SIAM J. MATH. ANAL.
Vol. 51, No. 5, pp. 3956–3981

DERIVATION OF LINEARIZED POLYCRYSTALS FROM A TWO-DIMENSIONAL SYSTEM OF EDGE DISLOCATIONS*

SILVIO FANZON†, MARIAPIA PALOMBARO†, AND MARCELLO PONSIGLIONE‡

Abstract. In this paper we show the emergence of polycrystalline structures as a result of elastic energy minimization. For this purpose, we consider a well-known variational model for two-dimensional systems of edge dislocations, within the so-called core radius approach, and we derive the Γ-limit of the elastic energy functional as the lattice space tends to zero. In the energy regime under investigation, the symmetric and skew part of the strain become decoupled in the limit, the dislocation measure being the curl of the skew part of the strain. The limit energy is given by the sum of a plastic term, acting on the dislocation density, and an elastic term, which depends on the symmetric strains. Minimizers under suitable boundary conditions are piecewise constant antisymmetric strain fields, representing in our model a polycrystal whose grains are mutually rotated by infinitesimal angles. In the energy regime under investigation, the symmetric and skew part of the strain become decoupled in the limit, the dislocation measure being the curl of the skew part of the strain. The limit energy is given by the sum of a plastic term, acting on the dislocation density, and an elastic term, which depends on the symmetric strains. Minimizers under suitable boundary conditions are piecewise constant antisymmetric strain fields, representing in our model a polycrystal whose grains are mutually rotated by infinitesimal angles.

Key words. geometric rigidity, linearization, polycrystals, dislocations, variational methods

AMS subject classifications. 74B15, 74N05, 74N15, 49J45

DOI. 10.1137/18M118726X

1. Introduction.

Many solids in nature exhibit a polycrystalline structure. A *single-phase polycrystal* is formed by many individual crystal grains, having the same underlying periodic atomic structure, but rotated with respect to each other. The region separating two grains with different orientation is called *grain boundary* (Figure 1). Since the grains are mutually rotated, the periodic crystalline structure is disrupted at grain boundaries. As a consequence, grain boundaries are regions where *dislocations* occur, inducing high energy concentration. Polycrystalline structures, which a priori may seem energetically not convenient, arise from the crystallization of a melt. As the temperature decreases, crystallization starts from a number of points within the melt. These single grains grow until they meet. Since their orientation is generally different, the grains are not able to arrange in a single crystal, and grain boundaries appear as local minimizers of the energy, in fact, as metastable configurations. After crystallization a grain growth phase occurs, and the solid tries to minimize the energy by reducing the boundary area. This process happens by atomic diffusion, and it is thermally activated [12, Chapter 5.7], [19].

The aim of this paper is to describe, and to some extent to predict, polycrystalline structures by variational principles. To this end, we first introduce a well-known variational semidiscrete model for edge dislocations. Then we derive by Γ-convergence, as the lattice spacing tends to zero, a total energy functional depending on the strain and on the dislocation density. Finally, we focus on the ground states of such energy,

*Received by the editors May 15, 2018; accepted for publication (in revised form) April 30, 2019; published electronically October 11, 2019.
https://doi.org/10.1137/18M118726X

†Department of Mathematics, University of Sussex, Brighton BN1 9QH, UK (S.Fanzon@sussex.ac.uk, M.Palombaro@sussex.ac.uk).
‡Dipartimento di Matematica, Sapienza Università di Roma, 00185 Rome, Italy (ponsigli@mat.uniroma1.it).

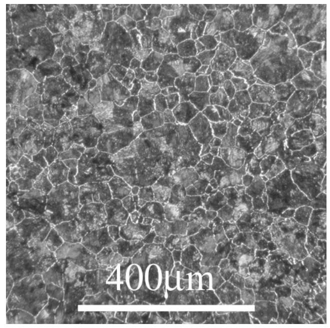

FIG. 1. *Section of an iron-carbon alloy. The darker regions are single crystal grains separated by grain boundaries represented by lighter lines (source* [20]*, licensed under CC BY-NC-SA* 2.0 *UK).*

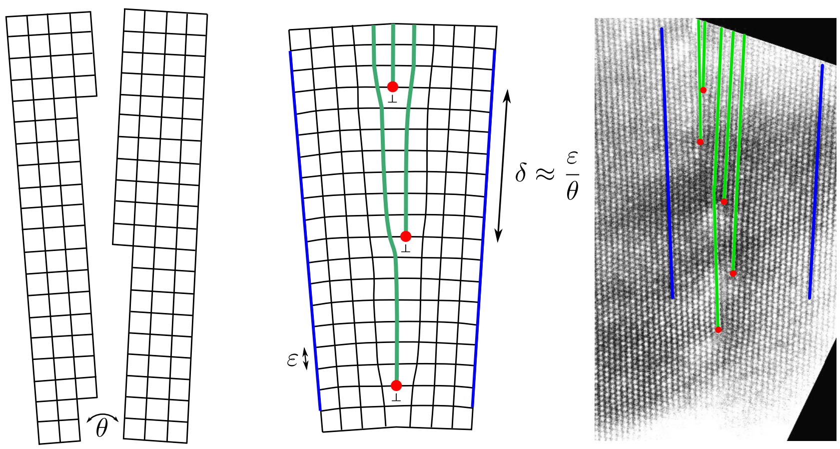

FIG. 2. *Left and center: schematic picture of a SATGB. Two grains mutually rotated by an angle θ are joined together. The lattice misfit (green lines) is accommodated by an array of edge dislocations spaced δ apart (red dots) (pictures after* [16]*). The blue lines show the rotation between the grains. Right: high-resolution transmission electron microscopy image of a SATGB in silicon (from* [8, section 7.2.2] *with permission of the author).*

neglecting the fundamental mechanisms driving the formation and evolution of grain boundaries. The main feature of the model proposed in this paper is that grain boundaries and the corresponding grain orientations are not introduced as internal variables of the energy; in fact, they spontaneously arise as a result of the only energy minimization under suitable boundary conditions.

Let us introduce our model by first discussing the case of two-dimensional small-angle tilt grain boundaries (abbreviated to SATGB). The atomic structure of SATGBs is well understood [12, Chapter 3.4], [17]. Indeed the lattice mismatch between two grains mutually tilted by a small angle θ is accommodated by a single array of edge dislocations at the grain boundary, evenly spaced at distance $\delta \approx \varepsilon/\theta$, where ε represents the atomic lattice spacing. Hence, the number of dislocations at a SATGB is of the order θ/ε (Figure 2). The elastic energy of a SATGB is given by the celebrated Read–Shockley formula introduced in [17]:

$$\text{Elastic Energy} = \mathrm{E}_0\theta(\mathrm{A} + |\log\theta|)\,, \tag{1}$$

where E_0 and A are positive constants depending only on the material.

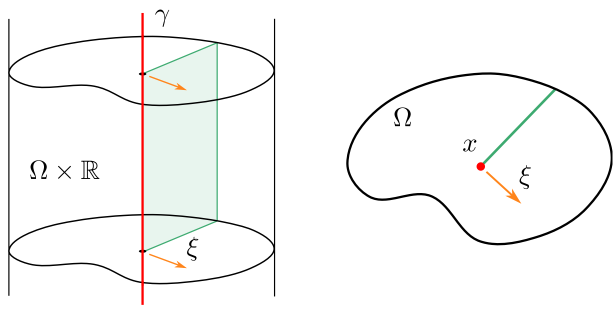

FIG. 3. *Left: domain $\Omega \times \mathbb{R}$ with the edge dislocation (γ, ξ). The green plane represents the extra half-plane of atoms corresponding to γ. Right: the section Ω of the crystal with the edge dislocation (x, ξ), $x := \gamma \cap \Omega$.*

Recently in [14], starting from a nonlinear elastic energy, the authors proved compactness properties and energy bounds in agreement with (1). In this paper we focus on lower-energy regimes, deriving by Γ-convergence, as the lattice spacing $\varepsilon \to 0$ and the number of dislocations $N_\varepsilon \to \infty$, a certain limit energy functional $\mathcal{F}$ that can be regarded as a linearized version of the Read–Shockley formula. We work in the setting of linearized planar elasticity as introduced in [9], and in particular we require good separation of the dislocation cores. Such good separation hypothesis will in turn imply that the number of dislocations at grain boundaries is of the order

$$N_\varepsilon \ll \frac{\theta}{\varepsilon}\,. \tag{2}$$

As a consequence, we cannot allow a number of dislocations sufficient to accommodate small rotations θ between grains, but rather we can have rotations by an infinitesimal angle $\theta \approx 0$, that is, antisymmetric matrices. In this respect our analysis represents the linearized counterpart of the Read–Shockley formula: grains are microrotated by infinitesimal angles, and the corresponding ground states can be seen as linearized polycrystals, whose energy is linear with respect to the number of dislocations at grain boundaries.

We now briefly introduce the setting of our problem following [9]. In *linearized planar elasticity*, the reference configuration is a bounded domain $\Omega \subset \mathbb{R}^2$, representing a horizontal section of an infinite cylindrical crystal $\Omega \times \mathbb{R}$. Following the *semidiscrete dislocation model* [3, 6, 9], dislocations are introduced as point defects of the strain $\beta\colon \Omega \to \mathbb{M}^{2\times 2}$, where $\mathbb{M}^{2\times 2}$ denotes the set of 2×2 real matrices. Specifically, a family of straight dislocation lines $\{\gamma_i\}_{i=1}^M$ orthogonal to the cross section Ω is identified with the points $x_i := \gamma_i \cap \Omega$. We then require

$$\operatorname{Curl} \beta = \sum_{i=1}^{M} \xi_i \, \delta_{x_i} \tag{3}$$

in the sense of distributions. Here $\xi_i \in \mathbb{R}^2$ is the Burgers vector associated to γ_i; it depends only on the underlying crystalline structure and not on the lattice spacing ε. (Since we are working in linearized elasticity, the Burgers vector can be rescaled by ε^{-1}.) As ξ_i and γ_i are orthogonal, (γ_i, ξ_i) defines an edge dislocation (Figure 3). Denote by $\mu := \sum_{i=1}^M \xi_i \delta_{x_i}$ the dislocation measure and by $B_r(x)$ the ball of radius $r > 0$ centered at $x \in \mathbb{R}^2$. The linear elastic energy for the pair (μ, β) satisfying (3) is defined as

$$E_\varepsilon(\mu,\beta) := \frac{1}{2}\int_{\Omega_\varepsilon(\mu)} \mathbb{C}\beta : \beta\, dx\,, \tag{4}$$

where $\Omega_\varepsilon(\mu) := \Omega \setminus \cup_{i=1}^M B_\varepsilon(x_i)$ and $\mathbb{C}$ is a fourth-order stress tensor, which is assumed to be positive definite on symmetric matrices. The energy induced by the dislocation distribution μ is obtained by minimizing (4) over the set of all strains satisfying (3).

Following [9], we make a technical hypothesis of good separation for the dislocation cores by introducing a small scale $\rho_\varepsilon \gg \varepsilon$, called *hard-core radius*: Any cluster of dislocations on a scale ρ_ε will be identified with a multiple dislocation $\xi\,\delta_x$, where ξ is the sum of the Burgers vectors corresponding to the dislocations in the cluster. Specifically, we will consider integer multiples of Burgers vectors and require that dislocation points are separated by at least $2\rho_\varepsilon$.

We now want to examine how the energy in (4) scales with ε. The energy contribution of a single dislocation core is of order $|\log\varepsilon|$ (see Proposition 3.1). For a system of N_ε dislocations with $N_\varepsilon \to \infty$ as $\varepsilon \to 0$, the relevant energy regime is then

$$E_\varepsilon \approx N_\varepsilon |\log\varepsilon|\,.$$

This scaling was already studied in [5] for $N_\varepsilon \le C$, where the authors do not assume any separation between the dislocation cores. The critical regime $N_\varepsilon \approx |\log\varepsilon|$ has been considered for Ginzburg–Landau vortices in [13] and for edge dislocations in [9], where the authors, assuming that the dislocations are well separated, characterize the Γ-limit of $\frac{E_\varepsilon}{|\log\varepsilon|^2}$. Recently the critical regime without good separation assumption was studied in [10], where the author performs a Γ-convergence analysis in the spirit of [5].

Our analysis focuses on the energy regime corresponding to

$$|\log\varepsilon| \ll N_\varepsilon \ll \frac{1}{\varepsilon}$$

(see section 2 for the precise assumptions on N_ε). We will see that such energy regime will account for grain boundaries that are mutually rotated by *infinitesimal* angles $\theta \approx 0$. To be more specific, one can split the contribution of E_ε into

$$E_\varepsilon(\mu,\beta) = E_\varepsilon^{\text{inter}}(\mu,\beta) + E_\varepsilon^{\text{self}}(\mu,\beta)\,,$$

where $E_\varepsilon^{\text{self}}$ is the self-energy concentrated in the hard-core region $\cup_i B_{\rho_\varepsilon}(x_i)$, while $E_\varepsilon^{\text{inter}}$ is the interaction energy computed outside the hard-core region. In Theorem 4.2 we will prove that the Γ-limit as $\varepsilon \to 0$ of the rescaled functionals E_ε with respect to the strains and the dislocation measures is of the form

$$\mathcal{F}(\mu,S,A) = \frac{1}{2}\int_\Omega \mathbb{C}S : S\,dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right)\,d|\mu|\,. \tag{5}$$

The first term of $\mathcal{F}$ comes from the interaction energy. It represents the elastic energy of the symmetric field S, which is the weak limit of the symmetric part of the strains rescaled by $\sqrt{N_\varepsilon|\log\varepsilon|}$. Instead, the antisymmetric part of the strain, rescaled by N_ε, weakly converges to an antisymmetric field A. Therefore, since $N_\varepsilon \gg |\log\varepsilon|$, the symmetric part of the strain is of lower order with respect to the antisymmetric part. The second term of $\mathcal{F}$ is the plastic energy, where the density φ is positively

1-homogeneous, and it can be defined as the relaxation of a cell-problem formula (see Proposition 3.1). The measure μ in (5) is the weak-$*$ limit of the dislocation measures rescaled by N_ε. Notice that A and μ come from the same rescaling N_ε, whereas the symmetric part S is of lower order, namely, $\sqrt{N_\varepsilon |\log\varepsilon|}$. As a consequence, the compatibility condition (3) passes to the limit as

$$\operatorname{Curl} A = \mu \, .$$

This implies that the *elastic* and *plastic* terms in $\mathcal{F}$ are *decoupled*. Indeed this is the main difference to the energy regime $N_\varepsilon \approx |\log\varepsilon|$ studied in [9]. Specifically, the macroscopic energy derived in [9] has the same structure as $\mathcal{F}$, but S, A, and μ live on the same scale $|\log\varepsilon|$. Therefore, the contributions of the elastic and plastic energy are coupled by the relation $\mu = \operatorname{Curl}\beta$, where $\beta = S + A$ represents the whole macroscopic strain.

