Bonn International Graduate School in Mathematics

The Cubic-to-Orthorhombic Phase Transition: Rigidity, Non-Rigidity and Scaling

Angkana Rüland, Bonn University

The Model

Introduction. The cubic-to-orthorhombic phase transition is an example of a martensitic phase transition occurring in certain shape-memory alloys, for instance in CuAlNi. Martensitic phase transitions are temperature- (or stress-) induced diffusionless, solid-solid transitions. Both due to their promising technological applications (e.g. in medicine and aeronautics) and their fascinating mathematical properties, these materials have been subject of very active research.

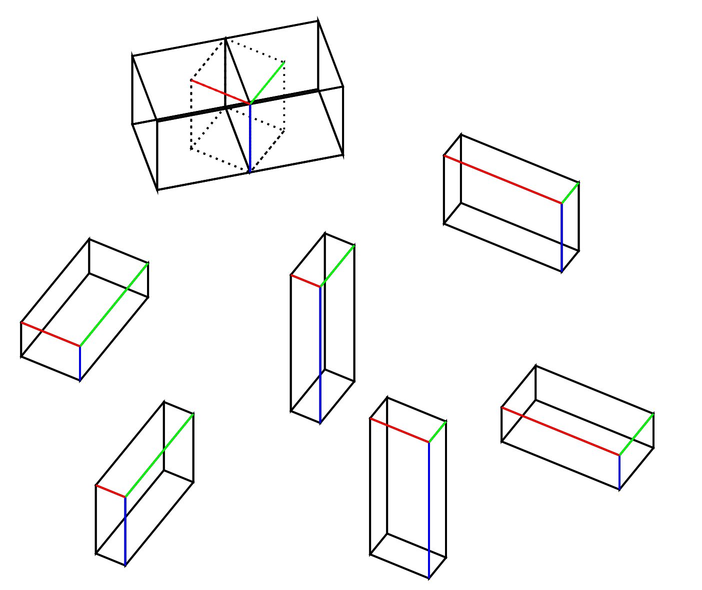

Figure 1: A microscopic interpretation of the cubic-to-orthorhombic phase transition.

Microscopically, the phase transition can be described as a deformation of the cubic high-temperature austenite lattice into less symmetric orthorhombic ones corresponding to the different variants of martensite (c.f. figure on the left). In the sequel we deal with the low temperature regime in the framework of the linear theory of elasticity. Our guiding questions are:

- **Non-Rigidity.** Which features does a mathematical model have to take into account in order to reflect the material properties?
- **Rigidity.** Which boundary conditions can be imposed without creating stresses? In other words, what are the solutions of the exactly stress-free model? Which patterns emerge?
- **Scaling.** Are these stress-free states energetically stable? What kind of scaling behavior do (not necessarily stress-free) microstructures depict?

The Linear, Stress-Free Setting. The stress-free strains associated with the cubic-to-orthorhombic phase transition are described by the following trace-free matrices

$$e_1 = \epsilon\begin{pmatrix} 1 & \delta & 0 \\ \delta & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \quad e_2 = \epsilon\begin{pmatrix} 1 & -\delta & 0 \\ -\delta & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \quad e_3 = \epsilon\begin{pmatrix} 1 & 0 & \delta \\ 0 & -2 & 0 \\ \delta & 0 & 1 \end{pmatrix},$$

$$e_4 = \epsilon\begin{pmatrix} 1 & 0 & -\delta \\ 0 & -2 & 0 \\ -\delta & 0 & 1 \end{pmatrix}, \quad e_5 = \epsilon\begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & \delta \\ 0 & \delta & 1 \end{pmatrix}, \quad e_6 = \epsilon\begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & -\delta \\ 0 & -\delta & 1 \end{pmatrix}.$$

Here δ and ϵ are dimensionless material parameters, typically of the size $\delta \sim 0.25$, $\epsilon \sim 0.04$, c.f. [Bha03]. Dealing with the stress-free setting first, we investigate the six-well problem, i.e. we are concerned with the structure of strains satisfying

$$e(\nabla u) := \frac{1}{2}(\nabla u + (\nabla u)^t) \in \{e_1, ..., e_6\}.$$

As we will see, this simple model does not describe the physically observed patterns correctly without imposing additional conditions.

