Twinned martensite configurations arising as ground states of a two-well discrete Hamiltonian

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In this paper we construct and analyze a two-well Hamiltonian on 2D atomic lattice considered with nonconvex interactions. Two wells of the Hamiltonian are given by two rank-one connected martensitic twins, respectively. Our combined analytical and numerical results show that the structure of ground states under appropriate boundary conditions is close to the macroscopically expected twinned configuration plus additional exponential boundary layers localized near the twinning interface. Besides, we proceed to continuum limit, show asymptotic piece-wise rigidity of minimizing sequences and derive the limiting form of their surface energy.

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1 Introduction

In the last decades there been produced an intensive mathematical research on the martensitic transformations in shape memory alloys using nonlinear elasticity models of continuum mechanics, see e.g. [1–4]. In several models the finite scale in the arising laminate structure of the twinned martensitic variants was obtained and analyzed by adding penalizing higher order gradient terms to the elastic energy [3,4]. In this paper we are trying to look on the problem from the microscopic point of view. Starting from the construction of an atomistic two-well Hamiltonian on 2D atomic lattice considered with nonconvex interactions and aimed to model the simple martensitic transformations we would like to describe the structure of its ground states and to derive the limiting form of their surface energy. The latter should come out naturally from the full microscopic energy given by the Hamiltonian.

Consider a 2D atomic lattice $\chi^N = \{u_{ij}|\ i,j = 1,...,N\} \subset \mathbb{R}^2$ where $u:\ [1,N]^2 \cap \mathbb{Z}^2 \to \mathbb{R}^2$ prescribes the deformation of N^2 atoms from their initial reference configuration taken on $\mathbb{Z}^2$:

$$u_{ij} := u(i,j) \text{ for } (i,j) \in [1,N]^2 \cup \mathbb{Z}^2.$$

Additionally we suppose the u is an orientation-preserving deformation, i.e. $u \in \mathcal{A}$ where

$$\begin{aligned}\mathcal{A} \ := \ \Big\{ u : \mathbb{Z}^2 \to \mathbb{R}^2 \Big|\ & \det(u(x_2)-u(x_1), u(x_3)-u(x_1)) \geq 0 \text{ for all } \{x_1,x_2,x_3\} \subset \mathbb{Z}^2 \\ & \text{such that } \operatorname{diam}(x_1,x_2,x_3) = \sqrt{2} \text{ and } \det(x_2-x_1, x_3-x_1) \geq 0 \Big\}.\end{aligned}$$

We define an atomistic two-well Hamiltonian $H_N(\chi^N)$ as follows.

$$\begin{aligned}H_N(\chi^N) \ := \ & \sum_{i,j=1}^{N} h(u_{ij}, u_{i\pm 1 j \pm 1}) = \sum_{i,j=1}^{N} \Big[\left((u_{ij\pm 1}-u_{ij})^2 - a^2\right)^2 + \left((u_{i\pm 1 j}-u_{ij})^2 - b^2\right)^2 + \\ & + \left((u_{ij\pm 1}-u_{ij})\cdot(u_{i\pm 1 j}-u_{ij})\right)^2 \Big] \times \Big[\left((u_{ij\pm 1}-u_{ij})^2 - b^2\right)^2 + \left((u_{i\pm 1 j}-u_{ij})^2 - a^2\right)^2 + \\ & + \left((u_{ij\pm 1}-u_{ij})\cdot(u_{i\pm 1 j}-u_{ij})\right)^2 \Big], \qquad (1)\end{aligned}$$

where parameters $a,\ b \in \mathbb{R}^+$ satisfy $ab = 1$. In this definition and below we use a summation agreement: the sign $\pm$ in a term indicates that the latter should be replaced by the sum of the terms with all possible sign combinations, e.g.

$$\begin{aligned}(u_{ij\pm 1}-u_{ij})\cdot(u_{i\pm 1 j}-u_{ij}) \ := \ & (u_{ij-1}-u_{ij})\cdot(u_{i-1 j}-u_{ij}) + (u_{ij-1}-u_{ij})\cdot(u_{i+1 j}-u_{ij}) + \\ & + (u_{ij+1}-u_{ij})\cdot(u_{i-1 j}-u_{ij}) + (u_{ij+1}-u_{ij})\cdot(u_{i+1 j}-u_{ij}) \qquad (2)\end{aligned}$$