In the second part of the paper we focus on the study of the Γ-limit $\mathcal{F}$. Precisely, we impose soft boundary conditions and compute (Theorem 5.1) the corresponding Γ-limit, which is given by

$$\mathcal{F}^{g_A}(\mu, S, A) = \frac{1}{2}\int_\Omega \mathbb{C}S : S\, dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu| + \int_{\partial\Omega} \varphi\left((g_A - A)\cdot t\right) ds \tag{6}$$

for suitable antisymmetric boundary values g_A. By imposing piecewise constant boundary conditions g_A and by reducing the problem to a minimization problem in BV, we show that $\mathcal{F}^{g_A}$ is minimized by strains that are *locally constant* and take values in the set of *antisymmetric matrices* (Theorem 6.1). More specifically, a minimizer is given by

$$\hat{A} = \sum_{i=1}^{k} A_i \, \chi_{\Omega_i} \, , \tag{7}$$

where $\{\Omega_i\}_{i=1}^k$ is a Caccioppoli partition of Ω and A_i are constant antisymmetric matrices. In this context the sets Ω_i represent the grains of the polycrystal, while the corresponding A_i represent their orientation. We call such configurations *linearized polycrystals*. Such definition is motivated by the fact that antisymmetric matrices can be considered as infinitesimal rotations, being the linearization about the identity of the set of rotations. The linear energy corresponding to $\hat{A}$ in (7) can be interpreted as a linearized version of the Read–Shockley formula in (1).

The paper is organized as follows. In section 2 we introduce the rigorous mathematical setting of the problem. In section 3 we recall some results from [9], which will be useful for the Γ-convergence analysis of the rescaled energy E_ε. The main Γ-convergence result will be proved in section 4. In section 5 we will include Dirichlet-type boundary conditions to the Γ-convergence analysis performed in the previous section, obtaining the functional $\mathcal{F}^{g_A}$ in (6). Finally, in section 6 we will show that the plastic part of $\mathcal{F}^{g_A}$ is minimized by linearized polycrystals by prescribing piecewise constant boundary conditions on the antisymmetric part of the limit strain.

2. Setting of the problem. Let $\Omega \subset \mathbb{R}^2$ be a bounded open domain with Lipschitz boundary, representing a horizontal section of an infinite cylindrical crystal $\Omega \times \mathbb{R}$. Define the class of Burgers vectors as $\mathcal{S} := \{b_1, \dots, b_s\}$. We will assume that $\mathcal{S}$ contains at least two linearly independent vectors so that $\operatorname{Span}_\mathbb{R} \mathcal{S} = \mathbb{R}^2$. We then define the set of slip directions

$$\mathbb{S} := \operatorname{Span}_\mathbb{Z} \mathcal{S} \, ,$$

which coincides with the set of Burgers vectors for multiple dislocations. An edge dislocation is identified with a point $x \in \Omega$ and a vector $\xi \in \mathbb{S}$. Let $\varepsilon > 0$ be a parameter representing the interatomic distance of the crystal, and denote by $\{N_\varepsilon\} \subset \mathbb{N}$ the number of dislocations present in the crystal at the scale ε. We will work in the supercritical regime

$$N_\varepsilon \gg |\log \varepsilon|\,, \tag{8}$$

in which the interaction energy is dominant with respect to the self-energy. As in [9], we assume good separation between dislocations by introducing a hard-core radius $\rho_\varepsilon \to 0$ satisfying

(i) $\lim_{\varepsilon\to 0} \rho_\varepsilon/\varepsilon^s = +\infty$ for every fixed $0 < s < 1$;

(ii) $\lim_{\varepsilon\to 0} N_\varepsilon \rho_\varepsilon^2 = 0$.

Condition (i) implies that the hard-core region contains almost all the self-energy (see Proposition 3.2), while (ii) guarantees that the area of the hard-core region tends to zero. Conditions (i), (ii), and (8) are compatible if

$$\rho_\varepsilon = \varepsilon^{t(\varepsilon)}, \qquad N_\varepsilon = \varepsilon^{-t(\varepsilon)}$$

for some positive $t(\varepsilon)$ converging to zero slowly enough (for instance, such that $t(\varepsilon)|\log\varepsilon| \ll \log(|\log\varepsilon|)$). The class of admissible dislocations is defined by

$$\begin{aligned}\mathcal{AD}_\varepsilon(\Omega) := \Big\{\mu \in &\mathcal{M}(\Omega;\mathbb{R}^2) :\ \mu = \sum_{i=1}^{M} \xi_i \delta_{x_i}\,,\ M\in\mathbb{N},\ \xi_i \in \mathbb{S}\,,\\ &B_{\rho_\varepsilon}(x_i) \subset \Omega\,,\ |x_j - x_k| \geq 2\rho_\varepsilon\,,\ \text{for every } i \text{ and } j\neq k\Big\}\,,\end{aligned}$$

where $\mathcal{M}(\Omega;\mathbb{R}^2)$ denotes the space of $\mathbb{R}^2$ valued Radon measures on Ω. For $r>0$ and $\mu = \sum_{i=1}^M \xi_i\delta_{x_i} \in \mathcal{AD}_\varepsilon(\Omega)$, define

$$\Omega_r(\mu) := \Omega \setminus \cup_{i=1}^M \overline{B_r(x_i)}\,.$$

The class of admissible strains associated to $\mu = \sum_{i=1}^M \xi_i\delta_{x_i} \in \mathcal{AD}_\varepsilon(\Omega)$ is given by

$$\begin{aligned}\mathcal{AS}_\varepsilon(\mu) :=\Big\{&\beta \in L^2(\Omega;\mathbb{M}^{2\times 2}) :\ \beta \equiv 0 \text{ in } \Omega\setminus\Omega_\varepsilon(\mu)\,,\ \operatorname{Curl}\beta = 0 \text{ in } \Omega_\varepsilon(\mu)\,,\\ &\int_{\partial B_\varepsilon(x_i)} \beta\cdot t\,ds = \xi_i\,,\ \int_{\Omega_\varepsilon(\mu)} \beta^{\mathrm{skew}}\,dx = 0\,,\ \text{for every } i=1,\dots,M\Big\}\,.\end{aligned} \tag{9}$$

The first condition in (9) is not restrictive, and it is introduced so that the strains are defined on the common domain Ω instead of $\Omega_\varepsilon(\mu)$. The second and third conditions replace (3). The identity $\operatorname{Curl}\beta = 0$ is intended in the sense of distributions with

$$\operatorname{Curl}\beta := (\partial_1\beta_{12} - \partial_2\beta_{11}, \partial_1\beta_{22} - \partial_2\beta_{21})\,. \tag{10}$$

The integrand $\beta\cdot t$ is intended in the sense of traces since $\beta \in H(\operatorname{Curl},\Omega_\varepsilon(\mu))$ (see [4, p. 204]), and t is the unit tangent vector to $\partial B_\varepsilon(x_i)$, obtained by $t := J\nu$, where

$$J := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{11}$$

and ν is the outer normal to $B_\varepsilon(x)$. Finally, $F^{\mathrm{skew}} := (F - F^T)/2$. The last condition in (9) is not restrictive and will guarantee the uniqueness of the minimizing strain.

The linear elastic energy associated to an admissible pair (μ, β) with $\mu \in \mathcal{AD}_\varepsilon(\Omega)$ and $\beta \in \mathcal{AS}_\varepsilon(\mu)$ is defined by

$$E_\varepsilon(\mu, \beta) := \int_{\Omega_\varepsilon(\mu)} W(\beta)\, dx = \int_\Omega W(\beta)\, dx\,, \tag{12}$$

where

$$W(F) := \frac{1}{2}\mathbb{C}F : F$$

is the strain energy density and $\mathbb{C}$ is the elasticity tensor satisfying

$$c^{-1}|F^{\mathrm{sym}}|^2 \le W(F) \le c|F^{\mathrm{sym}}|^2 \qquad \text{for every} \quad F \in \mathbb{M}^{2\times 2} \tag{13}$$

for some given constant $c > 0$. We remark that (13) is equivalent to

$$\frac{1}{2}\mathbb{C}F : F = \frac{1}{2}\mathbb{C}F^{\mathrm{sym}} : F^{\mathrm{sym}} \tag{14}$$

since the elasticity tensor satisfies the symmetry properties $\mathbb{C}_{ijkl} = \mathbb{C}_{klij} = \mathbb{C}_{ijlk} = \mathbb{C}_{jikl}$ (see [2]). Notice that for any fixed $\mu \in \mathcal{AD}_\varepsilon(\Omega)$ the energy $E_\varepsilon(\mu, \beta)$ admits a unique minimizer due to the last condition in (9). As already discussed in the introduction, the relevant scaling for the asymptotic study of E_ε is given by $N_\varepsilon|\log\varepsilon|$. Therefore, we introduce the scaled energy functional defined on the space $\mathcal{M}(\Omega; \mathbb{R}^2) \times L^2(\Omega; \mathbb{M}^{2\times 2})$ as

$$\mathcal{F}_\varepsilon(\mu, \beta) := \begin{cases} \dfrac{1}{N_\varepsilon|\log\varepsilon|}\, E_\varepsilon(\mu, \beta) & \text{if } \mu \in \mathcal{AD}_\varepsilon(\Omega)\,,\ \beta \in \mathcal{AS}_\varepsilon(\mu)\,, \\ +\infty & \text{otherwise.} \end{cases} \tag{15}$$

3. Preliminaries. In the present section we recall some results and notation from [9], which will be needed in the Γ-convergence analysis.

3.1. Cell formula for the self-energy. In this section we rigorously define the density function $\varphi\colon \mathbb{R}^2 \to [0, +\infty)$ appearing in the Γ-limit $\mathcal{F}$ introduced in (5). Following [9, section 4], for every $\xi \in \mathbb{R}^2$ and $0 < r_1 < r_2$, we define the space

$$\mathcal{AS}_{r_1,r_2}(\xi) := \left\{ \beta \in L^2(B_{r_2} \setminus B_{r_1}; \mathbb{M}^{2\times 2}) :\ \operatorname{Curl}\beta = 0,\ \int_{\partial B_{r_1}} \beta \cdot t\, ds = \xi \right\},$$

where B_r is the ball of radius r centered at the origin. Let $C_\varepsilon := B_1 \setminus B_\varepsilon$ with $0 < \varepsilon < 1$, and introduce $\psi_\varepsilon\colon \mathbb{R}^2 \to \mathbb{R}$ through the cell problem

$$\psi_\varepsilon(\xi) := \frac{1}{|\log\varepsilon|} \min\left\{ \int_{C_\varepsilon} W(\beta)\, dx :\ \beta \in \mathcal{AS}_{\varepsilon,1}(\xi) \right\}. \tag{16}$$

The existence of the minimum in (16) is a consequence of the classical Korn inequality and of (14). The following result holds (see [9, Corollary 6]).

Proposition 3.1. *Let $\varepsilon > 0$ and ψ_ε defined as in* (16)*. Then for every $\xi \in \mathbb{R}^2$ we have*

$$\lim_{\varepsilon\to 0} \psi_\varepsilon(\xi) = \psi(\xi)\,,$$

where $\psi\colon \mathbb{R}^2 \to [0, \infty)$ is defined by

$$\psi(\xi) := \lim_{\varepsilon\to 0} \frac{1}{|\log\varepsilon|} \int_{C_\varepsilon} W(\beta_0(\xi))\, dx \tag{17}$$

and $\beta_0(\xi)\colon \mathbb{R}^2 \to \mathbb{M}^{2\times 2}$ *is a distributional solution to*

$$\begin{cases} \operatorname{Div} \mathbb{C}\beta_0(\xi) = 0 & \text{in } \mathbb{R}^2, \\ \operatorname{Curl} \beta_0(\xi) = \xi\, \delta_0 & \text{in } \mathbb{R}^2. \end{cases}$$

Moreover, there exists a constant $c > 0$ *such that for every* $\xi \in \mathbb{R}^2$

$$c^{-1}|\xi|^2 \le \psi(\xi) \le c|\xi|^2\,. \tag{18}$$

We now want to formalize that the self-energy $\psi(\xi)$ is indeed concentrated in the hard-core region $B_{\rho_\varepsilon} \setminus B_\varepsilon$ of the dislocation $\xi\,\delta_0$. To this end, define the maps $\bar\psi_\varepsilon, \tilde\psi_\varepsilon\colon \mathbb{R}^2 \to \mathbb{R}$

$$\bar\psi_\varepsilon(\xi) := \frac{1}{|\log\varepsilon|} \min\left\{ \int_{B_{\rho_\varepsilon}\setminus B_\varepsilon} W(\beta)\,dx :\ \beta \in \mathcal{AS}_{\varepsilon,\rho_\varepsilon}(\xi) \right\} \tag{19}$$

(20)

$$\tilde\psi_\varepsilon(\xi) := \frac{1}{|\log\varepsilon|} \min\left\{ \int_{B_{\rho_\varepsilon}\setminus B_\varepsilon} W(\beta)\,dx :\ \beta \in \mathcal{AS}_{\varepsilon,\rho_\varepsilon}(\xi),\ \beta\cdot t = \hat\beta\cdot t \ \text{ on } \ \partial B_\varepsilon \cup \partial B_{\rho_\varepsilon} \right\}$$

for $\xi \in \mathbb{R}^2$, where $\hat\beta \in \mathcal{AS}_{\varepsilon,\rho_\varepsilon}(\xi)$ in (20) is a given strain such that

$$|\hat\beta(x)| \le K\,\frac{|\xi|}{|x|} \tag{21}$$

for some positive constant K. By (13), it is immediate to see that problems (19)–(20) are well-posed. The following result holds (see [9, Remark 7, Proposition 8]).

Proposition 3.2. *We have* $\bar\psi_\varepsilon(\xi) = \psi_\varepsilon(\xi)(1 + o(\varepsilon))$ *and* $\tilde\psi_\varepsilon(\xi) = \psi_\varepsilon(\xi)(1 + o(\varepsilon))$ *with* $o(\varepsilon) \to 0$ *as* $\varepsilon \to 0$ *uniformly with respect to* $\xi \in \mathbb{R}^2$*. In particular*

$$\lim_{\varepsilon\to 0} \bar\psi_\varepsilon(\xi) = \lim_{\varepsilon\to 0} \tilde\psi_\varepsilon(\xi) = \psi(\xi)$$

pointwise, where ψ *is the self-energy defined in* (17).