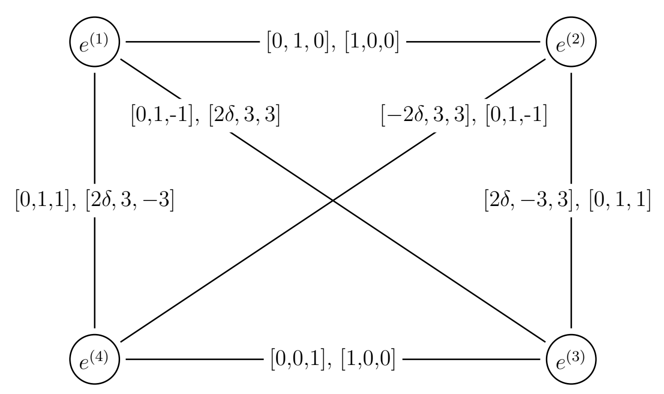

Figure 2: Possible rank-one connections, the remaining ones follow from symmetry.

Rigidity and Non-Rigidity

Non-Rigidity. Using the technique of convex integration in the framework developed by Müller and Šverák, [MŠ99], which was later extended by Kirchheim and Conti, we show that the six-well problem associated with the cubic-to-orthorhombic phase transition does not exhibit any rigidity properties in the class $C^{0,\alpha}$ for $\alpha \in [0,1)$:

Theorem 1 ([Rül13a]). *Let $e_1, ..., e_6 \in \mathbb{R}^{3\times3}_{sym}$, $\operatorname{tr}(e_i) = 0$ be such that $\dim(\operatorname{intconv}(e_1, ..., e_6)) = 5$ and assume that there exist $a_{ij} \in \mathbb{R}^3 \setminus \{0\}, n_{ij} \in \mathbb{S}^2$ with*

$$e_i - e_j = \frac{1}{2}(a_{ij} \otimes n_{ij} + n_{ij} \otimes a_{ij}) \text{ for } i \neq j.$$

Then for any Lipschitz domain Ω and any $M \in \mathbb{R}^{3\times3}$ such that $\frac{1}{2}(M + M^t) \in \operatorname{intconv}(e_1, ..., e_6)$ there exists a function $u : \mathbb{R}^3 \to \mathbb{R}^3$, $u \in C^{0,\alpha}$ for all $\alpha \in [0,1)$, satisfying

$$\nabla u = M \text{ on } \mathbb{R}^3 \setminus \bar{\Omega},$$
$$\frac{1}{2}(\nabla + \nabla^t)u \in \{e_1, ..., e_6\} \text{ in } \Omega \text{ a.e.}$$

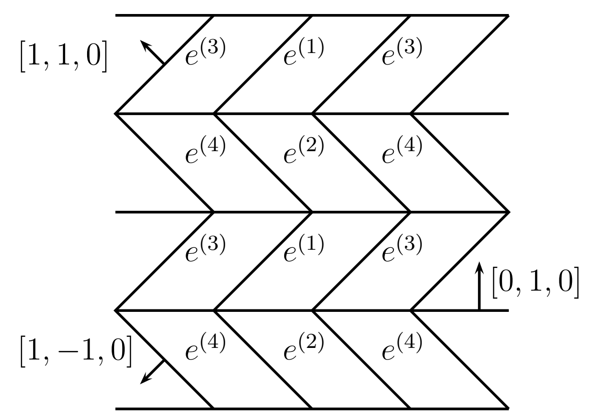

Figure 3: A crossing twin configuration.

The theorem reflects the fact that already in the *linear* situation the interior of the convex hull of the strains is "large enough". This is necessary in order to apply the oscillation strategy involved in the convex integration procedure which creates highly irregular configurations. The rather explicit construction strategy illustrates that the underlying phase distribution is extremely "wild": the associated surface energy of the constructions is unbounded.

Rigidity for Generic δ. Considering configurations for which the underlying phase distribution is given by a finite number of polygons, this "wildness" can be ruled out. In fact, all possible configurations are essentially two-dimensional:

Theorem 2 ([Rül13a]). *Let $e = e(\nabla u) : \Omega \to \mathbb{R}^{3\times3}_{sym}$, $e \in \{e_1, ..., e_6\}$, $\delta \notin \{\pm\frac{3}{2}, \pm3\}$. Assume that e is a piecewise constant strain. Then it, locally, forms only simple laminates or crossing twin configurations.*

Key ingredients of the proof are

- a characterization of zero-homogeneous strains via a blow-up procedure,
- combinatorial considerations (on a spherical graph),
- the strain equations for a reduced number of strains.

