A model for polycrystalline shape-memory alloys derived from microscopically motivated assumptions

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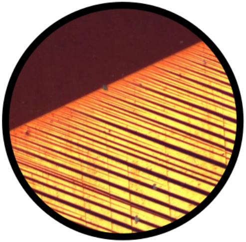
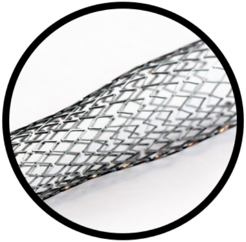
Polycrystals: microstructure and effective properties
March 26-28, 2018

Views on shape-memory alloys

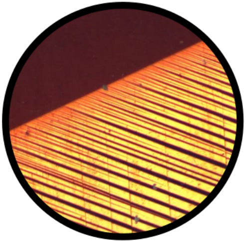
Microscopic picture



Macroscopic picture



Microscopic point of view



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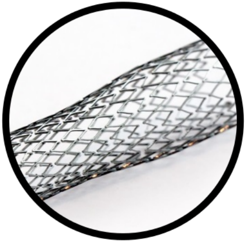

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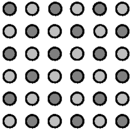
Microscopic point of view

On the microscopic level, we have

◦ high temperature:
atomic grid with high symmetry (usually cubic):
the so-called austenite, higher heat capacity



parent austenite
(cubic)

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- low temperature
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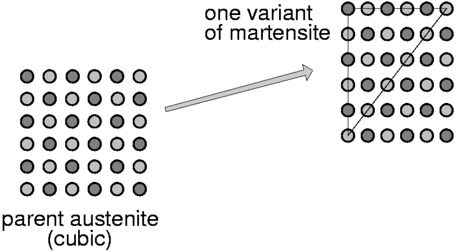

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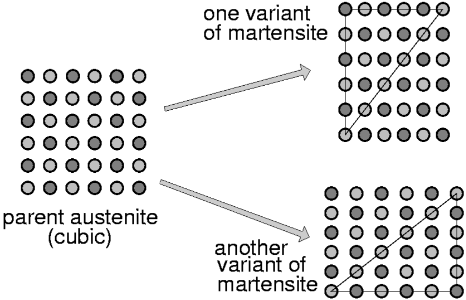

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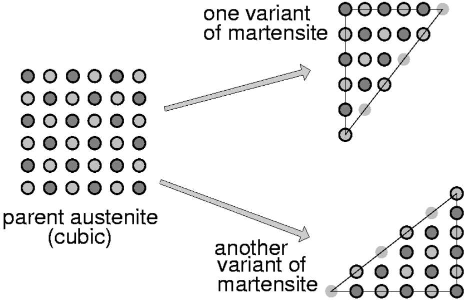

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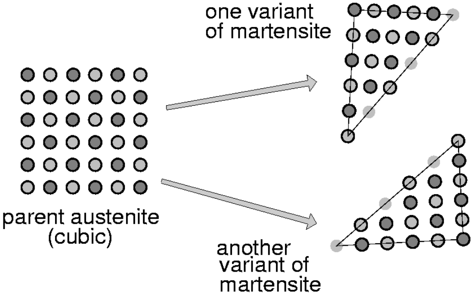

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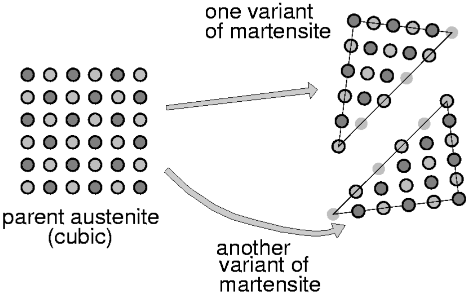

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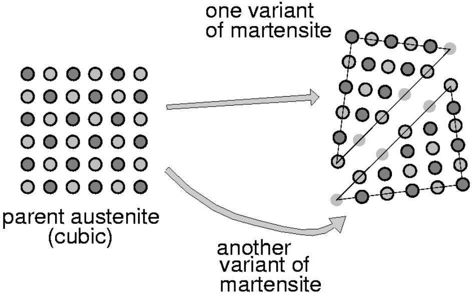

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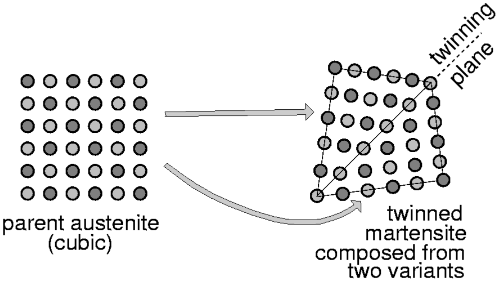
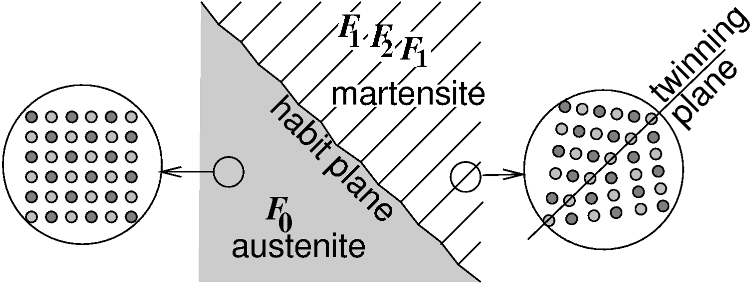


