Surface Energies Arising in Microscopic Modeling of Martensitic Transformations

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1 Introduction

2 The Model Hamiltonian

3 Results

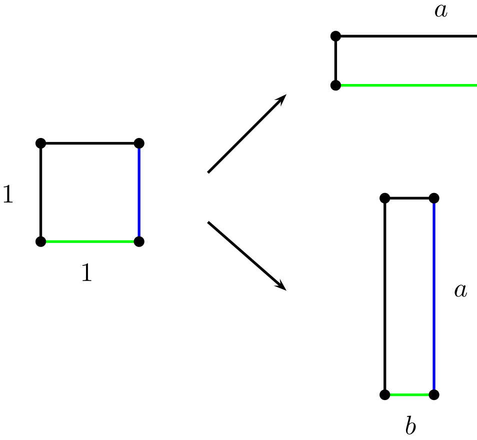
4 Ideas of Proof

5 Conclusion and Outlook

Questions and Objectives

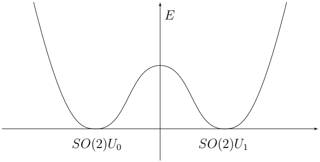
- Justification of continuum models as limits of discrete models (closer to first principles)? How are continuum models related to the atomistic Hamiltonians governing the behavior of the atoms in a crystal?
- Explanations of surface energies? Is it possible to extract surface energy contributions from a discrete Hamiltonian?
- Discrete elastic energies as regularizations of continuum energies? Comparability to singular perturbation problems?

The Square-to-Rectangular Phase Transition and Shape Memory Alloys

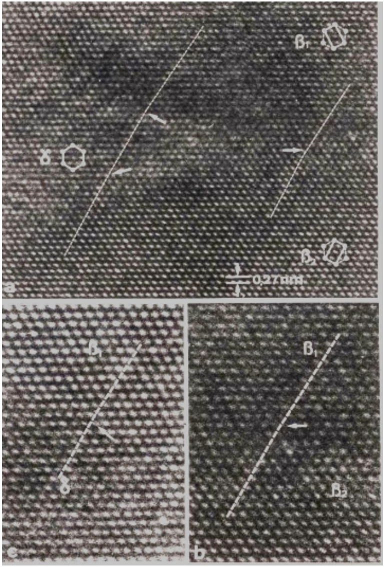


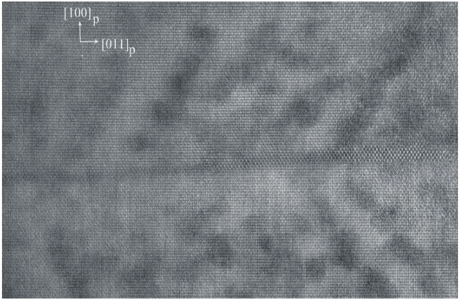
$$SO(2)\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix},$$

$$SO(2)\begin{pmatrix} b & 0 \\ 0 & a \end{pmatrix}.$$



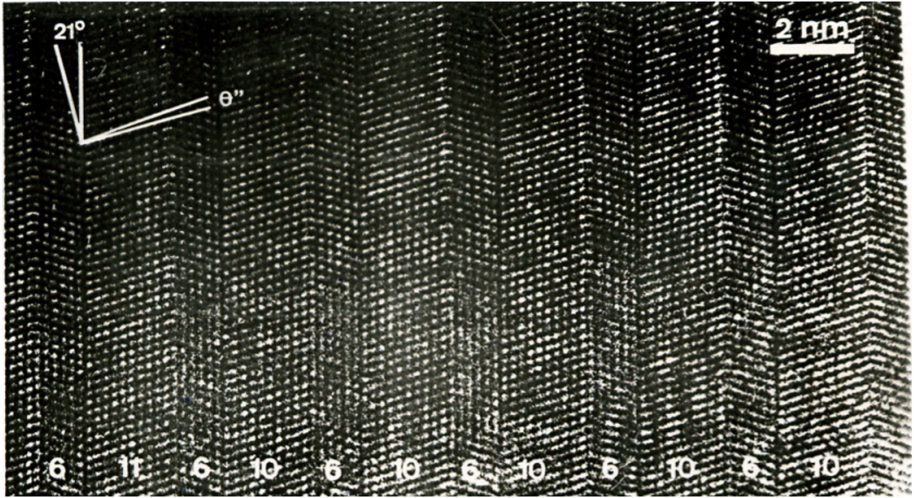
Experimental Observations: Diffuse Interfaces





