NSF-PIRE Summer School

Geometrically linear theory for shape memory alloys: the effect of interfacial energy

Felix Otto

Max Planck Institute for Mathematics in the Sciences

Leipzig, Germany

Goal of mini-course

Introduction to 3 recent works on
microstructure or absence thereof
in cubic-to-tetragonal phase transformation

Approximate rigidity of twins, periodic case

Capella, O.: A rigidity result for a perturbation of the geometrically linear three-well problem, CPAM 62, 2009

Approximate rigidity of twins, local case

Capella, O.: A quantitative rigidity result for the cubic-to-tetragonal

phase transition in the geometrically linear theory with interfacial energy, Proc. Roy. Soc. Edinburgh A, to appear

Optimal microstructure of Martensitic inclusions

Knüpfer, Kohn, O.: Nucleation barriers for the cubic-to-tetragonal phase transformation, CPAM, to appear

See www.mis.mpg.de for copies (Otto, Publications, Shape-Memory Alloys)

Structure of mini-course

- Chap 1. Kinematics

- Chap 2. 2-d models
  square-to-rectangular, hexagonal-to-rhombic

- Chap 3. 3-d models
  cubic-to-tetragonal, [cubic-to-orthorombic]

Structure of Chapter 1 on kinematics

Structure of Chapter 2 on 2-d models

Square-to-rectangular phase transformation

2.1 Derivation of the linearized two-well problem

2.2 Rigidity of twins

2.3 Elastic and interfacial energies

2.4 Derivation of a reduced model for twinned-Martensite to Austenite interface

2.5 Self-consistency of reduced model, lower bounds by interpolation, upper bounds by construction

Structure of Chapter 2 on 2-d models, cont

Hexagonal-to-rhombic phase transformation

2.6 Derivation of the linearized three-well problem

2.7 Twins and sextuple junctions

2.8 Loss of rigidity by convex integration

2.4 Derivation of a reduced model for the twinned-Martensite to Austenite interface

Phase indicator function: $\chi \in \{-1, 0, 1\}$, $\chi = \chi(x_1, x_2)$

Displacement field: $u = (u_1, u_2)$, $u = u(x_1, x_2)$

Interfacial energy:

$$\eta \Big(\text{length of interface between } \{\chi = 1\} \text{ and } \{\chi = -1\} \\ + \text{ length of interface between } \{\chi = 1\} \text{ and } \{\chi = 0\} \\ + \text{ length of interface between } \{\chi = -1\} \text{ and } \{\chi = 0\} \Big)$$

Elastic energy: $\displaystyle \int\int \left| \tfrac{1}{2}(\nabla + \nabla^t)u - \begin{pmatrix} 0 & \chi \\ \chi & 0 \end{pmatrix} \right|^2 dx_1 dx_2$

2.4 Derivation of a reduced model for the twinned-Martensite to Austenite interface

Simplification 1 Impose position of twinned-Martensite to Austenite interface

Simplification 2 Impose shear direction

∞ **Simplification 3** Anisotropic rescaling and limit

Simplification 1): Impose position of twinned-Martensite to Austenite interface

Position of interface $\{x_2 = 0\}$:

$$\chi \; \left\{ \begin{array}{ll} \in \{-1,1\} & \text{for } x_1 > 0 \\ = 0 & \text{for } x_1 < 0 \end{array} \right\}$$

Nondimensionalize length by restriction to $x_1 \in (-1,1)$,

regime of interest $\eta \ll 1$

Impose (artificial) L-periodicity in x_2

Interfacial energy $\eta \left(\frac{1}{2} \int_{(0,1)\times[0,L)} |\nabla \chi| + L \right)$

Simplification 2): Impose shear direction

Favor twin normal $n = \binom{0}{1}$
by imposing shear direction $a = \binom{2}{0}$. i. e.

$$u_2 \equiv 0 \quad \text{but} \quad u_1 = u_1(x_1, x_2)$$

Strain $\frac{1}{2}(\nabla + \nabla^t)u = \begin{pmatrix} \partial_1 u_1 & \frac{1}{2}\partial_2 u_1 \\ \frac{1}{2}\partial_2 u_1 & 0 \end{pmatrix}$

Elastic energy $\int_{-1}^{1}\int_{0}^{L}(\partial_1 u_1)^2 + 2(\frac{1}{2}\partial_2 u_1 - \chi)^2 dx_2 dx_1$

Simplification 3): Anisotropic rescaling and limit

$$\frac{1}{L}\Big(\frac{\eta}{2}\int_{(0,1)\times[0,L)}|\nabla\chi|$$
$$+\ \int_{(-1,1)\times(0,L)}(\partial_1 u_1)^2+2(\tfrac{1}{2}\partial_2 u_1-\chi)^2dx\Big)$$