Microscopic point of view

- Microstructure particularly appears on the austenite - martensite interface



Macroscopic point of view

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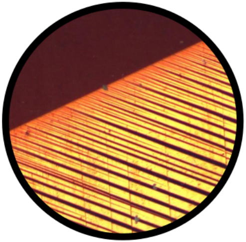

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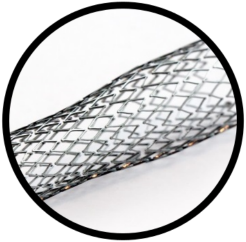
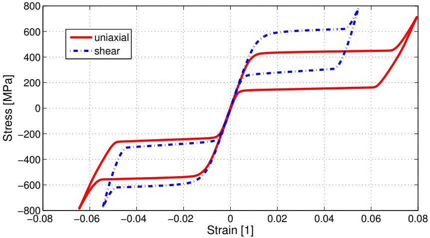


Macroscopic point of view

- One could start the phenomenological modelling “just” from the available measurement



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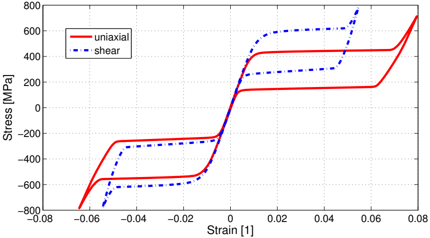

⇝ see Petr Sedlák’s talk for more experimental data

Macroscopic point of view

1. We need to model the hysteretic (inelastic) stress-strain behavior
2. The designed model needs to be simple, should allow for computations even on large specimens
3. Detailed knowledge of the processes on the microscopic level is not necessary (but we will need to reflect the microscopic knowledge)

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$\rightsquigarrow$ puts us into the setting of irreversible thermodynamics

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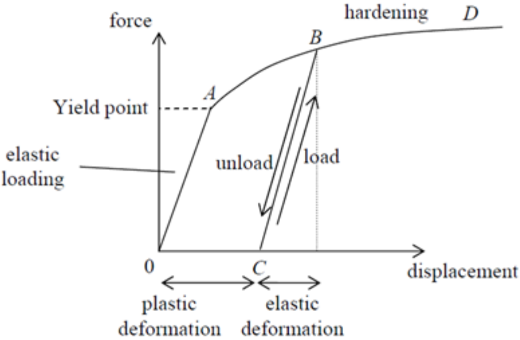
Aside: Modelling von-Mises plasticity

- A prototypical non-elastic behavior is plasticity



Aside: Modelling von-Mises plasticity

- The modelling ansatz (small-strain setting) is to divide the strain into its elastic and plastic part: $\varepsilon = \varepsilon^{\mathrm{el}} + \varepsilon^{in}$
- The stress σ (given e.g. by $\sigma = \mathbb{C}\varepsilon^{\mathrm{el}}$) is confined to a ball (region of elasticity)
- Plastic strain increases only if the stresses are at the boundary of the region of elasticity (Yield criterion)

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$$\Downarrow$$

The inelastic material properties are described by the inner variable and the main constitutive quantity for their modelling is the "shape" of the region of elasticity

Inspiration for shape-memory alloys

A number of models for polycrystalline shape-memory alloys have been designed building up on a similar principle:

1. The inner variables are

$$\varepsilon^{\mathrm{tr}} \text{ (transformation strain)} \quad \text{OR}$$

$$\xi \text{ (volume frac. of mart.) and } \varepsilon^{\mathrm{tr}}$$

2. The stress is given by $\sigma = \frac{\mathrm{d}\varphi}{\mathrm{d}\varepsilon^{\mathrm{el}}}$ with

$$\begin{aligned}\phi &= \underbrace{\frac{1}{2}\varepsilon^{\mathrm{el}}\mathbb{C}(\xi)\varepsilon^{\mathrm{el}}}_{\text{elastic part}} + \underbrace{\xi f^A(T) + (1-\xi) f^M(T)}_{\text{chemical part}} + \underbrace{\dots}_{\text{hardening,...}} \\ &= \frac{1}{2}\varepsilon^{\mathrm{el}}\mathbb{C}(\xi)\varepsilon^{\mathrm{el}} + \Delta s^{AM}(T-T_0)\xi \\ &\quad + u_0^A - s_0^A T + c^A\left[(T-T_0) - T\ln\left(\frac{T}{T_0}\right)\right]\end{aligned}$$

3. A region of elasticity or “dissipative forces” are prescribed

[Auricchio, Petrini, 2004], [Chemisky et al; 2011], [Panico, Brinson, 2007], [Sadjapour, Bhattacharya; 2007]

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Inspiration for shape-memory alloys

$$\Downarrow$$

The region of elasticity is of a high dimension (tensor as inner variable)

$$\Downarrow$$

maybe a different (“scalar”) modelling approach?

