Nucleation of austenite in martensite

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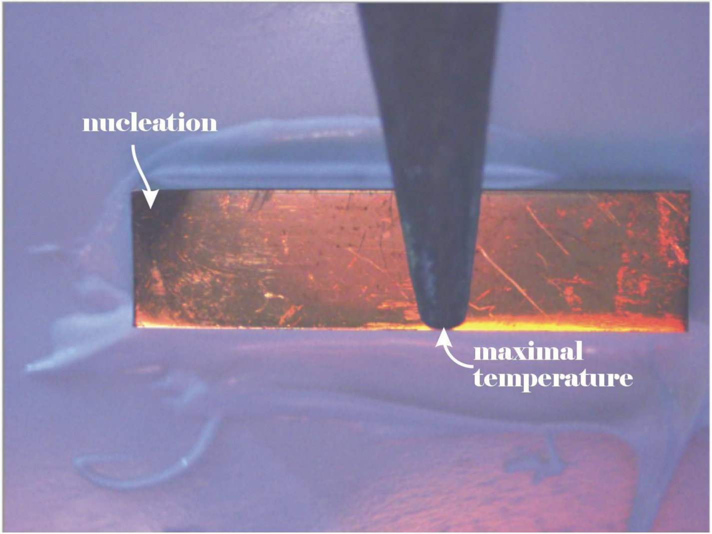
Experimental observations (H. Seiner)

- CuAlNi bar of dimension $12 \times 3 \times 3$mm.
- Orientation at austenite close to $(1,0,0),(0,1,0),(0,0,1)$.
- Mechanically stabilised into a pure phase of martensite containing a single variant.



Austenite was nucleated via a localized heat source.

Irrespective of the point of contact, the austenite always nucleated at a corner.

Introduction

We will follow the nonlinear elasticity model for martensitic transformations in which microstructures are identified with minimizing sequences for some energy functional

$$\mathcal{E}(y) := \int_\Omega \varphi(Dy(x))\,dx.$$

Any minimizing sequence of gradients Dy^j (assumed bounded in L^∞) will converge weak-* to some gradient Dy (up to a subsequence) which is the macroscopic deformation gradient.

However, in passing to this limit, a lot of information is lost and then, the use of gradient Young measures becomes a convenient way to describe microstructures.

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However, in passing to this limit, a lot of information is lost and then, the use of gradient Young measures becomes a convenient way to describe microstructures.

Any minimizing sequence of gradients, Dy^j, generates a family $\nu = (\nu_x)_{x\in\Omega}$ of probability measures such that for all continuous f

$$f\left(Dy^j\right) \overset{*}{\rightharpoonup} \langle \nu_x, f\rangle = \int_{M^{3\times 3}} f(A)\, d\nu_x(A) \text{ in } L^\infty \quad \text{(up to a subsequence).}$$

The problem then becomes that of minimising

$$I(\nu) = \int_\Omega \langle \nu_x, \varphi\rangle\, dx$$

over the set of ($W^{1,\infty}$) gradient Young measures. Any minimizer ν of I is generated by a minimizing sequence Dy^j of $\mathcal{E}$ (and vice versa) for which the macroscopic deformation gradient satisfies

$$Dy(x) = \bar{\nu}_x = \langle \nu_x, \mathrm{id}\rangle.$$

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Our work is also connected to the problem of necessary and sufficient conditions for an extremal (solution to the Euler-Lagrange equations) to be a strong local minimizer for

$$\mathcal{E}(y) := \int_{\Omega} \varphi(x, y(x), Dy(x))\, dx.$$

For the vectorial case and Ω smooth, known necessary conditions are:

- positivity of the second variation
- quasiconvexity in the interior (N.G. Meyers, '65)
- quasiconvexity at the boundary (J.M. Ball/J.E. Marsden, '84)

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In this work, we wish to make use of some notion of quasiconvexity to explain why the nucleation cannot occur in the interior or the faces and edges, as well as show how the austenite can compatibly nucleate from any corner.

For domains with edges and corners there are new associated quasiconvexity conditions.

