Microstructures in Shape-Memory Alloys

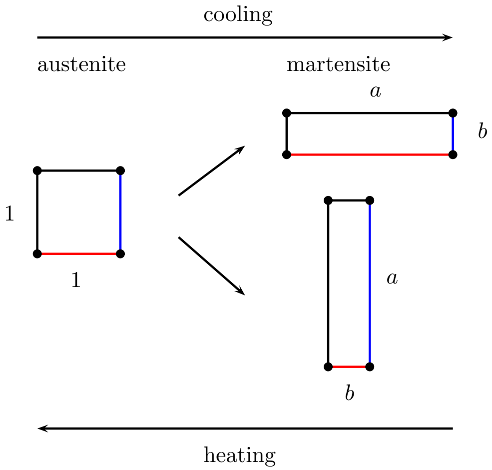
Rigidity, Flexibility and Some Numerical Experiments

Angkana Rüland
(joint work with J. M. Taylor, Ch. Zillinger, B. Zwicknagl)

Max Planck Institute for Mathematics in the Sciences

Polycrystals: Microstructure and Effective Properties Workshop
Oxford, 26-28.03.2018

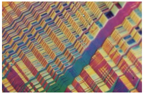
Solid-Solid Phase Transformations in SMA

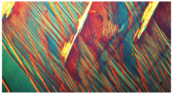


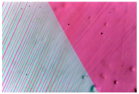
$$SO(2)\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$$

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

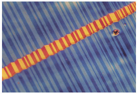
$SO(2) = \{2 \times 2$ rotation matrices$\}$


crossing twins


low hysteresis material


aust.-mart. interface

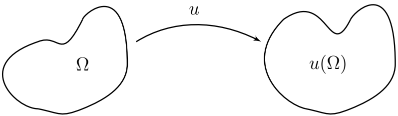

needles


crossing twins

The Phenomenological Theory

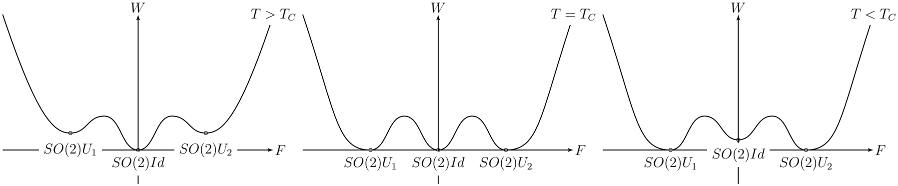
Ball & James: Minimize

$$\mathcal{E}(\nabla u, T) = \int_\Omega \underbrace{W_T(\nabla u)}_{\text{energy density}} \, dx,$$



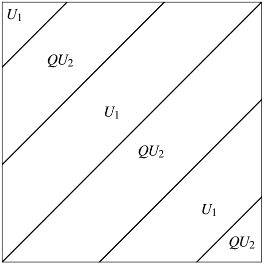
for deformations $u : \Omega \to \mathbb{R}^2$.

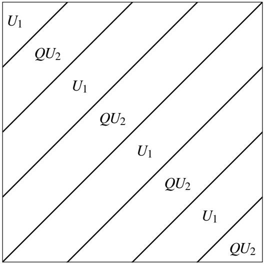
$$W_T(QF) = W_T(F) \text{ for all rotations } Q,$$
$$W_T(FR) = W_T(F) \text{ for all material symmetries } R.$$

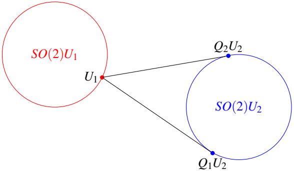


Differential Inclusion and Twins

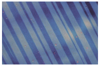
$$\nabla u \in SO(2)U_1 \cup SO(2)U_2$$







rank-one connections



$$U_1 - Q_1U_2 = \sqrt{2}\frac{a^2-b^2}{a^2+b^2}\begin{pmatrix} a \\ -b \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad Q_1 \in SO(2),$$

$$U_1 - Q_2U_2 = \sqrt{2}\frac{a^2-b^2}{a^2+b^2}\begin{pmatrix} a \\ b \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad Q_2 \in SO(2).$$