Now, we can define the density $\varphi\colon \mathbb{R}^2 \to [0, +\infty)$ as the relaxation of the self-energy ψ,

$$\varphi(\xi) := \inf\left\{ \sum_{k=1}^N \lambda_k \psi(\xi_k) :\ \sum_{k=1}^N \lambda_k \xi_k = \xi,\ N \in \mathbb{N},\ \lambda_k \ge 0,\ \xi_k \in \mathbb{S} \right\}. \tag{22}$$

The properties of φ are summarized in the following proposition.

Proposition 3.3. *The function* φ *defined in* (22) *is convex and positively* 1-*homogeneous. Moreover, there exists a constant* $c > 0$ *such that*

$$c^{-1}|\xi| \le \varphi(\xi) \le c|\xi|$$

for every $\xi \in \mathbb{R}^2$*. In particular, the infimum in* (22) *is actually a minimum.*

3.2. Korn-type inequality. Next we recall the generalized Korn inequality proved in [9, Theorem 11].

Theorem 3.4. *There exists a constant* $C > 0$*, depending only on* Ω*, with the following property: For every* $\beta \in L^1(\Omega; \mathbb{M}^{2\times 2})$ *with* $\operatorname{Curl}\beta \in \mathcal{M}(\Omega; \mathbb{R}^2)$ *we have*

$$\int_\Omega |\beta - A|^2\,dx \le C\left(\int_\Omega |\beta^{\rm sym}|^2\,dx + |\operatorname{Curl}\beta|(\Omega)^2 \right),$$

where A *is the constant* 2×2 *antisymmetric matrix defined by* $A := \frac{1}{|\Omega|}\int_\Omega \beta^{\rm skew}\,dx$*.*

3.3. Remarks on the distributional Curl. Here we recall some facts on the distributional Curl of admissible strains (see [9, Remark 1]). Let $\mu \in \mathcal{AD}_\varepsilon(\Omega)$, $\mu = \sum_{i=1}^M \xi_i \, \delta_{x_i}$, and $\beta \in \mathcal{AS}_\varepsilon(\mu)$. Recalling (10), we can define the scalar distribution $\operatorname{curl} \beta_{(i)}$ as

$$\langle \operatorname{curl} \beta_{(i)}, \varphi \rangle = - \int_\Omega \beta_{(i)} \cdot J \nabla \varphi \, dx \quad \text{for} \quad \varphi \in C_c^\infty(\Omega) \,, \tag{23}$$

where J is as in (11) and $\beta_{(i)}$ denotes the ith row of β. If $\beta_{(i)} \in L^2(\Omega;\mathbb{R}^2)$, then (23) implies that $\operatorname{curl} \beta_{(i)}$ is well defined also for $\varphi \in H_0^1(\Omega)$ and acts continuously on it, i.e., $\operatorname{Curl} \beta \in H^{-1}(\Omega;\mathbb{R}^2)$ for every $\beta \in \mathcal{AS}_\varepsilon(\mu)$, where $H^{-1}(\Omega;\mathbb{R}^2)$ is the dual of $H_0^1(\Omega;\mathbb{R}^2)$. Notice that the circulation condition

$$\int_{\partial B_\varepsilon(x_i)} \beta \cdot t \, ds = \xi_i \quad \text{for every} \quad i = 1, \dots, M$$

can be written as

$$\langle \operatorname{Curl} \beta, \varphi \rangle = \int_\Omega \varphi \, d\mu$$

for every $\varphi \in C^0(\Omega) \cap H_0^1(\Omega)$ such that $\varphi \equiv c_i$ in $B_\varepsilon(x_i)$ for all $x_i \in \operatorname{supp} \mu$.

4. Γ-convergence analysis. In this section we will study, by means of Γ-convergence, the behavior as $\varepsilon \to 0$ of the functionals $\mathcal{F}_\varepsilon \colon \mathcal{M}(\Omega;\mathbb{R}^2) \times L^2(\Omega;\mathbb{M}^{2\times 2}) \to \mathbb{R}$ defined in (15) in the energy regime $N_\varepsilon \gg |\log \varepsilon|$. In Theorem 4.2 we will prove that the Γ-limit for the sequence $\mathcal{F}_\varepsilon$ is given by $\mathcal{F} \colon (\mathcal{M}(\Omega;\mathbb{R}^2) \cap H^{-1}(\Omega;\mathbb{R}^2)) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}}) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}}) \to \mathbb{R}$ defined as

$$\mathcal{F}(\mu, S, A) := \begin{cases} \displaystyle\int_\Omega W(S) \, dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu| & \text{if } \operatorname{Curl} A = \mu, \\ +\infty & \text{otherwise}, \end{cases} \tag{24}$$

where φ is the energy density introduced in (22). Here $\mathbb{M}^{2\times 2}_{\mathrm{sym}}$ and $\mathbb{M}^{2\times 2}_{\mathrm{skew}}$ denote the space of 2×2 symmetric and antisymmetric matrices, respectively. In the next definition we introduce the topology under which the Γ-convergence result holds.

Definition 4.1. *We say that the family (also referred to as sequence in the following) $(\mu_\varepsilon, \beta_\varepsilon) \in \mathcal{M}(\Omega;\mathbb{R}^2) \times L^2(\Omega;\mathbb{M}^{2\times 2})$ is converging to a triplet $(\mu, S, A) \in \mathcal{M}(\Omega;\mathbb{R}^2) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}}) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})$ if*

$$\frac{\mu_\varepsilon}{N_\varepsilon} \overset{*}{\rightharpoonup} \mu \quad \textit{in} \quad \mathcal{M}(\Omega;\mathbb{R}^2) \tag{25}$$

$$\frac{\beta_\varepsilon^{\mathrm{sym}}}{\sqrt{N_\varepsilon |\log \varepsilon|}} \rightharpoonup S \qquad \textit{and} \qquad \frac{\beta_\varepsilon^{\mathrm{skew}}}{N_\varepsilon} \rightharpoonup A \quad \textit{weakly in} \quad L^2(\Omega;\mathbb{M}^{2\times 2}) \,. \tag{26}$$

Theorem 4.2. *The following Γ-convergence result holds true.*

(i) (Compactness) *Let $\varepsilon_n \to 0$, and assume that $(\mu_n, \beta_n) \in \mathcal{M}(\Omega;\mathbb{R}^2) \times L^2(\Omega;\mathbb{M}^{2\times 2})$ is such that $\sup_n \mathcal{F}_{\varepsilon_n}(\mu_n, \beta_n) \le E$ for some positive constant E. Then there exists*

$$(\mu, S, A) \in (\mathcal{M}(\Omega;\mathbb{R}^2) \cap H^{-1}(\Omega;\mathbb{R}^2)) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}}) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})$$

with $\operatorname{Curl} A = \mu$ *such that up to subsequences (not relabeled), (μ_n, β_n) converges to (μ, S, A) in the sense of Definition* 4.1.

(ii) (Γ-convergence) *As* $\varepsilon \to 0$, *the functionals* $\mathcal{F}_\varepsilon$ *defined in* (15) Γ*-converge with respect to the convergence of Definition* 4.1 *to the functional* $\mathcal{F}$ *defined in* (24).

Remark 4.3. Since A is antisymmetric, there exist $u \in L^2(\Omega)$ such that

$$A = \begin{pmatrix} 0 & u \\ -u & 0 \end{pmatrix} . \tag{27}$$

Notice that $\operatorname{Curl} A = Du$. Therefore, $\operatorname{Curl} A \in \mathcal{M}(\Omega;\mathbb{R}^2)$ implies that $u \in BV(\Omega)$ and curl $\mu = 0$. In particular, $\operatorname{curl}\operatorname{Curl} A = 0$. We also notice that, since the gradient of any vector-field is curl-free, it follows that any symmetric strain $\mathcal{E}$ satisfies $\operatorname{curl}\operatorname{Curl}\mathcal{E} = 0$, giving back the well-known Saint-Venant compatibility condition in defect-free linearized elasticity.

4.1. Compactness and Γ-liminf inequality. In this section we prove the compactness and Γ-liminf statements in Theorem 4.2. The proofs are similar to those in [9, Theorem 12]; therefore, we will only recall the main strategy and highlight the differences, which are due to the fact that in our setting β_n^{sym} and β_n^{skew} live on different scales.

Proof of compactness. Let $(\mu_n, \beta_n) \in \mathcal{M}(\Omega;\mathbb{R}^2) \times L^2(\Omega;\mathbb{M}^{2\times 2})$ be such that

$$\sup_n \mathcal{F}_{\varepsilon_n}(\mu_n, \beta_n) \le C\,. \tag{28}$$

Then $\mu_n := \sum_{i=1}^{M_n} \xi_{n,i}\delta_{x_{n,i}} \in \mathcal{AD}_{\varepsilon_n}(\Omega)$. First we show that, for sufficiently large n,

$$\frac{1}{N_{\varepsilon_n}}|\mu_n|(\Omega) = \frac{1}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}|\xi_{n,i}| \le C \tag{29}$$

for some constant $C > 0$. Since the function $y \mapsto \beta_n(x_{n,i}+y)$ belongs to $\mathcal{AS}_{\varepsilon_n,\rho_{\varepsilon_n}}(\xi_{n,i})$, by (28) and a change of variable we obtain

$$C \ge \mathcal{F}_{\varepsilon_n}(\mu_n,\beta_n) \ge \frac{1}{N_{\varepsilon_n}|\log\varepsilon_n|}\sum_{i=1}^{M_n}\int_{B_{\rho_{\varepsilon_n}}(x_{n,i})\setminus B_{\varepsilon_n}(x_{n,i})} W(\beta_n)\,dx \ge \frac{1}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}\bar{\psi}_{\varepsilon_n}(\xi_{n,i})\,,$$

where $\bar\psi_\varepsilon$ is defined in (19). Let ψ be the self-energy in (17), and set $c := \frac{1}{2}\min_{|\xi|=1}\psi(\xi)$. Notice that $c > 0$ by (18). By Proposition 3.2, $\bar\psi_\varepsilon \to \psi$ pointwise as $\varepsilon \to 0$; therefore, for sufficiently large n, we have $\bar\psi_{\varepsilon_n}(\xi) \ge c$ for every $\xi \in \mathbb{R}^2$ with $|\xi| = 1$. Hence,

$$\frac{1}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}\bar\psi_{\varepsilon_n}(\xi_{n,i}) = \frac{1}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}|\xi_{n,i}|^2\,\bar\psi_{\varepsilon_n}\left(\frac{\xi_{n,i}}{|\xi_{n,i}|}\right) \ge \frac{c}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}|\xi_{n,i}|^2 \ge \frac{c}{N_{\varepsilon_n}}\sum_{i=1}^{M_n}|\xi_{n,i}|$$

since the vectors $\xi_{n,i}$ are bounded away from zero. By combining the above estimates, we obtain (29) and (25).

Compactness for $\beta_n^{\mathrm{sym}}/\sqrt{N_{\varepsilon_n}|\log\varepsilon_n|}$ in $L^2(\Omega;\mathbb{M}^{2\times2})$ readily follows from (28), (12), and (13) since

$$CN_{\varepsilon_n}|\log\varepsilon_n| \ge CE_{\varepsilon_n}(\mu_n,\beta_n) \ge C\int_\Omega|\beta_n^{\mathrm{sym}}|^2\,dx\,. \tag{30}$$

We will now prove compactness for $\beta_n^{\mathrm{skew}}/N_{\varepsilon_n}$ in $L^2(\Omega;\mathbb{M}^{2\times2})$. Since the bounds (29)–(30) hold, the idea is to apply the generalized Korn inequality of Theorem 3.4

to obtain a uniform upper bound for $\beta_n^{\mathrm{skew}}/N_{\varepsilon_n}$ in $L^2(\Omega;\mathbb{M}^{2\times 2})$. In principle, in order to do that, we need to control $|\operatorname{Curl}\beta_n|(\Omega)$ in terms of $|\mu_n|(\Omega)$. However, instead of controlling $|\operatorname{Curl}\beta_n|(\Omega)$, following [9], it is possible to make use of the circulation condition for β_n and of the classical Korn inequality to define new strains $\tilde\beta_n\colon \Omega\to\mathbb{M}^{2\times 2}$ such that

$$\tilde\beta_n = \beta_n \quad \text{in} \quad \Omega_{\varepsilon_n}(\mu_n) \tag{31}$$

$$\int_\Omega |\tilde\beta_n^{\mathrm{sym}}|^2\,dx \le C\int_\Omega |\beta_n^{\mathrm{sym}}|^2\,dx \tag{32}$$

$$|\operatorname{Curl}\tilde\beta_n|(\Omega) = |\mu_n|(\Omega)\,. \tag{33}$$

Now we apply the generalized Korn inequality of Theorem 3.4 to $\tilde\beta_n$ and obtain

$$\int_\Omega |\tilde\beta_n - \tilde A_n|^2\,dx \le C\left(\int_\Omega |\tilde\beta_n^{\mathrm{sym}}|^2\,dx + (|\mu_n|(\Omega))^2\right) \le C\left(N_{\varepsilon_n}|\log\varepsilon_n| + N_{\varepsilon_n}^2\right) \le CN_{\varepsilon_n}^2\,,$$

where $\tilde A_n := \frac{1}{|\Omega|}\int_\Omega \tilde\beta_n^{\mathrm{skew}} \in \mathbb{M}^{2\times 2}_{\mathrm{skew}}$ and the last two inequalities follow from (32), (30), (29), and (8). Now recall that by hypothesis the average of β_n is a symmetric matrix and $\beta_n\equiv 0$ in $\Omega\setminus\Omega_{\varepsilon_n}(\mu_n)$. Therefore, by also recalling (31), we have

$$\int_{\Omega_{\varepsilon_n}(\mu_n)} |\beta_n|^2\,dx \le \int_{\Omega_{\varepsilon_n}(\mu_n)} |\beta_n - \tilde A_n|^2\,dx \le \int_\Omega |\tilde\beta_n - \tilde A_n|^2\,dx \le CN_{\varepsilon_n}^2\,.$$

The above estimate yields the desired compactness property for $\beta_n^{\mathrm{skew}}/N_{\varepsilon_n}$ in $L^2(\Omega;\mathbb{M}^{2\times 2})$ since (30) also holds.