Cubic-to-orthorhombic variants $\alpha, \beta, \gamma > 0$ and $\alpha \neq \gamma$

$$U_1 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} \\ 0 & \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix} \quad U_2 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} \\ 0 & \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}$$

$$U_3 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\alpha-\gamma}{2} \\ 0 & \beta & 0 \\ \frac{\alpha-\gamma}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix} \quad U_4 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\gamma-\alpha}{2} \\ 0 & \beta & 0 \\ \frac{\gamma-\alpha}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix}$$

$$U_5 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix} \quad U_6 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} & 0 \\ \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}$$

Setting up the problem

Let Ω be a bounded domain describing the CuAlNi bar at the austenite and assume that $\theta > \theta_c$. We wish to minimise

$$I(\nu) = \int_\Omega \langle \nu_x, W \rangle \, dx,$$

where

$$W(F) = \begin{cases} -\delta, & F \in SO(3) \\ 0, & F \in \bigcup_{i=1}^{6} SO(3)\, U_i \\ +\infty, & \text{otherwise.} \end{cases}$$

This functional is derived via the means of Γ - convergence and is used to make the problem more tractable.

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If we let $K := SO(3) \cup \bigcup_{i=1}^{6} SO(3)\, U_i$ and

$$\nu_x(SO(3)) = \int_{SO(3)} d\nu_x(A)$$ -the volume fraction of austenite at $x \in \Omega$,

then, equivalently,

$$I(\nu) = \begin{cases} -\delta \int_\Omega \nu_x(SO(3))\, dx, & \operatorname{supp}\nu \subset K \\ +\infty, & \text{otherwise.} \end{cases}$$

Letting U_s denote the mechanically stabilized martensitic variant, the homogeneous gradient Young measure

$$\nu = \delta_{U_s}$$

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Let $S \subset \Omega$ be a region where the nucleation will be allowed to take place.

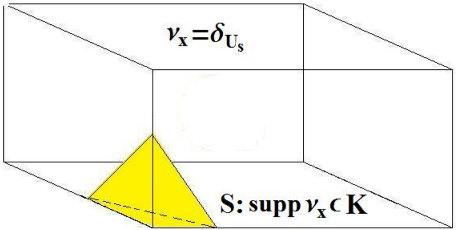
We perturb δ_{U_s} in this region and we let $\nu = (\nu_x)_{x \in \Omega}$ be a gradient Young measure such that

$$\nu_x = \delta_{U_s}, \qquad x \notin S$$

$$\operatorname{supp} \nu \subset K, \qquad x \in S.$$

Corner

S (yellow region) has parts of the three faces that meet at the given corner as a free boundary.



Aim: $\exists \nu_x$ as above such that

$$I(\nu) < I(\delta_{U_s}) = 0 \left(\Longleftrightarrow \int_\Omega \nu_x (SO(3)) > 0 \right).$$

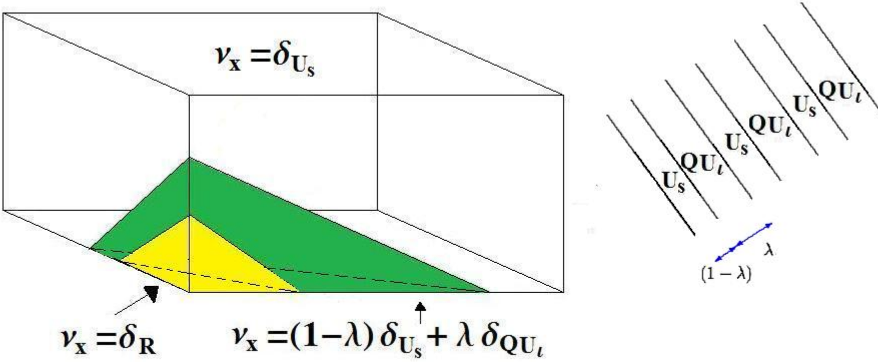
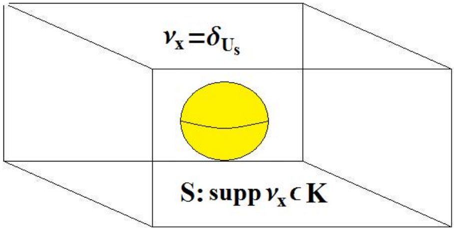


Figure: Nucleation from a corner; Yellow region occupied by austenite and green region by a simple laminate of martensite containing U_s.

Interior

S (yellow region) with no free boundary.