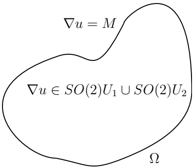
Flexibility

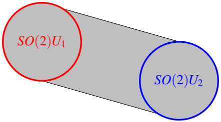
Theorem

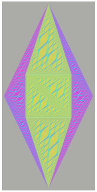
For any $\Omega \subset \mathbb{R}^2$ *and any* $M \in \text{int}(SO(2)U_1 \cup SO(2)U_2)^{lc}$ *there exists a deformation u such that*

$$\nabla u \in SO(2)U_1 \cup SO(2)U_2 \text{ a.e. in } \Omega,$$
$$\nabla u = M \text{ in } \mathbb{R}^2 \setminus \Omega.$$

- Dacorogna-Marcellini (relaxation property & Baire category)
- Müller-Šverák (convex integration)







Q: Are these solutions physically relevant?

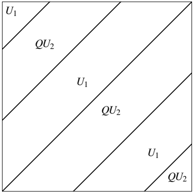
Rigidity

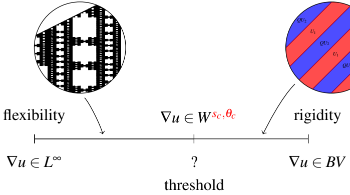
Theorem (Dolzmann-Müller, Rigidity)

Let $\Omega \subset \mathbb{R}^2$, $u : \Omega \to \mathbb{R}^2$ with $\nabla u \in BV(\Omega)$ and

$$\nabla u \in SO(2)U_1 \cup SO(2)U_2 \text{ a.e. in } \Omega.$$

Then ∇u is (locally) a laminate.





Extensions:

- Dacorogna-Marcellini-Paolini ($O(2)$, $O(n)$),
- Kirchheim & Conti-Dolzmann-Kirchheim (cubic-to-tetragonal),
- R '16 (cubic-to-orthorhombic).

Q: Is there a threshold behaviour between rigidity and flexibility?

Linear vs. Non-Linear Elasticity

Stress-free states

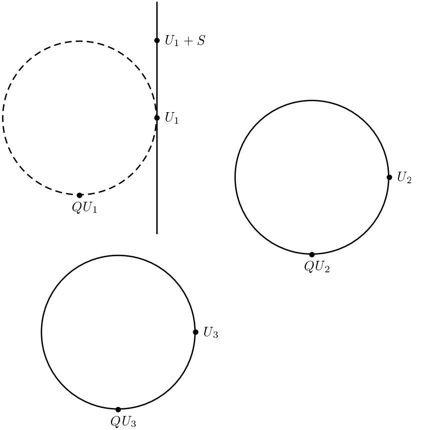
- non-linear:

$$(\nabla u)^t(\nabla u) \in \bigcup_{j=1}^{k} U_j^t U_j,$$

- linear:

$$e(\nabla v) := \frac{1}{2}(\nabla v + (\nabla v)^t) \in \bigcup_{j=1}^{k} (U_j^t U_j - Id),$$

where $u(x) = x + {\color{red}\epsilon} v(x)$.



- geometry linearises,
- material nonlinearity preserved.

Geometrically Linear m-Well Problems

- One-well problem:

$$e(\nabla v) := \frac{1}{2}(\nabla v + (\nabla v)^t) = 0 \text{ a.e. in } \Omega$$

$$\overset{\text{Liouville}}{\Rightarrow} \exists S \in Skew(n): \quad \nabla v = S \text{ a.e. in } \Omega.$$

- Two-well problem:

$$e(\nabla v) := \frac{1}{2}(\nabla v + (\nabla v)^t) \in \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \right\} \text{ a.e. in } \Omega$$

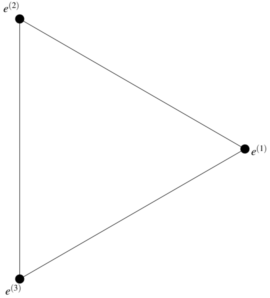
$$\overset{\text{Kohn}}{\Rightarrow} \exists f, g : \Omega \to \mathbb{R} \text{ s.t. } e_{11}(x_1, x_2) = f(x_1 + x_2)$$

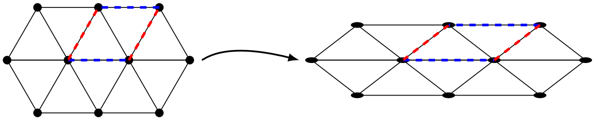
$$\text{or } e_{11}(x_1, x_2) = g(x_1 - x_2), \; x \in \Omega.$$

$\Rightarrow$ Laminate.

