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Article (Published Version)

PAMM · Proc. Appl. Math. Mech. **13**, 541 – 544 (2013) / **DOI** 10.1002/pamm.201310260

Dislocations in nanowire heterostructures: from discrete to continuum

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We discuss an atomistic model for heterogeneous nanowires, allowing for dislocations at the interface. We study the limit as the atomic distance converges to zero, considering simultaneously a dimension reduction and the passage from discrete to continuum. Employing the notion of Gamma-convergence, we establish the minimal energies associated to defect-free configurations and configurations with dislocations at the interface, respectively. It turns out that dislocations are favoured if the thickness of the wire is sufficiently large.

Dislocations represent an important class of defects in crystalline solids and their presence influences the behaviour of materials in many ways. For example, in semiconductor electronics dislocations play a crucial role in the development of nanowire heterostructures, which can be defined as the combination of two or more materials within the same nanowire structure. Indeed, a large lattice mismatch between the materials of interest may result in poor quality interfaces with high density of misfit dislocations. We present a rigorous discrete-to-continuum analysis showing that, for a given mismatch, formation of dislocations is energetically more favourable when the radius of the cross-section is sufficiently large. These results will appear in the forthcoming paper [7], to which we refer for a detailed discussion.

We consider a longitudinally heterostructured nanowire, which consists of two crystalline phases featuring different atomic distances. In our model each of the two phases has a different lattice structure already in the reference configuration. If the thickness of the nanowire is sufficiently large, the crystal develops edge dislocations at the interface.

A variational approach to this problem was first proposed in [4] in linearized elasticity. A rigorous justification in terms of Γ-convergence was given in [9] in the context of nonlinear continuum elasticity. In our work we show that the results proven in [9] can be recovered starting from a microscopic model and employing both methods from dimension reduction and techniques that are commonly used in the study of discrete systems, as done e.g. in [1, 12] for a different scaling of the energy.

In the present paper we focus on a two-dimensional model, where the reference configuration of each phase is a hexagonal Bravais lattice. The cells are then equilateral triangles with side that varies from phase to phase. An essential property for obtaining our result is that the nearest-neighbour interactions in this lattice provide a rigid structure. Although in this paper we consider for simplicity only the two-dimensional case, our approach can be applied to three-dimensional rigid lattices of Bravais or non-Bravais type, see [7].

The energy of a deformation of the discrete system is based on harmonic nearest-neighbour interactions and depends on four quantities, ε, k, λ, and ρ. The small parameter ε is here the equilibrium lattice distance between the atoms in the first phase. We perform an asymptotic analysis as $\varepsilon \to 0^+$, in a discrete-to-continuum framework.

In the reference configuration the specimen is a parallelogram of sides $2L$ and $k\varepsilon$, with $L > 0$ and $k \in \mathbb{N}$. Hence, k describes the thickness of the nanowire, which consists of $k+1$ lines of atoms, see Figure 1. Since the quantities L and k are independent of ε, the dimension of the system reduces to one as $\varepsilon \to 0^+$.

In the deformed configuration, the equilibrium lattice distance between the atoms in the second phase is $\lambda\varepsilon$, where $\lambda \in (0,1)$ is a constant, being a datum of the problem. In the reference configuration the lattice distance between the atoms of the second phase is instead $\rho\varepsilon$, with $\rho \in (0,1]$ (the most interesting case being $\rho \in [\lambda, 1]$). The parameter ρ is variable in the model, so we compare different reference configurations, with different structures of nearest neighbours.

In the case $\rho = 1$, which corresponds to a defect-free system, the coordination number of the lattice (i.e., the number of nearest neighbours of an internal atom) is constantly six. For different values of ρ, if k is sufficiently large, some atoms have more than six nearest neighbours and some have less than six; this corresponds to dislocations.