The result suggests that surface energy plays a crucial role in the pattern formation of the cubic-to-orthorhombic phase transition. In contrast to other phase transition models, the illustrated complementary results with and without surface energy already appear in the *linear* theory.

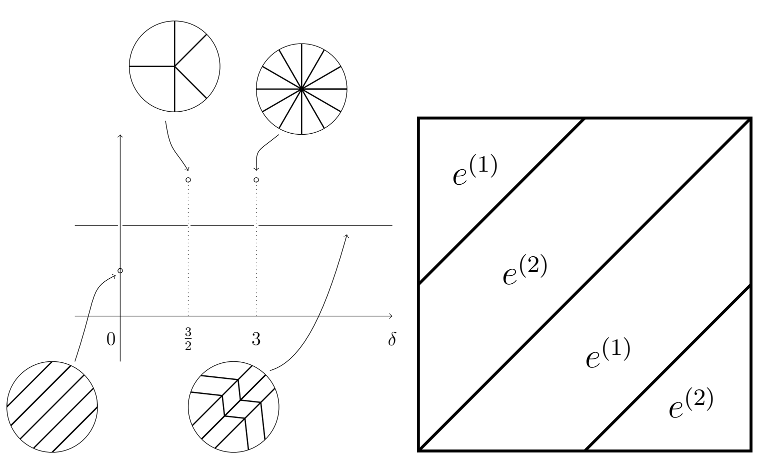

Figure 4: Different characteristic configurations depending on δ (left), an example of a simple laminate configuration (right).

An Energy Based Interpretation and a Reduced Model

Including Small Stresses. It is natural to investigate whether crossing twin constructions are stable with respect to small perturbations. Guided by the results on the stress-free setting, we expect the surface energy to play an important role. Hence, a natural energy functional measuring the smallness of the perturbations consists of two contributions: An elastic one, reflecting the material symmetry of the phase transition, and a higher order regularizing surface energy contribution.

As crossing twin constructions already emerge in the context of the four-well problem

$$e \in \{e_1, ..., e_4\},$$

we focus on this situation as a toy model for our full problem. Furthermore, we assume that the strain $e = e(y_1, y_2)$ only depends on two variables. These are chosen in such a way that crossing twin structures occur in the respective plane.

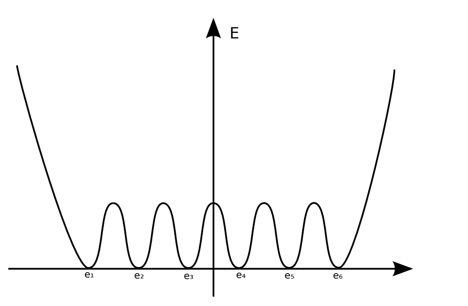

Figure 5: A cartoon of a possible elastic energy density.

The Elastic Energy. We make the ansatz:

$$E_{el}(e) = \mu \min_{\chi_i} \int_{\Omega} |e(\nabla u) - \chi_i e_i|^2 dx,$$
$$\chi_i \in \{0,1\}, \quad \sum_i \chi_i = 1.$$

Implicitly, this assumes that Hooke's law for the material is isotropic and that the second Lamé constant vanishes; μ has the dimension $\left[\frac{J}{m^3}\right]$.

The Surface Energy. As a second ingredient we consider:

$$E_{surf}(\chi) = \kappa \sum_i \int_{\Omega} |\nabla \chi_i| dx$$

This penalizes surface energy contributions in order to avoid the "wild" convex integration solutions. The parameter κ has the dimension $\left[\frac{J}{m^2}\right]$.

Non-Dimensionalization. After non-dimensionalization our energy turns into

$$E = \eta^{-\frac{2}{3}} E_{elast} + \eta^{\frac{1}{3}} E_{surf},$$

where $\eta = \frac{\kappa}{\mu L}$, L being the sample size. Setting

$$\bar{\chi}_1 := 1 - 2(\chi_3 + \chi_4), \ \bar{\chi}_2 := 1 - 2(\chi_2 + \chi_4), \ \bar{\chi}_3 := 1 - 2(\chi_2 + \chi_3),$$
$$\chi_1 + \chi_2 + \chi_3 + \chi_4 = 1, \ \ \chi_i \in \{0,1\}, \ \ \bar{\chi}_i \in \{-1,1\},$$

we prove the following stability result inspired by the papers of Capella and Otto on the cubic-to-tetragonal phase transition, c.f. [CO12].