Finally, we show that $\operatorname{Curl} A = \mu$. Let $\varphi\in C_0^1(\Omega)$ and $\varphi_n\in H_0^1(\Omega)$ be a sequence converging to φ uniformly and strongly in $H_0^1(\Omega)$ and such that $\varphi_n\equiv\varphi(x_{n,i})$ in $B_{\varepsilon_n}(x_{n,i})$ for every $x_{n,i}$ in $\operatorname{supp}\mu_n$. By the remarks in section 3.3, we then have

$$\frac{1}{N_{\varepsilon_n}}\int_\Omega \varphi_n\,d\mu_n = \frac{1}{N_{\varepsilon_n}}\langle \operatorname{Curl}\beta_n,\varphi_n\rangle = \frac{1}{N_{\varepsilon_n}}\int_\Omega \beta_n J\nabla\varphi_n\,dx\,.$$

Hence, by invoking (8), (25), and (26), we can pass to the limit in the above identity to obtain $\operatorname{Curl} A = \mu$. Moreover, since $A\in L^2(\Omega;\mathbb{M}^{2\times 2})$, by definition $\mu = \operatorname{Curl} A\in H^{-1}(\Omega;\mathbb{R}^2)$. ∎

Proof of Γ*-liminf inequality.* Let $\mu_\varepsilon\in\mathcal{AD}_\varepsilon(\Omega)$, $\beta_\varepsilon\in\mathcal{AS}_\varepsilon(\mu_\varepsilon)$, and (μ,S,A) be as in the hypothesis of Theorem 4.2. We have to show that

$$\liminf_{\varepsilon\to 0}\mathcal{F}_\varepsilon(\mu_\varepsilon,\beta_\varepsilon) \ge \mathcal{F}(\mu,S,A)\,. \tag{34}$$

To show (34), we follow [9] and decompose the energy in

$$\frac{1}{N_\varepsilon|\log\varepsilon|}\int_\Omega W(\beta_\varepsilon)\,dx = \frac{1}{N_\varepsilon|\log\varepsilon|}\int_{\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} W(\beta_\varepsilon)\,dx + \frac{1}{N_\varepsilon|\log\varepsilon|}\int_{\Omega\setminus\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} W(\beta_\varepsilon)\,dx\,.$$

We then study the two contributions separately. Recall that $\mu_\varepsilon = \sum_{i=1}^{M_\varepsilon}\xi_{\varepsilon,i}\delta_{x_{\varepsilon,i}}$. By hypothesis $\mu_\varepsilon/N_\varepsilon \overset{*}{\rightharpoonup} \mu$. Hence, $|\mu_\varepsilon|(\Omega)/N_\varepsilon$ is uniformly bounded, and $M_\varepsilon\le CN_\varepsilon$ for some uniform constant $C>0$. Moreover, $N_\varepsilon\rho_\varepsilon^2\to 0$ by hypothesis; therefore, $\chi_{\Omega_{\rho_\varepsilon}}\to 1$ strongly in $L^1(\Omega)$. By hypothesis $\beta_\varepsilon^{\mathrm{sym}}/\sqrt{N_\varepsilon|\log\varepsilon|}\rightharpoonup S$. Hence, also

$\beta_\varepsilon^{\rm sym}\chi_{\Omega_{\rho_\varepsilon}}/\sqrt{N_\varepsilon|\log\varepsilon|} \rightharpoonup S$. By invoking (14) and the weak lower semicontinuity of the energy, we get

$$\liminf_{\varepsilon\to 0}\frac{1}{N_\varepsilon|\log\varepsilon|}\int_{\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} W(\beta_\varepsilon)\,dx \geq \int_\Omega W(S)\,dx\,. \tag{35}$$

Let us consider the second integral in the energy decomposition. By Proposition 3.2,

$$\frac{1}{|\log\varepsilon|}\int_{\Omega\setminus\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} W(\beta_\varepsilon)\,dx \geq \sum_{i=1}^{M_\varepsilon}\bar\psi_\varepsilon(\xi_{\varepsilon,i}) = (1+o(\varepsilon))\sum_{i=1}^{M_\varepsilon}\psi(\xi_{\varepsilon,i})\,, \tag{36}$$

where $o(\varepsilon)\to 0$ as $\varepsilon\to 0$. By the properties of φ (Proposition 3.3), Reshetnyak's lower semicontinuity theorem ([1, Theorem 2.38]), and the assumption $\mu_\varepsilon/N_\varepsilon \overset{*}{\rightharpoonup} \mu$, we obtain

$$\liminf_{\varepsilon\to 0}\frac{1}{N_\varepsilon}\sum_{i=1}^{M_\varepsilon}\psi(\xi_{\varepsilon,i}) \geq \liminf_{\varepsilon\to 0}\frac{1}{N_\varepsilon}\sum_{i=1}^{M_\varepsilon}\varphi(\xi_{\varepsilon,i}) \geq \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right)\,d|\mu|\,. \tag{37}$$

From (35), (36), and (37) and from the energy decomposition, we infer (34). ◻

4.2. Γ-limsup inequality. In this section we prove the Γ-limsup inequality of Theorem 4.2. Even though the strategy of the proof is similar [9, Theorem 12], in our case we need finer estimates due to the fact that S and A live on different scales. Before proceeding with the proof, we need the following technical lemma to construct the recovery sequence for the measure μ. Let us first introduce some notation. For a sequence of atomic vector valued measures of the form $\nu_\varepsilon := \sum_{i=1}^{M_\varepsilon}\alpha_{\varepsilon,i}\delta_{x_{\varepsilon,i}}$ and a sequence $r_\varepsilon\to 0$, we define the corresponding diffused measures

$$\tilde\nu_\varepsilon^{r_\varepsilon} := \frac{1}{\pi r_\varepsilon^2}\sum_{i=1}^{M_\varepsilon}\alpha_{\varepsilon,i}\,\mathcal{H}^2 \llcorner B_{r_\varepsilon}(x_{\varepsilon,i})\,,\quad \hat\nu_\varepsilon^{r_\varepsilon} := \frac{1}{2\pi r_\varepsilon}\sum_{i=1}^{M_\varepsilon}\alpha_{\varepsilon,i}\,\mathcal{H}^1 \llcorner \partial B_{r_\varepsilon}(x_{\varepsilon,i})\,. \tag{38}$$

For $x_{\varepsilon,i}\in\operatorname{supp}\nu_\varepsilon$, define the functions $\tilde K_{\varepsilon,i}^{\alpha_{\varepsilon,i}}$, $\hat K_{\varepsilon,i}^{\alpha_{\varepsilon,i}}: B_{r_\varepsilon}(x_{\varepsilon,i})\to\mathbb{M}^{2\times 2}$ as

$$\tilde K_{\varepsilon,i}^{\alpha_{\varepsilon,i}}(x) := \frac{1}{2\pi r_\varepsilon^2}\,\alpha_{\varepsilon,i}\otimes J(x-x_{\varepsilon,i})\,,\quad \hat K_{\varepsilon,i}^{\alpha_{\varepsilon,i}}(x) := \frac{1}{2\pi}\,\alpha_{\varepsilon,i}\otimes J\frac{x-x_{\varepsilon,i}}{|x-x_{\varepsilon,i}|^2}\,, \tag{39}$$

where J is the counterclockwise rotation of $\pi/2$. Finally, define $\tilde K_\varepsilon^{\nu_\varepsilon}$, $\hat K_\varepsilon^{\nu_\varepsilon}:\Omega\to\mathbb{M}^{2\times 2}$ as

$$\tilde K_\varepsilon^{\nu_\varepsilon} := \sum_{i=1}^{M_\varepsilon}\tilde K_{\varepsilon,i}^{\alpha_{\varepsilon,i}}\chi_{B_{r_\varepsilon}(x_{\varepsilon,i})}\,,\quad \hat K_\varepsilon^{\nu_\varepsilon} := \sum_{i=1}^{M_\varepsilon}\hat K_{\varepsilon,i}^{\alpha_{\varepsilon,i}}\chi_{B_{r_\varepsilon}(x_{\varepsilon,i})}\,. \tag{40}$$

It is easy to show that

$$\operatorname{Curl}\tilde K_\varepsilon^{\nu_\varepsilon} = \tilde\nu_\varepsilon^{r_\varepsilon} - \hat\nu_\varepsilon^{r_\varepsilon}\,,\quad \operatorname{Curl}\hat K_\varepsilon^{\nu_\varepsilon} = \nu_\varepsilon - \hat\nu_\varepsilon^{r_\varepsilon}\,. \tag{41}$$

The following easy lemma will be used in some density argument in the construction of the recovery sequence.

LEMMA 4.4. *Let $n\in\mathbb{N}$, and set*

$$S_n := \left\{\xi := \sum_{k=1}^{M}\lambda_k\xi_k \text{ with } M\in\mathbb{N},\ \xi_k\in\mathbb{S}, \lambda_k>0 \text{ such that } z_j := \frac{n^2\lambda_j}{\sum\lambda_k}\in\mathbb{N} \text{ for all } j\right\}. \tag{42}$$

The union of such sets is dense in $\mathbb{R}^2$.

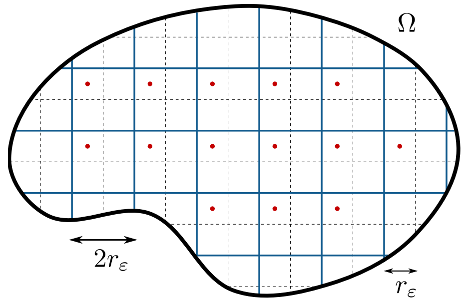

FIG. 4. *Approximating $\mu = \xi\, dx$ with the $2r_\varepsilon$-periodic atomic measure η_ε. The red dots represent Dirac masses $\xi\delta_{x_{\varepsilon,i}}$ in the support of η_ε.*

LEMMA 4.5. *Let conditions* (i), (ii), *and* (8) *of section* 2 *hold true. Then we have the following:*

(A) *Let $n \in \mathbb{N}$, $\xi \in S_n$ defined as in* (42)*, and let $\mu := \xi\, dx$. Set $\Lambda := \sum_{k=1}^M \lambda_k$, $r_\varepsilon := \frac{1}{2\sqrt{\Lambda N_\varepsilon}}$. Then there exists a sequence $\eta_\varepsilon = \sum_{k=1}^M \xi_k \eta_\varepsilon^k$ with $\eta_\varepsilon^k = \sum_{l=1}^{M_\varepsilon^k} \delta_{x_{\varepsilon,l}}$ such that $\eta_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$ and*

$$\frac{|\eta_\varepsilon^k|}{N_\varepsilon} \overset{*}{\rightharpoonup} \lambda_k\, dx \quad in \quad \mathcal{M}(\Omega;\mathbb{R}), \qquad \frac{\eta_\varepsilon}{N_\varepsilon} \overset{*}{\rightharpoonup} \mu \quad in \quad \mathcal{M}(\Omega;\mathbb{R}^2) \tag{43}$$

$$\left\| \frac{\tilde{\eta}_\varepsilon^{r_\varepsilon}}{N_\varepsilon} - \mu \right\|_{H^{-1}(\Omega;\mathbb{R}^2)} \le \frac{nC}{\sqrt{N_\varepsilon}} \tag{44}$$

for some constant C independent of n, where the measure $\tilde{\eta}_\varepsilon^{r_\varepsilon}$ is defined according to (38)*.*

(B) *Let μ, r_ε as in (A), let $g \in C^0(\overline{\Omega};\mathbb{R}^2)$, and set $\sigma := g(x)\, dx$. Then there exists a sequence η_ε satisfying all the properties in (A) and a sequence $\sigma_\varepsilon = \sum_{l=1}^{H_\varepsilon} \zeta_{\varepsilon,l}\delta_{y_{\varepsilon,l}}$ with $\zeta_{\varepsilon,l} \in \mathbb{S}$ such that supp$(\sigma_\varepsilon) \cap$ supp$(\eta_\varepsilon) = \emptyset$, $\eta_\varepsilon + \sigma_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$, and*

$$\frac{\sigma_\varepsilon}{\sqrt{N_\varepsilon|\log\varepsilon|}} \overset{*}{\rightharpoonup} \sigma \quad in \quad \mathcal{M}(\Omega;\mathbb{R}^2), \qquad \frac{\tilde{\sigma}_\varepsilon}{\sqrt{N_\varepsilon|\log\varepsilon|}} \to \sigma \quad in \quad H^{-1}(\Omega;\mathbb{R}^2), \tag{45}$$

where the measures $\tilde{\sigma}_\varepsilon^{r_\varepsilon}$ are defined according to (38)*.*

In particular there exists a constant $C > 0$ such that

$$H_\varepsilon \le C\sqrt{N_\varepsilon|\log\varepsilon|}, \qquad M_\varepsilon \le CN_\varepsilon, \tag{46}$$

where $M_\varepsilon := \sum_{k=1}^M M_\varepsilon^k$.

Proof.

Step 1. *Proof of (A), the case $M = 1$, and $\mu = \xi\, dx$ with $\xi \in \mathbb{S}$.* We cover $\mathbb{R}^2$ with squares of side length $2r_\varepsilon$. Divide each of them in four squares of side length r_ε, and plug a mass $\xi\,\delta_{x_{\varepsilon,i}}$ at the center of one of such r_ε-squares, obtaining in this way a measure ν_ε on $\mathbb{R}^2$, which is $2r_\varepsilon$ periodic. We notice that we leave some free space just in order to accomplish also point (B). Then we define η_ε as the restriction of ν_ε on all the $2r_\varepsilon$-squares contained in Ω (see Figure 4). Notice that $\eta_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$

since $r_\varepsilon \gg 2\rho_\varepsilon$ by condition (ii) in section 2. Also, the density of $\frac{1}{N_\varepsilon}\tilde{\eta}_\varepsilon^{r_\varepsilon} - \mu$ has zero average on each $2r_\varepsilon$-square so that it converges to zero weakly in $L^2(\Omega;\mathbb{R}^2)$ and (43) is verified.

Let $v_\varepsilon : \mathbb{R}^2 \to \mathbb{R}^2$ be the $2r_\varepsilon$-periodic solution to $\Delta v_\varepsilon = \frac{1}{N_\varepsilon}\tilde{\nu}_\varepsilon^{r_\varepsilon} - \mu$. By construction it is easy to see that

(47)
$$\left\|\frac{1}{N_\varepsilon}\tilde{\nu}_\varepsilon^{r_\varepsilon} - \mu\right\|_{H^{-1}(\Omega)} \le \|v_\varepsilon\|_{H^1(\Omega;\mathbb{R}^2)} \le Cr_\varepsilon, \qquad \left\|\frac{1}{N_\varepsilon}\tilde{\eta}_\varepsilon^{r_\varepsilon} - \frac{1}{N_\varepsilon}\tilde{\nu}_\varepsilon^{r_\varepsilon}\right\|_{H^{-1}(\Omega;\mathbb{R}^2)} \le Cr_\varepsilon.$$

These last estimates clearly imply (44).

Step 2. *Proof of* (*A*), *the general case* $\xi \in S_n$. Cover $\mathbb{R}^2$ with squares of side length $2nr_\varepsilon$, and divide each of them in four squares of side length nr_ε. As in Step 1, pick one of these nr_ε-squares in all $2nr_\varepsilon$-squares in a periodic manner. Finally, divide each of these selected nr_ε-squares in n^2 squares of side length r_ε. Now, plug at the centers of each of these n^2 squares a mass $\xi_k\,\delta_{x_{\varepsilon,i}}$ with $1 \le k \le M$ in such a way that the resulting measure ν_ε is $2nr_\varepsilon$-periodic and on each $2nr_\varepsilon$-square there are exactly z_k masses with weight ξ_k, where z_k is defined in (42). Then, defining η_ε as the restriction of ν_ε on the union of all $2nr_\varepsilon$-squares contained in Ω and arguing as in the proof of Step 1, we have that (43) holds true, while (47) holds true with C replaced by nC so that (44) follows.