1 Setting of the model

We now define an unbounded lattice depending only on the quantity $\rho \in (0,1]$. We set $\mathrm{w}_1 := (1,0)$, $\mathrm{w}_2 := (\frac{1}{2}, \frac{\sqrt{3}}{2})$, $\mathrm{w}_3 := \mathrm{w}_2 - \mathrm{w}_1$, and

$$\mathcal{L}_\rho := \mathcal{L}_1^- \cup \mathcal{L}_\rho^+ , \quad \mathcal{L}_1^- := \{\xi_1\mathrm{w}_1 + \xi_2\mathrm{w}_2 \colon \xi_1, \xi_2 \in \mathbb{Z},\ \xi_1 < 0\} , \quad \mathcal{L}_\rho^+ := \{\xi_1\mathrm{w}_1 + \xi_2\mathrm{w}_2 \colon \xi_1, \xi_2 \in \rho\mathbb{Z},\ \xi_1 \geq 0\} .$$

In order to define the nearest neighbours in $\mathcal{L}_\rho$, we fix a triangulation $\mathcal{T}_\rho$ associated with $\mathcal{L}_\rho$ and fulfilling the Delaunay property according to the definition below, see also [10].

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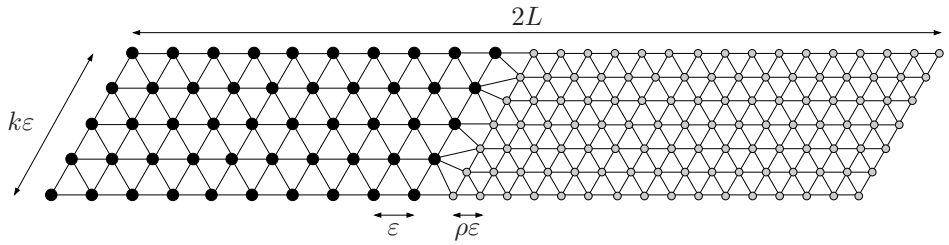

Fig. 1: A lattice with dislocations of type $\mathcal{L}_{\rho,\varepsilon}(k)$.

Definition 1.1 (Delaunay property; Nearest neighbours) Let $\mathcal{T}_\rho$ be a triangulation associated with $\mathcal{L}_\rho$, i.e., a partition of $\mathbb{R}^2$ in open nonempty triangles with vertices in $\mathcal{L}_\rho$. We say that $\mathcal{T}_\rho$ has the Delaunay property if, for every simplex of $\mathcal{T}_\rho$, its circumcircle contains no points of $\mathcal{L}_\rho$ in its interior. Two points $x, y \in \mathcal{L}_\rho$ are said to be nearest neighbours (and we write: $x,\ y$ NN) if they are vertices of one of the triangles of $\mathcal{T}_\rho$.

For the details of the construction of such a triangulation, we refer to [7]. We remark here that $\mathcal{L}_1$ is the two-dimensional hexagonal Bravais lattice generated by the vectors w_1 and w_2, and the previous definition gives the usual choice of nearest neighbours in $\mathcal{L}_1$, i.e., the nearest neighbours of an atom are the six atoms with distance one.

We also underline that the choice of a Delaunay triangulation is not essential for the following results: indeed, $\mathcal{T}_\rho$ can be any triangulation associated with $\mathcal{L}_\rho$, such that both the maximal number of nearest neighbours per atom and the length of the bonds in the reference configuration are bounded.

In order to model wires, we define bounded lattices. Given $L > 0$, $\varepsilon \in (0, 1]$, and $k \in \mathbb{N}$, we set

$$\Omega_{k\varepsilon} := \{\xi_1 \mathrm{w}_1 + \xi_2 \mathrm{w}_2 \colon \xi_1 \in (-L, L),\ \xi_2 \in (0, k\varepsilon)\}\,, \quad \mathcal{L}_{\rho,\varepsilon}(k) := (\varepsilon\mathcal{L}_\rho) \cap \overline{\Omega}_{k\varepsilon}\,.$$