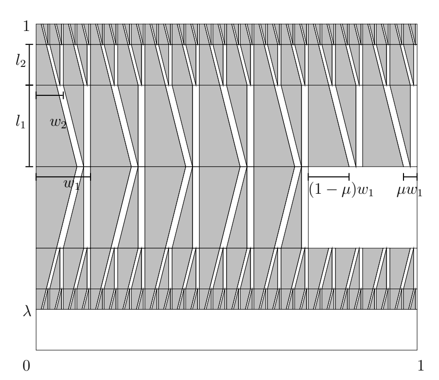

Figure 6: A branching microstructure.

Stability and Scaling

Theorem 3 ([Rül13b]). *Let $\bar{\chi}_i$, $E \ll 1$ be as above, let $\eta \leq 1$. Define $\theta_i := \langle \chi_i \rangle := \int_{\mathbb{T}^2} \chi_i dx$. Then*

1. *The following dichotomy holds*

$$\int_{\mathbb{T}^2} |\bar{\chi}_2 - f_{(100)}| dx \lesssim E^{\frac{1}{2}} \text{ or } \int_{\mathbb{T}^2} |\bar{\chi}_2 - f_{(010)}| dx \lesssim E^{\frac{1}{2}},$$

$$f_{(100)} = f(y_1) \in \{-1,1\} \text{ and } f_{(010)} = f(y_2) \in \{-1,1\}.$$

2. *If $\bar{\chi}_2 \sim f_{(100)}$ then*

$$|\theta_1(\theta_2 + \theta_4) - \theta_4(\theta_1 + \theta_3)| \lesssim E^{\frac{1}{4}}.$$

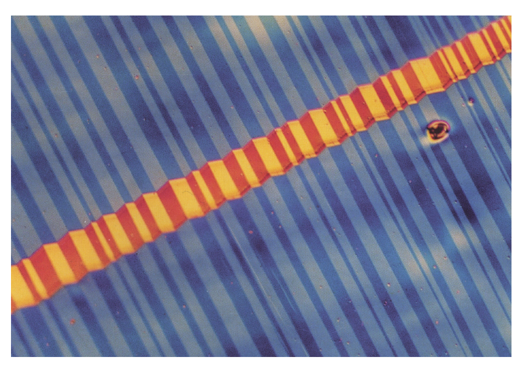

Figure 7: Crossing twin configurations in CuAlNi, [Bha03].

This result has a two-fold interpretation: On the one hand, it proves that the observed crossing twin configurations are stable among two-dimensional perturbations. On the other hand, it yields a lower bound on the scaling of "incompatible" microstructures. In this sense, the scaling result is sharp, as it is possible to find microstructures which display a scaling of $E \sim 1$.

References

[Bha03] Kaushik Bhattacharya. *Microstructure of martensite: why it forms and how it gives rise to the shape-memory effect.* Oxford series on materials modeling, Oxford University Press, 2003.

[CO12] Antonio Capella and Felix Otto. A quantitative rigidity result for the cubic-to-tetragonal phase transition in the geometrically linear theory with interfacial energy. *Proceedings of the Royal Society of Edinburgh: Section A Mathematics, 142 , pp 273-327 doi:10.1017/S0308210510000478*, 2012.

[MŠ99] Stefan Müller and Vladimír Šverák. Convex integration with constraints and applications to phase transitions and partial differential equations. *Journal of the European Mathematical Society*, 1:393–422, 1999. 10.1007/s100970050012.

[Rül13a] Angkana Rüland. The Cubic-to-Orthorhombic Phase Transition – Rigidity and Non-Rigidity Properties in the Linear Theory of Elasticity. *MPI-MIS Preprint, 45*, 2013.

[Rül13b] Angkana Rüland. A Rigidity Result for a Reduced Model of a Cubic-to-Orthorhombic Phase Transition in the Geometrically Linear Theory of Elasticity. *ArXiv Preprint*, 2013.

Mathematisches Institut der Universität Bonn
Endenicher Allee 60, 53115 Bonn
rueland@math.uni-bonn.de

Deutsche Telekom Stiftung