Aim: $\forall \nu_x$ as above

$$I(\nu) \geq I(\delta_{U_s}) = 0 \left(\Longleftrightarrow \int_\Omega \nu_x (SO(3)) = 0 \right).$$

Definition

A function $W : M^{3\times3} \longrightarrow \mathbb{R} \cup \{+\infty\}$ is quasiconvex at $F \in M^{3\times3}$ if for any homogeneous gradient Young measure μ with $\bar{\mu} = F$,

$$W(F) \leq \langle \mu, W \rangle.$$

Lemma

If the energy density W is quasiconvex at U_s then $I(\nu) \geq I(\delta_{U_s})$ so that nucleation cannot occur in the interior.

Remark: Using the minors' relations one can show that

$$\bar{\mu}_x = U_s \Longrightarrow \mu_x(SO(3)) = 0.$$

Here, this implies that W is quasiconvex at U_s so that, from the lemma above, nucleation cannot occur in the interior. Nevertheless, the same result will be used for faces and edges.

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Faces and Edges

For a face, we perturb δ_{U_s} in a region $S \subset \Omega$ with part of one face as a free boundary.

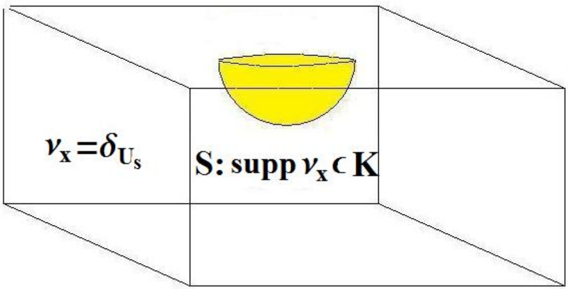

Figure: Nucleation from a face; region S in yellow.

For an edge, the set $S \subset \Omega$ where δ_{U_s} is perturbed has parts of two faces as a free boundary.

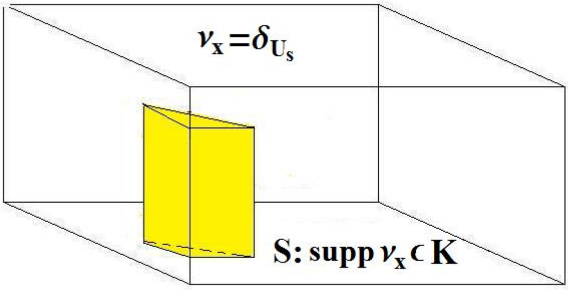

Figure: Nucleation from an edge; region S in yellow.

Both for the faces and edges, we wish to show that for all gradient Young measures as in the respective pictures,

$$I(\nu) \geq I(\delta_{U_s}).$$

(quasiconvexity at a face and an edge respectively)

To proceed we need a definition.

Definition

A vector $e \in S^2$ is called a maximal direction for U_s if

$$|U_s e| = \max_i \{1, |U_i e|\}.$$

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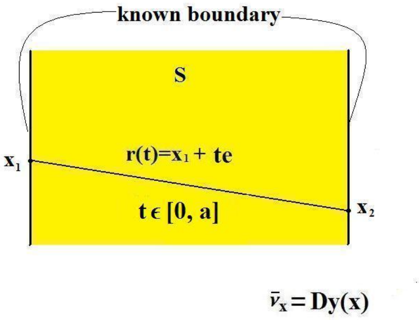


Figure: $r(t) \subset S$.

If e is a maximal direction for U_s

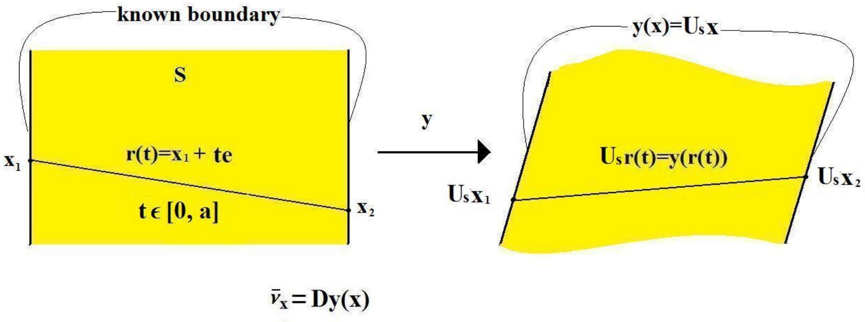
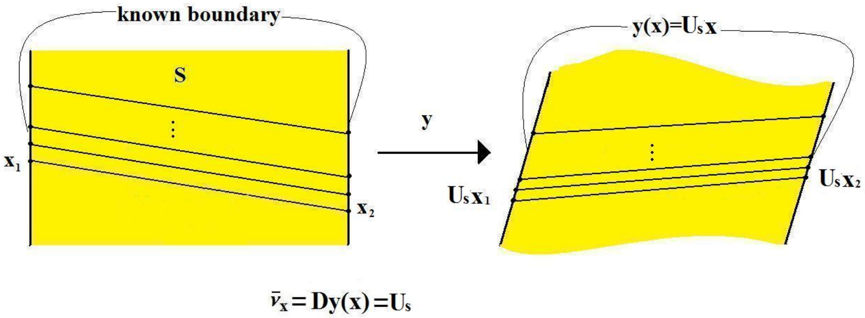