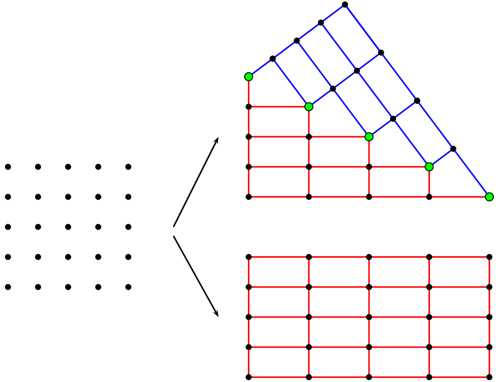
above: perovskite (Salje)
left: $Pb_3V_2O_8$ (Manolikas, van Tendeloo, Amelinckx)

Experimental Observations: Sharp Interfaces



NiMn (Baele, van Tendeloo, Amelinckx)

Deformations: Examples

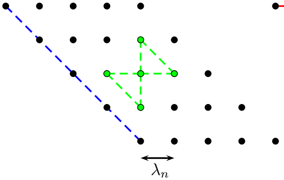


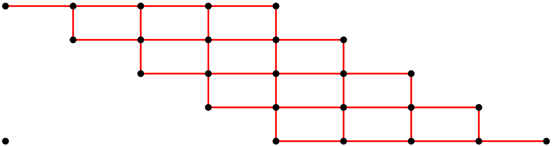
Homogeneous transformations to martensite are characterized by

- horizontal/vertical distances between neighboring atoms are given by a or b,
- neighboring horizontal/vertical inter-atomic distances are equal,
- angles of 90°.

interfaces between the martensitic variants $\rightsquigarrow$ violation of these properties.

Set-up





$$\Omega_n := \left\{ z \middle| z = s \begin{pmatrix} 1 \\ 0 \end{pmatrix} + t \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}, s, t \in [-1, 1] \right\} \cap [\lambda_n \mathbb{Z}]^2,$$

$$u_n : \Omega_n \to \mathbb{R}^2, \ u_n^{j,-n-j} = F \lambda_n \begin{pmatrix} j \\ -n-j \end{pmatrix},$$

$$u_n \in \mathcal{A}_n := \{ v : \Omega_n \to \mathbb{R}^2 | \det(v(x_2) - v(x_1), v(x_3) - v(x_1)) > 0$$

for all $x_1, x_2, x_3 \in \Omega_n$ such that $\operatorname{diam}(x_1, x_2, x_3) = \sqrt{2}\lambda_n$

and $\det(x_2 - x_1, x_3 - x_1) > 0 \}$.

Construction of a Model Hamiltonian

$$H_n(u) := \sum_{i,j=-n}^{n} \lambda_n^2 h\left(\frac{u^{ij}-u^{i\pm1j}}{\lambda_n}, \frac{u^{ij}-u^{ij\pm1}}{\lambda_n}\right)$$

$$= \sum_{i,j=-n}^{n} \lambda_n^2 \left[\left(\left(\frac{u^{ij\pm1}-u^{ij}}{\lambda_n}\right)^2 - a^2\right)^2 + \left(\left(\frac{u^{i\pm1j}-u^{ij}}{\lambda_n}\right)^2 - b^2\right)^2\right.$$

$$\left. + \left(\left(\frac{u^{ij\pm1}-u^{ij}}{\lambda_n}\right)\cdot\left(\frac{u^{i\pm1j}-u^{ij}}{\lambda_n}\right)\right)^2\right] \times$$

$$\times \left[\left(\left(\frac{u^{ij\pm1}-u^{ij}}{\lambda_n}\right)^2 - b^2\right)^2 + \left(\left(\frac{u^{i\pm1j}-u^{ij}}{\lambda_n}\right)^2 - a^2\right)^2\right.$$

$$\left. + \left(\left(\frac{u^{ij\pm1}-u^{ij}}{\lambda_n}\right)\cdot\left(\frac{u^{i\pm1j}-u^{ij}}{\lambda_n}\right)\right)^2\right].$$