Step 3. *Proof of* (*B*). We have at disposal CN_ε squares of side length nr_ε, left free from the constructions in Step 2. Clearly, we can plug masses with weights in $\mathbb{S}$ at the center of $c\sqrt{N_\varepsilon|\log\varepsilon|}$ of such free squares in such a way that (45) holds true. $\square$

We are now ready to prove the Γ-limsup inequality of Theorem 4.2.

Proof of Γ-*limsup inequality of Theorem* 4.2. Let

$$(\mu, S, A) \in (\mathcal{M}(\Omega;\mathbb{R}^2) \cap H^{-1}(\Omega;\mathbb{R}^2)) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\rm sym}) \times L^2(\Omega;\mathbb{M}^{2\times 2}_{\rm skew})$$

with $\operatorname{Curl} A = \mu$. We will construct a recovery sequence in three steps.

Step 1. *The case* $\mu = \xi\,dx$ *with* $S \in C^1(\overline{\Omega};\mathbb{M}^{2\times 2}_{sym})$. In this step we assume that $\mu := \xi\,dx$, $A \in L^2(\Omega;\mathbb{M}^{2\times 2}_{\rm skew})$ with $\operatorname{Curl} A = \mu$ and $S \in C^1(\overline{\Omega};\mathbb{M}^{2\times 2}_{\rm sym})$. We will construct a recovery sequence $\mu_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$, $\beta_\varepsilon \in \mathcal{AS}_\varepsilon(\mu_\varepsilon)$ such that $(\mu_\varepsilon, \beta_\varepsilon)$ converges to (μ, S, A) in the sense of Definition 4.1 and

$$\limsup_{\varepsilon\to 0} \frac{1}{N_\varepsilon|\log\varepsilon|}\int_\Omega W(\beta_\varepsilon)\,dx \le \int_\Omega (W(S) + \varphi(\xi))\,dx\,. \tag{48}$$

By Proposition 3.3, there exist $\lambda_k \ge 0$, $\xi_k \in \mathbb{S}$, $M \in \mathbb{N}$ such that $\xi = \sum_{k=1}^M \lambda_k \xi_k$ and

$$\varphi(\xi) = \sum_{k=1}^M \lambda_k \psi(\xi_k)\,, \tag{49}$$

where φ is the self-energy defined in (22). By standard density arguments in Γ-convergence, we will assume without loss of generality that $\xi \in S_n$ is as in (42) for some $n \in \mathbb{N}$.

Set $\sigma := \operatorname{Curl} S$. Since $S \in C^1(\overline{\Omega};\mathbb{M}^{2\times 2}_{\rm sym})$, $\sigma = g(x)\,dx$ for some continuous function $g\colon \overline{\Omega} \to \mathbb{R}^2$. Let $\eta_\varepsilon := \sum_{i=1}^{M_\varepsilon} \xi_{\varepsilon,i}\delta_{x_{\varepsilon,i}}$, $\sigma_\varepsilon := \sum_{i=1}^{H_\varepsilon} \zeta_{\varepsilon,i}\delta_{y_{\varepsilon,i}}$ and $r_\varepsilon := C/\sqrt{N_\varepsilon}$ be the sequences given by Lemma 4.5 (B). Set $\mu_\varepsilon := \eta_\varepsilon + \sigma_\varepsilon$. By (43), (45), and the hypothesis $N_\varepsilon \gg |\log\varepsilon|$, μ_ε is a recovery sequence for μ.

Let $\tilde\eta_\varepsilon^{r_\varepsilon}, \hat\eta_\varepsilon^{r_\varepsilon}, \tilde\sigma_\varepsilon^{r_\varepsilon}, \hat\sigma_\varepsilon^{r_\varepsilon}$ be defined according to (38). Notice that $\hat K_{\varepsilon,i}^{\xi_{\varepsilon,i}} \in \mathcal{AS}_{\varepsilon,\rho_\varepsilon}(\xi_{\varepsilon,i})$ and it satisfies (21). Therefore, by Proposition 3.2, there exist strains $\hat A_{\varepsilon,i}$ such that

(i) $\hat A_{\varepsilon,i} \in \mathcal{AS}_{\varepsilon,\rho_\varepsilon}(\xi_{\varepsilon,i})$,

(ii) $\hat A_{\varepsilon,i} \cdot t = \hat K_{\varepsilon,i}^{\xi_{\varepsilon,i}} \cdot t$ on $\partial B_\varepsilon(x_{\varepsilon,i}) \cup \partial B_{\rho_\varepsilon(x_{\varepsilon,i})}$,

and

$$\frac{1}{|\log\varepsilon|}\int_{B_{\rho_\varepsilon}(x_{\varepsilon,i})\setminus B_\varepsilon(x_{\varepsilon,i})} W(\hat A_{\varepsilon,i})\,dx = \psi(\xi_{\varepsilon,i})(1+o(\varepsilon)). \tag{50}$$

Now extend $\hat A_{\varepsilon,i}$ to be $\hat K_{\varepsilon,i}^{\xi_{\varepsilon,i}}$ in $B_{r_\varepsilon}(x_{\varepsilon,i})\setminus B_{\rho_\varepsilon}(x_{\varepsilon,i})$ and zero in $\Omega\setminus(B_{r_\varepsilon}(x_{\varepsilon,i})\setminus B_\varepsilon(x_{\varepsilon,i}))$. Set

$$\hat S_\varepsilon := \sum_{l=1}^{H_\varepsilon} \hat K_\varepsilon^{\zeta_{\varepsilon,i}}\,\chi_{B_{r_\varepsilon}(y_{\varepsilon,i})\setminus B_\varepsilon(y_{\varepsilon,i})}\,, \quad \hat A_\varepsilon := \sum_{i=1}^{M_\varepsilon} \hat A_{\varepsilon,i}\,. \tag{51}$$

Hence, recalling definition (38) we have

$$\operatorname{Curl}\hat S_\varepsilon = -\hat\sigma_\varepsilon^{r_\varepsilon} + \hat\sigma_\varepsilon^{\varepsilon}\,, \quad \operatorname{Curl}\hat A_\varepsilon = -\hat\eta_\varepsilon^{r_\varepsilon} + \hat\eta_\varepsilon^{\varepsilon}\,. \tag{52}$$

Define $Q_\varepsilon := J\,\nabla u_\varepsilon$, $R_\varepsilon := J\,\nabla v_\varepsilon$, where u_ε, v_ε solve

$$\begin{cases} \Delta u_\varepsilon = \tilde\sigma_\varepsilon^{r_\varepsilon} - \sqrt{N_\varepsilon|\log\varepsilon|}\,\sigma & \text{in } \Omega, \\ \frac{u_\varepsilon}{\partial\nu} = C_{u,\varepsilon} & \text{on } \partial\Omega; \end{cases} \qquad \begin{cases} \Delta v_\varepsilon = \tilde\eta_\varepsilon^{r_\varepsilon} - N_\varepsilon\mu & \text{in } \Omega \\ \frac{v_\varepsilon}{\partial\nu} = C_{v,\varepsilon} & \text{on } \partial\Omega\,, \end{cases} \tag{53}$$

where the constants $C_{u,\varepsilon}$, $C_{v,\varepsilon}$ satisfy the compatibility condition

$$\int_{\partial\Omega} C_{u,\varepsilon}\,ds = \int_\Omega \tilde\sigma_\varepsilon^{r_\varepsilon} - \sqrt{N_\varepsilon|\log\varepsilon|}\,dx, \qquad \int_{\partial\Omega} C_{v,\varepsilon}\,ds = \int_\Omega \tilde\eta_\varepsilon^{r_\varepsilon} - N_\varepsilon\mu\,dx.$$

In this way,

$$\operatorname{Curl} Q_\varepsilon = \tilde\sigma_\varepsilon^{r_\varepsilon} - \sqrt{N_\varepsilon|\log\varepsilon|}\,\sigma, \qquad \operatorname{Curl} R_\varepsilon = \tilde\eta_\varepsilon^{r_\varepsilon} - N_\varepsilon\mu\,. \tag{54}$$

Notice that by construction $\frac{1}{\sqrt{N_\varepsilon|\log\varepsilon|}}(|C_{u,\varepsilon}|+|C_{v,\varepsilon}|) \to 0$ as $\varepsilon\to 0$. Therefore, using also (44), (45), and standard elliptic estimates, we have

$$\frac{Q_\varepsilon}{\sqrt{N_\varepsilon|\log\varepsilon|}} \to 0, \quad \frac{R_\varepsilon}{\sqrt{N_\varepsilon|\log\varepsilon|}} \to 0 \qquad \text{in} \quad L^2(\Omega;\mathbb{M}^{2\times 2})\,. \tag{55}$$

Also notice that

$$\frac{Q_\varepsilon + R_\varepsilon}{\sqrt{N_\varepsilon|\log\varepsilon|}}\cdot t \to 0 \quad \text{in} \quad H^{-1/2}(\partial\Omega;\mathbb{R}^2)\cap L^1(\partial\Omega;\mathbb{R}^2)\,. \tag{56}$$

We can now define the candidate recovery sequence as

$$\mu_\varepsilon = \eta_\varepsilon + \sigma_\varepsilon, \qquad \beta_\varepsilon := (S_\varepsilon + A_\varepsilon)\,\chi_{\Omega_\varepsilon(\mu_\varepsilon)}\,, \tag{57}$$

where

$$S_\varepsilon := \sqrt{N_\varepsilon\,|\log\varepsilon|}\,S + \hat S_\varepsilon - \tilde K_\varepsilon^{\sigma_\varepsilon} + Q_\varepsilon \tag{58}$$

$$A_\varepsilon := N_\varepsilon A + \hat A_\varepsilon - \tilde K_\varepsilon^{\eta_\varepsilon} + R_\varepsilon\,. \tag{59}$$

By definition and (41), (52), and (54), it is immediate to check that

$$\operatorname{Curl} S_\varepsilon = \hat{\sigma}^\varepsilon_\varepsilon\,, \quad \operatorname{Curl} A_\varepsilon = \hat{\eta}^\varepsilon_\varepsilon \quad \text{in} \ \ \Omega\,.$$

Recalling that $\mu_\varepsilon = \eta_\varepsilon + \sigma_\varepsilon$, we deduce that

$$\operatorname{Curl} \beta_\varepsilon = \hat{\eta}^\varepsilon_\varepsilon + \hat{\sigma}^\varepsilon_\varepsilon = \hat{\mu}^\varepsilon_\varepsilon \quad \text{in} \ \ \Omega\,, \qquad \operatorname{Curl} \beta_\varepsilon \llcorner \Omega_\varepsilon(\mu_\varepsilon) = 0.$$

Moreover, the circulation condition $\int_{\partial B_\varepsilon(x)} \beta_\varepsilon \cdot t\, ds = \mu_\varepsilon(x)$ is satisfied for every point $x \in \operatorname{supp} \mu_\varepsilon$. Hence, $\beta_\varepsilon \in \mathcal{AS}_\varepsilon(\mu_\varepsilon)$.

In order for $(\mu_\varepsilon, \beta_\varepsilon)$ to be the desired recovery sequence, we need to prove that

$$\frac{\beta^{\mathrm{sym}}_\varepsilon}{\sqrt{N_\varepsilon |\log \varepsilon|}} \rightharpoonup S \qquad \text{weakly in} \quad L^2(\Omega; \mathbb{M}^{2\times 2}) \tag{60}$$

$$\frac{\beta^{\mathrm{skew}}_\varepsilon}{N_\varepsilon} \rightharpoonup A \qquad \text{weakly in} \quad L^2(\Omega; \mathbb{M}^{2\times 2}) \tag{61}$$

$$\lim_{\varepsilon\to 0} \frac{1}{N_\varepsilon |\log \varepsilon|} \int_\Omega W(\beta_\varepsilon)\, dx = \int_\Omega (W(S) + \varphi(\xi))\, dx\,. \tag{62}$$

In view of (55)–(59), in order to prove (60), (61) we have to show that

$$\frac{\hat{A}_\varepsilon}{\sqrt{N_\varepsilon\, |\log \varepsilon|}} \rightharpoonup 0 \quad \text{in} \quad L^2(\Omega; \mathbb{M}^{2\times 2}) \tag{63}$$

$$\frac{\hat{S}_\varepsilon}{\sqrt{N_\varepsilon\, |\log \varepsilon|}},\ \frac{\tilde{K}^{\sigma_\varepsilon}_\varepsilon}{\sqrt{N_\varepsilon\, |\log \varepsilon|}},\ \frac{\tilde{K}^{\eta_\varepsilon}_\varepsilon}{\sqrt{N_\varepsilon\, |\log \varepsilon|}} \to 0 \quad \text{in} \quad L^2(\Omega; \mathbb{M}^{2\times 2})\ . \tag{64}$$

We have

$$\begin{aligned} \int_{\Omega_{\rho_\varepsilon}(\mu_\varepsilon)} \frac{|\hat{A}_\varepsilon|^2}{N_\varepsilon |\log \varepsilon|}\, dx &\le \frac{C}{N_\varepsilon |\log \varepsilon|} \sum_{i=1}^{M_\varepsilon} \int_{B_{r_\varepsilon}(x_{\varepsilon,i}) \setminus B_{\rho_\varepsilon}(x_{\varepsilon,i})} |x - x_{\varepsilon,i}|^{-2}\, dx \\ &\le C\, \frac{M_\varepsilon (\log r_\varepsilon - \log \rho_\varepsilon)}{N_\varepsilon |\log \varepsilon|} \le C\, \frac{\log r_\varepsilon - \log \rho_\varepsilon}{|\log \varepsilon|} \to 0 \end{aligned} \tag{65}$$

as $\varepsilon \to 0$, where the last inequality follows from (46). Moreover, by (65), (43), (50), (49), and the definition of μ^k_ε given by Lemma 4.5, we have

$$\begin{aligned} \lim_{\varepsilon\to 0} \frac{1}{N_\varepsilon |\log \varepsilon|} \int_\Omega W(\hat{A}_\varepsilon)\, dx &= \lim_{\varepsilon\to 0} \frac{1}{N_\varepsilon} \sum_{i=1}^{M_\varepsilon} \psi(\xi_{\varepsilon,i})(1 + o(\varepsilon)) \\ &= \lim_{\varepsilon\to 0} \frac{1}{N_\varepsilon} \sum_{k=1}^{M} |\eta^k_\varepsilon|(\Omega)\, \psi(\xi_k)(1 + o(\varepsilon)) = |\Omega| \sum_{k=1}^{M} \lambda_k \psi(\xi_k) = \int_\Omega \varphi(\xi)\, dx\,. \end{aligned} \tag{66}$$

From (13), (65), and (66), we conclude that $\hat{A}_\varepsilon / \sqrt{N_\varepsilon |\log \varepsilon|}$ is bounded in $L^2(\Omega; \mathbb{M}^{2\times 2})$ and its energy is concentrated in the hard-core region. We easily deduce that (63) holds true.

