Bounds and estimates on the effective energy

of shape memory alloys

Michaël Peigney

Laboratoire Navier
(Ecole des Ponts ParisTech, IFSTTAR, CNRS)
University Paris-Est, France

Introduction

Three length scales are involved :

- the microscopic scale of the austenite/martensite microstructure.
- the mesoscopic scale, corresponding to the typical length scale of a grain.
- the macroscopic scale, corresponding to an assemblage of numerous grains.

Microscopic free energy (geometrically linear theory)

The microscopic free energy Ψ^0 is modelled as a multiwell function of the form

$$\Psi^0(\varepsilon) = \min_{1 \leq i \leq k} \Psi_i^0(\varepsilon)$$

where

$$\Psi_i^0(\varepsilon) = \frac{1}{2}(\varepsilon - \varepsilon_i^0) : \boldsymbol{L}^0 : (\varepsilon - \varepsilon_i^0) + w_i^0$$

represents the free energy of phase i.

Elastic energy minimization

- The mesoscopic free energy of the reference single crystal is the relaxation (or quasi-convexification) of Ψ^0
- The macroscopic free energy is obtained by homogenization, and depends on the texture of the polycrystal.
- The exact expressions of the mesoscopic and the macroscopic free energy remains elusive in the general case.

Single crystal : lower bound on the energy

Polycrystal : lower bound on the energy

Simple examples

Computational aspects

Upper bounds and estimates

Mesoscopic free energy

The mesoscopic free energy of the reference single crystal is

$$Q\Psi^0(\bar{\varepsilon}) = \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_\Omega \Psi^0(\varepsilon)\, dx$$

where

$$\mathcal{K}(\bar{\varepsilon}) = \{\varepsilon | \exists \boldsymbol{u}(\boldsymbol{x}) \text{ such that } \varepsilon = (\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u})/2 \text{ in } \Omega; \boldsymbol{u}(\boldsymbol{x}) = \bar{\varepsilon}.\boldsymbol{x} \text{ on } \partial\Omega\}$$

Mesoscopic free energy

Following Kohn(1991), we have

$$Q\Psi^0(\bar{\varepsilon}) = \inf_{\boldsymbol{\theta} \in \mathcal{T}} Q\Psi^0(\bar{\varepsilon}, \boldsymbol{\theta})$$

where $\mathcal{T} = \{\boldsymbol{\theta} = (\theta_1 \cdots, \theta_k) \in \mathbb{R}_k | \theta_i \geq 0; \sum_{i=1}^{k} \theta_i = 1\}$ and

$$Q\Psi^0(\bar{\varepsilon}, \boldsymbol{\theta}) = \inf_{\chi_i} \inf_{\boldsymbol{\varepsilon} \in \mathcal{K}(\bar{\boldsymbol{\varepsilon}})} \frac{1}{|\Omega|} \int_\Omega \sum_{i=1}^{k} \chi_i(\boldsymbol{x}) \Psi_i^0(\varepsilon)\, d\boldsymbol{x}$$

The first infimum is taken over characteristic functions χ_i compatible with volume fractions $\boldsymbol{\theta}$. Such functions satisfy

$$\chi_i(\boldsymbol{x}) \in \{0, 1\};\ 1 = \sum_{i=1}^{k} \chi_i(\boldsymbol{x});\ \theta_i = \frac{1}{|\Omega|} \int_\Omega \chi_i(\boldsymbol{x})\, d\boldsymbol{x}$$

A general lower bound on $Q\Psi^0$

- For arbitrary *comparison potential* $\mathrm{U}(\varepsilon)$ and *polarization* $\boldsymbol{\tau}$, introduce the Legendre transform :

$$(\Psi_i^0 - \mathrm{U})_*(\boldsymbol{\tau}) = \sup_{\varepsilon} \varepsilon : \boldsymbol{\tau} - \Psi_i^0(\varepsilon) + \mathrm{U}(\varepsilon)$$

- From that definition, we obtain

$$\sum_{i=1}^{k} \chi_i(\boldsymbol{x})\Psi_i^0(\varepsilon) \geq \varepsilon : \boldsymbol{\tau} - \sum_{i=1}^{k} \chi_i(\boldsymbol{x})(\Psi_i^0 - \mathrm{U})_*(\boldsymbol{\tau}) + \mathrm{U}(\varepsilon)$$

- Taking '$\inf_{\chi_i} \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \int_\Omega$' yields

$$Q\Psi^0(\bar{\varepsilon}, \boldsymbol{\theta}) \geq \bar{\varepsilon} : \boldsymbol{\tau} - \sum_{i=1}^{k} \theta_i(\Psi_i^0 - \mathrm{U})_*(\boldsymbol{\tau}) + \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_\Omega \mathrm{U}(\varepsilon)\, dx$$

Choice of comparison potential U

$$Q\Psi^0(\bar{\varepsilon},\boldsymbol{\theta}) \geq \bar{\varepsilon} : \boldsymbol{\tau} - \sum_{i=1}^k \theta_i (\Psi_i^0 - \mathrm{U})_*(\boldsymbol{\tau}) + \inf_{\boldsymbol{\varepsilon}\in\mathcal{K}(\bar{\boldsymbol{\varepsilon}})} \frac{1}{|\Omega|}\int_\Omega \mathrm{U}(\varepsilon)\, d\boldsymbol{x}$$

Choosing $\mathrm{U}(\varepsilon) = 0$ gives the *convexification* lower bound :

$$Q\Psi^0(\bar{\varepsilon}) \geq \inf_{\boldsymbol{\theta}\in\mathcal{T}} C\Psi^0(\bar{\varepsilon},\boldsymbol{\theta})$$

with

$$C\Psi^0(\bar{\varepsilon},\boldsymbol{\theta}) = \frac{1}{2}(\bar{\varepsilon} - \varepsilon^0(\boldsymbol{\theta})) : \boldsymbol{L}^0 : (\bar{\varepsilon} - \varepsilon^0(\boldsymbol{\theta})) + \sum_{i=1}^k \theta_i w_i^0$$

and $\varepsilon^0(\boldsymbol{\theta}) = \sum_{i=1}^k \theta_i \varepsilon_i^0$

Choice of comparison potential U

$$Q\Psi^0(\bar{\varepsilon}, \boldsymbol{\theta}) \geq \bar{\varepsilon} : \boldsymbol{\tau} - \sum_{i=1}^{k} \theta_i (\Psi_i^0 - \mathrm{U})_*(\boldsymbol{\tau}) + \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_\Omega \mathrm{U}(\varepsilon)\, dx$$