The Hamiltonian is aimed to describe a martensitic cubic to tetragonal transformation in $\mathbb{R}^2$. It easy to see that $H(\chi^N) \geq 0$ and zeros of the first and second square brackets in (1) are given by two rank-one connected affine deformations that are produced via transformation matrices

$$U_0 := \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \text{ and } U_1 := \begin{bmatrix} b & 0 \\ 0 & a \end{bmatrix}, \qquad (3)$$

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respectively and correspond to two twinned martensitic variants. In this paper we put onto the atomic lattice $\chi^N = \{u_{ij}|\, i,j = 1,...,N\}$ an additional constraint $u \in \mathcal{A}_\tau$ where

$$\mathcal{A}_\tau := \Big\{ u \in \mathcal{A} \Big|\ u(i+1,j) - u(i,j+1) = \tau \text{ for all } (i,j) \in \mathbb{Z}^2 \Big\}.$$

It implies that χ^N is represented via a 2D atomic chain extended N times by the vector $\tau := [a,\, b]$. This is a reasonable assumption when one expects the ground states to (1) to stay close to two twinned martensitic variants which are produced by the transformations in (3) and are separated by a single linear interface prescribed by τ. It allows us to reduce (1) to a function on the generating 2D chain. Namely,

$$\begin{aligned} H_N(\chi^N) \;&=\; N\sum_{j=1}^{N} h(u_j, u_{j\pm1}) = N\sum_{j=1}^{N} \Big[\big((u_{j\pm1}-u_j)^2 - a^2\big)^2 + \big((u_{j\pm1}-u_j \pm \tau)^2 - b^2\big)^2 + \\ &\quad + \big((u_{j\pm1}-u_j)\cdot(u_{j\pm1}-u_j \pm \tau)\big)^2 \Big] \times \Big[\big((u_{j\pm1}-u_j)^2 - b^2\big)^2 + \big((u_{j\pm1}-u_j \pm \tau)^2 - a^2\big)^2 + \\ &\quad + \big((u_{j\pm1}-u_j)\cdot(u_{j\pm1}-u_j \pm \tau)\big)^2 \Big], \end{aligned} \tag{4}$$

where we denote the atoms of the generating 2D chain as $u_j := u(1,j)$ for $j \in [1,N] \cap \mathbb{Z}$. In this paper we investigate the global minimizers of the reduced Hamiltonian (4) among all atomic lattices $\chi^N = \{u_{ij}|\, i,j = 1,...,N\}$ with the deformation $u \in \mathcal{A}_\tau$ satisfying Dirichlet boundary conditions prescribed by linear deformations $F^\pm \in \mathbb{M}^{2\times2}$ with $\det(F^\pm) > 0$. Namely, we assume that u may be extended to the whole $\mathbb{Z}^2$ so that for the generating chain it holds

$$u_j = F^- \begin{bmatrix} j \\ 0 \end{bmatrix} \text{ if } j \le 1 \text{ and } u_j = F^+ \begin{bmatrix} j \\ 0 \end{bmatrix} \text{ if } j \ge N. \tag{5}$$

2 Rigidity of minimizers and limiting form for the surface energy

The next main theorem shows that the minimizing sequences to (4) considered with (5) converge to a piece-wise constant deformation coinciding on each of its continuity subintervals with a rotation of one of two martensitic variants produced by one of the transformations in (3).

Theorem 2.1 *Let $\chi^N = \{u_{ij}|\, i,j = 1,...,N\}$ with $u \in \mathcal{A}_\tau$ be a sequence of minimizers to (4)–(5) and let $u_a^N :\ (0,1)^2 \to \mathbb{R}^2$ be a piece-wise linear approximation of $u^N(N\cdot, N\cdot)/N$. Then there exists numbers $K \in \mathbb{N}$ and $p > 2$ such that*

