty$ and a corresponding sequence $(h_n, \sigma_n, H_n) \in X_{e_0}$ of global minimizers for (61), with γ replaced by γ_n, such that $\sigma_n = 0$. In particular $H_n = e_{0,n} Du_{h_n}$, where u_{h_n} is the elastic equilibrium in Ω_{h_n} (see (21)). It follows that (h_n, u_{h_n}) is a global minimizer of

$$\min\left\{G_n(h,u) :\ (h,0,Du) \in X_1,\ |\Omega_h| = d\right\},$$

where

$$G_n(h,u) := \frac{1}{\gamma_n} \int_{\Omega_h} W(E(u))\,dz + \mathcal{H}^1(\Gamma_h) + 2\mathcal{H}^1(\Sigma_h)\,.$$

Arguing exactly as in Step 1 of the proof of Theorem 2.18 we can show that $\sup_{[0,\ell)} |h_n - d/\ell| \to 0$. We claim that

$$h_n = d/\ell \qquad \text{for } n \text{ large enough.} \tag{3.5}$$

To this aim, we argue by contradiction assuming $\sup_{x\in[0,\ell]} |h_n(x) - d/\ell| > 0$ for a (not relabeled) subsequence, Note that we may rewrite the functional G_n as

$$G_n(h,u) := \int_{\Omega_h} W_n(E(u))\,dz + \mathcal{H}^1(\Gamma_h) + 2\mathcal{H}^1(\Sigma_h)\,,$$

where W_n is defined as in (12), with μ and λ replaced by $\mu_n := \mu\frac{1}{\gamma_n}$ and $\lambda_n := \lambda\frac{1}{\gamma_n}$, respectively. Since $\mu_n \to 0$ and $\lambda_n \to 0$, we may apply the local minimality result in [25, Theorem 2.9], to conclude that there exist n_0 and $\delta > 0$ such that

$$G_{n_0}(d/\ell, u_{d/\ell}) < G_{n_0}(k, u_k) \tag{3.6}$$

whenever $k \in AP(0,\ell)$, $|\Omega_k| = d$, and $0 < \sup_{x\in[0,\ell]} |k(x) - d/\ell| \le \delta$.

Take $n > n_0$ so large that

$$0 < \sup_{x\in[0,\ell]} |h_n(x) - d/\ell| \le \delta \quad \text{and} \quad \frac{\gamma_{n_0}}{\gamma_n} < 1\,.$$

From the inequalities above and (65), we get

$$\begin{aligned} G_n(d/\ell, u_{d/\ell}) &= \frac{\gamma_{n_0}}{\gamma_n} G_{n_0}(d/\ell, u_{d/\ell}) + \left(1 - \frac{\gamma_{n_0}}{\gamma_n}\right)\mathcal{H}^1(\Gamma_{d/\ell}) \\ &< \frac{\gamma_{n_0}}{\gamma_n} G_{n_0}(h_n, u_{h_n}) + \left(1 - \frac{\gamma_{n_0}}{\gamma_n}\right)\big(\mathcal{H}^1(\Gamma_{h_n}) + 2\mathcal{H}^1(\Sigma_{h_n})\big) \\ &= G_n(h_n, u_{h_n}), \end{aligned}$$

thus contradicting the minimality of (h_n, u_{h_n}). This proves claim (64). In turn, by Proposition 3.3 we deduce that for n sufficiently large $\sigma_n \neq 0$, in contrast with our initial contradiction assumption. □

References

[1] Alicandro R.; De Luca L.; Garroni A.; Ponsiglione M., *Metastability and dynamics of discrete topological singularities in two dimensions: a Γ-convergence approach.* Arch. Rational Mech. Anal. **214** (2014), 269–330.

[2] Ambrosio L.; Fusco N.; Pallara D., *Functions of bounded variation and free discontinuity problems.* Oxford Mathematical Monographs. The Clarendon Press, Oxford University Press, New York, 2000.

[3] Ariza M.P.; Ortiz M., *Discrete crystal elasticity and discrete dislocations in crystals.* Arch. Rational Mech. Anal. **178** (2005), 149–226.

[4] Asaro R.J.; Tiller W.A., *Interface morphology development during stress corrosion cracking: Part I: Via surface diffusion.* Metall. Trans. **3** (1972), 1789–1796.