Proof. Saint Venant compatibility: $\partial_{11} e_{22} + \partial_{22} e_{11} = \partial_{12} e_{12} \rightsquigarrow$ wave equation for e_{11} combined with two-valuedness: $e_{11} \in \{\pm 1\}$.

The Hexagonal-to-Rhombic Transformation



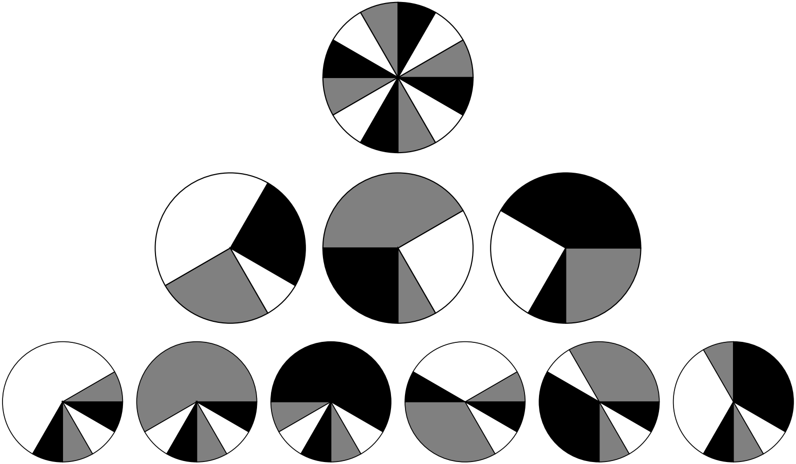


$$e(\nabla u) \in \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}, \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix} \right\}$$

($Mg_2Al_4Si_5O_{18}$, $Pb_3(VO_4)_2$)

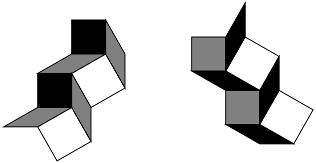
Properties

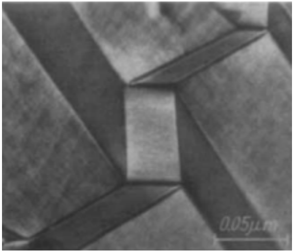
- $K^{lc} := \mathrm{conv}\{e^{(1)}, e^{(2)}, e^{(3)}\}$ [Bhattacharya, 2D & trace-free]
- very flexible: many stress-free microstructures; no rigidity result known.



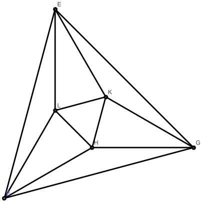
Concatenated Microstructures

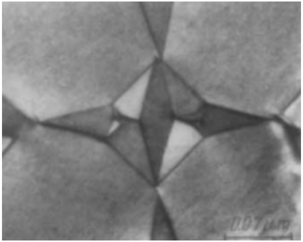
Crossing Twins:





Star Deformation:





[Kitano & Kifune]

The Main Result

Theorem (R.-Zillinger-Zwicknagl '16)