(i) *$u_a^N \to u$ in $W^{1,p}((0,1)^2, \mathbb{R}^2)$;*

(ii) *for each $k \in 1,...,K$ there exist $m_k \in \{1,2\}$, $x_k \in (0,1)$ and $R_k \in SO(2)$ such that*

$$\nabla u \equiv R_k U_{m_k} \text{ in } (x_k, x_{k+1}) \times (0,1). \tag{6}$$

The proof of the theorem will be given elsewhere. We concentrate here on one of its important consequences. Namely, it allows us to define the limiting form of the energy of minimizing sequences basing on their derived piece-wise rigid structure. Let us first define the boundary $B_i^\pm(\varphi)$ and internal layer $C_i(\varphi)$ energies as follows. Let $\varphi \in (-\varphi_\tau,\, \varphi_\tau)$, where $\varphi_\tau \in \mathbb{R}$ is an angle depending on the vector τ. For $m = 0, 1$ define minima of problems on half-lines as

$$B_m^+(\varphi) \;:=\; \inf_{N\in\mathbb{N}} \min \Big\{ H_N(\chi^N) :\ u_j = R_\varphi U_m \begin{bmatrix} j \\ 0 \end{bmatrix} + \tau_1 \text{ if } j \ge N \Big\}, \tag{7}$$

$$B_m^-(\varphi) \;:=\; \inf_{N\in\mathbb{N}} \min \Big\{ H_N(\chi^N) :\ u_j = R_\varphi U_m \begin{bmatrix} j \\ 0 \end{bmatrix} + \tau_1 \text{ if } j \le -N \Big\}, \tag{8}$$

$$\tag{9}$$

For $m = 0, 1$ define minima of problems on the full line as

$$C_m(\varphi) = \inf_{N\in\mathbb{N}} \min \Big\{ H_N(\chi^N) :\ u_j = R_\varphi U_{[(m+1) \bmod 2]} \begin{bmatrix} j \\ 0 \end{bmatrix} + \tau_1 \text{ if } j \ge N \text{ and } u_j = U_m \begin{bmatrix} j \\ 0 \end{bmatrix} \text{ if } j \le -N \Big\}. \tag{10}$$

Note that both boundary and internal layer energies are uniquely defined by the relative angle φ between two affine deformations applied far away from the layer. In the latter case φ is the prescribed relative angle between two martensitic variants, produced by U_0 and U_1, respectively.

Next, for $\{\varphi_1, ..., \varphi_m\} \in (-\varphi_\tau,\, \varphi_\tau)^m \subset \mathbb{R}^m$ consider a function

$$E(\varphi_1, ..., \varphi_K) = \min_{m=0,1} \Big\{ B_m^+(\varphi_1) + \sum_{k=2}^{K-1} C_{[(k-m) \bmod 2]}(\varphi_k) + B_{[(K-m) \bmod 2]}^-(\varphi_m) \Big\} \tag{11}$$

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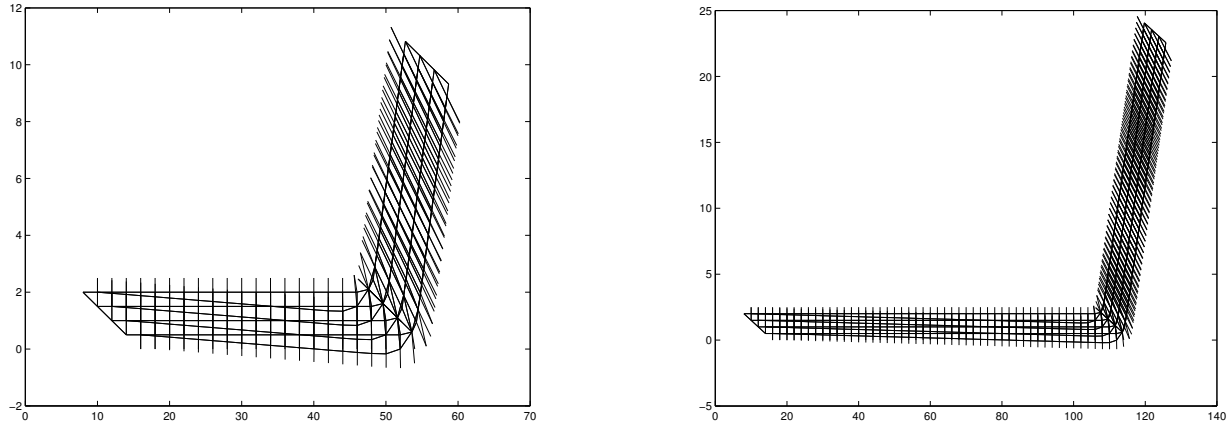

Fig. 1: Twins appearing as local minimizers ($N = 40$ and $N = 100$)