We define also the sublattices corresponding to the two crystalline phases of the material:

$$\mathcal{L}^-_{1,\varepsilon}(k) := \{\xi_1 \mathrm{w}_1 + \xi_2 \mathrm{w}_2 \in \mathcal{L}_{\rho,\varepsilon}(k) \colon \xi_1 < 0\}\,, \quad \mathcal{L}^+_{\rho,\varepsilon}(k) := \{\xi_1 \mathrm{w}_1 + \xi_2 \mathrm{w}_2 \in \mathcal{L}_{\rho,\varepsilon}(k) \colon \xi_1 \geq 0\}\,.$$

We set also $\mathcal{T}_{\rho,\varepsilon} := \{\varepsilon T \colon T \in \mathcal{T}_\rho\}$. The nearest neighbours in $\mathcal{L}_{\rho,\varepsilon}(k)$ are defined in the following way: $x, y \in \mathcal{L}^+_{\rho,\varepsilon}(k)$ are nearest neighbours if $x/\varepsilon, y/\varepsilon$ satisfy the same property in $\mathcal{L}_\rho$.

The admissible deformations are piecewise affine on the triangulation $\mathcal{T}_{\rho,\varepsilon}$ and fulfill the non-interpenetration condition (common in the treatment of atomistic systems, see e.g. [3, 6]): namely, the deformation gradient is required to preserve local orientation. We set

$$\mathcal{A}_{\rho,\varepsilon}(\Omega_{k\varepsilon}) := \left\{u_\varepsilon \in C^0(\overline{\Omega}_{k\varepsilon}; \mathbb{R}^2) \colon u_\varepsilon \text{ piecewise affine, } \nabla u_\varepsilon \text{ constant on } \Omega_{k\varepsilon} \cap T\ \ \forall\, T \in \mathcal{T}_{\rho,\varepsilon}\,,\ \det \nabla u_\varepsilon > 0 \text{ a.e. in } \Omega_{k\varepsilon}\right\}.$$

The energy of a deformation $u_\varepsilon \in \mathcal{A}_{\rho,\varepsilon}(\Omega_{k\varepsilon})$ is defined as

$$\mathcal{E}^\lambda_\varepsilon(u_\varepsilon, \rho, k) := \tfrac{1}{2} \sum_{\substack{x,\, y \text{ NN} \\ x \in \mathcal{L}^-_{1,\varepsilon}(k) \\ y \in \mathcal{L}_{\rho,\varepsilon}(k)}} \left(\left|\frac{u_\varepsilon(x) - u_\varepsilon(y)}{\varepsilon}\right| - 1\right)^2 + \tfrac{1}{2} \sum_{\substack{x,\, y \text{ NN} \\ x \in \mathcal{L}^+_{\rho,\varepsilon}(k) \\ y \in \mathcal{L}_{\rho,\varepsilon}(k)}} \left(\left|\frac{u_\varepsilon(x) - u_\varepsilon(y)}{\varepsilon}\right| - \lambda\right)^2.$$

For more general choices of the interaction energy we refer to [7].

In the characterization of the limiting functional, we consider the rescaled domain $\frac{1}{\varepsilon}\Omega_{k\varepsilon}$ and the limit as $\varepsilon \to 0^+$, so we set

$$\Omega_{k,\infty} := \{\xi_1 \mathrm{w}_1 + \xi_2 \mathrm{w}_2 \colon \xi_1 \in (-\infty, +\infty),\ \xi_2 \in (0, k)\} = \mathbb{R} \times \left(0, \tfrac{\sqrt{3}}{2}k\right)\,, \quad \mathcal{L}_{\rho,\infty}(k) := \mathcal{L}_\rho \cap \overline{\Omega}_{k,\infty}\,,$$

as well as

$$\mathcal{L}^-_{1,\infty}(k) := \{\xi_1 \mathrm{w}_1 + \xi_2 \mathrm{w}_2 \in \mathcal{L}_{\rho,\infty}(k) \colon \xi_1 < 0\}\,, \quad \mathcal{L}^+_{\rho,\infty}(k) := \{\xi_1 \mathrm{w}_1 + \xi_2 \mathrm{w}_2 \in \mathcal{L}_{\rho,\infty}(k) \colon \xi_1 \geq 0\}\,.$$