Ansatz for rescaling

$$x_2=\eta^\alpha\hat{x}_2 \implies \partial_2=\eta^{-\alpha}\hat{\partial}_2. \quad L=\eta^\alpha\hat{L},$$
$$u_1=2\eta^\alpha\hat{u}_1 \implies \partial_2 u_1=2\hat{\partial}_2\hat{u}_1, \quad \partial_1 u_1=2\eta^\alpha\partial_1\hat{u}_1.$$

$$\frac{1}{\hat{L}}\Big(\frac{\eta}{2}\int_{(0,1)\times[0,L)}\Big|\begin{pmatrix}\partial_1\chi\\ \eta^{-\alpha}\hat{\partial}_2\chi\end{pmatrix}\Big|$$
$$+\int_{(-1,1)\times(0,L)}4\eta^{2\alpha}(\partial_1\hat{u}_1)^2+2(\hat{\partial}_2\hat{u}_1-\chi)^2d\hat{x}\Big)$$

Seek nontrivial limit: elastic part

Elastic energy density: $4\eta^{2\alpha}(\partial_1\widehat{u}_1)^2 + 2(\widehat{\partial}_2\widehat{u}_1 - \chi)^2$

Penalization of $\widehat{\partial}_2\widehat{u}_1 - \chi \quad \gg \quad$ penalization of $\partial_1\widehat{u}_1$

Neclegting $\partial_1\widehat{u}_1$ no option — otherwise no elastic effect

Hence *constraint* $\widehat{\partial}_2\widehat{u}_1 - \chi = 0$ in limit.

Seek nontrivial limit: interfacial part

Interfacial energy density: $\frac{\eta}{2}\left|\begin{pmatrix}\partial_1\chi \\ \eta^{-\alpha}\widehat{\partial}_2\chi\end{pmatrix}\right|$

Penalization of $\widehat{\partial}_2\chi$ $\quad\gg\quad$ penalization of $\partial_1\chi$

Constraint $\widehat{\partial}_2\chi = 0$ no option — otherwise no twin

Hence have to neglect penalization of $\partial_1\chi$

Interfacial energy density $\frac{\eta^{1-\alpha}}{2}|\widehat{\partial}_2\chi|$ in limit.

Seek nontrivial limit: choice of α

Total energy density $4\eta^{2\alpha}(\partial_1 \hat{u}_1)^2 + \frac{\eta^{1-\alpha}}{2}|\hat{\partial}_2 \chi|$

For balance need $\eta^{2\alpha} \sim \eta^{1-\alpha} \Rightarrow \alpha = \frac{1}{3}$

Rescaling of energy density: $\frac{1}{L}E = \eta^{\frac{2}{3}} \frac{1}{\hat{L}} \hat{E}$

Prediction from $\frac{1}{L}E = \eta^{\frac{2}{3}} \frac{1}{\hat{L}} \hat{E}$: energy density $\sim \eta^{\frac{2}{3}}$

Prediction from $x_2 = \eta^{\frac{1}{3}} \hat{x}_2$: twin width $\sim \eta^{\frac{1}{3}}$

... provided limit model makes sense for $\hat{L} \gg 1$

Limit model is singular

Minimize $4\int_{-1}^{1}\int_{0}^{\widehat{L}}(\partial_1\hat{u}_1)^2 d\widehat{x}_2 dx_1 + \frac{1}{2}\int_0^1\int_{[0,\widehat{L})}|\widehat{\partial}_2\chi|dx_1$ subject to

$$\widehat{\partial}_2\hat{u}_1 = \chi \left\{ \begin{array}{cl} \in \{-1,1\} & \text{for } x_1 > 0 \\ = 0 & \text{for } x_1 < 0 \end{array} \right\}.$$

$\frac{1}{2}\int_{[0,\widehat{L})}|\widehat{\partial}_2\chi|$ just counts transitions between 1 and -1

Infinite twin refinement:

$$\begin{aligned}
\text{Elastic energy} &\Longrightarrow \hat{u}_1 = \text{const} = 0 \quad \text{for } x_1 < 0 \\
&\Longrightarrow \hat{u}_1(x_1,\cdot) \to 0 \quad \text{as } x_1 \downarrow 0 \\
&\Longrightarrow \chi(x_1,\cdot) \rightharpoonup 0 \quad \text{as } x_1 \downarrow 0 \\
&\Longrightarrow \int_{[0,\widehat{L})}|\widehat{\partial}_2\chi(x_1,\cdot)| \uparrow \infty \quad \text{as } x_1 \downarrow 0 \\
\text{Interfacial energy} &\Longrightarrow \int_0^1\int_{[0,\widehat{L})}|\widehat{\partial}_2\chi(x_1,\cdot)|dx_1 < \infty
\end{aligned}$$

... does limit model have finite energy?