Figure: Necessary deformation of $r(t) \subset S$ under y



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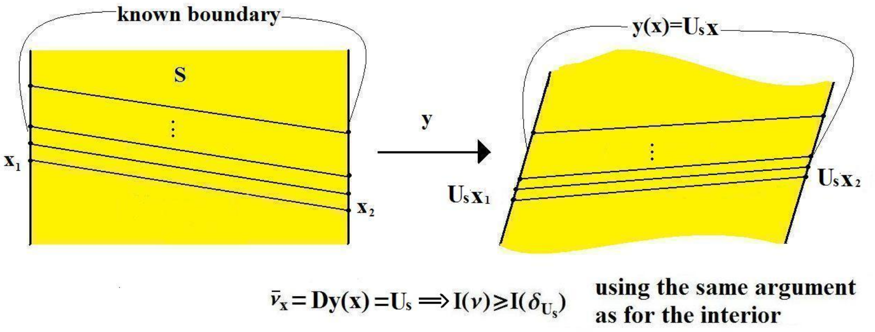

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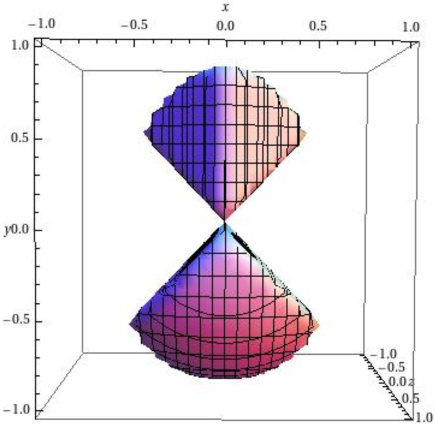

Figure: Set of maximal directions for U_1.

Adding new directions

Although these directions can cover some domains, they are not enough to cover the specimen used in the experiment.

For this reason, we develop a method similar to the above and add more directions using the inverse transformation.

For this, we need another definition.

Definition

A vector $e \in S^2$ is a maximal direction for U_s^{-1} if

$$|\mathrm{cof}\ U_s e| = \max_i \{1,\ |\mathrm{cof}\ U_i e|\}.$$

For the method to be applicable we need to employ the non-linear elasticity framework of Ciarlet and Nečas by adding a constraint on the admissible deformations. This is

$$\int_{\Omega} \det Dy\,(x)\;\,dx \leq \operatorname{vol}\, y\,(\Omega)$$

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Using injectivity a.e. along with other results, we can improve the regularity to ensure that the minimiser is bi-Lipschitz and that (roughly speaking) the boundary of the image of S, $y(S)$, does not come into contact with itself.

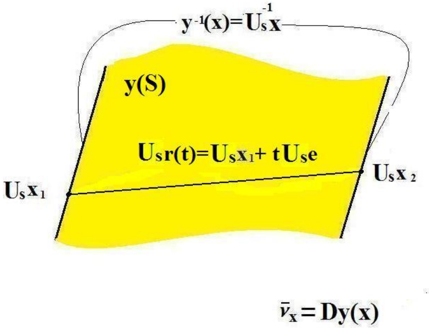
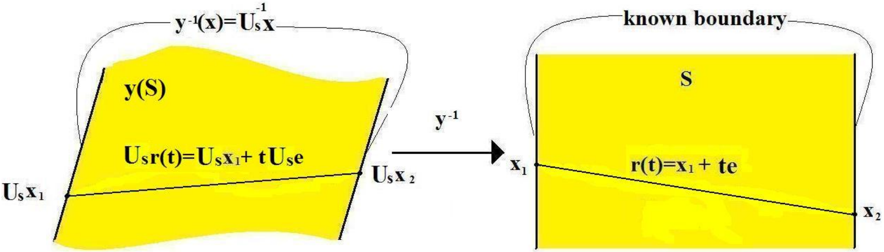