By definition, two elements of $\mathcal{L}_{\rho,\infty}(k)$ are nearest neighbours if they are such in $\mathcal{L}_\rho$. As before we set

$$\mathcal{A}_{\rho,\infty}(\Omega_{k,\infty}) := \left\{u \in C^0(\overline{\Omega}_{k,\infty}; \mathbb{R}^2) \colon u \text{ piecewise affine, } \nabla u \text{ constant on } \Omega_{k,\infty} \cap T\ \ \forall\, T \in \mathcal{T}_\rho\,,\ \det \nabla u > 0 \text{ a.e. in } \Omega_{k,\infty}\right\}.$$

and

$$\mathcal{E}^\lambda_\infty(u, \rho, k) := \tfrac{1}{2} \sum_{\substack{x,\, y \text{ NN} \\ x \in \mathcal{L}^-_{1,\infty}(k) \\ y \in \mathcal{L}_{\rho,\infty}(k)}} (|u(x) - u(y)| - 1)^2 + \tfrac{1}{2} \sum_{\substack{x,\, y \text{ NN} \\ x \in \mathcal{L}^+_{\rho,\infty}(k) \\ y \in \mathcal{L}_{\rho,\infty}(k)}} (|u(x) - u(y)| - \lambda)^2\,.$$

for every $u \in \mathcal{A}_{\rho,\infty}(\Omega_{k,\infty})$.

2 The limiting variational problem

In this section we present the passage from the discrete two-dimensional energy introduced before to a one-dimensional continuous approximation. We outline our main results and refer to [7] for further details.

A fundamental tool in our proofs is the rigidity estimate of Friesecke, James, and Müller [5], which states that for every bounded Lipschitz domain $U \subset \mathbb{R}^2$ there exists a constant $C(U)$, depending on the shape of the domain, such that for each $u \in H^1(U;\mathbb{R}^2)$ there exists $R \in SO(2)$ with

$$\|\nabla u - R\|_{L^2(U;\mathbb{M}^{2\times 2})} \le C(U)\|\mathrm{dist}(\nabla u, SO(2))\|_{L^2(U)}\,.$$

This estimate can be applied to our setting because we have chosen a rigid lattice (i.e., each cell of the lattice is a rigid polygon, namely a triangle) and because we suppose the admissible deformations to preserve orientation locally (non-interpenetration). Using these assumptions it is possible to prove that the discrete energy $\mathcal{E}_\varepsilon^\lambda(u_\varepsilon,\rho,k)$ controls from above both $\|\mathrm{dist}(\nabla u_\varepsilon, SO(2))\|_{L^2(U)}$ and $\|\mathrm{dist}(\nabla u_\varepsilon, \frac{\lambda}{\rho}SO(2))\|_{L^2(V)}$ in certain subdomains U and V of $\Omega_{k\varepsilon}$. For discussions on rigidity in discrete systems we refer e.g. to [11] and references therein.

Let now $\rho \in (0,1]$ and $k \in \mathbb{N}$ be fixed. In order to derive the continuum model as $\varepsilon \to 0^+$, we rescale the deformations in such a way that they belong to the same function space: given $u_\varepsilon \in \mathcal{A}_{\rho,\varepsilon}(\Omega_{k\varepsilon})$ we define $\tilde u_\varepsilon(y) := u_\varepsilon(A_\varepsilon y)$, where $A_\varepsilon := \begin{pmatrix} 1 & \frac{\varepsilon-1}{\sqrt{3}} \\ 0 & \varepsilon \end{pmatrix}$. Notice that, for every $x \in \Omega_{k\varepsilon}$, the point $A_\varepsilon^{-1}x$ is an element of the domain Ω_k, independent of ε. Accordingly, we set