Generalized standard materials (GSM)

- The constitutive properties of the material are encoded in two scalar potentials:

$$\begin{aligned} \phi(\varepsilon, \xi, \varepsilon^{\mathrm{tr}}) &\quad \text{energy} \\ d(\varepsilon, \xi, \varepsilon^{\mathrm{tr}}, \dot{\xi}, \dot{\varepsilon}^{\mathrm{tr}}) &\quad \text{dissipation potential} \end{aligned}$$

- The generalized thermodynamic forces are given by

$$A \in \partial_{\dot{\xi}, \dot{\varepsilon}^{\mathrm{tr}}} d(\varepsilon, \xi, \varepsilon^{\mathrm{tr}}, \dot{\xi}, \dot{\varepsilon}^{\mathrm{tr}})$$

- To ensure thermodanymical consistency (second law of thermodynamics) the dissipation potential is convex and zero for zero rates

Plasticity in the GSM network

- For von-Mises plasticity we set

$$\phi(\varepsilon, \varepsilon_{\mathrm{pl}}) = \frac{1}{2}\varepsilon_{\mathrm{el}}\mathbb{C}\varepsilon_{\mathrm{el}}$$
$$d(\dot{\varepsilon}_{\mathrm{pl}}) = \alpha|\dot{\varepsilon}_{\mathrm{pl}}|$$

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$$\Downarrow$$

We will restrict our modelling only to rate-independent processes in shape-memory alloys

From dissipation potential to a dissipation distance

For our modelling we will use yet another approach and define

$$\delta(\alpha_A,\alpha_B) := \inf\left\{ \int_{\alpha_A \to \alpha_B} d(\alpha,\dot{\alpha})\,\mathrm{d}\Gamma;\ \text{over all smooth paths from } \alpha_A \text{ to } \alpha_B \right\}$$

a dissipation distance between two states α_A, α_B

Since the dissipation is independent of the speed, we can find a path that leads to minimal dissipation between two states ⇝ this defines the dissipation distance

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- If the dissipation distance is derived from a potential, we have that

$$d(\alpha, \dot{\alpha}) = \lim_{\epsilon \to 0^+} \frac{1}{\epsilon} \delta(\alpha, \alpha + \epsilon \dot{\alpha})$$

(*but otherwise the “reverse” relation is unclear*)

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a dissipation distance between two states α_A, α_B For thermodynamical consistency we will need that

- $\delta(\cdot, \cdot) \geq 0$
- δ is convex in the second variable
- it fulfills the triangle inequality

$$\delta(\alpha_A, \alpha_B) \leq \delta(\alpha_A, \alpha_C) + \delta(\alpha_C, \alpha_B)$$

for all admissible states of the system α_A, α_B, α_C.

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In our modelling, we will see the dissipation distance as the dissipation between two states within a small time increment.

Recalling: variables, energy

- For the inner variables we will take

  $$\varepsilon^{\mathrm{in}} = \xi\varepsilon^{\mathrm{tr}} \text{ (inelastic strain)} \quad \text{AND} \quad \xi \text{ (volume frac.)}$$

  with the constraints

  $$\langle\varepsilon^{\mathrm{in}}\rangle \le \xi \quad \text{AND} \quad 0 \le \xi \le 1.$$

  $\rightsquigarrow$ this corresponds to the fact that only some microstructures can be reached without elasticity

- For the energy we take the standard form

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Recalling: variables, energy

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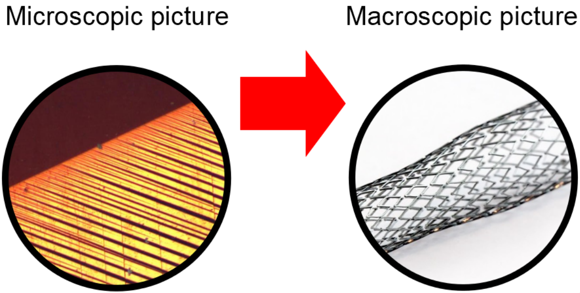

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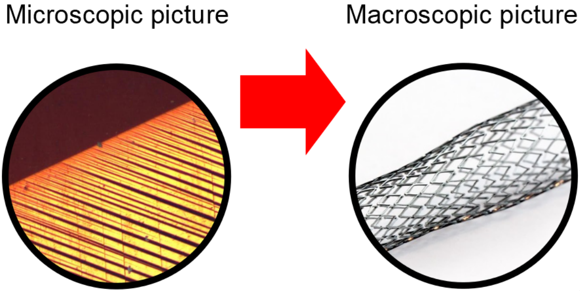

But what is missing is the microstructure formation

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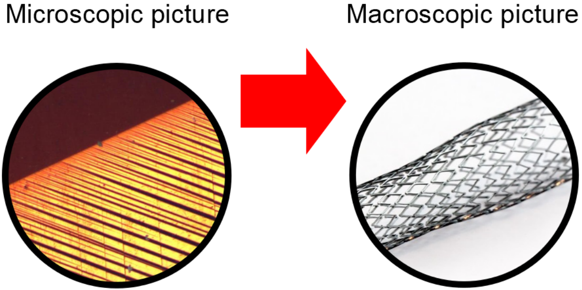

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$$\Downarrow$$

We will try to take this into account for the dissipation distance

Transformation-favourable martensite

Transformation-favourable martensite-forward

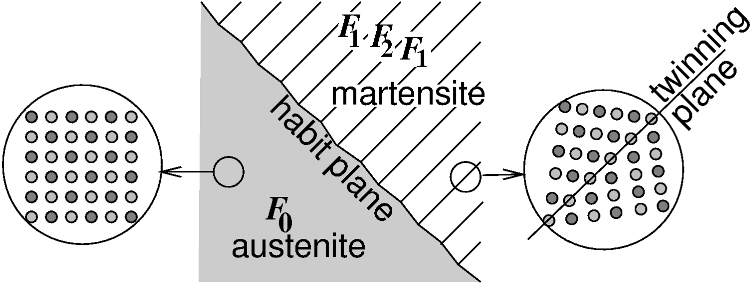
Austenite transforms to martensite always through formation of a particular martensitic structure – transformation favorable martensite (TFM) – that is characterized by zero net macroscopic strain at the moment of creation. Immediate subsequent reorientation of TFM is possible.