2.5 Self consistency of reduced model, upper bounds by construction, lower bounds by interpolation

Proposition 2 [Kohn, Müller]

Functional:

$$E = 4\int_{-1}^{1}\int_{0}^{L}(\partial_1 u_1)^2 dx_2 dx_1 + \frac{1}{2}\int_{0}^{1}\int_{[0,L)}|\partial_2\chi| dx_1.$$

Admissible configurations: u_1, χ L-periodic in x_2 with

$$\partial_2 u_1 = \chi \left\{ \begin{array}{cc} \in \{-1,1\} & \text{for } x_1 > 0 \\ = 0 & \text{for } x_1 < 0 \end{array} \right\}.$$

Then $\exists$ universal $C < \infty$ such that

i) upper bound $\quad \forall\, L\, \exists\, (u_1, \chi) \quad E \leq CL,$

ii) lower bound $\quad \forall\, L, (u_1, \chi) \quad E \geq \frac{1}{C}L.$

Proof of Proposition 2 i) (Construction)

W. l. o. g. $L = 1$.

Step 1 Building block for branched structure on $(0,1) \times (0,1)$

Step 2 Rescaling $\rightsquigarrow$ construction on $(0,H) \times (0,1)$

Step 3 Concatenation $\rightsquigarrow$ construction on $(0,1) \times (0,1)$

Proof of Proposition 2 i) (lower bound)

Lemma 7

$\exists$ universal $C < \infty$

$\forall$ L-periodic $u_1(x_2), \chi(x_2)$ related by $\partial_2 u_1 = \chi$ with

$$\int_0^L \chi^2 dx_1 \leq C \left(\int_0^L u_1^2 dx_2 \right)^{\frac{1}{3}} \left(\int_0^L |\partial_2 \chi| dx_2 \sup_{x_2} |\chi| \right)^{\frac{2}{3}}.$$

Holds in any d as $\quad \|\chi\|_{L^2} \leq C(d) \||\nabla|^{-1}\chi\|_{L^2}^{\frac{1}{3}} \|\nabla\chi\|_{L^1}^{\frac{1}{3}} \|\chi\|_{L^\infty}^{\frac{1}{3}}$

Simpler version of $\quad \|\chi\|_{L^{\frac{4}{3}}} \leq C(d) \||\nabla|^{-1}\chi\|_{L^2}^{\frac{2}{3}} \|\nabla\chi\|_{L^1}^{\frac{1}{3}}$

(Cohen-Dahmen-Daubechies-Devore)

2.8 Loss of rigidity by convex integration

Proposition 3 [Müller, Sverák]

$\forall\, M$ s. t. $\frac{1}{2}(M + M^t) \in \operatorname{int}\operatorname{conv}\{E_0, E_1, E_2\}$

$\forall\, \Omega \subset \mathbb{R}^2$ open, bdd.

$\exists\, u\colon \mathbb{R}^2 \to \mathbb{R}^2$ with $\nabla u \in L^2_{loc}$

$$\begin{aligned} \nabla u &= M \quad \text{in } \mathbb{R}^2 - \bar{\Omega}, \\ \frac{1}{2}(\nabla + \nabla^t)u &\in \{E_0, E_1, E_2\} \quad \text{a. e. on } \Omega. \end{aligned}$$

Step 1: Conti's construction = Lemma 5

Consider for $\lambda = \frac{1}{4}$:

$$M_0 = \frac{1}{\lambda}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\ M_1 = \frac{1}{1-\lambda}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},\ M_2 = \frac{1}{1-\lambda^2}\begin{pmatrix} 1 & -\lambda \\ \lambda & -1 \end{pmatrix},$$

$$M_3 = \frac{1}{1-\lambda^2}\begin{pmatrix} -1 & -\lambda \\ \lambda & 1 \end{pmatrix},\ M_4 = \frac{1}{\lambda}\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix},\ \Omega = (-1,1)^2.$$

Then $\exists\ \Omega_0, \cdots \Omega_4 \subset \Omega$ finite $\bigcup$ of convex, open sets
$\exists\ u\colon \mathbb{R}^2 \to \mathbb{R}^2$ Lipschitz s. t.

