Surface Energies Arising in Microscopic Modeling of Martensitic Transformations

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Introduction

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)
NiMn (Baele, van Tendeloo, Amelinckx)
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 \( 90^\circ \).

Interfaces between the martensitic variants \( \rightsquigarrow \) violation of these properties.
\[ \Omega_n := \left\{ z \mid z = s \begin{pmatrix} 1 \\ 0 \end{pmatrix} + t \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}, s, t \in [-1, 1] \right\} \cap [\lambda_n \mathbb{Z}]^2, \]

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

\[ u_n \in \mathcal{A}_n := \left\{ v : \Omega_n \to \mathbb{R}^2 \mid \det(v(x_2) - v(x_1), v(x_3) - v(x_1)) > 0 \right\} \]

for all \( x_1, x_2, x_3 \in \Omega_n \) such that \( \text{diam}(x_1, x_2, x_3) = \sqrt{2} \lambda_n \) and \( \det(x_2 - x_1, x_3 - x_1) > 0 \).
Construction of a Model Hamiltonian

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

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

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

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

\[ + \left. \left( \left( \frac{u_{ij\pm1} - u_{ij}}{\lambda_n} \right) \cdot \left( \frac{u_{i\pm1j} - u_{ij}}{\lambda_n} \right) \right)^2 \right]. \]
Construction of a Model Hamiltonian

\[ H_n(u) := \sum_{i,j=-n}^{n} \lambda_n^2 h \left( \frac{u_{ij} - u_{i\pm j}}{\lambda_n}, \frac{u_{ij} - u_{ij\pm 1}}{\lambda_n} \right) \]

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.
The Model Hamiltonian

Martensitic Twins

\[ H_n(u) \leq c\lambda_n \]

\[
U_0 - QU_1 = \sqrt{2 \frac{a^2 - b^2}{a^2 + b^2}} \left( \begin{array}{c} a \\ -b \end{array} \right) \otimes \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ 1 \end{array} \right), \quad Q \in SO(2),
\]

\[
U_0 - \tilde{Q}U_1 = \sqrt{2 \frac{a^2 - b^2}{a^2 + b^2}} \left( \begin{array}{c} a \\ b \end{array} \right) \otimes \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ -1 \end{array} \right), \quad \tilde{Q} \in SO(2).
\]
The Chain Hamiltonian

Additional “chain” assumption:

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

\[ \leadsto \text{corresponding adaptations for Hamiltonian} \]

\[ H_n(u_n) = \lambda_n^2 \sum_{i,j=-n}^{n} h \left( \frac{u_n^i - u_n^{i\pm1}}{\lambda_n}, \tau_n^i, \tau_n^{i\pm1}, j \right). \]
The Model Hamiltonian

**Set-up**

\[ H_n(u_n) := \sum_{i,j} \lambda_n^2 h(u_i^{\pm 1} - u^i, \tau^i_n, \tau^{i\pm 1}_n, j) \leq C \lambda_n, \]

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

\[ F_\mu = \mu QU_0 + (1 - \mu)U_1, \quad Q \in SO(2), \mu \in [0, 1]. \]
Rigidity

Proposition

Let $F_\mu := \mu U_0 + (1 - \mu) QU_1$ with $\mu \in [0, 1]$. Let $\{u_n\}_{n \in \mathbb{N}} \in \mathcal{A}^{F_\mu}_{\eta, \tau}$ 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 $s \in \{1, \ldots, K - 1\}$ 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

\[ C(V_2, V_3, r^*) := \lim_{n \to \infty} \inf \min_{\tau_i, u^i} \left\{ \sum_{i \in \mathbb{Z}} \frac{1}{n} \sum_{j=-n}^{n} h(u^i_n - u^i_{n+1}, \tau^i_n, \tau^i_{n+1}, j) : \right. \]

\[ u \in A^r_{n, \tau}, \quad u_{i-j} = V_2 \left( \begin{pmatrix} i \end{pmatrix} \begin{pmatrix} j \end{pmatrix} \right) + r_1, \quad i \leq -n, \quad |j| \leq n, \]

\[ u_{i-j} = V_3 \left( \begin{pmatrix} i \end{pmatrix} \begin{pmatrix} j \end{pmatrix} \right) + r_2, \quad r^* = r_2 - r_1, \quad i \geq n, \quad |j| \leq n \} \]
Surface Energies

Proposition

\[ H_n^1 := \lambda_n^{-1} H_n \rightharpoonup E_{surf} \text{ with respect to the } L^\infty \text{ topology.} \]

Here,

\[ E_{surf}(u) := \begin{cases} 
E^K (F_\mu, \nabla u(x_1-, 0), \ldots, \nabla u(x_{(K-1)}-, 0), F_\mu), 
& \text{if } u \in W^{1,\infty}_0(\Omega) + F_\mu x, \ \nabla u \in \{U_0, QU_1\} 
\text{ in } \Omega(x_j, x_{j+1}), u \text{ satisfies the b.c.,} \\
\infty, & \text{else,} 
\end{cases} \]

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

\[
\sum_{i,j=-n}^{n} \frac{1}{n} h(u^{i\pm1,j\pm1} - u^{ij}) \leq C \quad \epsilon = \frac{1}{n} \quad \int_{\Omega} \frac{1}{\epsilon} W(\nabla u) + \epsilon |\nabla^{2}u|^{2} dx \leq C
\]
Compactness: Good Layers

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

- \( j_{-1}^n \in [-n, -n + 2\delta n] \), \( j_0^n \in [-\delta n, \delta n] \), \( j_1^n \in [n - 2\delta n, n] \),

- \( \lambda_n \sum_{i=-n}^n h \left( \frac{u_i - u_{i+1}^n}{\lambda_n}, \tau_i^n, \tau_{i+1}^n,j_l^n \right) \lesssim n^{-\alpha} \),

- \( \# \left\{ i \in [-n, n] : h \left( \frac{u_i - u_{i+1}^n}{\lambda_n}, \tau_i^n, \tau_{i+1}^n,j_l^n \right) \geq n^{-\alpha} \right\} \lesssim \delta^{-1} n^\alpha \),

- there exists a number \( M_\delta > 0 \), independent of \( n \) with

\[
\# \left\{ i \in [-n, n] : h \left( \frac{u_i - u_{i+1}^n}{\lambda_n}, \tau_i^n, \tau_{i+1}^n,j_l^n \right) \geq \tilde{c} \right\} \leq M_\delta.
\]

Chain structure:

- \( L^\infty \) bound:

\[
|\nabla u_i^n| \leq c < \infty
\]

for all \( i, j \in \{-n, \ldots, n\} \).
Most points “simultaneously good” points:

\[
h \left( \frac{u_n^i - u_n^{i \pm 1}}{\lambda_n}, \tau_n^i, \tau_n^{i \pm 1}, j^n \right) \leq n^{-\alpha}
\]

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

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

or

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

Up to subsequences,

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

- $x_s^n \to x_s$, $s \in \{1, \ldots, K\}$,
- $u_n \rightharpoonup u$ 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 $l \in \{1, \ldots, K^n_s\}$, either

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

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

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

Results for the full 2D model:

- Rigidity (one sided comparability to spin system).
- Sharp-interface limit:
  \[ H_n^1 := \lambda_n^{-1} H_n \Gamma \to \tilde{E}_{surf} \]
  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?