We choose $\mathrm{U}(\varepsilon) = \frac{1}{2}\varepsilon : \boldsymbol{K} : \varepsilon$ with $\boldsymbol{K}$ such that

- $\boldsymbol{L}^0 - \boldsymbol{K} \succ 0$
- $\boldsymbol{K}$ 'quasiconvex', i.e. :

$$\bar{\varepsilon} : \boldsymbol{K} : \bar{\varepsilon} \leq \frac{1}{|\Omega|} \int_\Omega \varepsilon : \boldsymbol{K} : \varepsilon\, dx \quad \forall \varepsilon \in \mathcal{K}(\bar{\varepsilon})$$

A lower bound on $Q\Psi^0(\bar{\varepsilon}, \theta)$

After some manipulation, we find :

$$Q\Psi^0(\bar{\varepsilon}, \boldsymbol{\theta}) \geq \frac{1}{2}\bar{\varepsilon} : \boldsymbol{K} : \bar{\varepsilon} + \bar{\varepsilon} : \boldsymbol{\tau} + F^r(\boldsymbol{\theta}; \boldsymbol{K}, \boldsymbol{\tau})$$

where

$$\begin{aligned} F^r(\boldsymbol{\theta}; \boldsymbol{K}, \boldsymbol{\tau}) \geq \quad & -\tfrac{1}{2}\boldsymbol{\tau} : (\boldsymbol{L}^0 - \boldsymbol{K})^{-1} : \boldsymbol{\tau} + \sum_{i=1}^{k} \theta_i w_i^0 \\ & -\boldsymbol{\tau} : (\boldsymbol{L}^0 - \boldsymbol{K})^{-1} : \boldsymbol{L}^0 : \varepsilon^0(\boldsymbol{\theta}) + \tfrac{1}{2} \sum_{i=1}^{k} \theta_i \varepsilon_i^0 : \boldsymbol{M}^0(\boldsymbol{K}) : \varepsilon_i^0 \end{aligned}$$

(quadratic in $\boldsymbol{\tau}$)

and

$$\varepsilon^0(\boldsymbol{\theta}) = \sum_{i=1}^{k} \theta_i \varepsilon_i^0 \ , \ \ \boldsymbol{M}^0(\boldsymbol{K}) = \boldsymbol{L}^0 - \boldsymbol{L}^0 : (\boldsymbol{L}^0 - \boldsymbol{K})^{-1} : \boldsymbol{L}^0$$

A lower bound on $Q\Psi^0$

Optimizing with respect to $\boldsymbol{\tau}$ yields

$$Q\Psi^0(\bar{\varepsilon}) \geq \inf_{\boldsymbol{\theta}\in\mathcal{T}} \{C\Psi^0(\bar{\varepsilon},\boldsymbol{\theta}) + g(\boldsymbol{\theta})\}$$

where

$$g(\boldsymbol{\theta}) = \frac{1}{2}\sum_{i,j=1}^{k} \theta_i\theta_j(\varepsilon_i^0 - \varepsilon_j^0) : \boldsymbol{M}^0(\boldsymbol{K}) : (\varepsilon_i^0 - \varepsilon_j^0)$$

A family of quasiconvex tensors $\boldsymbol{K}$

Let ε^* be the adjugate of ε, i.e :

$$\varepsilon^*_{ii} = \varepsilon_{jj}\varepsilon_{kk} - \varepsilon^2_{jk} \ , \ \varepsilon^*_{jk} = \varepsilon_{ji}\varepsilon_{ki} - \varepsilon_{jk}\varepsilon_{ii}$$

Define $\boldsymbol{K}(\boldsymbol{a})$ by

$$\frac{1}{2}\boldsymbol{\varepsilon} : \boldsymbol{K}(\boldsymbol{a}) : \boldsymbol{\varepsilon} = -\boldsymbol{a} : \boldsymbol{\varepsilon}^*$$

The tensors $\boldsymbol{K}(\boldsymbol{a})$ are quasiconvex for $\boldsymbol{a} \succeq 0$.

Using that family of tensors, we obtain

$$g(\boldsymbol{\theta}) = \sup_{\boldsymbol{K} \in \mathcal{C}} \frac{1}{4} \sum_{i,j} \theta_i \theta_j (\boldsymbol{\varepsilon}^0_i - \boldsymbol{\varepsilon}^0_j) : \boldsymbol{M}^0(\boldsymbol{K}) : (\boldsymbol{\varepsilon}^0_i - \boldsymbol{\varepsilon}^0_j)$$

with

$$\mathcal{C} = \{\boldsymbol{K}(\boldsymbol{a}) : \boldsymbol{a} \succeq 0, \boldsymbol{L}^0 - \boldsymbol{K}(\boldsymbol{a}) \succ 0\}$$

Summary

$$Q\Psi^0(\bar{\varepsilon}) \geq \inf_{\boldsymbol{\theta}\in\mathcal{T}} \{C\Psi^0(\bar{\varepsilon},\boldsymbol{\theta}) + g(\boldsymbol{\theta})\}$$

with

$$g(\boldsymbol{\theta}) = \sup_{\boldsymbol{K}\in\mathcal{C}} \frac{1}{4}\sum_{i,j} \theta_i\theta_j(\varepsilon_i^0 - \varepsilon_j^0) : \boldsymbol{M}^0(\boldsymbol{K}) : (\varepsilon_i^0 - \varepsilon_j^0)$$

and

$$\mathcal{C} = \{\boldsymbol{K}(\boldsymbol{a}) : \boldsymbol{a} \succeq 0, \boldsymbol{L}^0 - \boldsymbol{K}(\boldsymbol{a}) \succ 0\}$$

- coincides with the solution of Kohn(1991) for the two-well problem
- g is identically null if all the transformation strains ε_i^0 are pairwise compatible.

Polycrystal

$$Q\Psi(\varepsilon, \boldsymbol{x}) = \sum_{r=1}^{n} \chi^r(\boldsymbol{x}) Q\Psi^r(\varepsilon) \qquad Q\Psi^r(\varepsilon) = Q\Psi^0(\boldsymbol{R}^{r,T} \varepsilon \boldsymbol{R}^r)$$

- The texture of the polycrystal is described by characteristic functions χ^r $(r = 1, \cdots, n)$, such that the domain $\Omega^r = \{\boldsymbol{x} \in \Omega | \chi^r(\boldsymbol{x}) = 1\}$ is occupied by grains with the same orientation relative to a reference single crystal.