Construction of a Model Hamiltonian

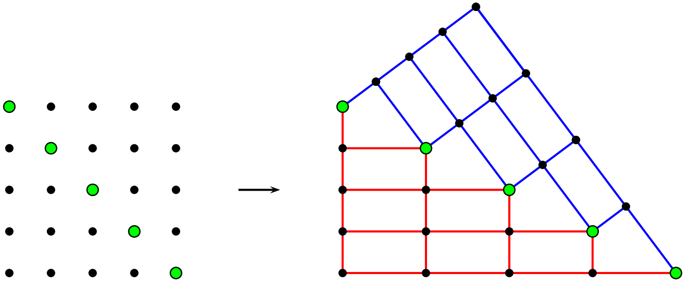
$$H_n(u) := \sum_{i,j=-n}^{n} \lambda_n^2 h\left(\frac{u^{ij}-u^{i\pm1j}}{\lambda_n}, \frac{u^{ij}-u^{ij\pm1}}{\lambda_n}\right)$$

Advantages and Disadvantages

- based on geometric quantities,
- has $SO(2)U_0 \cup SO(2)U_1$ as wells,
- controls distance from wells,
- controls discrete second derivatives.

- ad hoc, no "first principles" justification for explicit form,
- uses underlying reference configuration,
- no defects allowed.

Martensitic Twins



$$H_n(u) \leq c\lambda_n$$

$$U_0 - QU_1 = \sqrt{2}\frac{a^2-b^2}{a^2+b^2}\begin{pmatrix} a \\ -b \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \; Q \in SO(2),$$

$$U_0 - \tilde{Q}U_1 = \sqrt{2}\frac{a^2-b^2}{a^2+b^2}\begin{pmatrix} a \\ b \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \; \tilde{Q} \in SO(2).$$

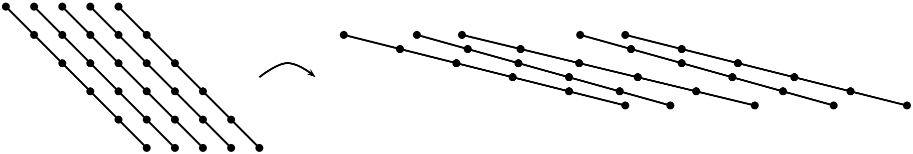
The Chain Hamiltonian

Additional "chain" assumption:

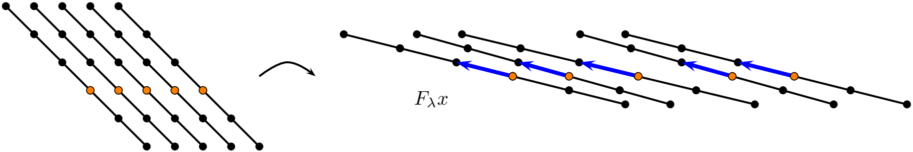
$$u_n^{i+1j} - u_n^{ij+1} = -\lambda_n \tau^{i+j+1}, \quad \tau^i \in SO(2)\begin{pmatrix} -a \\ b \end{pmatrix},$$

$\rightsquigarrow$ corresponding adaptations for Hamiltonian

$$H_n(u_n) = \lambda_n^2 \sum_{i,j=-n}^{n} h\left(\frac{u_n^i - u_n^{i\pm 1}}{\lambda_n}, \tau_n^i, \tau_n^{i\pm 1}, j\right).$$