$$\begin{aligned} \nabla u &= 0 \quad \text{in } \mathbb{R}^2 - \bar{\Omega}, \\ \nabla u &= M_i \quad \text{in } \Omega_i, \\ |\Omega_0| &= \tfrac{1}{2}\lambda|\Omega|. \end{aligned}$$

Step 2: Deformation and rotation of Conti's construction

$\forall\, M, M_0, M_1$ s. t. $M = \frac{1}{4}M_0 + \frac{3}{4}M_1$ with

$$M_1 - M_0 = a \otimes n \quad \text{for some } a \in \mathbb{R}^2, n \in S^1, a \cdot n = 0$$

$\forall\, \epsilon > 0 \quad \exists\, \tilde{M}_1, \cdots, \tilde{M}_4$ s. t.

$|\tilde{M}_1 - M_1|,\ |\tilde{M}_{2/3} - M_2|,\ |\tilde{M}_4 - M| < \epsilon,$ where $M_2 := \frac{1}{5}M_0 + \frac{4}{5}M_1$.

$\exists\, \Omega \subset \mathbb{R}^2$ open, bdd., $\tilde{\Omega}_1, \cdots, \tilde{\Omega}_4 \subset \Omega$ finite $\bigcup$ of convex, open sets
$\exists\, u\colon \mathbb{R}^2 \to \mathbb{R}^2$ Lipschitz with

$$\begin{aligned} \nabla u &= M \quad \text{in } \mathbb{R}^2 - \bar{\Omega}, \\ \nabla u &= \tilde{M}_i \quad \text{in } \tilde{\Omega}_i, \\ \nabla u &= M_0 \quad \text{in } \Omega - (\tilde{\Omega}_1 \cup \cdots \cup \tilde{\Omega}_4), \\ |\tilde{\Omega}_1 \cup \cdots \cup \tilde{\Omega}_4| &\le \tfrac{7}{8}|\Omega|. \end{aligned}$$

Step 3: Application to hexagonal-to-rhombic

$\forall\, M$ s. t. $\frac{1}{2}(M + M^t) \in \text{int conv}\{E_0, E_1, E_2\}$

$\exists\, \tilde{M}_1, \cdots, \tilde{M}_4$ s. t. $\frac{1}{2}(\tilde{M}_i + \tilde{M}_i^t) \in \text{int conv}\{E_0, E_1, E_2\}$

$\exists\, \Omega \subset \mathbb{R}^2$ open, bdd., $\tilde{\Omega}_1, \cdots, \tilde{\Omega}_4 \subset \Omega$ finite $\bigcup$ of convex, open sets

$\exists\, u\colon \mathbb{R}^2 \to \mathbb{R}^2$ Lipschitz with

$$\begin{aligned} \nabla u &= M \quad \text{in } \mathbb{R}^2 - \bar{\Omega}, \\ \nabla u &= \tilde{M}_i \quad \text{in } \tilde{\Omega}_i, \\ \tfrac{1}{2}(\nabla + \nabla^t)u &\in \{E_0, E_1, E_2\} \quad \text{in } \Omega - (\tilde{\Omega}_1 \cup \cdots \cup \tilde{\Omega}_4), \\ |\tilde{\Omega}_1 \cup \cdots \cup \tilde{\Omega}_4| &\le \tfrac{7}{8}|\Omega|. \end{aligned}$$

Step 4: Concatenation

$\forall\, M$ s. t. $\frac{1}{2}(M + M^t) \in \text{int conv}\{E_0, E_1, E_2\}$

$\forall\, \Omega \subset \mathbb{R}^2$ open, bbd

$\exists\, \tilde{M}_1, \cdots, \tilde{M}_4$ s. t. $\frac{1}{2}(\tilde{M}_i + \tilde{M}_i^t) \in \text{int conv}\{E_0, E_1, E_2\}$

$\exists\, \tilde{\Omega}_1, \cdots, \tilde{\Omega}_4 \subset \Omega$ countable $\bigcup$ of convex, open sets

$\exists\, u \colon \mathbb{R}^2 \to \mathbb{R}^2$ Lipschitz with

$$\begin{aligned} \nabla u &= M \quad \text{in } \mathbb{R}^2 - \bar{\Omega}, \\ \nabla u &= \tilde{M}_i \quad \text{in } \tilde{\Omega}_i, \\ \tfrac{1}{2}(\nabla + \nabla^t)u &\in \{E_0, E_1, E_2\} \quad \text{in } \Omega - (\tilde{\Omega}_1 \cup \cdots \cup \tilde{\Omega}_4), \\ |\tilde{\Omega}_1 \cup \cdots \cup \tilde{\Omega}_4| &\leq \tfrac{7}{8}|\Omega|. \end{aligned}$$