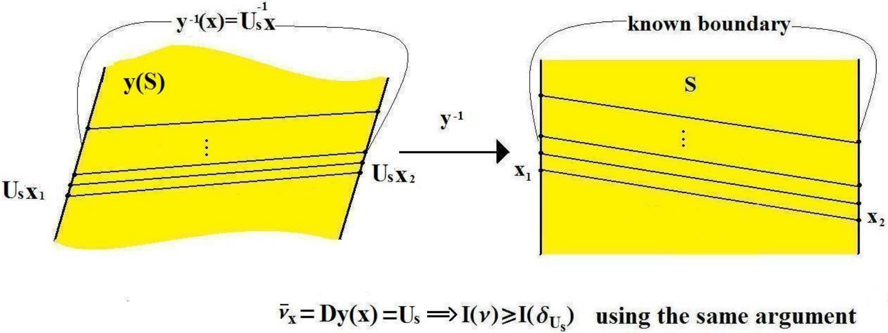
Figure: $U_s r(t) \subset y(S)$.

If $U_s e$ is a maximal direction for U_s^{-1}



$\bar{\nu}_x = Dy(x)$

Figure: Necessary deformation of $U_s r(t) \subset y(S)$ under y^{-1}



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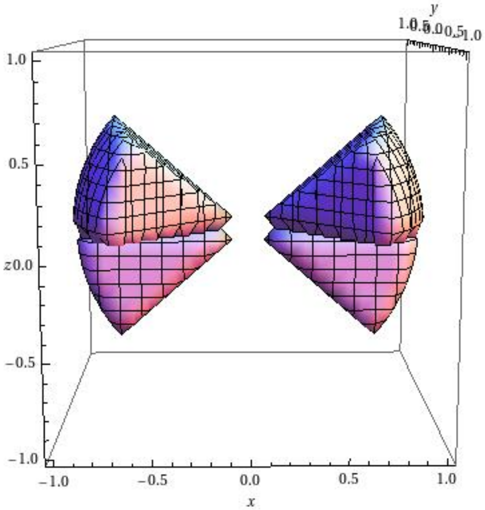

Figure: Vectors e such that $U_1 e$ is a maximal direction for U_1^{-1}.

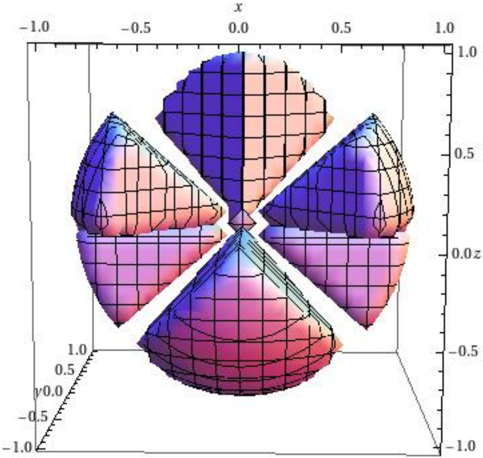

Figure: All vectors e with e maximal for U_1 or $U_1 e$ maximal for U_1^{-1}.

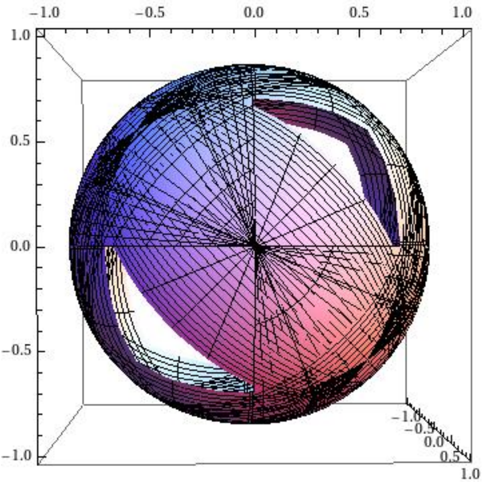

Figure: Normals to all possible faces the method can cover.

Conclusion

For the specimen in H. Seiner's experiment and for any U_s we can cover the entire domain and conclude that, indeed, the nucleation can only occur at a corner.

Moreover, for each $s = 1, \ldots, 6$ the sets of maximal directions for U_s and U_s^{-1} (as well as their union) contain sets of three linearly independent vectors.

This means that for any parallelepiped with edges parallel to these directions, nucleation can only be initiated at a corner making the method applicable to several other domains.

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