Set-up



$$H_n(u_n) := \sum_{i,j} \lambda_n^2 h(u^{i\pm1} - u^i, \tau_n^i, \tau_n^{i\pm1}, j) \leq C\lambda_n,$$

$$u_n^{j,-n-j} = \lambda_n F_\mu \begin{pmatrix} j \\ -n-j \end{pmatrix},\ u_n \in \mathcal{A}_{n,\tau}^{F_\mu},$$

$$F_\mu = \mu Q U_0 + (1-\mu)U_1,\ Q \in SO(2), \mu \in [0,1].$$

Rigidity

Proposition

Let $F_\mu := \mu U_0 + (1-\mu) Q U_1$ *with* $\mu \in [0,1]$. *Let* $\{u_n\}_{n\in\mathbb{N}} \in \mathcal{A}_{n,\tau}^{F_\mu}$ *s.t.*

$$\limsup_{n\to\infty} \lambda_n^{-1} H_n(u_n) < \infty.$$

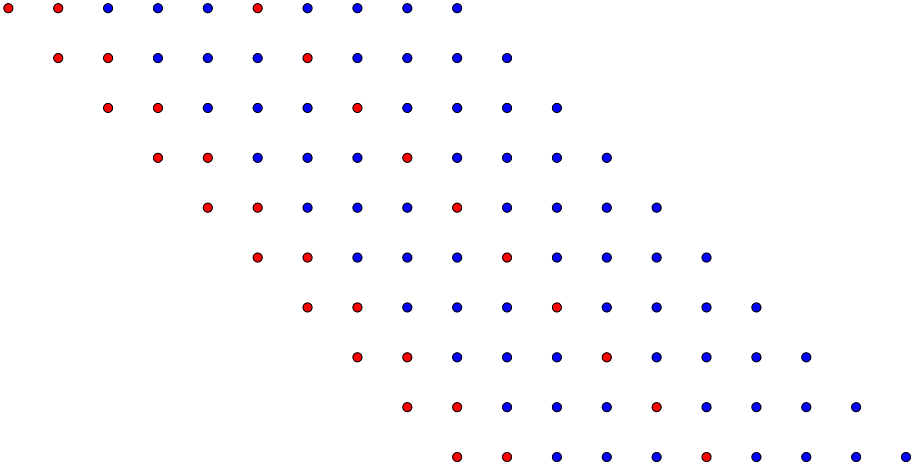
Then there exists a number $K \in \mathbb{N}$ *and a subsequence such that*

- $u_n \to u$ *in* $W^{1,4}(\Omega, \mathbb{R}^2)$,
- *for each* $s \in \{1, \dots, K-1\}$ *there exists* $m_s \in \{0,1\}$, $x_s \in [-1,1]$ *such that*

  $$\nabla u(z) = Q^{m_s} U_{m_s},$$

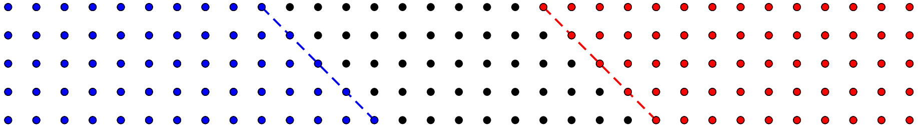
  for $z \in \Omega(x_s, x_{s+1})$ *where* $Q^0 = Id$, $Q^1 := Q$ *and* $x_K = 1$,
- $\bigcup_{s=1}^{K-1} [x_s, x_{s+1}] = [-1,1]$.