Transformation-favourable martensite-reverse

A necessary condition for initialisation of a reverse transformation in any amount of martensite is formation of TFM within it.

Transformation-favourable martensite

What we have in mind....



.... when an austenite-martensite interface is formed, the martensite has to form twins/microstructure at the interface for compatibility.

Transformation-favourable martensite

However,...

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Transformation-favourable martensite-reverse

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$$\Downarrow$$

this is an oversimplification!

On the microscopic level...

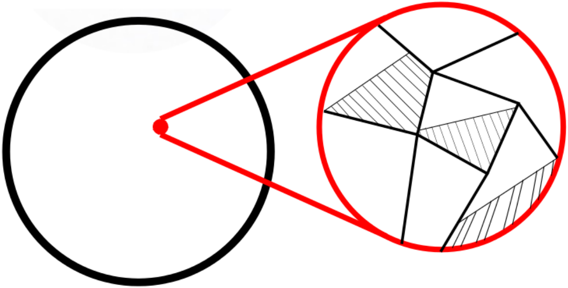
- Even for monoclinic SMAs (like NiTi) no twinned structure actually has zero-net strain.

$$\Downarrow$$

How can we actually interpret this assumption?

On the microscopic level...

Averaging...



- in every material point there are many grains with very different microstructures

On the microscopic level...

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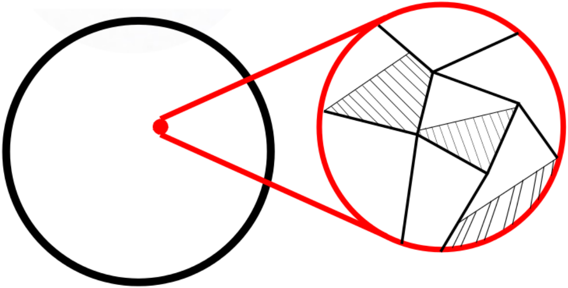

- in every material point there are many grains with very different microstructures

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However, there is no rigorous proof that the average has to be of zero-net strain

On the microscopic level...

Looking just from the dissipation point of view...

- The assumption is that there is no dissipation connected to reorientation when transforming from austenite to TFM (and back)
- in the simplified case of phenomenological modelling this is achieved by the zero-net strain assumption
- $\rightsquigarrow$ also other phenomenological models assume that the twinned structure is of zero-net inelastic strain

[Lexcellent et al; 2006], [Popov, Lagoudas; 2007]

On the microscopic level...

The best argument is of course that the derived model compares well to experiment

$$\Downarrow$$

see Petr Sedlák's talk!

Implications on the dissipation distance

- We can split the dissipation distance into a transformation part and a reorientation part:

$$\delta = \delta^{\mathrm{tr}} + \delta^{\mathrm{reo}}.$$

$$\Downarrow$$

Notice: Here this split is a consequence of formation of TFM

[Zaki, Moumni;2009], [Chemisky et al.; 2011]

Transformation part of dissipation distance

Assumption on transformation part of dissipation distance

The transformation part of dissipation distance is proportional to the absolute value of the difference between its initial and final volume fraction of martensite. The positive proportionality factor may depend (linearly) on the volume fraction.

$$\Downarrow$$

$$\delta^{\mathrm{tr}}(\xi_A, \xi_B) = c(\xi_A, \xi_B)|\xi_B - \xi_A|$$

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$\rightsquigarrow$ for thermodynamical consistency (triangle inequality) the form of $c(\xi_A, \xi_B)$ is not arbitrary

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$$\Downarrow$$

$$\delta^{\mathrm{tr}}(\xi_A, \xi_B) = c(\xi_A, \xi_B)|\xi_B - \xi_A|$$

$\rightsquigarrow$ for thermodynamical consistency (triangle inequality) the form of $c(\xi_A, \xi_B)$ is not arbitrary
Here, we take

$$\xi_B \geq \xi_A : \quad \delta^{\mathrm{tr}}(\xi_A, \xi_B) = \Delta s^{AM} \left[(T_0 - M_{\mathrm{s}}) + \frac{\xi_A + \xi_B}{2}(M_{\mathrm{s}} - M_{\mathrm{f}}) \right] |\xi_B - \xi_A|,$$

$$\xi_B < \xi_A : \quad \delta^{\mathrm{tr}}(\xi_A, \xi_B) = \Delta s^{AM} \left[(A_{\mathrm{f}} - T_0) + \frac{\xi_A + \xi_B}{2}(A_{\mathrm{s}} - A_{\mathrm{f}}) \right] |\xi_B - \xi_A|.$$

Reorientation part of dissipation distance

Assumption on the reorientation part of the dissipation distance

If martensite is subject to reorientation, the corresponding dissipation distance is proportional to the norm of the difference between its final and initial inelastic strain

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this already allows us to deduce the dissipation when no phase transition is occurring....

Austenite-to-martensite transition

If $\xi_B > \xi_A$ austenite-to-martensite:

- In the small step we look at austenite transforms to TFM $\rightsquigarrow$ dissipation-free
- Additionally other portions of martensite may reorient

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but how much TFM is formed and how does this effect the inelastic strain?

