Microstructure formation in shape memory alloys

Konstantinos Koumatos

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**Figure:** Cubic-to-tetragonal

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The most successful model (Ball/James, Chipot/Kinderlehrer) is based on nonlinear elasticity and leads to the following variational problem:

Minimise

\[ I_\theta (y) := \int_\Omega \varphi (Dy (x), \theta) \, dx. \]

subject to appropriate boundary data \( y|_{\partial \Omega_1} = y_0 \).

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Small-energy deformations are driven by the zero set of $\varphi$:

$$K(\theta) = \{ A : \varphi(A, \theta) = 0 \} = \{ \text{energy-minimising deformation gradients at } \theta \}. $$

This is entirely determined by the break of symmetry in the lattice!

Denoting the martensitic variants by $U_1, \ldots, U_N$, we assume that

$$K(\theta) = \begin{cases} 
\alpha(\theta) \text{SO}(3), & \theta > \theta_c \\
\text{SO}(3) \cup \bigcup_{i=1}^n \text{SO}(3) U_i, & \theta = \theta_c \\
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In the context of vector valued functions, the existence of a minimiser for $I_\theta (y)$ is roughly equivalent to the energy density $\varphi$ being *quasiconvex*.

**Definition**

We say that $\varphi : M^{n \times n} \to \mathbb{R}$ is *quasiconvex* if for all $F \in M^{3 \times 3}$ and for some bounded and open set $E \subset \mathbb{R}^n$ with $\mathcal{L}^n (\partial E) = 0$

$$\varphi (F) \leq \frac{1}{\mathcal{L}^n (E)} \int_E \varphi (F + Dy (x)) \, dx$$

for all $y \in W^{1,\infty}_0 (E, \mathbb{R}^n)$, whenever the integral exists.

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Typical energy-densities fail to be quasiconvex and so one expects that the infimum of the energy is not in general attained.

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The answer is yes and the set is the \textit{quasiconvex hull} of $K - K^{qc}$.

For a SMA it provides the set of all affine deformations recoverable upon heating.

However, calculating quasiconvex hulls is usually far from trivial. Very little is known about the structure of these sets and in cases applicable to shape memory materials, we can only solve the \textit{two well problem}, i.e.

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**Figure:** Classical austenite-martensite interface in CuAlNi (C.H. Chu and R.D. James).
Nevertheless, $K^{qc}$ typically contains objects far more complicated than simple laminates.
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**Figure:** Parallelogram microstructure in CuAlNi (H. Seiner)
Compatible interfaces with the austenite are still possible; these are called non-classical.

J.M. Ball and R.D. James have provided an extensive theoretical investigation of non-classical interfaces for the cubic-to-tetragonal case by analysing the inclusion

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Figure: Non-classical interface between austenite and a parallelogram microstructure of martensite in CuAlNi (H. Seiner)
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Figure: Curved austenite-martensite interface in CuAlNi resulting from the inhomogeneity of the volume fractions (H. Seiner)

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- the analysis of microstructures and non-classical interfaces,
- the investigation of curved interfaces,
- mechanisms of nucleation (motivated by an experiment of H. Seiner/related to quasiconvexity conditions for the energy density) and
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