Step 5: Iteration via replacement

$\forall\ M$ s. t. $\frac{1}{2}(M + M^t) \in \text{int conv}\{E_0, E_1, E_2\}$

$\forall N \in \mathbb{N} \quad \forall\ \Omega \subset \mathbb{R}^2$ open, bbd

$\exists\ \tilde{M}_1, \cdots, \tilde{M}_{4^N}$ s. t. $\frac{1}{2}(\tilde{M}_i + \tilde{M}_i^t) \in \text{int conv}\{E_0, E_1, E_2\}$

$\exists\ \tilde{\Omega}_1, \cdots, \tilde{\Omega}_{4^N} \subset \Omega$ countable $\bigcup$ of convex, open sets

$\exists\ u \colon \mathbb{R}^2 \to \mathbb{R}^2$ Lipschitz with

$$
\begin{aligned}
\nabla u &= M \quad \text{in } \mathbb{R}^2 - \bar{\Omega}, \\
\nabla u &= \tilde{M}_i \quad \text{in } \tilde{\Omega}_i, \\
\tfrac{1}{2}(\nabla + \nabla^t)u &\in \{E_0, E_1, E_2\} \quad \text{in } \Omega - (\tilde{\Omega}_1 \cup \cdots \cup \tilde{\Omega}_{4^N}), \\
|\tilde{\Omega}_1 \cup \cdots \cup \tilde{\Omega}_{4^N}| &\leq (\tfrac{7}{8})^N |\Omega|.
\end{aligned}
$$

3.1 3-d models, cubic-to-tetragonal phase transformation

3 stress-free strains = Martensitic variants:

$$E_1 := \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ E_2 := \begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ E_3 := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

6 Martensitic twins with normals:

$n \in \{(0,1,1),(0,1,-1),(1,0,1),(-1,0,1),(1,1,0),(1,-1,0)\}$

No twin between Austenite $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

and three Martensitic variants E_1, E_2, E_3

cf. Lemma 3

Rigidity of twins

Dolzmann & Müller, Meccanica '95

Proposition 4 (Dolzmann & Müller)

Let $u\colon \mathbb{R}^3 \supset B_1 \to \mathbb{R}^3$ be Lipschitz with

$$\frac{1}{2}(\nabla + \nabla^t)u \in \{E_1, E_2, E_3\} \quad \text{a. e. in } B_1.$$

Then $u =$ one of the six Martensitic twins on B_δ

(with $\delta > 0$ universal).

Approximate rigidity of twins

Elastic + interfacial energy on B_1:

$$\begin{aligned} E \ := \ & \int_{B_1} |\tfrac{1}{2}(\nabla + \nabla^t)u - (\chi_1 E_1 + \chi_2 E_2 + \chi_3 E_3)|^2 dx \\ + \ & \eta \int_{B_1} |\nabla \chi_1| + |\nabla \chi_2| + |\nabla \chi_3| \end{aligned}$$

Admissible phase functions $\chi_i \in \{0,1\}$, $\chi_1 + \chi_2 + \chi_3 \leq 1$

Proposition 5 (Capella & O.)

$$\text{Suppose} \quad E \ll \eta^{2/3}.$$

Then $(u, \chi_1, \chi_2, \chi_3) \approx$
Austenite or one of the six Martensitic twins.

Optimal Martensitic inclusions

Energy in whole space

$$E := \int_{\mathbb{R}^3} |\tfrac{1}{2}(\nabla + \nabla^t)u - (\chi_1 E_1 + \chi_2 E_2 + \chi_3 E_3)|^2 dx + \int_{\mathbb{R}^3} |\nabla \chi_1| + |\nabla \chi_2| + |\nabla \chi_3|$$

Volume of Martensitic inclusion $V := \int_{\mathbb{R}^3} \chi_1 + \chi_2 + \chi_3 dx$

Proposition 6 (Knüpfer & Kohn & O.)

$$\min_{(u,\chi_1,\chi_2,\chi_3) \text{ of volume } V} E \sim V^{9/11}.$$

... energy barriers to nucleation

Future directions

Cubic-to-tetragonal:

Nucleation barriers at faces, edges, corners of sample

Cubic-to-orthorhombic (similar to hexagonal-to-rhombic ?): crossing twins rigid (for finite interfacial energy)? [Rüland]

Cubic-to-orthorhombic: Nucleation barrier for materials with nearly compatible Austenite-Martensite [Zhang-James-Müller, Zwicknagl]