[5] Bella P.; Goldman M.; Zwicknagl B., *Study of island formation in epitaxially strained films on unbounded domains.* Arch. Ration. Mech. Anal. **218** (2015), 163–217.

[6] Blass T.; Fonseca I.; Leoni G.; Morandotti M., *Dynamics for systems of screw dislocations.* SIAM J. Appl. Math., **75** (2015), 393–419..

[7] Boyer F.; Fabrie P., *Mathematical tools for the study of the incompressible Navier-Stokes equations and related models.* Vol. 183. Springer Science and Business Media, New York, 2012.

[8] Bonacini M., *Epitaxially strained elastic films: the case of anisotropic surface energies.* ESAIM Control Optim. Calc. Var. **19** (2013), 167–189.

[9] Bonacini M., *Stability of equilibrium configurations for elastic films in two and three dimensions.* Adv. Calc. Var. **8** (2015), 117–153.

[10] Bonnetier E.; Chambolle A., *Computing the equilibrium configuration of epitaxially strained crystalline films.* SIAM J. Appl. Math. **62** (2002), 1093–1121.

[11] Bonnetier E.; Falk R.S.; Grinfeld M.A., *Analysis of a one-dimensional variational model of the equilibrium shape of a deformable crystal.* M2AN Math. Model. Numer. Anal. **33** (1999), 573–591.

[12] Braides A.; Chambolle A.; Solci M., *A relaxation result for energies defined on pairs set-function and applications.* ESAIM: Control, Optimisation and Calculus of Variations, **13** (2007), 717–734.

[13] Cermelli P.; Leoni G., *Renormalized energy and forces on dislocations.* SIAM J. Math. Anal. **37** (2005), 1131–1160.

[14] Chambolle A.; Larsen C.J., *C^∞ regularity of the free boundary for a two-dimensional optimal compliance problem.* Calc. Var. Partial Differential Equations **18** (2003), 77–94.

[15] Chambolle A.; Solci M., *Interaction of a bulk and a surface energy with a geometrical constraint.* SIAM J. Math. Anal. **39** (2007), 77–102.

[16] Conti S.; Garroni A.; Ortiz M., *The line-tension approximation as the dilute limit of linearelastic dislocations.* Arch. Ration. Mech. Anal. **218** (2015), 699–755.