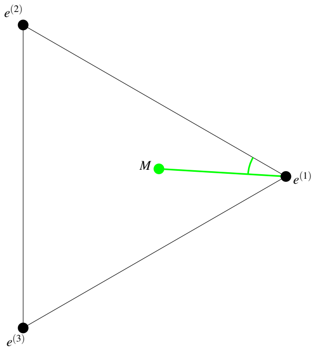
Let $\Omega \subset \mathbb{R}^2$ *be a bounded Lipschitz domain. Let* $K = \{e^{(1)}, e^{(2)}, e^{(3)}\}$ *and let* $e(M) = \frac{1}{2}(M + M^t) \in \text{intconv}(K)$*. Then there exists* $\theta_0 \in (0,1)$ *depending on* $\frac{dist(e(M), \partial\, \text{conv}(K))}{dist(e(M), K)}$ *and a deformation* $u : \mathbb{R}^2 \to \mathbb{R}^2$ *with* $u \in W^{1,\infty}_{loc}(\mathbb{R}^2)$

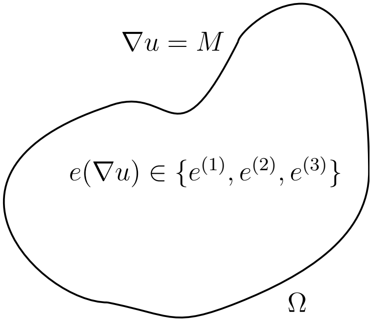
$$\nabla u = M \text{ a.e. in } \mathbb{R}^2 \setminus \Omega,$$
$$e(\nabla u) \in K \text{ a.e. in } \Omega,$$

and for all $s \in (0,1), p \in (1,\infty)$ *with* $0 < sp < \theta_0$

$$\nabla u \in W^{s,p}_{loc}(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2).$$

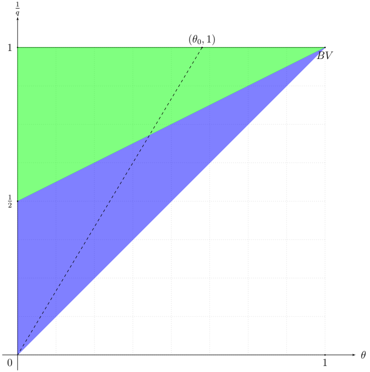
Remarks





- Solution has "fractal structure".
- Argument exploits $2D$ structure.
- Argument exploits geometrically linear structure.
- No rigidity counterpart for this model.
- Optimal dependence of exponent?

Ingredients of the Proof – Interpolation



Theorem (Cohen-Dahmen-Daubechies-DeVore '03)

Let $p \in [2, \infty)$ and assume that for some $\theta \in (0,1)$

$$\frac{1}{q} = \frac{1-\theta}{p} + \theta.$$

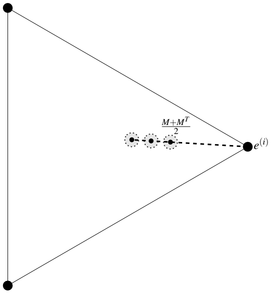
Then,

$$\|u\|_{W^{\theta,q}(\mathbb{R}^n)} \leq C \|u\|_{L^p(\mathbb{R}^n)}^{1-\theta} \|u\|_{BV(\mathbb{R}^n)}^{\theta}.$$

Remark:

- Original result in [CDDD03] formulated for Besov spaces.
- Similar (slightly weaker) result available for $p \in (1,2)$.

Quantitative Convex Integration



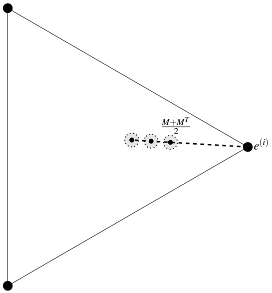
1. $M \in \mathbb{R}^{2\times 2}$:
   $e(M) \in \text{intconv}(e^{(1)}, e^{(2)}, e^{(3)})$.
2. Replacement construction (similar to tent construction) along rank-one line (with skew control) $\rightsquigarrow M_1, M_2, M_3, M_4$.
3. Covering + iteration.