$$\widetilde{\mathcal{A}}_{\rho,\varepsilon}(\Omega_k) := \big\{\tilde u_\varepsilon \in C^0(\overline{\Omega}_k;\mathbb{R}^2)\colon \tilde u_\varepsilon \text{ piecewise affine, } \nabla\tilde u_\varepsilon \text{ constant on } \Omega_k \cap (A_\varepsilon^{-1}T)\ \forall T \in \mathcal{T}_{\rho,\varepsilon}\,,\ \det\nabla\tilde u_\varepsilon > 0 \text{ a.e. in } \Omega_k\big\}\,.$$

We study the Γ-limit of the sequence of functionals $\{\widetilde{\mathcal{E}}_\varepsilon^\lambda(\cdot,\rho,k)\}$ defined by

$$\widetilde{\mathcal{E}}_\varepsilon^\lambda(\tilde u_\varepsilon,\rho,k) := \mathcal{E}_\varepsilon^\lambda(u_\varepsilon,\rho,k) \quad \text{for } \tilde u_\varepsilon \in \widetilde{\mathcal{A}}_{\rho,\varepsilon}(\Omega_k)\,,$$

where $u_\varepsilon(x) := \tilde u_\varepsilon(A_\varepsilon^{-1}x) \in \mathcal{A}_{\rho,\varepsilon}(\Omega_{k\varepsilon})$ as before. For the definition of Γ-convergence we refer e.g. to [2].

The first step for characterizing the Γ-limit is a compactness result. Let $\{\tilde u_\varepsilon\} \subset \widetilde{\mathcal{A}}_{\rho,\varepsilon}(\Omega_k)$ be a sequence such that $\limsup_{\varepsilon\to 0^+}\widetilde{\mathcal{E}}_\varepsilon^\lambda(\tilde u_\varepsilon,\rho,k) \le C$. Thanks to the L^∞-bound on $\nabla u_\varepsilon = \nabla\tilde u_\varepsilon A_\varepsilon^{-1}$ and to the scaling of the domain, one can extract a subsequence (not relabeled) such that $\nabla\tilde u_\varepsilon A_\varepsilon^{-1} \overset{*}{\rightharpoonup} (\partial_1\tilde u \,|\, d_2)$ weakly* in $L^\infty(\Omega_k;\mathbb{M}^{2\times 2})$ for some functions $\tilde u \in W^{1,\infty}(\Omega_k;\mathbb{R}^2)$ and $d_2 \in L^\infty(\Omega_k;\mathbb{R}^2)$, where $(\partial_1\tilde u \,|\, d_2)$ is the matrix whose columns are $\partial_1\tilde u$ and d_2. Since the dimension of the space reduces, it turns out that $\tilde u$ is independent of w_2, i.e., $\partial_{\mathrm{w}_2}\tilde u = 0$. We then apply the rigidity estimate in a family of subdomains with the same shape (so that the constant in the inequality does not depend on the domain). Hence we prove that d_2 is also independent of w_2, i.e., $\partial_{\mathrm{w}_2} d_2 = 0$, and the following inclusions hold: $(\partial_1\tilde u \,|\, d_2) \in \mathrm{co}(SO(2))$ a.e. in Ω_k^- and $(\partial_1\tilde u \,|\, d_2) \in \mathrm{co}(\frac{\lambda}{\rho}SO(2))$ a.e. in Ω_k^+, where

$$\Omega_k^- := \{\xi_1\mathrm{w}_1 + \xi_2\mathrm{w}_2\colon \xi_1 \in (-L,0),\ \xi_2 \in (0,k)\}\,,\quad \Omega_k^+ := \{\xi_1\mathrm{w}_1 + \xi_2\mathrm{w}_2\colon \xi_1 \in (0,L),\ \xi_2 \in (0,k)\}\,,$$

and $\mathrm{co}(\cdot)$ denotes the convex hull.