The macroscopic (or effective) energy of the polycrystal is

$$\Psi^{eff}(\bar{\varepsilon}) = \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_{\Omega} \sum_{r=1}^{n} \chi^r(\boldsymbol{x}) Q\Psi^r(\varepsilon)\, d\boldsymbol{x}$$

Bounding $\Psi^{eff}(\bar{\varepsilon})$ from below

$$\Psi^{eff}(\bar{\varepsilon}) = \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_\Omega \sum_{r=1}^{n} \chi^r(\boldsymbol{x}) Q\Psi^r(\varepsilon)\, d\boldsymbol{x}$$

- Consider a given strain field ε in $\mathcal{K}(\bar{\varepsilon})$:
  - Step 1 : Get a pointwise lower bound on $Q\Psi^r(\varepsilon(\boldsymbol{x}))$
  - Step 2 : Bound the total energy $\int_\Omega \sum_r \chi^r Q\Psi^r(\varepsilon, \boldsymbol{x}) dx$
  - Step 3 : Make that point independent of ε

Step 1 - Pointwise lower bound on $Q\Psi^r(\varepsilon(\boldsymbol{x}))$

- Consider a given strain field ε in $\mathcal{K}(\bar{\varepsilon})$. For a given $\boldsymbol{x}$ in Ω, we have

$$Q\Psi^r(\varepsilon(\boldsymbol{x})) = \inf_{\boldsymbol{\theta}\in\mathcal{T}} Q\Psi(\varepsilon(\boldsymbol{x}),\boldsymbol{\theta}) \geq \inf_{\boldsymbol{\theta}\in\mathcal{T}} Q\Psi^r_-(\varepsilon(\boldsymbol{x}),\boldsymbol{\theta})$$

where

$$Q\Psi^r_-(\varepsilon(\boldsymbol{x}),\boldsymbol{\theta}) = \sup_{\boldsymbol{K}\in\mathcal{C}} \sup_{\boldsymbol{\tau}} \frac{1}{2}\varepsilon(\boldsymbol{x}) : \boldsymbol{K} : \varepsilon(\boldsymbol{x}) + \varepsilon : \boldsymbol{\tau} + F^r(\boldsymbol{\theta};\boldsymbol{K},\boldsymbol{\tau})$$

Step 1 - Pointwise lower bound on $Q\Psi^r(\varepsilon(\boldsymbol{x}))$

- Consider a given strain field ε in $\mathcal{K}(\bar{\varepsilon})$. For a given $\boldsymbol{x}$ in Ω, we have

$$Q\Psi^r(\varepsilon(\boldsymbol{x})) = \inf_{\boldsymbol{\theta}\in\mathcal{T}} Q\Psi(\varepsilon(\boldsymbol{x}), \boldsymbol{\theta}) \geq \inf_{\boldsymbol{\theta}\in\mathcal{T}} Q\Psi^r_-(\varepsilon(\boldsymbol{x}), \boldsymbol{\theta})$$

  where

$$Q\Psi^r_-(\varepsilon(\boldsymbol{x}), \boldsymbol{\theta}) = \sup_{\boldsymbol{K}\in\mathcal{C}} \sup_{\boldsymbol{\tau}} \frac{1}{2}\varepsilon(\boldsymbol{x}) : \boldsymbol{K} : \varepsilon(\boldsymbol{x}) + \varepsilon : \boldsymbol{\tau} + F^r(\boldsymbol{\theta}; \boldsymbol{K}, \boldsymbol{\tau})$$

- There exists $\boldsymbol{\Theta}^r(\boldsymbol{x}) \in \mathcal{T}$ such that

$$\inf_{\boldsymbol{\theta}\in\mathcal{T}} Q\Psi^r_-(\varepsilon(\boldsymbol{x}), \boldsymbol{\theta}) = Q\Psi^r_-(\varepsilon(\boldsymbol{x}), \boldsymbol{\Theta}^r(\boldsymbol{x}))$$

Step 1 - Pointwise lower bound on $Q\Psi^r(\varepsilon(\boldsymbol{x}))$

- Consider a given strain field ε in $\mathcal{K}(\bar{\varepsilon})$. For a given $\boldsymbol{x}$ in Ω, we have

$$Q\Psi^r(\varepsilon(\boldsymbol{x})) = \inf_{\boldsymbol{\theta}\in\mathcal{T}} Q\Psi(\varepsilon(\boldsymbol{x}),\boldsymbol{\theta}) \geq \inf_{\boldsymbol{\theta}\in\mathcal{T}} Q\Psi^r_-(\varepsilon(\boldsymbol{x}),\boldsymbol{\theta})$$

  where

$$Q\Psi^r_-(\varepsilon(\boldsymbol{x}),\boldsymbol{\theta}) = \sup_{\boldsymbol{K}\in\mathcal{C}} \sup_{\boldsymbol{\tau}} \frac{1}{2}\varepsilon(\boldsymbol{x}) : \boldsymbol{K} : \varepsilon(\boldsymbol{x}) + \varepsilon : \boldsymbol{\tau} + F^r(\boldsymbol{\theta};\boldsymbol{K},\boldsymbol{\tau})$$

- There exists $\boldsymbol{\Theta}^r(\boldsymbol{x}) \in \mathcal{T}$ such that

$$\inf_{\boldsymbol{\theta}\in\mathcal{T}} Q\Psi^r_-(\varepsilon(\boldsymbol{x}),\boldsymbol{\theta}) = Q\Psi^r_-(\varepsilon(\boldsymbol{x}),\boldsymbol{\Theta}^r(\boldsymbol{x}))$$

- Hence

$$Q\Psi^r(\varepsilon(\boldsymbol{x})) \geq \sup_{\boldsymbol{K}\in\mathcal{C}} \sup_{\boldsymbol{\tau}} \frac{1}{2}\varepsilon(\boldsymbol{x}) : \boldsymbol{K} : \varepsilon(\boldsymbol{x}) + \varepsilon(\boldsymbol{x}) : \boldsymbol{\tau} + F^r(\boldsymbol{\Theta}^r(\boldsymbol{x});\boldsymbol{K},\boldsymbol{\tau})$$