We pass to the proof of (64). One can readily see that

$$\int_\Omega \frac{|\tilde{K}^{\sigma_\varepsilon}_\varepsilon|^2}{N_\varepsilon |\log \varepsilon|}\, dx \le \frac{C}{N_\varepsilon |\log \varepsilon|} \sum_{i=1}^{M_\varepsilon} \frac{1}{r_\varepsilon^4} \int_{B_{r_\varepsilon}(x_{\varepsilon,i})} |x - x_{\varepsilon,i}|^2\, dx = C\, \frac{M_\varepsilon}{N_\varepsilon |\log \varepsilon|} \to 0$$

as $\varepsilon \to 0$ by (46). The statement for $\tilde{K}_\varepsilon^{\eta_\varepsilon}$ can be proved in a similar way. Finally, since $H_\varepsilon \ll N_\varepsilon$ by (46) and (8), we have

$$\int_\Omega \frac{|\hat{S}_\varepsilon|^2}{N_\varepsilon |\log \varepsilon|}\, dx \le C\, \frac{H_\varepsilon(\log r_\varepsilon - \log \varepsilon)}{N_\varepsilon |\log \varepsilon|} \to 0\,,$$

which concludes the proof of (64).

We are left to prove (62). By the symmetries of the elasticity tensor $\mathbb{C}$ (see (14)) and definition (57), we have

$$\frac{W(\beta_\varepsilon)}{N_\varepsilon |\log \varepsilon|} = W\Bigg(S + \frac{\hat{S}_\varepsilon}{\sqrt{N_\varepsilon |\log \varepsilon|}} - \frac{\tilde{K}_\varepsilon^{\sigma_\varepsilon}}{\sqrt{N_\varepsilon |\log \varepsilon|}} + \frac{Q_\varepsilon}{\sqrt{N_\varepsilon |\log \varepsilon|}} \\ + \frac{\hat{A}_\varepsilon}{\sqrt{N_\varepsilon |\log \varepsilon|}} - \frac{\tilde{K}_\varepsilon^{\eta_\varepsilon}}{\sqrt{N_\varepsilon |\log \varepsilon|}} + \frac{R_\varepsilon}{\sqrt{N_\varepsilon |\log \varepsilon|}} \Bigg)\,.$$

From (64) and (55), we get

$$\lim_{\varepsilon \to 0} \frac{1}{N_\varepsilon |\log \varepsilon|} \int_\Omega W(\beta_\varepsilon)\, dx = \lim_{\varepsilon \to 0} \int_\Omega W\left(S + \frac{\hat{A}_\varepsilon}{\sqrt{N_\varepsilon |\log \varepsilon|}} \right) dx\,.$$

By recalling (63), (66), and (63) and by the Hölder inequality we deduce (62).

Step 2. *The case $\mu = \sum_{l=1}^L \chi_{\Omega_l} \xi_l \, dx$ and $S \in C^1(\overline{\Omega}; \mathbb{M}^{2\times 2}_{sym})$.* In this step we assume that $S \in C^1(\overline{\Omega}; \mathbb{M}^{2\times 2}_{\mathrm{sym}})$ and $A \in L^2(\Omega; \mathbb{M}^{2\times 2}_{\mathrm{skew}})$ with $\mu := \operatorname{Curl} A$ locally constant, i.e., $\mu = \sum_{l=1}^L \chi_{\Omega_l} \xi_l \, dx$ with $\xi_l \in \mathbb{R}^2$ and with $\Omega_l \subset \Omega$, which are Lipschitz pairwise disjoint domains such that $|\Omega \setminus \cup_{l=1}^L \Omega_l| = 0$. We will construct the recovery sequence by combining the previous step with classical localization arguments of Γ-convergence.

Let $S_l := S \llcorner \Omega_l$, $A_l := A \llcorner \Omega_l$, $\mu_l := \mu \llcorner \Omega_l = \xi_l \, dx$. Denote by $(\mu_{l,\varepsilon}, \beta_{l,\varepsilon})$ the recovery sequence for (μ_l, S_l, A_l) given by Step 1. We can now define $\mu_\varepsilon \in \mathcal{M}(\Omega; \mathbb{R}^2)$ and $\beta_\varepsilon \colon \Omega \to \mathbb{M}^{2\times 2}$ as

$$\beta_\varepsilon := \sum_{l=1}^L \chi_{\Omega_l}\, \beta_{l,\varepsilon}\,, \quad \mu_\varepsilon := \sum_{l=1}^L \mu_{l,\varepsilon}\,.$$

By construction $\mu_\varepsilon \in \mathcal{AD}_\varepsilon(\Omega)$, and β_ε satisfies the circulation condition on every $\partial B_\varepsilon(x_\varepsilon)$ with $x_\varepsilon \in \operatorname{supp} \mu_\varepsilon$. Also notice that on each set Ω_l belonging to the partition of Ω, we have

$$\operatorname{Curl} \beta_\varepsilon \llcorner \Omega_l(\mu_\varepsilon) = 0\,.$$

However $\operatorname{Curl} \beta_\varepsilon$ could concentrate on the intersection region between two elements of the partition $\{\Omega_l\}_{l=1}^L$. To overcome this problem, it is sufficient to notice that by construction

$$\left\| \frac{\operatorname{Curl} \beta_\varepsilon \llcorner \Omega_\varepsilon(\mu_\varepsilon)}{\sqrt{N_\varepsilon |\log \varepsilon|}} \right\|_{H^{-1}(\Omega;\mathbb{R}^2)} \le \sum_{l=1}^L \left\| \frac{\beta_{l,\varepsilon} - \sqrt{N_\varepsilon |\log \varepsilon|} S - N_\varepsilon A}{\sqrt{N_\varepsilon |\log \varepsilon|}} \cdot t \right\|_{H^{-1/2}(\partial \Omega_l;\mathbb{R}^2)} \\ = \sum_{l=1}^L \left\| \frac{Q_{l,\varepsilon} + R_{l,\varepsilon}}{\sqrt{N_\varepsilon |\log \varepsilon|}} \cdot t \right\|_{H^{-1/2}(\partial \Omega_l;\mathbb{R}^2)}\,,$$

where $Q_{l,\varepsilon}$, $R_{l,\varepsilon}$ are defined according to (53) with Ω replaced by Ω_l. Therefore, by (56),

$$\frac{\operatorname{Curl}\beta_\varepsilon \llcorner \Omega_\varepsilon(\mu_\varepsilon)}{\sqrt{N_\varepsilon|\log\varepsilon|}} \to 0 \quad \text{strongly in} \quad H^{-1}(\Omega;\mathbb{R}^2)\,.$$

Hence, we can add a vanishing perturbation to β_ε (on the scale $\sqrt{N_\varepsilon|\log\varepsilon|}$) in order to obtain the desired recovery sequence in $\mathcal{AS}_\varepsilon(\mu_\varepsilon)$.

Step 3. *The general case.* Let (μ, S, A) be in the domain of the Γ-limit $\mathcal{F}$. In view of Step 2 and by standard density arguments of Γ-convergence, it is sufficient to find sequences (μ_n, S_n, A_n) such that μ_n is locally constant as in Step 2,

$$S_n \in C^1(\overline{\Omega};\mathbb{M}^{2\times 2}_{\rm sym})\,,\ A_n \in L^2(\Omega;\mathbb{M}^{2\times 2}_{\rm skew}) \ \text{ with } \ \operatorname{Curl} A_n = \mu_n, \tag{67}$$

and such that

$$S_n \to S,\ A_n \to A \text{ in } L^2(\Omega;\mathbb{M}^{2\times 2})\,, \quad \mu_n \overset{*}{\rightharpoonup} \mu \text{ in } \mathcal{M}(\Omega;\mathbb{R}^2)\,, \quad |\mu_n|(\Omega) \to |\mu|(\Omega), \tag{68}$$

where S and A are the symmetric and antisymmetric part of β, respectively. In fact, we have to show that (68) implies

$$\lim_{n\to\infty} \mathcal{F}(\mu_n, \beta_n) = \mathcal{F}(\mu, S, A)\,. \tag{69}$$

Since $S_n \to S$ strongly in $L^2(\Omega;\mathbb{M}^{2\times 2})$,

$$\lim_{n\to\infty} \int_\Omega W(S_n)\,dx = \int_\Omega W(S)\,dx\,.$$

Also, $|\mu_n|(\Omega) \to |\mu|(\Omega)$ implies

$$\lim_{n\to\infty} \int_\Omega \varphi\left(\frac{d\mu_n}{d|\mu_n|}\right) d|\mu_n| = \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu|$$

by Reshetnyak's Theorem ([1, Theorem 2.39]) so that (69) is proved.

Let us then proceed to the construction of the sequences S_n, A_n, and μ_n satisfying properties (67)–(68). Clearly, we can approximate S in $L^2(\Omega;\mathbb{M}^{2\times 2}_{\rm sym})$ with a sequence $S_n \in C^1(\overline{\Omega};\mathbb{M}^{2\times 2}_{\rm sym})$. Then, by Remark (4.3), writing A as in (27) we have that u is in $BV(\Omega)\cap L^2(\Omega)$. Therefore, by standard density results in BV we can find a sequence of piecewise affine functions u_n with

$$u_n \to u \text{ in } L^2(\Omega), \qquad Du_n \overset{*}{\rightharpoonup} Du = \mu, \qquad |Du_n|(\Omega) \to |Du|(\Omega) = |\mu|(\Omega).$$

Setting $\mu_n := Du_n$ and A_n, as in (27) with u replaced by u_n, it is readily seen that μ_n is piecewise constant and that (67) and (68) hold true, and this concludes the proof of the Γ-limsup inequality. ∎

Remark 4.6. Recalling (56) and inspecting the density arguments in Step 3 above, we notice that we can provide a recovery sequence β_ε for the limit strain $\beta = S + A$ such that

$$\frac{\beta_\varepsilon}{N_\varepsilon}\cdot t \to A\cdot t \text{ in } H^{-1/2}(\partial\Omega;\mathbb{R}^2)\cap L^1(\partial\Omega;\mathbb{R}^2). \tag{70}$$

5. Relaxed Dirichlet-type boundary conditions. The aim of this section is to add a Dirichlet-type boundary condition to the Γ-convergence statement of Theorem 4.2. Fix a boundary condition

$$g_A \in L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}}) : \operatorname{Curl} g_A \in H^{-1}(\Omega;\mathbb{R}^2)\cap \mathcal{M}(\Omega;\mathbb{R}^2). \tag{71}$$

The rescaled energy functionals $\mathcal{F}^{g_A}_\varepsilon : \mathcal{M}(\Omega;\mathbb{R}^2)\times L^2(\Omega;\mathbb{M}^{2\times 2}) \to \mathbb{R}$, taking into account the boundary conditions, are defined by

$$\mathcal{F}^{g_A}_\varepsilon(\mu,\beta) := \frac{1}{N_\varepsilon|\log\varepsilon|}\,E_\varepsilon(\mu,\beta) + \int_{\partial\Omega}\varphi\Big(\Big(g_A - \frac{\beta}{N_\varepsilon}\Big)\cdot t\Big)\,ds \tag{72}$$

if $\mu \in \mathcal{AD}_\varepsilon(\Omega)$, $\beta\in\mathcal{AS}_\varepsilon(\mu)$, and $+\infty$ otherwise, while the candidate Γ-limit is the functional

$$\mathcal{F}^{g_A} : (H^{-1}(\Omega;\mathbb{R}^2)\cap\mathcal{M}(\Omega;\mathbb{R}^2))\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}})\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})\to\mathbb{R} \tag{73}$$

with

$$\mathcal{F}^{g_A}(\mu,S,A) := \int_\Omega W(S)\,dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right)d|\mu| + \int_{\partial\Omega}\varphi((g_A - A)\cdot t)\,ds \tag{74}$$

if $\operatorname{Curl} A = \mu$ and $\mathcal{F}^{g_A}(\mu,S,A) := \infty$ otherwise. Here ds coincides with $\mathcal{H}^1 \llcorner \partial\Omega$, while t is the unit tangent to $\partial\Omega$ defined as the $\pi/2$ counterclockwise rotation of the outer normal ν to Ω. The boundary terms appearing in the definition of $\mathcal{F}^{g_A}_\varepsilon$ and $\mathcal{F}^{g_A}$ are intended in the sense of traces of BV functions (see [1]). Indeed, since A and g_A are antisymmetric, there exist $u, a\in L^2(\Omega)$ such that

$$A = \begin{pmatrix} 0 & u \\ -u & 0\end{pmatrix}, \quad g_A = \begin{pmatrix} 0 & a\\ -a & 0\end{pmatrix}.$$

Notice that $\operatorname{Curl} A = Du$ and $\operatorname{Curl} g_A = Da$ in the sense of distributions. Therefore, as already observed in Remark 4.3, conditions $\operatorname{Curl} A, \operatorname{Curl} g_A \in \mathcal{M}(\Omega;\mathbb{R}^2)$ imply that $a, u\in BV(\Omega)$. Hence, a and u admit traces on $\partial\Omega$ that belong to $L^1(\partial\Omega;\mathbb{R}^2)$. By noting that

$$\int_{\partial\Omega}\varphi((g_A - A)\cdot t)\,ds = \int_{\partial\Omega}\varphi((u-a)\nu)\,ds,$$

where ν is the inner normal to Ω, we conclude that the definition of $\mathcal{F}^{g_A}$ is well-posed, as is the definition of $\mathcal{F}^{g_A}_\varepsilon$.

We are now ready to state the Γ-convergence result with boundary conditions.

THEOREM 5.1. *The following Γ-convergence statement holds with respect to the convergence of Definition* 4.1.

(i) (Compactness) *Let $\varepsilon_n\to 0$, and assume that $(\mu_n,\beta_n)\in\mathcal{M}(\Omega;\mathbb{R}^2)\times L^2(\Omega;\mathbb{M}^{2\times 2})$ is such that $\sup_n \mathcal{F}^{g_A}_{\varepsilon_n}(\mu_n,\beta_n)\le C$ for some $C>0$. Then there exists*

$$(\mu,S,A)\in(H^{-1}(\Omega;\mathbb{R}^2)\cap\mathcal{M}(\Omega;\mathbb{R}^2))\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{sym}})\times L^2(\Omega;\mathbb{M}^{2\times 2}_{\mathrm{skew}})$$

with $\operatorname{Curl} A=\mu$ *such that up to subsequences (not relabeled), (μ_n,β_n) converges to (μ,S,A) in the sense of Definition* 4.1.