Rigidity



Surface Energies

$$C(V_2, V_3, r^*) := \liminf_{n\to\infty} \min_{\tau_i, u^i} \Big\{ \sum_{i\in\mathbb{Z}} \frac{1}{n} \sum_{j=-n}^{n} h\left(u_n^i - u_n^{i\pm 1}, \tau_n^i, \tau_n^{i\pm 1}, j\right) :$$
$$u \in \mathcal{A}_{n,\tau}^r,\ u^{i-jj} = V_2 \begin{pmatrix} i-j \\ j \end{pmatrix} + r_1,\ i \leq -n,\ |j| \leq n,$$
$$u^{i-jj} = V_3 \begin{pmatrix} i-j \\ j \end{pmatrix} + r_2,\ r^* = r_2 - r_1,\ i \geq n,\ |j| \leq n \Big\}.$$



Surface Energies

Proposition

$$H_n^1 := \lambda_n^{-1} H_n \overset{\Gamma}{\to} E_{surf} \text{ with respect to the } L^\infty \text{ topology.}$$

Here,

$$E_{surf}(u) := \begin{cases} E^K(F_\mu, \nabla u(x_1-,0), ..., \nabla u(x_{(K-1)}-,0), F_\mu), \\ \quad \text{if } u \in W_0^{1,\infty}(\Omega) + F_\mu x,\ \nabla u \in \{U_0, QU_1\} \\ \quad \text{in } \Omega(x_j, x_{j+1}), u \text{ satisfies the b.c.,} \\ \infty, \quad \text{else,} \end{cases}$$

$$E^K(V_0, ..., V_K) := \inf_r \Big\{ B^+(V_0, V_1, r_0) + \sum_{s=1}^{K-2} C(V_s, V_{s+1}, r_s) \\ + B^-(V_{K-1}, V_K, r_{K-1}) \Big\}.$$

Comparison with Literature

Discrete:

- Blanc, Le Bris, Lions (2002): From molecular models to continuum mechanics.
- Braides,Cicalese (2007): Surface energies in nonconvex discrete systems.
- Luckhaus, Mugnai (2009): On a mesoscopic many-body Hamiltonian describing elastic shears and dislocations.

Continuous:

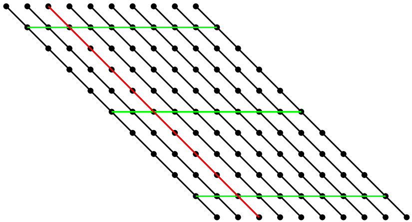
- Conti, Schweizer (2006): Rigidity and Gamma Convergence for Solid-Solid Phase Transitions with SO(2) Invariance.

$$\sum_{i,j=-n}^{n} \frac{1}{n} h(u^{i\pm 1, j\pm 1} - u^{ij}) \leq C \quad \overset{\epsilon = \frac{1}{n}}{\rightsquigarrow} \quad \int_{\Omega} \frac{1}{\epsilon} W(\nabla u) + \epsilon |\nabla^2 u|^2 dx \leq C$$

Compactness: Good Layers

There exist j_{-1}^n, j_0^n, j_1^n s.t.

- $j_{-1}^n \in [-n, -n+2\delta n],\ j_0^n \in [-\delta n, \delta n],\ j_1^n \in [n-2\delta n, n]$,
- $\lambda_n \sum_{i=-n}^{n} h\left(\frac{u_n^i - u_n^{i\pm1}}{\lambda_n}, \tau_n^i,\ \tau_n^{i\pm1}, j_l^n\right) \lesssim n^{-\alpha}$,
- $\#\left\{i \in [-n,n]:\ h\left(\frac{u_n^i - u_n^{i\pm1}}{\lambda_n}, \tau_n^i,\ \tau_n^{i\pm1}, j_l^n\right) \geq n^{-\alpha}\right\} \lesssim \delta^{-1} n^{\alpha}$,
- there exists a number $M_\delta > 0$, independent of n with $\#\left\{i \in [-n,n]:\ h\left(\frac{u_n^i - u_n^{i\pm1}}{\lambda_n}, \tau_n^i,\ \tau_n^{i\pm1}, j_l^n\right) \geq \tilde{c}\right\} \leq M_\delta$.