Step 2 - Lower bound on the total energy $\int_\Omega Q\Psi(\varepsilon, \boldsymbol{x})dx$

- Consider a piecewise constant function $\boldsymbol{\tau}(\boldsymbol{x})$:

$$\boldsymbol{\tau}(\boldsymbol{x}) = \sum_{r=1}^{n} \chi^r(\boldsymbol{x})\boldsymbol{\tau}^r$$

- We have

$$\frac{1}{|\Omega|}\int_\Omega \sum_{r=1}^{n} \chi^r(\boldsymbol{x}) Q\Psi^r(\varepsilon(\boldsymbol{x}))\, d\boldsymbol{x} \geq \frac{1}{|\Omega|}\int_\Omega \sum_{r=1}^{n} \chi^r(\boldsymbol{x})(\varepsilon : \boldsymbol{\tau}^r + \frac{1}{2}\varepsilon : \boldsymbol{K} : \varepsilon)\, d\boldsymbol{x} + \sum_r c_r F^r(\frac{\bar{\boldsymbol{\Theta}}^r}{c_r}; \boldsymbol{K}, \boldsymbol{\tau}^r)$$

where

$$\bar{\Theta}^r = \frac{1}{|\Omega|}\int_\Omega \chi^r(\boldsymbol{x})\Theta^r(\boldsymbol{x})\, d\boldsymbol{x}, \quad c_r = \frac{1}{|\Omega|}\int_\Omega \chi^r(\boldsymbol{x})\, d\boldsymbol{x}$$

- $\bar{\boldsymbol{\Theta}} = \{\bar{\Theta}_i^r\}_{1\leq i\leq k}^{1\leq r\leq n}$ depends on ε and belongs to the set $\mathcal{T}^{eff}$ defined by

$$\mathcal{T}^{eff} = \{\bar{\boldsymbol{\theta}} \in \mathbb{R}_k^n | \bar{\theta}_i^r \geq 0; \sum_{i=1}^{k} \bar{\theta}_i^r = c^r \ \forall r\}$$

Step 3 - Make the bound independent of $\boldsymbol{\varepsilon}$

- Set

$$W(\bar{\varepsilon}; \boldsymbol{K}, \{\boldsymbol{\tau_r}\}) = \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_\Omega \sum_{r=1}^{n} \chi^r(\boldsymbol{x})(\varepsilon : \boldsymbol{\tau}^r + \frac{1}{2}\varepsilon : \boldsymbol{K} : \varepsilon)\, d\boldsymbol{x}$$

We have

$$\frac{1}{|\Omega|} \int_\Omega \sum_{r=1}^{n} \chi^r(\boldsymbol{x}) Q\Psi^r(\varepsilon(\boldsymbol{x}))\, d\boldsymbol{x} \geq W(\bar{\varepsilon}; \boldsymbol{K}, \{\boldsymbol{\tau_r}\}) + \sum_r c_r F^r(\frac{\bar{\boldsymbol{\Theta}}^r}{c_r}; \boldsymbol{K}, \boldsymbol{\tau}^r)$$

Step 3 - Make the bound independent of ε

- Set

$$W(\bar{\varepsilon};\boldsymbol{K},\{\boldsymbol{\tau_r}\}) = \inf_{\varepsilon\in\mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|}\int_\Omega \sum_{r=1}^n \chi^r(\boldsymbol{x})(\varepsilon:\boldsymbol{\tau}^r + \frac{1}{2}\varepsilon:\boldsymbol{K}:\varepsilon)\,d\boldsymbol{x}$$

We have

$$\frac{1}{|\Omega|}\int_\Omega \sum_{r=1}^n \chi^r(\boldsymbol{x}) Q\Psi^r(\varepsilon(\boldsymbol{x}))\,d\boldsymbol{x} \geq W(\bar{\varepsilon};\boldsymbol{K},\{\boldsymbol{\tau_r}\}) + \sum_r c_r F^r(\frac{\bar{\boldsymbol{\Theta}}^r}{c_r};\boldsymbol{K},\boldsymbol{\tau}^r)$$

- Since $\bar{\boldsymbol{\Theta}} \in \mathcal{T}^{eff}$, we have

$$\frac{1}{|\Omega|}\int_\Omega \sum_{r=1}^n \chi^r(\boldsymbol{x}) Q\Psi^r(\varepsilon(\boldsymbol{x}))\,d\boldsymbol{x} \geq W(\bar{\varepsilon};\boldsymbol{K},\{\boldsymbol{\tau_r}\}) + \inf_{\bar{\boldsymbol{\theta}}\in\mathcal{T}^{eff}} \sum_r c_r F^r(\frac{\bar{\boldsymbol{\theta}}^r}{c_r};\boldsymbol{K},\boldsymbol{\tau}^r)$$

The RHS is independent of ε

Summary

$$\Psi^{eff}(\bar{\varepsilon}) \geq W(\bar{\varepsilon}; \boldsymbol{K}, \{\boldsymbol{\tau}_r\}) + \inf_{\bar{\boldsymbol{\theta}} \in \mathcal{T}^{eff}} \sum_{r=1}^{n} c_r F^r\left(\frac{\bar{\boldsymbol{\theta}}^r}{c_r}; \boldsymbol{K}, \boldsymbol{\tau}^r\right)$$

with

$$W(\bar{\varepsilon}; \boldsymbol{K}, \{\boldsymbol{\tau}_r\}) = \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_\Omega \sum_{r=1}^{n} \chi^r(\boldsymbol{x})(\varepsilon : \boldsymbol{\tau}^r + \frac{1}{2}\varepsilon : \boldsymbol{K} : \varepsilon)\, d\boldsymbol{x}.$$

$$F^r(\boldsymbol{\theta}; \boldsymbol{K}, \boldsymbol{\tau}) = -\tfrac{1}{2}\boldsymbol{\tau} : (\boldsymbol{L}^r - \boldsymbol{K})^{-1} : \boldsymbol{\tau} + \sum_{i=1}^{k} \theta_i w_i^0$$

$$-\boldsymbol{\tau} : (\boldsymbol{L}^r - \boldsymbol{K})^{-1} : \boldsymbol{L}^r : \varepsilon^r(\boldsymbol{\theta}) + \tfrac{1}{2} \sum_{i=1}^{k} \theta_i \varepsilon_i^r : \boldsymbol{M}^r(\boldsymbol{K}) : \varepsilon_i^r$$