We adopt the assumption that the inelastic strain does not change during the austenite-to-martensite transition
$\rightsquigarrow$ this gives the following form of the dissipation distance:

$$\delta^{\mathrm{reo}}(\varepsilon_A^{\mathrm{in}}, \xi_A, T_B, \varepsilon_B^{\mathrm{in}}, \xi_B) = \sigma^{\mathrm{reo}}(T_B)\|\varepsilon_B^{\mathrm{in}} - \varepsilon_A^{\mathrm{in}}\|.$$

$\sigma^{\mathrm{reo}}(T_B)$ is the proportionality factor

Reorientation part - reverse transformation

- if martensite transforms to austenite ($\xi_B < \xi_A$), some portion of the inelastic strain has to transform to TFM first (to allow the transition)
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how big are the individual portions?

$$\Downarrow$$

we assume that the fraction is given by the volume fraction of the disappearing martensite

Reorientation part - reverse transformation

With this assumptions we arrive at

$$\delta^{\mathrm{reo}}(\varepsilon_A^{\mathrm{in}}, \xi_A, T_B, \varepsilon_B^{\mathrm{in}}, \xi_B) = \underbrace{\sigma^{\mathrm{reo}}(T_B) \left\| \frac{\xi_A - \xi_B}{\xi_A} \varepsilon_A^{\mathrm{in}} - 0 \right\|}_{\text{trf. to TFM}} + \underbrace{\sigma^{\mathrm{reo}}(T_B) \left\| \varepsilon_B^{\mathrm{in}} - \frac{\xi_B}{\xi_A} \varepsilon_A^{\mathrm{in}} \right\|}_{\text{remaining reorient.}}$$

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...or rewriting as

$$\delta^{\text{reo}}(\varepsilon_A^{\text{in}}, \xi_A, T_B, \varepsilon_B^{\text{in}}, \xi_B) = \sigma^{\text{reo}}(T_B)\left[\left\|\frac{\xi_B}{\xi_A}\varepsilon_A^{\text{in}} - \varepsilon_A^{\text{in}}\right\| + \left\|\varepsilon_B^{\text{in}} - \frac{\xi_B}{\xi_A}\varepsilon_A^{\text{in}}\right\|\right]$$

Comments

- In addition to the assumption on TFM we had to assume how "big" the portion of inelastic strain is that is due to TFM $\rightsquigarrow$ complicated microstructure is represented by just one tensor
- During forward transformation the inelastic strain is unchanged
  $\rightsquigarrow$ *Heuristic idea:* Material can accommodate the transformation, the forward transformation is "preferred"
- During reverse transformation the assumption can be also read as: no TFM is in the material, all has to be formed
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$$\Downarrow$$

Nevertheless, also other settings would be compatible with the TFM idea...

Summing up

Altogether, we have the following energy and dissipation distance in one material point:

$$\begin{aligned}
\phi(T,\varepsilon,\varepsilon^{\mathrm{in}},\xi,\eta) &= \frac{1}{2}K\mathrm{tr}(\varepsilon)^2 + G(\xi,\eta)\|\mathrm{dev}(\varepsilon)-\varepsilon^{\mathrm{in}}\|^2 \\
&\quad + \Delta s^{AM}(T-T_0)\xi \\
&\quad + u_0^A - s_0^A T + c^A\left[(T-T_0) - T\ln\left(\frac{T}{T_0}\right)\right], \\
\delta(T,\varepsilon_A^{\mathrm{in}},\xi_A,\varepsilon_B^{\mathrm{in}},\xi_B) &= \begin{cases} c(\xi_A,\xi_b)|\xi_B-\xi_A| & +\,\sigma^{\mathrm{reo}}\|\varepsilon_B^{\mathrm{in}}-\varepsilon_A^{\mathrm{in}}\| \\ & \text{if } \xi_B \geq \xi_A, \\ c(\xi_A,\xi_b)|\xi_B-\xi_A| & +\,\sigma^{\mathrm{reo}}\left[\|\frac{\xi_B}{\xi_A}\varepsilon_A^{\mathrm{in}}-\varepsilon_A^{\mathrm{in}}\|\right. \\ \left.+\|\varepsilon_B^{\mathrm{in}}-\frac{\xi_B}{\xi_A}\varepsilon_A^{\mathrm{in}}\|\right] & \text{if } \xi_B < \xi_A. \end{cases}
\end{aligned}$$

Thermodynamical consistency

Notice that the proposed dissipation distance

$$\delta(T, \varepsilon^{\mathrm{in}}_A, \xi_A, \varepsilon^{\mathrm{in}}_B, \xi_B) \quad = \quad \begin{cases} c(\xi_A, \xi_b)|\xi_B - \xi_A| & + \, \sigma^{\mathrm{reo}} \|\varepsilon^{\mathrm{in}}_B - \varepsilon^{\mathrm{in}}_A\| \\ & \text{if } \xi_B \geq \xi_A, \\ & \\ c(\xi_A, \xi_b)|\xi_B - \xi_A| & + \, \sigma^{\mathrm{reo}} \Big[\| \frac{\xi_B}{\xi_A} \varepsilon^{\mathrm{in}}_A - \varepsilon^{\mathrm{in}}_A \| \\ + \| \varepsilon^{\mathrm{in}}_B - \frac{\xi_B}{\xi_A} \varepsilon^{\mathrm{in}}_A \| \Big] & \text{if } \xi_B < \xi_A. \end{cases}$$