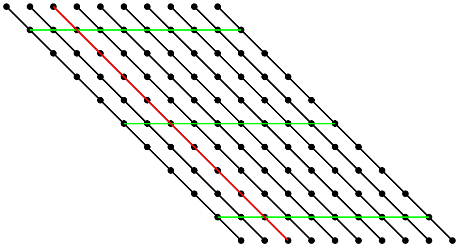
Chain structure:

- L^∞ bound:

$$|\nabla u_n^{ij}| \leq c < \infty$$

for all $i, j \in \{-n, \dots, n\}$.

Compactness: Simultaneously Good Points



Most points "simultaneously good" points:

$$h\left(\frac{u_n^i - u_n^{i\pm1}}{\lambda_n}, \tau_n^i, \tau_n^{i\pm1}, j_l^n\right) \leq n^{-\alpha}$$

for all $l \in \{-1, 0, 1\}$.

For each "simultaneously good" $i \in [-n, n]$ there exists $Q_{i,n} \in SO(2)$ such that either

$$||\nabla u_n^{i-jj} - Q_{i,n}U_0||_{C(\Omega_{i-jj})} \lesssim n^{-\alpha/4} \quad \text{for all} \quad j \in [-n, n],$$

$$\text{or } ||\nabla u_n^{i-jj} - Q_{i,n}U_1||_{C(\Omega_{i-jj})} \lesssim n^{-\alpha/4} \quad \text{for all} \quad j \in [-n, n].$$

Compactness: Conclusion

Up to subsequences,

- there exist $K \in \mathbb{N}$, $x_1, ..., x_K \in (-1, 1)$ independent of n,
- and for any n there exist associated points $x_1^n, ..., x_K^n \in (-1, 1)$ and $y_{s,1}^n, ..., y_{s,K_s^n}^n \in (x_s^n, x_{s+1}^n)$

such that

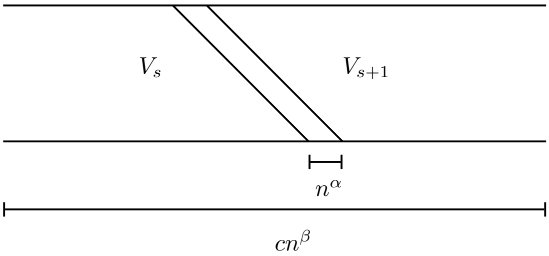
- $x_s^n \to x_s, \ s \in \{1, ..., K\}$,
- $u_n \rightharpoonup u$ in $W^{1,4}(\Omega)$,
- in the interval (x_s^n, x_{s+1}^n) the following dichotomy holds: For each i with $\lambda_n i \in (y_{s,l}^n, y_{s,l+1}^n) \subset (x_s^n, x_{s+1}^n)$ and $l \in \{1, ..., K_s^n\}$, either

$$\mathrm{dist}(\nabla u_n^{i-jj}, SO(2)U_0) \lesssim n^{-\alpha/4} \quad \text{or} \quad \mathrm{dist}(\nabla u_n^{i-jj}, SO(2)U_1) \lesssim n^{-\alpha/4}$$

for all $j \in [-n, n]$.

Gamma-Limit

- Idea: Use infimizing sequences, modify boundary conditions.
- Difficulties: Ensure boundary conditions without violating admissibility (in particular non-interpenetration condition).
- Techniques:
  - averaging,
  - cutting.



The Full 2D Model and Further Questions

$$H_n(u) \quad := \sum_{i,j=-n}^{n} \lambda_n^2 h\left(\frac{u^{ij}-u^{i\pm1j}}{\lambda_n}, \frac{u^{ij}-u^{ij\pm1}}{\lambda_n}\right)$$

Results for the full 2D model:

- Rigidity (one sided comparability to spin system).
- Sharp-interface limit:

$$H_n^1 := \lambda_n^{-1} H_n \xrightarrow{\Gamma} \tilde{E}_{surf}$$

with respect to the L^1 topology.

Further questions:

- More general m-well problem, e.g. three wells?
- Higher dimensional problem, e.g. 3D?
- Form of the energy densities?
- Minimizers of the energy densities? Relation to diffuse/sharp interfaces?