Convex bound

Choice 1

$$\boldsymbol{K} = 0 \text{ and } \boldsymbol{\tau}^r = \boldsymbol{\tau} \text{ independent of } r$$

- We have $W(\bar{\varepsilon}) = \bar{\varepsilon} : \boldsymbol{\tau}$
- Optimizing with respect to $\boldsymbol{\tau}$ gives

$$\Psi^{eff}(\bar{\varepsilon}) \geq \inf_{\bar{\boldsymbol{\theta}} \in \mathcal{T}^{eff}} \{C\Psi^{eff}(\bar{\varepsilon}, \bar{\boldsymbol{\theta}})\}$$

with

$$C\Psi^{eff}(\bar{\varepsilon}, \bar{\boldsymbol{\theta}}) = \frac{1}{2}(\bar{\varepsilon} - \sum_{r,i} \bar{\theta}_i^r \varepsilon_i^r) : \left(\sum_r c_r \boldsymbol{L}_r^{-1}\right)^{-1} : (\bar{\varepsilon} - \sum_{r,i} \bar{\theta}_i^r \varepsilon_i^r) + \sum_{r,i} \bar{\theta}_i^r w_i^0$$

Bound depending on one-point statistics

Choice 2

$\boldsymbol{K}$ quasiconvex and $\boldsymbol{\tau}^r = \boldsymbol{\tau}$ independent of r

- We have

$$W(\bar{\varepsilon}) \geq \bar{\varepsilon} : \boldsymbol{\tau} + \frac{1}{2}\bar{\varepsilon} : \boldsymbol{K} : \bar{\varepsilon}$$

- Optimizing with respect to $\boldsymbol{\tau}$ gives

$$\psi^{eff}(\bar{\varepsilon}, \bar{\boldsymbol{\theta}}) \geq \frac{1}{2}\bar{\varepsilon} : \boldsymbol{K} : \bar{\varepsilon} + \frac{1}{2}\boldsymbol{f} : \left(\sum_{r=1}^{n} c^r \left(\boldsymbol{L}^r - \boldsymbol{K}\right)^{-1}\right)^{-1} : \boldsymbol{f}$$
$$+ \sum_{r,i} \bar{\theta}_i^r w_i^0 + \tfrac{1}{2} \sum_{r=1}^{n} \sum_{i=1}^{k} \bar{\theta}_i^r \varepsilon_i^r : \boldsymbol{M}^r(\boldsymbol{K}) : \varepsilon_i^r$$

with $\boldsymbol{f} = \bar{\varepsilon} - \sum_r (\boldsymbol{L}^r - \boldsymbol{K})^{-1} : \boldsymbol{L}^r : \varepsilon^r(\bar{\boldsymbol{\theta}})$ and $\varepsilon^r(\bar{\boldsymbol{\theta}}) = \sum_i \bar{\boldsymbol{\theta}}_i^r \varepsilon_i^r$

Bound depending on one-point statistics

Choice 2

$\boldsymbol{K}$ quasiconvex and $\boldsymbol{\tau}^r = \boldsymbol{\tau}$ independent of r

- Case of equal elastic moduli $\boldsymbol{L}_1 = \cdots = \boldsymbol{L}_n (= \boldsymbol{L}_0)$:

$$\Psi^{eff}(\bar{\varepsilon}) \geq \inf_{\bar{\boldsymbol{\theta}} \in \mathcal{T}^{eff}} C\Psi^{eff}(\bar{\varepsilon}, \bar{\boldsymbol{\theta}}) + g(\bar{\boldsymbol{\theta}})$$

with

$$C\Psi^{eff}(\bar{\varepsilon}, \bar{\boldsymbol{\theta}}) = \frac{1}{2}(\bar{\varepsilon} - \sum_{r,i} \bar{\theta}_i^r \varepsilon_i^r) : \boldsymbol{L}^0 : (\bar{\varepsilon} - \sum_{r,i} \bar{\theta}_i^r \varepsilon_i^r) + \sum_{r,i} \bar{\theta}_i^r w_i^0$$

$$g(\bar{\boldsymbol{\theta}}) = \frac{1}{4} \sum \bar{\theta}_i^r \bar{\theta}_j^s (\varepsilon_i^r - \varepsilon_j^s) : \boldsymbol{M}^0(\boldsymbol{K}) : (\varepsilon_i^r - \varepsilon_j^s)$$

Bound depending on two-point statistics

Choice 3

$$\boldsymbol{K} = \tilde{\boldsymbol{L}} + \tilde{\boldsymbol{K}} \text{ with } \tilde{\boldsymbol{K}} \text{ quasiconvex and } \tilde{\boldsymbol{L}} > 0$$

- We have

$$W(\bar{\varepsilon}) = \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_\Omega \sum_{r=1}^{n} \chi^r(\boldsymbol{x})(\varepsilon : \boldsymbol{\tau}^r + \frac{1}{2}\varepsilon : \boldsymbol{K} : \varepsilon)\, d\boldsymbol{x}$$

Bound depending on two-point statistics

Choice 3

$$\boldsymbol{K} = \tilde{\boldsymbol{L}} + \tilde{\boldsymbol{K}} \text{ with } \tilde{\boldsymbol{K}} \text{ quasiconvex and } \tilde{\boldsymbol{L}} > 0$$

- We have

$$W(\bar{\varepsilon}) \geq (1/2)\bar{\varepsilon} : \tilde{\boldsymbol{K}} : \bar{\varepsilon} + \tilde{W}(\bar{\varepsilon})$$

where

$$\tilde{W}(\bar{\varepsilon}) = \inf_{\boldsymbol{\varepsilon} \in \mathcal{K}(\bar{\boldsymbol{\varepsilon}})} \frac{1}{|\Omega|} \int_\Omega \sum_{r=1}^{n} \chi^r(\boldsymbol{x})(\varepsilon : \boldsymbol{\tau}^r + \frac{1}{2}\varepsilon : \tilde{\boldsymbol{L}} : \varepsilon)\, d\boldsymbol{x}$$

Bound depending on two-point statistics

Choice 3

$$\boldsymbol{K} = \tilde{\boldsymbol{L}} + \tilde{\boldsymbol{K}} \text{ with } \tilde{\boldsymbol{K}} \text{ quasiconvex and } \tilde{\boldsymbol{L}} > 0$$