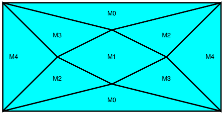
Proposition (Interpolation Bounds)

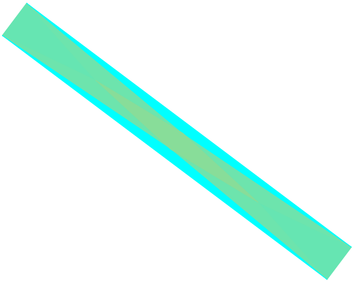
Let u_k be obtained from the convex integration algorithm. Then it is possible to ensure that $\|u_k\|_{W^{1,\infty}(\Omega)} \leq C$ and

$$\|\nabla u_{k+1} - \nabla u_k\|_{L^1(\mathbb{R}^2)} \leq C v_0^k,$$
$$\|\nabla u_{k+1} - \nabla u_k\|_{BV(\mathbb{R}^2)} \leq C \epsilon_0^{-k}.$$

Quantitative Convex Integration





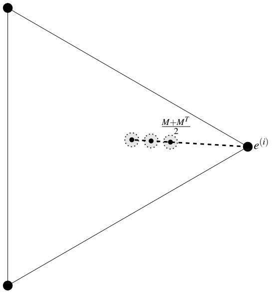


Proposition (Interpolation Bounds)

Let u_k be obtained from the convex integration algorithm. Then it is possible to ensure that $\|u_k\|_{W^{1,\infty}(\Omega)} \leq C$ and

$$\|\nabla u_{k+1} - \nabla u_k\|_{L^1(\mathbb{R}^2)} \leq C v_0^k,$$
$$\|\nabla u_{k+1} - \nabla u_k\|_{BV(\mathbb{R}^2)} \leq C \epsilon_0^{-k}.$$

Quantitative Convex Integration



1. $M \in \mathbb{R}^{2\times 2}$:
   $e(M) \in \text{intconv}(e^{(1)}, e^{(2)}, e^{(3)})$.
2. Replacement construction (similar to tent construction) along rank-one line (with skew control) $\rightsquigarrow M_1, M_2, M_3, M_4$.
3. Covering + iteration.

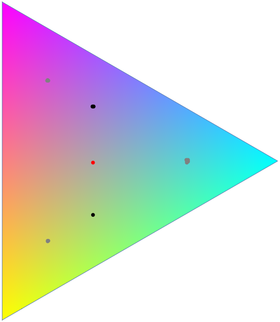
Proposition (Interpolation Bounds)

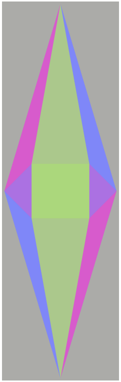
Let u_k be obtained from the convex integration algorithm. Then it is possible to ensure that $\|u_k\|_{W^{1,\infty}(\Omega)} \leq C$ and

$$\|\nabla u_{k+1} - \nabla u_k\|_{L^1(\mathbb{R}^2)} \leq C v_0^k,$$

$$\|\nabla u_{k+1} - \nabla u_k\|_{BV(\mathbb{R}^2)} \leq C \epsilon_0^{-k}.$$

Remarks and Improvements





Improvements in [RZZ '17]:

- Different convex integration scheme $\Rightarrow$ uniformity of regularity exponent sp.
- Applies to a “general” set-up; includes 3D geometrically linear transformations and $O(n)$ inclusions.

Surface Energies

$$E_{\epsilon} = \min_{\nabla u = M \text{ a.e. in } \mathbb{R}^n \backslash \overline{\Omega}} \left\{ \int_{\Omega} \text{dist}^2(\nabla u, K) dx + \epsilon^2 \int_{\Omega} |\nabla^2 u|^2 dx \right\}.$$

Theorem (Taylor-R.-Zillinger '18)

Assume that there exist constants $C > 1$, $\mu \in (0, \frac{1}{2})$ such that for all $\epsilon \in (0, \epsilon_0)$ it holds $E_{\epsilon} \geq C\epsilon^{2\mu}$. Suppose that u is a solution to

$$\nabla u \in K \text{ a.e. in } \Omega, \; \nabla u = M \text{ a.e. in } \mathbb{R}^n \setminus \overline{\Omega}.$$

If $v(x) := u(x) - Mx - b \in H^{s+1}(\mathbb{R}^n)$ for some $b \in \mathbb{R}^n$, $s \in \mathbb{R}$ and $\nabla v \in L^{\infty}(\mathbb{R}^n)$, then $s \leq \mu$.