Nucleation of austenite in martensite

Konstantinos Koumatos

OxMOS,
Mathematical Institute, University of Oxford,
Supported by EPSRC

29/09/10
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 $L^\infty$) 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.
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 $L^\infty$) 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.
Any minimizing sequence of gradients, \(Dy^j\), generates a family \(\nu = (\nu_x)_{x \in \Omega}\) of probability measures such that for all continuous \(f\)

\[
f (Dy^j) \rightharpoonup^* \langle \nu_x, f \rangle = \int_{M^{3\times3}} f (A) \, d\nu_x (A) \quad \text{in } L^\infty \quad \text{(up to a subsequence)}.
\]

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 \(\nu\) of \(I\) is generated by a minimizing sequence \(Dy^j\) of \(\mathcal{E}\) (and vice versa) for which the macroscopic deformation gradient satisfies

\[
Dy (x) = \bar{\nu}_x = \langle \nu_x, \text{id} \rangle.
\]

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

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

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 $\nu$ of $I$ is generated by a minimizing sequence $Dy^j$ of $E$ (and vice versa) for which the macroscopic deformation gradient satisfies

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

We will follow this approach.
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 $\Omega$ 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)

Recently Y. Grabovsky and T. Mengesha (2009), provided a generalization of the Weierstrass theory showing that a strengthened version of the above conditions is sufficient for $\varphi$ sufficiently smooth.
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 $\Omega$ 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)

Recently Y. Grabovsky and T. Mengesha (2009), provided a generalization of the Weierstrass theory showing that a strengthened version of the above conditions is sufficient for $\varphi$ sufficiently smooth.
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 \( \alpha \neq \gamma \)

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

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

\[
U_5 = \begin{pmatrix}
\frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\
\frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\
0 & 0 & \beta
\end{pmatrix} \quad U_6 = \begin{pmatrix}
\frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} & 0 \\
\frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} & 0 \\
0 & 0 & \beta
\end{pmatrix}
\]
Let \( \Omega \) 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 \( \Gamma \)-convergence and is used to make the problem more tractable.
Let $\Omega$ 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 $\Gamma$-convergence and is used to make the problem more tractable.
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,

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

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

$$\nu = \delta U_s$$

will correspond to a pure phase of $U_s$. 
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,

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

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

$$\nu = \delta U_s$$

will correspond to a pure phase of $U_s$. 
Let $S \subset \Omega$ be a region where the nucleation will be allowed to take place.

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

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

$$\text{supp}\ \nu \subset K, \quad x \in S.$$
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
\[
I(\nu) < I(\delta_U) = 0 \iff \int_{\Omega} \nu_X(SO(3)) > 0.
\]
Nucleation from a corner; Yellow region occupied by austenite and green region by a simple laminate of martensite containing $U_s$. 

\[ \nu_x = \delta_{U_s} \]

\[ \nu_x = (1-\lambda) \delta_{U_s} + \lambda \delta_{QU_t} \]
Interior

S (yellow region) with no free boundary.

\[ \forall \nu \text{ as above} \]

\[ I(\nu) \geq I(\delta_{U_s}) = 0 \iff \int_{\Omega} \nu_x (SO(3)) = 0. \]

Aim: \( \forall \nu_x \) as above
**Definition**

A function $W : M^{3 \times 3} \rightarrow \mathbb{R} \cup \{+\infty\}$ is quasiconvex at $F \in M^{3 \times 3}$ if for any homogeneous gradient Young measure $\mu$ 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

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

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.
Definition
A function \( W : M^{3 \times 3} \longrightarrow \mathbb{R} \cup \{+\infty\} \) is quasiconvex at \( F \in M^{3 \times 3} \) if for any homogeneous gradient Young measure \( \mu \) 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

\[
\bar{\mu}_x = U_s \Rightarrow \mu_x (SO (3)) = 0.
\]

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.
For a face, we perturb $\delta U_s$ 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 $\delta_{U_s}$ 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

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

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

Figure: $\mathbf{r}(t) \subset S$.
If $e$ is a maximal direction for $U_s$

\[ r(t) = x_1 + te \]
\[ t \in [0, a] \]

\[ \bar{v}_x = D\bar{y}(x) \]

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

Introduction

Setting up the problem

Corner

Interior

Faces and Edges

Adding more directions

Conclusion

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

$$\bar{y}_x = Dy(x) = U_s$$
Experimental observations

Introduction

Setting up the problem

Corner

Interior

Faces and Edges

Adding more directions

Conclusion

Konstantinos Koumatos

Nucleation of austenite in martensite

\[ \tilde{v}_x = D\gamma(x) = U_x \implies I(\nu) \geq I(\delta_{U_x}) \] using the same argument as for the interior

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

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

$$\int_{\Omega} \det D y (x) \, dx \leq \text{vol} \, y (\Omega)$$

and ensures the a.e. injectivity of the minimisers.
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

$$\int_{\Omega} \det D y (x) \, dx \leq \text{vol} \, y (\Omega)$$

and ensures the a.e. injectivity of the minimisers.

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.
Konstantinos Koumatos

Nucleation of austenite in martensite

\[ y^{-1}(x) = U_s^{-1}x \]

\[ U_{sr}(t) = U_s x_1 + t U_s e \]

\[ \bar{y}_x = D y(x) \]

**Figure:** \( U_s r(t) \subset y(S) \).
If $U_s e$ is a maximal direction for $U_s^{-1}$

$$y^{-1}(x) = U_s x$$

$$U s r(t) = U s x_1 + t U s e$$

$$x_1$$

$$x_2$$

$$\bar{y}_x = D y(x)$$

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

\[ \nu = D(y(x)) = U_s \Rightarrow I(\nu) \geq I(\delta_{U_s}) \text{ using the same argument} \]

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

The end
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.

The end
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.

The end