- is non-negative (and zero if no change of state occurs)
- is convex in the *B*-variables
- satisfies the triangle inequality

Global formulation

The derived energy and dissipation distance hold for *one material point*. For the whole specimen (Ω) we have to integrate (here u is the underlying deformation and $\alpha := (\varepsilon^{\mathrm{in}}, \xi)$ are the dissipative variables):

$$\mathcal{E}(t,u,\alpha) := \int_\Omega \phi(t,\varepsilon(u),\alpha) + \underbrace{\nu\|\nabla\alpha(t)\|^2}_{\text{regularization term}} - \underbrace{F_{\mathrm{vol}}(t)\cdot u}_{\text{volume force}}\,\mathrm{d}x \\ - \int_{\Gamma_{\mathrm{N}}} \underbrace{F_{\mathrm{surf}}\cdot u}_{\text{surface force}}(t)\,\mathrm{d}S,$$

$$\begin{aligned} \mathcal{D}(t,\alpha,\tilde{\alpha}) &:= \mathcal{D}^{\mathrm{tr}}(t,\alpha,\tilde{\alpha}) + \mathcal{D}^{\mathrm{reo}}(t,\alpha,\tilde{\alpha}) \\ &= \int_\Omega \delta^{\mathrm{tr}}(t,\alpha,\tilde{\alpha})\mathrm{d}x + \int_\Omega \delta^{\mathrm{reo}}(t,\alpha,\tilde{\alpha})\mathrm{d}x. \end{aligned}$$

Global formulation

The variables are limited to the following sets:

$$\mathcal{Q} := \big\{ (u, \alpha) \in \mathcal{U} \times \mathcal{V} \times \mathcal{Z} \;\; \text{with } \alpha = (\varepsilon^{\mathrm{in}}, \xi) \big\}$$

where

$$\begin{aligned}
\mathcal{U} &:= \{ u \in W^{1,2}(\Omega, \mathbb{R}^3) : u = 0 \text{ on } \Gamma_{\mathrm{D}} \} \\
\mathcal{V} &:= \{ (\varepsilon^{\mathrm{in}}, \xi) \in W^{1,2}(\Omega, \mathbb{R}^{3\times 3}) \times W^{1,2}(\Omega) \;\; : \\
&\qquad \varepsilon^{\mathrm{in}} \text{ is a traceless, symmetric matrix,} \\
&\qquad \langle \varepsilon^{\mathrm{in}}(x) \rangle \leq \xi(x) \text{ for a.a.} x \in \Omega \\
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the triple $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$ defines the rate-independent system under consideration

Energetic solution

With the energy and dissipation distance given, we can define an an energetic solution for the problem:

- ideally fitted for rate-independent processes
- a global, derivative-free solution concept (avoids subdifferential calculation)
- based on energy conservation and the idea that for any time instant the found state is “the best possible”

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$$\Downarrow$$

In other words, as soon as a process is admissible from the thermodynamic point of view, it will happen immediately

Energetic solution

Definition of an energetic solution

Let $\mathcal{E}, \mathcal{D}$ be given as above and let $(u_0, \alpha_0) \in \mathcal{Q}$. Then triplet $(u(t), \alpha(t), \eta(t)) : [0, \mathcal{T}] \mapsto \mathcal{Q}$ is called an *energetic solution* to the rate-independent system $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$ if $\partial_t \mathcal{E}(t, u(t)) \in L^1([0, \mathcal{T}])$ and if the following conditions are satisfied:

- **Stability condition:** (for all $(\tilde{u}, \tilde{\alpha}, \tilde{\eta}) \in \mathcal{Q}$)

$$\mathcal{E}(t, u(t), \alpha(t), \eta(t)) \leq \mathcal{E}(t, \tilde{u}, \tilde{\alpha}, \tilde{\eta}) + \mathcal{D}(t, \alpha(t), \tilde{\alpha})$$

- **Energy balance:**

$$\begin{aligned}&\mathcal{E}(t, u(t), \alpha(t), \eta(t)) + \mathrm{Diss}_{\mathcal{D}}(\alpha, [0, \mathcal{T}])\\ &\quad = \mathcal{E}(0, u(0), \alpha(0), \eta(0)) + \int_0^{\mathcal{T}} \partial_t \mathcal{E}(s, u(s)) \mathrm{d}s.\end{aligned}$$

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$\mathrm{Diss}_{\mathcal{D}}(\alpha, [0, \mathcal{T}])$ is the overall dissipated energy

- For smooth processes it is given by

$$\mathrm{Diss}_{\mathcal{D}}(\alpha; [0, \mathcal{T}]) = \int_0^{\mathcal{T}} \int_\Omega d(t, \alpha(t), \dot{\alpha}(t)) \mathrm{d}x \mathrm{d}t,$$

  $\rightsquigarrow \delta$ is the dissipation potential.