In the second step, we take a rescaling of the domain in both variables, obtaining $\frac{1}{\varepsilon}\Omega_{k\varepsilon}$, which tends to the strip $\Omega_{k,\infty}$ introduced above as $\varepsilon \to 0^+$. An application of the rigidity estimate then shows that one can restrict to deformations $v \in \mathcal{A}_{\rho,\infty}(\Omega_{k,\infty})$ that are in equilibrium far from the interface, i.e., such that $\nabla v = I$ if $x_1 \in (-\infty,-M)$ and $\nabla v = \frac{\lambda}{\rho}R$ if $x_1 \in (M,+\infty)$ for some $M > 0$ and $R \in SO(2)$. Therefore, for every $R \in SO(2)$, we define the minimum cost of such deformations as

$$\gamma^\lambda(\rho,k,R) := \inf\big\{\mathcal{E}_\infty^\lambda(v,\rho,k)\colon M > 0,\ v \in \mathcal{A}_{\rho,\infty}(\Omega_{k,\infty}), \nabla v = I \text{ for } x_1 < -M\,,\ \nabla v = \tfrac{\lambda}{\rho}R \text{ for } x_1 > M\big\}\,.$$

It is possible to prove that $\gamma^\lambda(\rho,k,R) = \gamma^\lambda(\rho,k,I)$ for every $R \in SO(2)$; hence, we write

$$\gamma^\lambda(\rho,k) := \gamma^\lambda(\rho,k,I)\,.$$

For each convergent sequence with equibounded energy we obtain that $\liminf_{\varepsilon\to 0^+}\widetilde{\mathcal{E}}_\varepsilon^\lambda(\tilde u_\varepsilon,\rho,k) \ge \gamma^\lambda(\rho,k)$, which gives the so-called Γ-$\liminf$ inequality. As for the upper bound, we introduce the set

$$\mathcal{A} := \big\{\tilde u \in W^{1,\infty}(\Omega_k;\mathbb{R}^2)\colon \partial_{\mathrm{w}_2}\tilde u = 0 \text{ a.e. in } \Omega_k\,, |\partial_1\tilde u| \le 1 \text{ a.e. in } \Omega_k^-\,, |\partial_1\tilde u| \le \tfrac{\lambda}{\rho} \text{ a.e. in } \Omega_k^+\big\}\,.$$

Given $\tilde u \in \mathcal{A}$, by [8, Theorem 4.1] one can construct a measurable function $d_2 \in L^\infty(\Omega_k;\mathbb{R}^2)$, independent of w_2, such that $(\partial_1\tilde u \,|\, d_2) \in \mathrm{co}(SO(2))$ a.e. in Ω_k^- and $(\partial_1\tilde u \,|\, d_2) \in \mathrm{co}(\frac{\lambda}{\rho}SO(2))$ a.e. in Ω_k^+. Moreover, we prove that there exists a sequence $\{\tilde u_\varepsilon\} \subset \widetilde{\mathcal{A}}_{\rho,\varepsilon}(\Omega_{k\varepsilon})$ such that $\nabla\tilde u_\varepsilon A_\varepsilon^{-1} \overset{*}{\rightharpoonup} (\partial_1\tilde u \,|\, d_2)$ weakly* in $L^\infty(\Omega_k;\mathbb{M}^{2\times 2})$ and $\limsup_{\varepsilon\to 0^+}\widetilde{\mathcal{E}}_\varepsilon^\lambda(\tilde u_\varepsilon,\rho,k) \le \gamma^\lambda(\rho,k)$. It follows that the domain of the Γ-limit of the sequence $\{\widetilde{\mathcal{E}}_\varepsilon^\lambda(\cdot,\rho,k)\}$ is $\mathcal{A}$ and that the Γ-limit is constant on $\mathcal{A}$.