- We have

$$W(\bar{\varepsilon}) \geq (1/2)\bar{\varepsilon} : \tilde{\boldsymbol{K}} : \bar{\varepsilon} + \tilde{W}(\bar{\varepsilon})$$

$$\tilde{W}(\bar{\varepsilon}) = \frac{1}{2}\bar{\varepsilon} : \tilde{\boldsymbol{L}} : \bar{\varepsilon} + \sum_r c^r \boldsymbol{\tau}^r : \bar{\varepsilon} - \frac{1}{2}\sum_{r,s} \boldsymbol{\tau}^r : \boldsymbol{A}^{rs} : \boldsymbol{\tau}^s$$

with

$$\boldsymbol{A}^{rs} = \frac{1}{|\Omega|}\int_\Omega \chi^r(\boldsymbol{x})(\boldsymbol{\Gamma}\chi^s)(\boldsymbol{x})\, d\boldsymbol{x}$$

and Γ is a singular integral operator (related to Green functions) (Willis 1981).

Case of equal elastic moduli

We obtain

$$\Psi^{eff}(\bar{\varepsilon}) \geq \inf_{\bar{\boldsymbol{\theta}}\in\mathcal{T}^{eff}} C\Psi^{eff}(\bar{\varepsilon},\bar{\boldsymbol{\theta}}) + h(\bar{\varepsilon},\bar{\boldsymbol{\theta}})$$

with

$$h(\bar{\varepsilon},\bar{\boldsymbol{\theta}}) = \frac{1}{2}\sum_r \tilde{\boldsymbol{\tau}}^r : (\boldsymbol{L}^0 - \boldsymbol{K})^{-1} : \boldsymbol{L}^0 : (c^r \varepsilon(\bar{\boldsymbol{\theta}}) - \varepsilon^r(\bar{\boldsymbol{\theta}})) + \frac{1}{4}\sum_{r,s,i,j} \bar{\theta}_i^r \bar{\theta}_j^s (\varepsilon_i^r - \varepsilon_j^s) : \boldsymbol{M}^0(\boldsymbol{K}) : (\varepsilon_i^r - \varepsilon_j^s)$$

where $\boldsymbol{K} = \tilde{\boldsymbol{K}} + \tilde{\boldsymbol{L}}$ and $\{\tilde{\boldsymbol{\tau}}^r\}$ is solution of

$$c^r(\boldsymbol{L}^0 - \boldsymbol{K})^{-1} : \tilde{\boldsymbol{\tau}}^r + \sum_s \boldsymbol{A}^{rs} : \tilde{\boldsymbol{\tau}}^s = c^r\bar{\varepsilon} - (\boldsymbol{L}^0 - \boldsymbol{K})^{-1} : \boldsymbol{L}^0 : \varepsilon^r(\bar{\boldsymbol{\theta}})$$

Case of ellipsoidal symmetry

- Assume the probability of finding orientation r at point $\boldsymbol{x}$ and orientation s at $\boldsymbol{x}'$ is a function of $|\boldsymbol{Z}.(\boldsymbol{x}-\boldsymbol{x}')|$ where $\boldsymbol{Z}$ is a constant symmetric positive tensor.
- The tensors $\boldsymbol{A}^{rs}$ take the form (Willis 1977,1981)

$$\boldsymbol{A}^{rs} = c^r(\delta_{rs} - c^s)\boldsymbol{P}(\tilde{\boldsymbol{L}})$$

- The term $h(\bar{\varepsilon}, \bar{\boldsymbol{\theta}})$ becomes independent of $\bar{\varepsilon}$ and equal to

$$h(\bar{\boldsymbol{\theta}}) = \frac{1}{4}\sum_{r,s,i,j} \bar{\theta}_i^r\bar{\theta}_j^s(\varepsilon_i^r - \varepsilon_j^s) : \boldsymbol{M}^0(\boldsymbol{K}) : (\varepsilon_i^r - \varepsilon_j^s) + \frac{1}{2}\sum_r \frac{1}{c_r}\boldsymbol{h}^r : (\boldsymbol{L}^0 - \boldsymbol{K} + (\boldsymbol{L}^0 - \boldsymbol{K}) : \boldsymbol{P} : (\boldsymbol{L}^0 - \boldsymbol{K}))^{-1} : \boldsymbol{h}^r$$

where $\boldsymbol{h}^r = \boldsymbol{L}^0 : (c^r\varepsilon(\bar{\boldsymbol{\theta}}) - \varepsilon^r(\bar{\boldsymbol{\theta}}))$.

Lower bounds for polycrystals [M.P.,J.Mech.Phys.Solids, 2009]

Convex bound

$$\Psi^{eff}(\bar{\varepsilon}) \geq \inf_{\bar{\boldsymbol{\theta}} \in \mathcal{T}^{eff}} C\Psi^{eff}(\bar{\varepsilon}, \bar{\boldsymbol{\theta}})$$

Non convex bound, 1-point statistics

$$\Psi^{eff}(\bar{\varepsilon}) \geq \inf_{\bar{\boldsymbol{\theta}} \in \mathcal{T}^{eff}} C\Psi^{eff}(\bar{\varepsilon}, \bar{\boldsymbol{\theta}}) + g(\bar{\boldsymbol{\theta}})$$

Non convex bound, 2-point statistics

$$\Psi^{eff}(\bar{\varepsilon}) \geq \inf_{\bar{\boldsymbol{\theta}} \in \mathcal{T}^{eff}} C\Psi^{eff}(\bar{\varepsilon}, \bar{\boldsymbol{\theta}}) + h(\bar{\boldsymbol{\theta}})$$

Lower bounds on the mixing energy

- Bound depending on 1-point statistics

$$g(\bar{\boldsymbol{\theta}}) = \sup_{\boldsymbol{K}\in\mathcal{C}} \frac{1}{4} \sum_{r,s,i,j} \bar{\theta}_i^r \bar{\theta}_j^s (\varepsilon_i^r - \varepsilon_j^s) : \boldsymbol{M}^0(\boldsymbol{K}) : (\varepsilon_i^r - \varepsilon_j^s)$$

where $\mathcal{C}$ is a family of quasiconvex tensors such that $\boldsymbol{L}^0 \succ \boldsymbol{K}$ for any $\boldsymbol{K} \in \mathcal{C}$