- For processes with jumps, we have that

$$\mathrm{Diss}^{\mathrm{tr}}(\alpha; [0, \mathcal{T}]) := \sup \Big\{ \sum_{i=1}^{N} \mathcal{D}^{\mathrm{tr}}(\alpha(t_{i-1}), \alpha(t_i)) \; : \\ \text{a.p.p.} \;\; 0 = t_0 \leq t_1 \leq \ldots \leq t_N = \mathcal{T} \Big\},$$

- If the dissipation distance depends on time (*as the reorientation part through temperature*) in has to be defined via a suitable Radon measure

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Existence of an energetic solution

Theorem (MF, BB, PS, '14)

Let $\mathcal{E}, \mathcal{D}$ *be defined by as above, let the prescribed forces be "sufficiently smooth" and let initial conditions* $(u_0, \alpha_0, \eta_0) \in \mathcal{Q}$ *satisfy the stability condition. Then there exists an energetic solution of the rate-independent system* $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$*.*

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$$\Downarrow$$

For the proof, we highlight just some steps...

Time-incremental minimization

Discrete level

We call $(u_\tau^k, \alpha_\tau^k) \in \mathcal{Q}$ a discrete energetic solution to rate-independent system $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$ at time-level $k = 1, \ldots, N(\tau)$ if it solves

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with $(u_\tau^0, \alpha_\tau^0) = (u_0, \alpha_0) \in \mathcal{Q}$ defined through the initial condition.

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$$\Downarrow$$

at every time-step we minimize the energy + dissipation from the last step

Convexity of the energy

- to assure existence of solutions to (TIP) it is important that $\mathcal{E}$ and $\mathcal{D}$ are *convex*
- for the dissipation distance this comes directly from thermodynamical consistency (*convexity in the second variable*)
- for the energy this is due to the choice of variables

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Convexity of the energy

Recall the energy function

$$\begin{aligned}\phi(T,\varepsilon,\varepsilon^{\mathrm{in}},\xi) \quad &= \quad \frac{1}{2}K\,\mathrm{tr}(\varepsilon)^2 + G(\xi)\|\mathrm{dev}(\varepsilon)-\varepsilon^{\mathrm{in}}\|^2 \\ &\quad + \Delta s^{AM}(T-T_0)\xi \\ &\quad + u_0^A - s_0^A T + c^A\left[(T-T_0) - T\ln\left(\frac{T}{T_0}\right)\right],\end{aligned}$$

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$$\Downarrow$$

if we used the *transformation strain* instead of the *inelastic* one, we would have

$$\begin{aligned}\phi(T,\varepsilon,\varepsilon^{\mathrm{in}},\xi) &= \frac{1}{2}K\,\mathrm{tr}(\varepsilon)^2 + G(\xi)\|\mathrm{dev}(\varepsilon) - \xi\varepsilon^{\mathrm{tr}}\|^2 \\ &\quad + \Delta s^{AM}(T - T_0)\xi \\ &\quad + u_0^A - s_0^A T + c^A\left[(T - T_0) - T\ln\left(\frac{T}{T_0}\right)\right],\end{aligned}$$

which is no longer convex...

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- The explicit dependence $G = G(\xi)$ affects the overall convexity of the energy.
- We use a form $G(\xi) \sim \frac{1}{\xi}$ so that the overall energy is of the form $\frac{y^2}{x} \rightsquigarrow$ convex for $x \geq 0$.

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Aside: Notes on implementation

The time-incremental problem

$$\begin{aligned}&\text{Minimize } \mathcal{E}(t_k, u, \alpha) + \mathcal{D}(t_k, \alpha_\tau^{k-1}, \alpha)\\ &\text{subject to } (u, \alpha) \in \mathcal{Q}\end{aligned} \tag{TIP}$$

is also the basis for numerical implementation

[Bourdin; 2007], [Bourdin, Francfort, Marigo; 2008]

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$$\Downarrow$$

This will converge to a critical point (and due to convexity) a minimizer.

[Bourdin; 2007], [Bourdin, Francfort, Marigo; 2008]

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is also the basis for numerical implementation

Advantages of the split:

1. The elasticity problem (for u) can be solved by standard packages in FEM
2. The problem for the inner variables actually splits and can be solved individually for each material (Gauß) point $\rightsquigarrow$ this allows to use a *derivative-free* method like the Nelder-Mead algorithm

[Bourdin; 2007], [Bourdin, Francfort, Marigo; 2008]

Discrete stability and two-sided energy inequality

Recall the time-incremental problem

$$\begin{aligned} &\text{Minimize } \mathcal{E}(t_k, u, \alpha,) + \mathcal{D}(t_k, \alpha_\tau^{k-1}, \alpha) \\ &\text{subject to } (u, \alpha) \in \mathcal{Q} \end{aligned} \qquad \text{(TIP)}$$

Discrete stability and two-sided energy inequality

From this we obtain the discrete stability condition

$$\mathcal{E}(t_k, u_k, \alpha_k,) \leq \mathcal{E}(t_k, \tilde{u}, \tilde{\alpha},) + \mathcal{D}(t_k, \alpha_k, \tilde{\alpha}) \quad \forall\, (\tilde{u}, \tilde{\alpha}) \in \mathcal{Q}$$

Discrete stability and two-sided energy inequality

From this we obtain the discrete stability condition

$$\mathcal{E}(t_k, u_k, \alpha_k,) \leq \mathcal{E}(t_k, \tilde{u}, \tilde{\alpha},) + \mathcal{D}(t_k, \alpha_k, \tilde{\alpha}) \quad \forall\, (\tilde{u}, \tilde{\alpha}) \in \mathcal{Q}$$

And the energy inequalities

$$\begin{aligned}\int_{t_{k-1}}^{t_k} \partial \mathcal{E}_t(s, u_k(s))\mathrm{d}s &\leq \mathcal{E}(t_k, u_k, \alpha_k,) + \mathcal{D}(t_k, \alpha_{k-1}, \alpha_k) \\ &\quad - \mathcal{E}(t_{k-1}, u_{k-1}, \alpha_{k-1}) \\ &\leq \int_{t_{k-1}}^{t_k} \partial_t \mathcal{E}(s, u_{k-1}(s))\mathrm{d}s.\end{aligned}$$

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$$\Downarrow$$

here it is important that the dissipation distance satisfies the triangle inequality!