Theorem 2.1 *The sequence of functionals* $\{\widetilde{\mathcal{E}}^{\lambda}_{\varepsilon}(\cdot,\rho,k)\}$ Γ*-converges, as* $\varepsilon \to 0^+$*, to the functional*

$$\widetilde{\mathcal{E}}^{\lambda}(u,\rho,k) = \begin{cases} \gamma^{\lambda}(\rho,k) & \text{if } u \in \mathcal{A}\,, \\ +\infty & \text{otherwise,} \end{cases}$$

with respect to the weak convergence in* $W^{1,\infty}(\Omega_k;\mathbb{R}^2)$.

3 Energetical comparison between defect-free and dislocated configurations

The continuum theory derived from the discrete system introduced above gives a variational characterization of the minimum cost $\gamma^{\lambda}(\rho,k)$ of the transitions between the equilibria of the discrete energy. We then obtain some interesting consequences.

Indeed, our analysis allows us to study such cost as a function of the parameters ρ and k (which were fixed in the passage to the limit as $\varepsilon \to 0^+$). In particular we compare the defect-free model ($\rho = 1$) with a model with $\rho \neq 1$ (for instance, $\rho = \lambda$). If $\rho \neq 1$ and k is large enough, the coordination number is not constant in the lattice, so the system contains dislocations. We study the asymptotic behavior of $\gamma^{\lambda}(\rho,k)$ as $k \to +\infty$.

The use of different reference configurations is motivated by the fact that the nearest neighbours are defined in the undeformed lattices, as usual in the mechanics of discrete systems. However, we assume that the crystal minimizes the total interaction energy between atoms allowing for possible defects: the nearest neighbours should be defined from the resulting deformation. Therefore, we regard the reference configuration as a variable of the problem and compare the continuum energies corresponding to different values of ρ.

If $\rho = 1$, a rescaling argument and an application of the rigidity estimate show that the growth of $\gamma^{\lambda}(\rho,k)$ is quadratic in k. This suggests that, in order to minimize the interaction energy $\mathcal{E}^{\lambda}_{\infty}(\cdot,\rho,k)$ without introducing defects, one should stretch a number of bonds of the order of k^2. We state here the result and refer to [7] for the proof.

Proposition 3.1 (Estimate in the defect-free case, $\rho = 1$) *There exist* $C_1, C_2 > 0$ *such that for every* $k \in \mathbb{N}$

$$C_1 k^2 \leq \gamma^{\lambda}(1,k) \leq C_2 k^2\,.$$

We compare the defect-free case with a possible configuration of nearest neighbours with dislocations, given for instance by setting $\rho = \lambda$. Thanks to the uniform bounds on the maximal number of nearest neighbours per atom and on the length of the bonds in $\mathcal{L}_{\rho}$, it turns out that the cost of the deformation $u\colon \mathcal{L}_{\rho,\infty}(k) \to \mathbb{R}^2\colon u(x) := x$ is linear in k, so the growth of $\gamma^{\lambda}(\rho,k)$ is at most linear in k.

Proposition 3.2 (Estimate for $\rho = \lambda$) *There exists a positive constant* C_{λ} *such that for every* k

$$\gamma^{\lambda}(\lambda,k) \leq C_{\lambda} k\,.$$

We recall that k is a mesoscale parameter corresponding to the number of lines of triangles in $\mathcal{L}^{-}_{1,\varepsilon}(k)$. If k is sufficiently large, from the previous estimates it follows that $\gamma^{\lambda}(\lambda,k) < \gamma^{\lambda}(1,k)$. Hence, assuming that the atoms of the crystal choose the configuration that minimizes the total interaction energy, one sees that the preferred configuration will contain defects (i.e., the coordination number will not be constant in the crystal) when the thickness of the nanowire is sufficiently large.

Acknowledgements This research was supported by the DFG grant SCHL 1706/2-1. M.P. acknowledges the Department of Mathematics of the University of Würzburg, to which she was affiliated when this work began.

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