(ii) (Γ-convergence) *As $\varepsilon\to 0$ the energy functionals $\mathcal{F}^{g_A}_\varepsilon$ defined in* (72) *Γ-converge with respect to the convergence of Definition* 4.1 *to $\mathcal{F}^{g_A}$ defined in* (74).

The compactness statement readily follows from the compactness of Theorem 4.2 since $\mathcal{F}^{g_A}_\varepsilon(\mu,\beta) \geq \mathcal{F}_\varepsilon(\mu,\beta)$. Let us proceed with the proof of the Γ-convergence result.

Proof of Γ-$\limsup$ *inequality of Theorem* 5.1. Let (μ, S, A) be given in the domain of the Γ-limit $\mathcal{F}^{g_A}$. We will construct a recovery sequence in two steps, relying on Theorem 4.2.

Step 1. *Approximation of the boundary values.* For $\delta > 0$ fixed, set $\omega_\delta := \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) > \delta\}$ so that $\omega_\delta \subset\subset \Omega$, and assume without loss of generality that w_δ is Lipschitz. Define $S_\delta \in L^2(\Omega; \mathbb{M}^{2\times 2}_{\mathrm{sym}})$ and $A_\delta \in L^2(\Omega; \mathbb{M}^{2\times 2}_{\mathrm{skew}})$ as

$$A_\delta := \begin{cases} A & \text{in } \omega_\delta\,, \\ g_A & \text{in } \Omega \setminus \omega_\delta\,, \end{cases} \qquad S_\delta := \begin{cases} S & \text{in } \omega_\delta\,, \\ 0 & \text{in } \Omega \setminus \omega_\delta\,. \end{cases}$$

Further, let $\mu_\delta \in \mathcal{M}(\Omega; \mathbb{R}^2)$ be such that

$$\mu_\delta := \mu \llcorner \omega_\delta + \operatorname{Curl} g_A \llcorner (\Omega \setminus \omega_\delta) + (g_A - A)\cdot t\ \mathcal{H}^1 \llcorner \partial\omega_\delta\,.$$

Notice that

$$\operatorname{Curl} A_\delta = \mu_\delta \quad \text{and} \quad \mu_\delta \in H^{-1}(\Omega; \mathbb{R}^2)\,;$$

therefore, $(\mu_\delta, S_\delta, A_\delta)$ belongs to the domain of the functional $\mathcal{F}$. Also note that

$$\begin{gathered} S_\delta \to S\,,\ A_\delta \to A \ \text{ in } \ L^2(\Omega; \mathbb{M}^{2\times 2})\,, \\ \mu_\delta \overset{*}{\rightharpoonup} \mu \ \text{ in } \ \mathcal{M}(\Omega; \mathbb{R}^2)\,,\ |\mu_\delta|(\Omega) \to |\mu|(\Omega) + \int_{\partial\Omega} |(g_A - A)\cdot t|\, ds \end{gathered} \tag{75}$$

as $\delta \to 0$. Therefore, by Reshetnyak's Theorem (see [1, Theorem 2.39]), we have

$$\lim_{\delta\to 0} \mathcal{F}(\mu_\delta, S_\delta, A_\delta) = \mathcal{F}^{g_A}(\mu, S, A)\,. \tag{76}$$

It will now be sufficient to construct dislocation measures $\mu_{\delta,\varepsilon}$ and strains $\beta_{\delta,\varepsilon}$ such that $(\mu_{\delta,\varepsilon}, \beta_{\delta,\varepsilon})$ converges to $(\mu_\delta, S_\delta, A_\delta)$ in the sense of Definition 4.1 and that

$$\lim_{\varepsilon\to 0} \mathcal{F}^{g_A}_\varepsilon(\mu_{\delta,\varepsilon}, \beta_{\delta,\varepsilon}) = \mathcal{F}(\mu_\delta, S_\delta, A_\delta)\,.$$

By taking a diagonal sequence $(\mu_{\delta_\varepsilon,\varepsilon}, \beta_{\delta_\varepsilon,\varepsilon})$ and using (75), (76), the thesis will follow.

Step 2. *Recovery sequence for strains satisfying the boundary condition.* Let us now proceed to construct the sequence $(\mu^{g_\varepsilon}_{\delta,\varepsilon}, \beta^{g_\varepsilon}_{\delta,\varepsilon})$ as stated in the previous step. From Theorem 4.2, there exists a sequence $(\mu_{\delta,\varepsilon}, \beta_{\delta,\varepsilon})$ converging to (μ, S, A) in the sense of Definition 4.1 and such that

$$\lim_{\varepsilon\to 0} \mathcal{F}_\varepsilon(\mu_{\delta,\varepsilon}, \beta_{\delta,\varepsilon}) = \mathcal{F}(\mu, S, A)\,. \tag{77}$$

Moreover (see Remark 4.6), we can assume that β_ε satisfies (70), from which (77) easily follows. $\square$

Proof of Γ-$\liminf$ *inequality of Theorem* 5.1. Let (μ, S, A) be in the domain of the Γ-limit $\mathcal{F}^{g_A}$. Assume that $(\mu_\varepsilon, \beta_\varepsilon)$ converges to (μ, S, A) in the sense of Definition 4.1. By combining an extension argument with the Γ-$\liminf$ inequality in Theorem 4.2 we will show that

$$\mathcal{F}^{g_A}(\mu, S, A) \leq \liminf_{\varepsilon\to 0} \mathcal{F}^{g_A}_\varepsilon(\mu_\varepsilon, \beta_\varepsilon)\,.$$

Fix $\delta > 0$, and define $U_\delta := \{x \in \mathbb{R}^2 : \operatorname{dist}(x, \Omega) < \delta\}$. By standard reflexion arguments one can extend g_A to $\tilde g_A \in L^2(U_\delta; \mathbb{M}^{2\times 2}_{\mathrm{skew}})$ in such a way that $\tilde\mu_A := \operatorname{Curl} \tilde g_A$ is a measure on U_δ satisfying $|\tilde\mu_A|(\partial\Omega) = 0$. Recall the functions $\tilde\beta_\varepsilon$ defined in the proof of compactness in section 4.1 (with ε_n replaced by ε), and set

$$\hat\beta_\varepsilon := \begin{cases} \tilde\beta_\varepsilon & \text{in } \Omega\,, \\ N_\varepsilon \tilde g_A & \text{in } U_\delta \setminus \Omega\,, \end{cases} \qquad \hat\beta := \begin{cases} A & \text{in } \Omega\,, \\ \tilde g_A & \text{in } U_\delta \setminus \Omega\,. \end{cases}$$

By construction we have $\frac{\hat\beta_\varepsilon}{N_\varepsilon} \rightharpoonup \hat\beta$ in $L^1(U_\delta)$ so that

$$\hat\mu_\varepsilon := \frac{\operatorname{Curl} \hat\beta_\varepsilon}{N_\varepsilon} \overset{*}{\rightharpoonup} \mu + ((g_A - A)\cdot t)\mathcal{H}^1 \llcorner \partial\Omega + \operatorname{Curl} \tilde g_A \llcorner (U_\delta \setminus \Omega)\,.$$

Recalling (33), (36), and (37), we conclude

$$\begin{aligned}
\liminf_{\varepsilon\to 0} \mathcal{F}^{g_A}_\varepsilon(\mu_\varepsilon, \beta_\varepsilon) &\geq \liminf_{\varepsilon\to 0} \frac{1}{\sqrt{N_\varepsilon |\log\varepsilon|}} \int_\Omega W(\beta^{\mathrm{sym}}_\varepsilon)\, dx \\
&\quad + \liminf_{\varepsilon\to 0} \frac{1}{N_\varepsilon} \int_\Omega \varphi\left(\frac{d\mu_\varepsilon}{d|\mu_\varepsilon|}\right) d|\mu_\varepsilon| + \int_{\partial\Omega} \varphi\Big(\Big(g_A - \frac{\beta_\varepsilon}{N_\varepsilon}\Big)\cdot t\Big)\, ds \\
&\geq \int_\Omega W(S)\, dx + \liminf_{\varepsilon\to 0} \int_{U_\delta} \varphi\left(\frac{d\hat\mu_\varepsilon}{d|\hat\mu_\varepsilon|}\right) d|\hat\mu_\varepsilon| - \int_{U_\delta\setminus\Omega} \varphi\left(\frac{d \operatorname{Curl} \tilde g_A}{d|\operatorname{Curl} \tilde g_A|}\right) d|\operatorname{Curl} \tilde g_A| \\
&\geq \int_\Omega W(S)\, dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu| + \int_{\partial\Omega} \varphi((g_A - A)\cdot t)\, ds = \mathcal{F}^{g_A}_\varepsilon(\mu, S, A). \qquad \square
\end{aligned}$$

6. Linearized polycrystals as minimizers of the Γ-limit. Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with Lipschitz continuous boundary. Let $k \in \mathbb{N}$ be fixed, and let $\{U_i\}_{i=1}^k$ be a Caccioppoli partition of Ω (see [1, section 4.4]). Moreover, fix $m_1, \dots, m_k \in \mathbb{R}_+$ with $m_i < m_{i+1}$, and define the piecewise constant function $a \in BV(\Omega)$ as

$$a := \sum_{i=1}^k m_i \chi_{U_i}\,. \tag{78}$$

In particular, (78) implies that $a \in L^\infty(\Omega)$ and $Da \in \mathcal{M}(\Omega; \mathbb{R}^2)$. We can now define the piecewise constant boundary condition $g_A \in L^\infty(\Omega; \mathbb{M}^{2\times 2}_{\mathrm{skew}})$ as

$$g_A := \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix}. \tag{79}$$

Notice that $g_A \in L^2(\Omega; \mathbb{M}^{2\times 2}_{\mathrm{skew}})$ and $\operatorname{Curl} g_A = Da$; hence, $\operatorname{Curl} g_A \in H^{-1}(\Omega; \mathbb{R}^2) \cap \mathcal{M}(\Omega; \mathbb{R}^2)$. In this way g_A is an admissible boundary condition for $\mathcal{F}^{g_A}$, as required in (71).

We wish to minimize the Γ-limit (74) with boundary condition g_A prescribed by (78)–(79). Since the elastic energy and plastic energy are decoupled in $\mathcal{F}^{g_A}$ and there is no boundary condition fixed on the elastic part of the strain S, we have

$$\inf \mathcal{F}^{g_A}(\operatorname{Curl} A, S, A) = \inf \mathcal{F}^{g_A}(\operatorname{Curl} A, 0, A)\,.$$

Therefore, it is sufficient to study

$$\inf\left\{\int_\Omega \varphi(\operatorname{Curl} A)+\int_{\partial\Omega}\varphi((g_A-A)\cdot t)\,ds:\ A\in L^2(\Omega;\mathbb{M}^{2\times 2}_{\rm skew}),\right.$$
$$\left.\operatorname{Curl} A\in H^{-1}(\Omega;\mathbb{R}^2)\cap\mathcal{M}(\Omega;\mathbb{R}^2)\right\}, \tag{80}$$

where $\varphi\colon \mathbb{R}^2\to[0,\infty)$ is the density defined in (22) and

$$\int_\Omega \varphi(\mu):=\int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right)\,d|\mu| \tag{81}$$

is the anisotropic φ-total variation for a measure $\mu\in\mathcal{M}(\Omega;\mathbb{R}^2)$. Note that (81) is well-posed since φ satisfies the properties given in Proposition 3.3.

For $A\in L^2(\Omega;\mathbb{M}^{2\times 2}_{\rm skew})$, we have that

$$A=\begin{pmatrix}0 & u\\ -u & 0\end{pmatrix} \tag{82}$$

for some $u\in L^2(\Omega)$. Moreover, $\operatorname{Curl} A=Du$; therefore, condition $\operatorname{Curl} A\in\mathcal{M}(\Omega;\mathbb{R}^2)$ implies $u\in BV(\Omega)$. We claim that (80) is equivalent to the following minimization problem:

$$\inf\left\{\int_\Omega \varphi(Du)+\int_{\partial\Omega}\varphi((u-a)\nu)\,ds:\ u\in BV(\Omega)\right\}. \tag{83}$$

Indeed, we already showed that if A is a competitor for (80), then the function u, given by (82), belongs to $BV(\Omega)$, and it is a competitor for (83). Conversely, assume that $u\in BV(\Omega)$, and define A through (82). Since $u\in BV(\Omega)$, $\operatorname{Curl} A=Du\in\mathcal{M}(\Omega;\mathbb{R}^2)$. Moreover, recall that the immersion $BV(\Omega)\hookrightarrow L^2(\Omega)$ is continuous; therefore, $u\in L^2(\Omega)$, which implies $A\in L^2(\Omega;\mathbb{M}^{2\times 2})$ so that $\operatorname{Curl} A\in H^{-1}(\Omega;\mathbb{R}^2)$. This shows that (80) and (83) are equivalent.

The main result of this section states that, given the piecewise constant boundary condition a defined in (78), there exists a piecewise constant minimizer $\tilde u$ to (83). In our model the function $\tilde u$ corresponds to a linearized polycrystal.

THEOREM 6.1. *There exists a locally constant minimizer $\tilde u\in BV(\Omega)$ to* (83)*, i.e.,*

$$\tilde u=\sum_{i=1}^k m_i\chi_{\Omega_i},$$

where $\{\Omega_i\}_{i=1}^k$ is a Caccioppoli partition of Ω and the values m_i are the ones of (78)*.*

The proof of this theorem relies on the anisotropic coarea formula. For the reader's convenience we briefly recall it here. For $E\subset\Omega$ of finite perimeter, the anisotropic φ-perimeter of E in Ω is defined as

$$\operatorname{Per}_\varphi(E,\Omega):=\int_\Omega \varphi(D\chi_E).$$

Since φ satisfies the properties of Proposition 3.3, the anisotropic coarea formula holds true for every $u\in BV(\Omega)$:

$$\int_\Omega \varphi(Du)=\int_{-\infty}^{\infty}\operatorname{Per}_\varphi(E_t,\Omega)\,dt, \tag{84}$$

where E_t is the level set $E_t:=\{x\in\Omega:\ u(x)>t\}$, defined for every $t\in\mathbb{R}$.

Proof of Theorem 6.1.