Aside: Using the two-sided energy inequality in non-convex problems

In non-convex situations (with many local minima) it is advantageous to verify the energy inequality

$$\begin{aligned}\int_{t_{k-1}}^{t_k} \partial\mathcal{E}_t(s, u_k(s))\mathrm{d}s &\leq \mathcal{E}(t_k, u_k, \alpha_k,) + \mathcal{D}(t_k, \alpha_{k-1}, \alpha_k) \\ &\quad - \mathcal{E}(t_{k-1}, u_{k-1}, \alpha_{k-1}) \\ &\leq \int_{t_{k-1}}^{t_k} \partial_t\mathcal{E}(s, u_{k-1}(s))\mathrm{d}s.\end{aligned}$$

in every step ($\rightsquigarrow$ particularly the “first” inequality)

[B., 2009]

Aside: Using the two-sided energy inequality in non-convex problems

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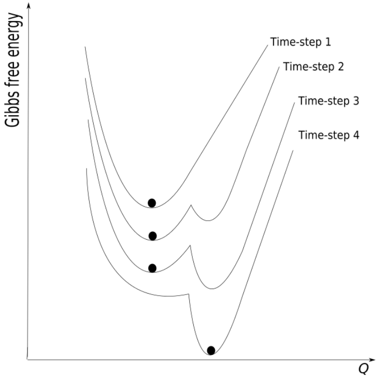
in every step ($\rightsquigarrow$ particularly the "first" inequality)

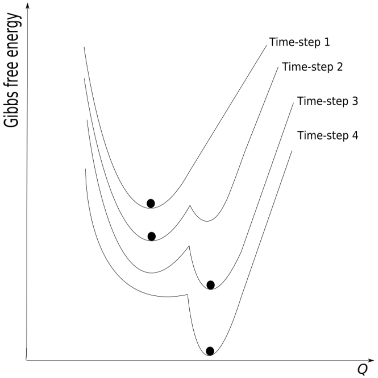
$$\Downarrow$$

this helps to identify whether the found minimum would not have been optimal already in the last time-step.

[B., 2009]

Aside: Using the two-sided energy inequality in non-convex problems





[B., 2009]

Convergence

- Based on the a-priori estimates we choose convergent sub-sequences for $\tau \to 0$
- The converges is pointwise for every time-step
- Here we additionaly have to cope with the fact that the dissipation distance depends on time (through temperature)

Obtained result

Theorem (MF, BB, PS, '14)

Let $\mathcal{E}, \mathcal{D}$ be defined by as above, let the prescribed forces be "sufficiently smooth" and let initial conditions $(u_0, \alpha_0, \eta_0) \in \mathcal{Q}$ satisfy the stability condition. Then there exists an energetic solution of the rate-independent system $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$, that is

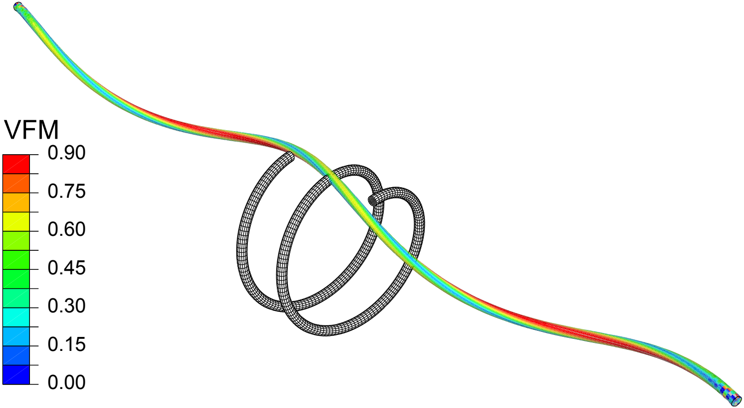
- **Stability condition:** *(for all $(\tilde{u}, \tilde{\alpha}, \tilde{\eta}) \in \mathcal{Q}$)*

$$\mathcal{E}(t, u(t), \alpha(t)) \leq \mathcal{E}(t, \tilde{u}, \tilde{\alpha}) + \mathcal{D}(t, \alpha(t), \tilde{\alpha})$$

- **Energy balance:**

$$\begin{aligned}\mathcal{E}(t, u(t), \alpha(t)) &+ \mathrm{Diss}_{\mathcal{D}}(\alpha, [0, \mathcal{T}]) \\ &= \mathcal{E}(0, u(0), \alpha(0)) + \int_0^{\mathcal{T}} \partial_t \mathcal{E}(s, u(s)) \mathrm{d}s.\end{aligned}$$

A numerical calculation



Reference

Frost, M., Benešová, B., Sedlák, P.: A microscopically motivated constitutive model for shape memory alloys: formulation, analysis and computations, Math. Mech. Solids, 21(3) (2016), 358-382.

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Thank you for your attention!