[17] De Luca L.; Garroni A.; Ponsiglione M., *Γ-convergence analysis of systems of edge dislocations: the self energy regime.* Arch. Rational Mech. Anal. **206** (2012), 885910.
[18] De Maria B.; Fusco. N., *Regularity properties of equilibrium configurations of epitaxially strained elastic films.* Topics in modern regularity theory, CRM Series **13**, Ed. Norm., Pisa, 2012, 169–204.
[19] Elder K.R.; Provatas N.; Berry J.; Stefanovic P.; Grant M., *Phase-field crystal modeling and classical density functional theory of freezing.* Phys. Rev. B **75** (2007), 064107.
[20] Fanzon S.; Palombaro M.P.; Ponsiglione M., *A variational model for dislocations at semi-coherent interfaces.* J. Nonlinear Sci., to appear.
[21] Fonseca I.; Fusco N.; Leoni G.; Morini M., *Equilibrium configurations of epitaxially strained crystalline films: existence and regularity results.* Arch. Ration. Mech. Anal. **186** (2007), 477–537.
[22] Fonseca I.; Fusco N.; Leoni G.; Morini M., *Motion of elastic thin films by anisotropic surface diffusion with curvature regularization.* Arch. Ration. Mech. Anal. **205** (2012), 425–466.
[23] Fonseca I.; Fusco N.; Leoni G.; Morini M., *Motion of three-dimensional elastic films by anisotropic surface diffusion with curvature regularization.* Anal. PDE **8** (2015), 373–423.
[24] Fung Y.C., *A first course in Continuum Mechanics.* Prentice-Hall, Inc, Englewood Cliffs, N.J., 1969.
[25] Fusco N.; Morini M., *Equilibrium configurations of epitaxially strained elastic films: second order minimality conditions and qualitative properties of solutions.* Arch. Rational Mech. Anal. **203** (2012), 247–327.
[26] Gao H.; Nix W.D., *Surface roughening of heteroepitaxial thin fillms.* Annu. Rev. Mater. Sci. **29** (1999), 173–209.
[27] Geers M.G.D.; Peerlings R.H.J.; Peletier M.A.; Scardia L., *Asymptotic behaviour of a pile-up of infinite walls of edge dislocations.* Arch. Ration. Mech. Anal. **209** (2013), 495–539.
[28] Garroni A.; Leoni G.; Ponsiglione M.*Gradient theory for plasticity via homogenization of discrete dislocations.* J. Eur. Math. Soc. **12** (2010), 1231–1266.
[29] Goldman M.; Zwicknagl B., *Scaling law and reduced models for epitaxially strained crystalline films.* SIAM J. Math. Anal. **46** (2014), 1–24.
[30] Grinfeld M.A., *Instability of the separation boundary between a non-hydrostatically stressed elastic body and a melt.* Soviet Physics Doklady **31** (1986), 831–834.
[31] Grinfeld M.A., *Stress driven instabilities in crystals: mathematical models and physical manifestation.* J. Nonlinear Sci. **3** (1993), 35–83.
[32] Grisvard P., *Singularités en elasticité.* Arch. Rational Mech. Anal. **107** (1989), 157–180.
[33] Haataja M.; Müller J.; Rutenberg A.D.; Grant M., *Dislocations and morphological instabilities: Continuum modeling of misfitting heteroepitaxial films.* Phys. Rev. B **65** (2002), 165414.
[34] Hudson T.; Ortner C., *Existence and stability of a screw dislocation under anti-plane deformation.* Arch. Rational Mech. Anal. **213** (2014), 887–929.
[35] Hudson T.; Ortner C., *Analysis of Stable Screw Dislocation Configurations in an Antiplane Lattice Model.* SIAM J. Math. Anal. **47** (2015), 291–320.
[36] Jesson D.E.; Pennycook S.J.; Baribeau J.-M.; Houghton D.C., *Direct imaging of surface cusp evolution during strained-layer epitaxy and implications for strain relaxation.* Phys. Rev. Lett. **71** (1993), 1744–1748.
[37] Koch H.; Leoni G.; Morini M., *On Optimal regularity of Free Boundary Problems and a Conjecture of De Giorgi.* Comm. Pure Applied Math. **58** (2005), 1051–1076.
[38] Lazzaroni G., Palombaro M., Schlömerkemper A., *Rigidity of three-dimensional lattices and dimension reduction in heterogeneous nanowires.* Preprint 2015.
[39] Monk P.; *Finite element methods for Maxwell's equations.* Oxford University Press, 2003.
[40] Mora M.G.; Peletier M.; Scardia L., *Convergence of interaction-driven evolutions of dislocations with Wasserstein dissipation and slip-plane confinement.* Preprint 2014.
[41] Nabarro F.R.N., *Theory of crystal dislocations.* Clarendon Press, Oxford, 1967.
[42] Nicaise S., *About the Lamé system in a polygonal or a polyhedral domain and a coupled problem between the Lamé system and the plate equation. I. Regularity of the solutions.* Ann. Scuola Norm. Sup. Pisa Cl. Sci. (4) **19** (1992), 327–361.
[43] Nitsche J.A., *On Korn's second inequality.* RAIRO-Analyse numérique, **15**(1981), 237–248.
[44] Piovano P., *Evolution of elastic thin films with curvature regularization via minimizing movements.* Calc. Var. Partial Differential Equations **49** (2014), 337–367.
[45] Ponsiglione M., *Elastic energy stored in a crystal induced by screw dislocations: from discrete to continuous.* SIAM J. Math. Anal. **39** (2007), 449–469.
[46] Spencer B.J., *Asymptotic derivation of the glued-wetting-layer model and contact-angle condition for Stranski-Krastanow islands.* Physical Review B **59** (1999), no. 3, 2011-2017.

[47] Spencer B.J.; Meiron D.I., *Nonlinear evolution of stress-driven morphological instability in a two-dimensional semi-infinite solid.* Acta Metall. Mater. **42** (1994), 3629–3641.
[48] Spencer B. J.; Tersoff J., *Equilibrium shapes and properties of epitaxially strained islands.* Physical Review Letters **79** (1997), 4858-4861.
[49] Tersoff J.; LeGoues F.K., *Competing relaxation mechanisms in strained layers.* Phys. Rev. Lett. **72** (1994), 3570–3574.