Step 1. *Equivalent minimization problem.* We start by rewriting (83) as a boundary value problem in BV. Let $\Omega' := \{x \in \mathbb{R}^2 : \operatorname{dist}(x,\Omega) < 1\}$ so that $\Omega \subset\subset \Omega'$. Consider a piecewise constant extension $\tilde{a} \in BV(\Omega')$ of the function $a \in BV(\Omega)$ defined in (78); that is,

$$\tilde{a} = \sum_{i=1}^{k} m_i \, \chi_{U_i'} \,,$$

where $\{U_i'\}_{i=1}^k$ is a Caccioppoli partition of Ω', agreeing with $\{U_i\}_{i=1}^k$ on Ω. This is possible since the extension can be chosen such that $|D\tilde{a}|(\partial\Omega) = 0$; that is, we are not creating any jump on $\partial\Omega$. Consider the new minimization problem

$$I := \inf \left\{ \int_{\Omega'} \varphi(Du) : \, u \in BV(\Omega'), \; u = \tilde{a} \text{ a.e. in } \Omega' \setminus \Omega \right\} . \tag{85}$$

Finding a solution to (85) is equivalent to finding a solution to (83). Indeed, if $u \in BV(\Omega')$ is such that $u = \tilde{a}$ in $\Omega' \setminus \Omega$, then

$$Du = Du \llcorner \Omega + (u^\Omega - a^\Omega) \, \nu \, \mathcal{H}^1 \llcorner \partial\Omega + D\tilde{a} \llcorner (\Omega' \setminus \Omega) \,, \tag{86}$$

where $u^\Omega, a^\Omega \in L^1(\partial\Omega)$ are the traces of u and a on $\partial\Omega$. Notice that we can use a^Ω in (86) because the extension $\tilde{a}$ is such that $|D\tilde{a}|(\partial\Omega) = 0$; hence, we have $\tilde{a}^+_{\partial\Omega} = \tilde{a}^-_{\partial\Omega} = a^\Omega \; \mathcal{H}^{n-1}$-a.e. in $\partial\Omega$.

Step 2. *Existence of a minimizer for* (85)*.* Let $u_j \in BV(\Omega')$ be a minimizing sequence for (85), that is, $u_j = \tilde{a}$ a.e. on $\Omega' \setminus \Omega$ and

$$\lim_{j\to\infty} \int_{\Omega'} \varphi(Du_j) = I \, . \tag{87}$$

By standard truncation arguments we can assume that $\|u_j\|_\infty \le \max_i |m_i|$. In particular, from (87), we deduce that $\sup_j \|u_j\|_{BV(\Omega')} < \infty$. By compactness in BV, there exists $\tilde{u} \in BV(\Omega')$ such that, up to subsequences, $u_j \to \tilde{u}$ in $L^1(\Omega')$ and $Du_j \overset{*}{\rightharpoonup} D\tilde{u}$ weakly in $\mathcal{M}(\Omega';\mathbb{R}^2)$. Since $u_j = \tilde{a}$ a.e. on $\Omega' \setminus \Omega$, the strong convergence in L^1 implies that (up to subsequences) $u_j \to \tilde{u}$ a.e. in Ω' so that $\tilde{u} = \tilde{a}$ a.e. in $\Omega' \setminus \Omega$. From Reshetnyak's lower semicontinuity theorem we conclude that

$$\int_{\Omega'} \varphi(D\tilde{u}) \le \liminf_{j\to\infty} \int_{\Omega'} \varphi(Du_j) = I$$

so that $\tilde{u}$ is a minimizer for (85).

Step 3. *Existence of a piecewise constant minimizer for* (83)*.* Let u be a minimizer for (85). By a standard truncation argument we can assume that $m_1 \le u \le m_k$ a.e. on Ω'. Formula (84) then reads

$$\int_{\Omega'} \varphi(Du) = \sum_{i=1}^{k-1} \int_{m_i}^{m_{i+1}} \operatorname{Per}_\varphi(E_t, \Omega') \, dt \,, \tag{88}$$

where $E_t := \{x \in \Omega' \colon u(x) > t\}$ for $t \in \mathbb{R}$. By the mean value theorem, for every $i = 1, \ldots, k-1$, there exists $t_i \in (m_i, m_{i+1})$ such that

$$\int_{m_i}^{m_{i+1}} \operatorname{Per}_\varphi(E_t, \Omega') \, dt \ge (m_{i+1} - m_i) \operatorname{Per}_\varphi(E_{t_i}, \Omega') \, . \tag{89}$$

We define the piecewise constant function

$$\tilde{u}(x) := m_i \qquad \text{if } x \in E_{t_{i-1}} \setminus E_{t_i}$$

for $i = 1, \dots, k$, where we have set $E_{t_0} := \Omega'$ and we notice that $E_{t_k} = \emptyset$ set theoretically. Since the sets E_t have finite perimeter in Ω', we have that $\tilde{u} \in BV(\Omega')$. Moreover, by construction, $\tilde{u} = \tilde{a}$ on $\Omega' \backslash \Omega$ so that $\tilde{u}$ is a piecewise constant competitor for (85). It is immediate to compute that

$$D\tilde{u} = \sum_{i=1}^{k-1} (m_{i+1} - m_i)\, \nu_{E_{t_i}}\, \mathcal{H}^1 \llcorner \partial^* E_{t_i}$$

so that

$$\begin{aligned} \int_{\Omega'} \varphi(D\tilde{u}) &= \sum_{i=1}^{k-1} (m_{i+1} - m_i) \int_{\partial^* E_{t_i}} \varphi(\nu_{E_{t_i}})\, d\mathcal{H}^1 \\ &= \sum_{i=1}^{k-1} (m_{i+1} - m_i)\, \mathrm{Per}_\varphi(E_{t_i}, \Omega')\,. \end{aligned} \tag{90}$$

By minimality of u and (88)–(90) we conclude that $\tilde{u}$ is a locally constant minimizer for (85). Hence, $\tilde{u}|_\Omega$ is a locally constant minimizer for (83). ∎

7. Conclusions and perspectives. The aim of this paper is to describe polycrystalline structures from a variational point of view. Grain boundaries and the corresponding grain orientations are not introduced as internal variables of the energy, but they spontaneously arise as a result of energy minimization, under suitable boundary conditions.

We work under the hypothesis of linear planar elasticity as in [9] with the reference configuration $\Omega \subset \mathbb{R}^2$ representing a section of an infinite cylindrical crystal. The elastic energy functional depends on the lattice spacing ε of the crystal, and we allow N_ε edge dislocations in the reference configuration with $N_\varepsilon \to \infty$ as $\varepsilon \to 0$. Each dislocation contributes by a factor $|\log \varepsilon|$ to the elastic energy so that the natural rescaling for the energy functional is $N_\varepsilon |\log \varepsilon|$. We work in the energy regime

$$|\log \varepsilon| \ll N_\varepsilon \ll \frac{1}{\varepsilon}\,,$$

which accounts for grain boundaries that are mutually rotated by an infinitesimal angle $\theta \approx 0$. After rescaling the elastic energy of such system of dislocations and sending the lattice spacing ε to zero, in Theorem 4.2 we derive by Γ-convergence a macroscopic energy functional of the form

$$\mathcal{F}(\mu, S, A) = \frac{1}{2} \int_\Omega \mathbb{C} S : S\, dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu|\,,$$

where $\mathbb{C}$ is the linear elasticity tensor and φ is a positively 1-homogeneous density function, defined through a suitable cell-problem. The elastic energy is computed on S, which represents the elastic part of the macroscopic strain. The plastic energy depends only on the dislocation measure μ, which is coupled to the plastic part A of the macroscopic strain through the relation $\mu = \mathrm{Curl}\, A$. As a consequence, μ is a curl-free vector Radon measure. The contributions of elastic energy and plastic energy are decoupled in the Γ-limit $\mathcal{F}$ due to the fact that S and A live on different scales: $\sqrt{N_\varepsilon|\log\varepsilon|}$ and N_ε, respectively.

Once the Γ-limit $\mathcal{F}$ is obtained, we impose a piecewise constant Dirichlet boundary condition on A and minimize $\mathcal{F}$ under such constraint. In Theorem 6.1 we prove that $\mathcal{F}$ admits piecewise constant minimizers of the form

$$\hat{A} = \sum_{i=1}^{k} A_i\,\chi_{\Omega_i}\,,$$

where the A_i's are antisymmetric matrices and $\{\Omega_i\}$ is a Caccioppoli partition of Ω. We interpret $\hat{A}$ as a linearized polycrystal with Ω_i representing a single grain having orientation A_i. This interpretation is motivated by the fact that antisymmetric matrices can be considered as infinitesimal rotations. The (linear) energy corresponding to $\hat{A}$ can be seen as a linearized version of the Read–Shockley formula for small angle tilt grain boundaries, i.e.,

$$E = E_0\,\theta(1+|\log\theta|)\,, \tag{91}$$

where $E_0 > 0$ is a constant depending only on the material and θ is the angle formed by two grains. Indeed, the Read–Shockley formula is obtained in [17] by computing the elastic energy for an evenly spaced array of $1/\varepsilon$ dislocations at the grain boundaries. Our energy regime accounts only for $N_\varepsilon \ll 1/\varepsilon$ dislocations; therefore, we do not have enough dislocations to create true rotations between grains. Nevertheless, we still observe polycrystalline structures, but the rotation angles between grains are infinitesimal.

Recently, Lauteri and Luckhaus [14] proved some compactness properties and energy bounds in agreement with the Read–Shockley formula. It would be desirable to understand if our Γ-limit can be deduced from their model as the angle θ between grains tends to zero. Moreover, it would be interesting to push our Γ-convergence analysis to energy regimes of order $\frac{|\log\varepsilon|}{\varepsilon}$, corresponding to $N_\varepsilon \approx \frac{1}{\varepsilon}$. In this regime true rotations should emerge, and the Read–Shockley formula could be possibly derived by Γ-convergence. At present, our technical assumption on good separation between dislocations is not compatible with such an energy regime.

Another natural question is whether the minimizer $\hat{A}$ is unique or at least if all the minimizers are piecewise constant. We suspect that, by enforcing piecewise constant boundary conditions, generically all minimizers are piecewise constant.

A further problem is to deduce our Γ-limit $\mathcal{F}$ by starting from a nonlinear energy computed on small deformations $v = x + \varepsilon u$ in the energy regime $N_\varepsilon \gg |\log\varepsilon|$. A similar analysis was already performed in [15] (see also [18, 11]), where the authors derive the Γ-limit obtained in [9] starting from a nonlinear energy under the assumption that $N_\varepsilon \approx |\log\varepsilon|$. It seems possible to adapt the techniques used in [15] to our case. This problem is currently under investigation by the authors.

Finally, a further step forward in our analysis is the following: In this paper the formation of polycrystalline structures is driven by relaxed boundary conditions as usual for minimization problems in BV spaces. It would be interesting to deal with true boundary conditions, which we expect to lead to the same Γ-limit F^{g_A} defined in (73). Moreover, it would be interesting to replace boundary conditions by forcing terms. For instance, bulk forces in competition with surface energies at grain boundaries should result in polycrystals exhibiting some intrinsic length scale. This is the case of semicoherent interfaces, separated by periodic nets of dislocations (see [7]).

REFERENCES

[1] L. Ambrosio, N. Fusco, and D. Pallara, *Functions of Bounded Variation and Free Discontinuity Problems*, Oxford Science Publications, New York, 2000.

[2] D. J. Bacon, D. M. Barnett, and R. O. Scattergood, *Anisotropic continuum theory of lattice defects*, Progress in Materials Science, 23 (1978), pp. 51–262.

[3] P. Cermelli and G. Leoni, *Renormalized energy and forces on dislocations*, SIAM J. Math. Anal., 37 (2005), pp. 1131–1160, https://doi.org/10.1137/040621636.

[4] R. Dautray and J.-L. Lions, *Mathematical Analysis and Numerical Methods for Science and Technology*, Vol. 3, Springer, Berlin, 1988.

[5] L. De Luca, A. Garroni, and M. Ponsiglione, *Γ-convergence analysis of systems of edge dislocations: The self energy regime*, Arch. Ration. Mech. Anal., 206 (2012), pp. 885–910.

[6] V. S. Deshpande, A. Needleman, and E. Van der Giessen, *Finite strain discrete dislocation plasticity*, J. Mech. Phys. Solids, 51 (2003), pp. 2057–2083.

[7] S. Fanzon, M. Palombaro, and M. Ponsiglione, *A variational model for dislocations at semi-coherent interfaces*, J. Nonlinear Sci., 27 (2017), pp. 1436–1461, https://doi.org/10.1007/s00332-017-9366-5.

[8] H. Foell, *Defects in Crystals*, University of Kiel, https://www.tf.uni-kiel.de/matwis/amat/def_en/.

[9] A. Garroni, G. Leoni, and M. Ponsiglione, *Gradient theory for plasticity via homogenization of discrete dislocations*, J. Eur. Math. Soc. (JEMS), 12 (2010), pp. 1231–1266.

[10] J. Ginster, *Plasticity as the Γ-Limit of a Two-Dimensional Dislocation Energy: The Critical Regime without the Assumption of Well-Separateness*, preprint, 2018, https://arxiv.org/pdf/1805.12195.pdf.

[11] J. Ginster, *Strain-Gradient Plasticity as the Γ-Limit of a Nonlinear Dislocation Energy with Mixed Growth*, preprint, 2018, https://arxiv.org/pdf/1806.05067.pdf.

[12] G. Gottstein, *Physical Foundations of Materials Science*, Springer, Berlin, 2013.

[13] R. Jerrard and H. Soner, *Limiting behavior of the Ginzburg-Landau functional*, Funct. Anal., 192 (1992), pp. 524–561.

[14] G. Lauteri and S. Luckhaus, *An Energy Estimate for Dislocation Configurations and the Emergence of Cosserat-Type Structures in Metal Plasticity*, preprint, 2017, https://arxiv.org/abs/1608.06155.

[15] S. Müller, L. Scardia, and C. Zeppieri, *Geometric rigidity for incompatible fields and an application to strain-gradient plasticity*, Indiana Univ. Math. J., 63 (2014), pp. 1365–1396.

[16] W. T. Read, *Dislocations in Crystals*, McGraw-Hill, New York, 1953.

[17] W. T. Read and W. Shockley, *Dislocation models of crystal grain boundaries*, Phys. Rev., 78 (1950), pp. 275–289, https://doi.org/10.1103/PhysRev.78.275.

[18] L. Scardia and C. Zeppieri, *Line-tension model for plasticity as the Γ-limit of a nonlinear dislocation energy*, SIAM J. Math. Anal., 44 (2012), pp. 2372–2400.

[19] J. Taylor and W. Cahn, *A unified approach to motion of grain boundaries, relative tangential translation along grain boundaries, and grain rotation*, Acta Materialia, 52 (2004), pp. 4887–4898.

[20] Webpage, *Atomic Scale Structure of Materials*, DoITPoMS TLP, University of Cambridge, https://www.doitpoms.ac.uk/tlplib/atomic-scale-structure/poly.php.