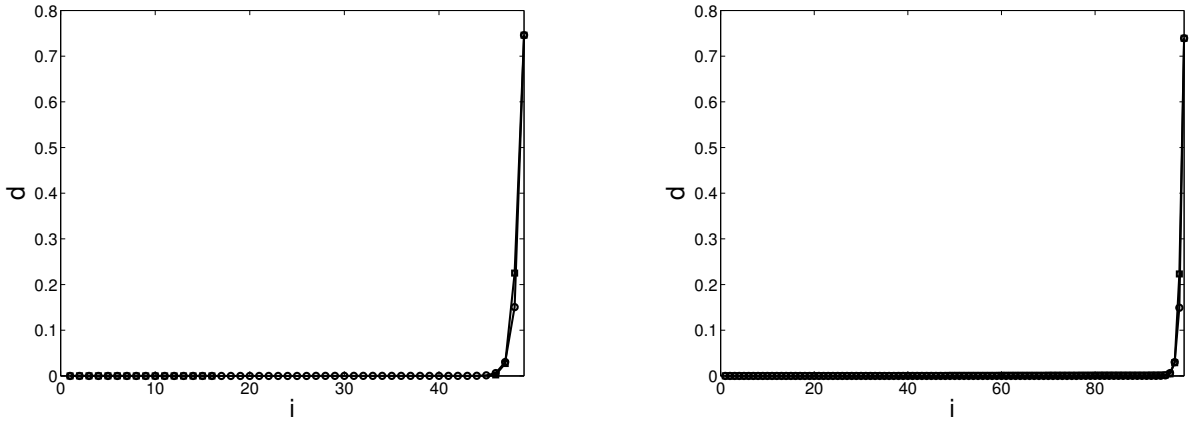

Fig. 2: Absolute deviation from the twinned configuration (13) ($N = 100$ and $N = 200$). Square points–deviation, round points– its approximation by an exponent.

and a minimizing sequence χ^N with the properties stated in Theorem 2.1. Then the following asymptotics holds for the energy of χ^N:

$$H_N(\chi^N) = N \inf_K \min_{\varphi_1,...,\varphi_K} E(\varphi_1, ..., \varphi_K) + O(1) \text{ as } N \to \infty, \tag{12}$$

i.e. the leading order energy scales like N and is given by (11). In turn, (11) prescribes the surface energy of χ^N. Note that in (12) one needs to minimize on overall number of boundary and internal layers K as it is a priori not given explicitly by Theorem 2.1. We conjecture that for a generic type of boundary conditions (5) one obtains after this minimization that $K = 3$.

3 Comparison with numerics

In this section we present the results of our numerical simulations finding local minimizers to (4)–(5) taken with $F^- = U_0$ and $F^+ = R_T U_1$. Matrix $R_T \in SO(2)$ is determined uniquely by the condition that $F^\pm$ should be rank one connected. The numerics is based on a local optimization Newton type algorithm. Taking the atomic lattice $\chi^N = \{u_{ij} |\, i, j = 1, ..., N\}$ with $u \in \mathcal{A}_\tau$ corresponding to the twinned configuration of two martensitic variants, i.e. such that

$$u_j = U_0 \begin{bmatrix} j \\ 0 \end{bmatrix} \text{ if } j \le [N/2] \text{ and } u_j = R_T U_1 \begin{bmatrix} j \\ 0 \end{bmatrix} \text{ if } j \ge [N/2], \tag{13}$$

we initially preoptimized the position of the middle atom in (13). Namely, we optimized its position w.r.t. (4) having given the fixed location of its neighbors as in (13). Next, the resulting configuration we used as an initial guess for the Newton algorithm and we found a closely located local minimizer of (4)–(5). The results on Fig. 1 show existence of a such minimizer with a straight twinning interface coinciding with that one of (13) and prescribed by vector τ. Note that the deviation from the the twinned configuration quickly decreases as number of atoms N tends to infinity. On Fig. 2 we plot the absolute deviation in atom positions of the found local minimizer from the twinned configuration (13). One finds that the deviation decreases exponentially starting from the middle atom lying on the twinning interface. Note, that the decay is not given exactly by a

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simple exponent but nevertheless is nicely approximated by it. Surprisingly, the middle atoms of the found local minimizer and initial (13) lying on the twinning interface coincide (deviation is zero). This can be due to the fact that initially we locally preoptimized the position of the middle atom in (13) as was described above. Interestingly, this simple preoptimization step finds the exact position of this atom on the twinning interface.

Acknowledgements GK acknowledges the postdoctoral scholarship at the Max-Planck-Institute for Mathematics in the Natural Sciences, Leipzig.

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