- Bound depending on 2-point statistics

$$\begin{aligned} h(\bar{\boldsymbol{\theta}}) = & \sup_{(\tilde{\boldsymbol{K}},\tilde{\boldsymbol{L}})} \frac{1}{4} \sum_{r,s,i,j} \bar{\theta}_i^r \bar{\theta}_j^s (\varepsilon_i^r - \varepsilon_j^s) : \boldsymbol{M}^0(\boldsymbol{K}) : (\varepsilon_i^r - \varepsilon_j^s) \\ & + \tfrac{1}{2} \sum_r \frac{1}{c_r} \boldsymbol{h}^r : (\boldsymbol{L}^0 - \boldsymbol{K} + (\boldsymbol{L}^0 - \boldsymbol{K}) : \boldsymbol{P}(\tilde{\boldsymbol{L}}) : (\boldsymbol{L}^0 - \boldsymbol{K}))^{-1} : \boldsymbol{h}^r \end{aligned}$$

where the sup is taken over pairs $(\tilde{\boldsymbol{K}}, \tilde{\boldsymbol{L}})$ satisfying

$$\tilde{\boldsymbol{K}} \in \mathcal{C}, \quad \tilde{\boldsymbol{L}} \succ 0, \quad \boldsymbol{L}^0 \succ \tilde{\boldsymbol{L}} + \tilde{\boldsymbol{K}}$$

Example 1 : 'minimal' polycrystal

- 2 orientations (isotropically distributed)
  - Orientation 1 : austenite + 1 variant of martensite

$$\operatorname{tr} \boldsymbol{\varepsilon}^{tr} = 0$$

  - Orientation 2 : austenite only

- The elasticity tensor $\boldsymbol{L}^0$ is isotropic and incompressible ($\nu^0 \to 1/2$)

Lower bounds on the mixing energy

$$g(\theta) = \sup_{\tilde{\boldsymbol{K}}} \quad \tfrac{1}{2}\theta(1-\theta)\varepsilon^{\boldsymbol{tr}} : \boldsymbol{M}^0(\tilde{\boldsymbol{K}}) : \varepsilon^{\boldsymbol{tr}}$$

$$h(\theta) = \sup_{\tilde{\boldsymbol{K}},\tilde{\boldsymbol{L}}} \quad \{\tfrac{1}{2}\theta(1-\theta)\varepsilon^{\boldsymbol{tr}} : \boldsymbol{M}^0(\boldsymbol{K}) : \varepsilon^{\boldsymbol{tr}}$$

$$+2\mu_0^2\frac{c_2}{c_1}\theta^2\varepsilon^{\boldsymbol{tr}} : (\boldsymbol{L}^0 - \boldsymbol{K} + (\boldsymbol{L}^0 - \boldsymbol{K}) : \boldsymbol{P}(\tilde{\boldsymbol{L}}) : (\boldsymbol{L}^0 - \boldsymbol{K}))^{-1} : \varepsilon^{\boldsymbol{tr}}\}$$

where $\boldsymbol{K} = \tilde{\boldsymbol{K}} + \tilde{\boldsymbol{L}}$

Optimization with respect to :

- Isotropic and incompressible elasticity tensors $\tilde{\boldsymbol{L}}$
  $\rightarrow$ 1 scalar parameter $\tilde{\mu}$
- $\tilde{\boldsymbol{K}}=\boldsymbol{K}(\boldsymbol{a})$ with tensors $\boldsymbol{a}$ having the same eigenbasis as $\varepsilon^{\boldsymbol{tr}}$
  $\rightarrow$ 3 scalar parameters

Eig $\boldsymbol{\varepsilon}^{tr} = \frac{\sqrt{3}}{2}\{-1, 0, 1\}$ Bound h on the mixing energy

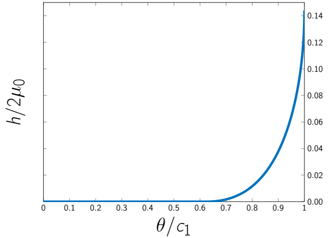
- It can be shown that the optimal value of $\boldsymbol{a}$ is

$$\boldsymbol{a} = 0 \quad (\text{ i.e. } \tilde{\boldsymbol{K}} = 0)$$

- Carrying out the optimization with respect to $\tilde{\mu}$ gives

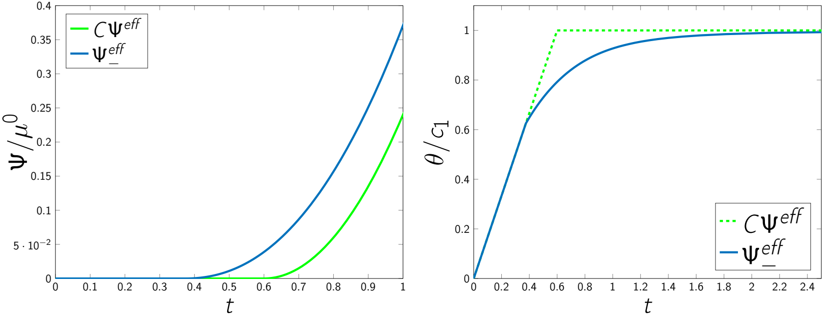
$$\frac{h(\theta)}{\mu_0} = \begin{cases} 0 & \text{for } \theta \leq \frac{2c_1}{5-3c_1} \\ \frac{\theta}{6}\frac{(5\Delta - 6c_1(1-\theta)^2}{5c_1(c_1(3-2\theta)-\theta-2\Delta)} & \text{for } \theta \geq \frac{2c_1}{5-3c_1} \end{cases}$$

with $\Delta = \sqrt{6c_2(c_1-\theta)\theta}$.



Eig $\varepsilon^{tr} = \frac{\sqrt{3}}{2}\{-1,0,1\}$ Bound Ψ_{-}^{eff} on the effective energy

$$\Psi_{-}^{eff}(\bar{\varepsilon}) = \inf_{0\le\theta\le c_1} \frac{1}{2}(\bar{\varepsilon} - \theta\varepsilon^{tr}) : \boldsymbol{L}^0 : (\bar{\varepsilon} - \theta\varepsilon^{tr}) + \lambda_T\theta + h(\theta)$$



$$\bar{\varepsilon} = t\varepsilon^{tr},\ \lambda_T = 0,\ c_1 = 0.6$$

- Transformation hardening due to elastic interaction between grains

$\operatorname{Eig} \varepsilon^{tr} = \frac{1}{2}\{-1,-1,2\}$ Bound on the mixing energy

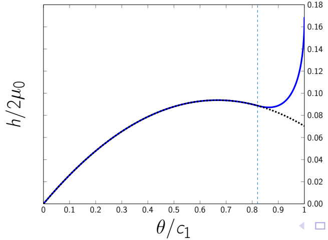
- For $\theta \leq \frac{8c_1}{15-7c_1}$:

$$g(\theta) = h(\theta) = \frac{3}{8}\mu_0(1-\theta)\theta$$

- For $\theta \geq \frac{8c_1}{15-7c_1}$:

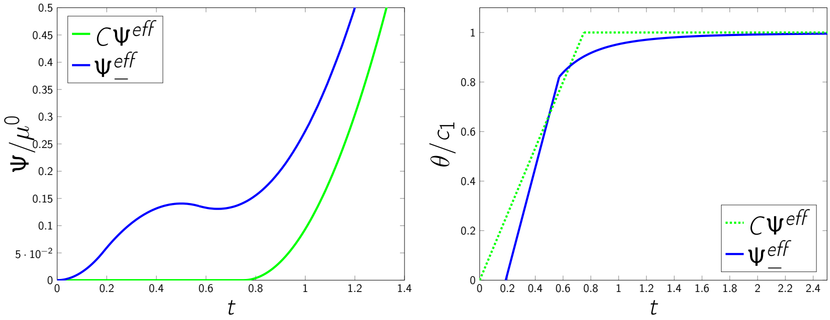
$$g(\theta) = \frac{3}{8}\mu_0(1-\theta)\theta, \quad h(\theta) = \frac{\mu_0 P(D, c_1, \theta)}{40c_1(7(c_1-\theta)-2D)(D-4\theta c_2)}$$

with $D = \sqrt{14c_2(c_1-\theta)\theta}$ and $P(D, c_1, \theta)$ is a polynomial



Eig $\boldsymbol{\varepsilon^{tr}} = \frac{1}{2}\{-1,-1,2\}$ Bound on the effective energy

$$\Psi_{-}^{eff}(\bar{\varepsilon}) = \inf_{0\le\theta\le c_1} \frac{1}{2}(\bar{\varepsilon} - \theta\boldsymbol{\varepsilon^{tr}}) : \boldsymbol{L}^0 : (\bar{\varepsilon} - \theta\boldsymbol{\varepsilon^{tr}}) + \lambda_T\theta + h(\theta)$$



$$\bar{\varepsilon} = t\boldsymbol{\varepsilon^{tr}},\ \lambda_T = 0,\ c_1 = 0.75$$

- The non compatibility has an influence on the onset of transformation

Example 2

- 2 orientations (isotropically distributed)
  - Orientation 1 : austenite + 2 compatible variants of martensite

$$\boldsymbol{\varepsilon}_{\mathbf{1}}^{\boldsymbol{tr}} = \operatorname{diag} \eta(-1,-1,2), \boldsymbol{\varepsilon}_{\mathbf{2}}^{\boldsymbol{tr}} = \operatorname{diag} \eta(2,-1,-1)$$

  - Orientation 2 : austenite only
- The elasticity tensor $\boldsymbol{L}^0$ is isotropic and incompressible.

Lower bounds on the mixing energy

$$g(\theta_1, \theta_2) = \sup_{\tilde{\boldsymbol{K}}} \cdots$$

$$h(\theta_1, \theta_2) = \sup_{\tilde{\boldsymbol{K}}, \tilde{\boldsymbol{L}}} \cdots$$

Optimization with respect to :

- Isotropic and incompressible elasticity tensors $\tilde{\boldsymbol{L}}$

  $\rightarrow$ 1 scalar parameter $\tilde{\mu}$

- $\tilde{\boldsymbol{K}} = \boldsymbol{K}(\boldsymbol{a})$ with tensors $\boldsymbol{a}$ having the same eigenbasis as $\varepsilon_{\boldsymbol{i}}^{\boldsymbol{tr}}$

  $\rightarrow$ 3 scalar parameters

Lower bounds on the mixing energy

$$g(\theta_1, \theta_2) = \sup_{\tilde{\boldsymbol{K}}} \cdots$$

→ can be solved exactly

$$h(\theta_1, \theta_2) = \sup_{\tilde{\boldsymbol{K}}, \tilde{\boldsymbol{L}}} \cdots$$

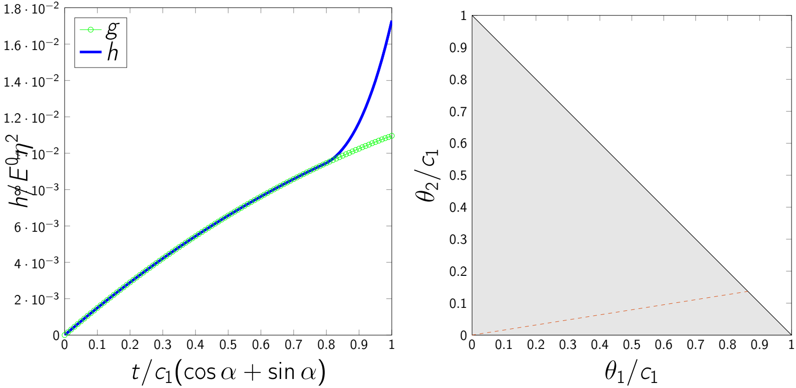
→ needs to be solved numerically

Optimization with respect to :

- Isotropic and incompressible elasticity tensors $\tilde{\boldsymbol{L}}$
- $\tilde{\boldsymbol{K}} = \boldsymbol{K}(\boldsymbol{a})$ with tensors $\boldsymbol{a}$ having the same eigenbasis as $\varepsilon_{\boldsymbol{i}}^{\boldsymbol{tr}}$

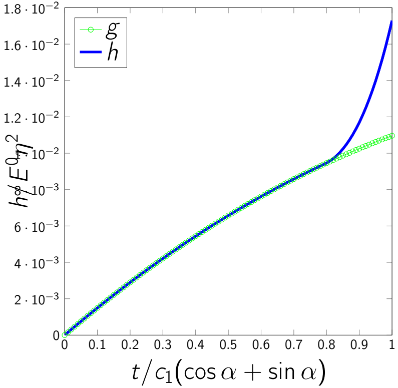
Lower bound on the mixing energy $(c_1 = 0.2)$

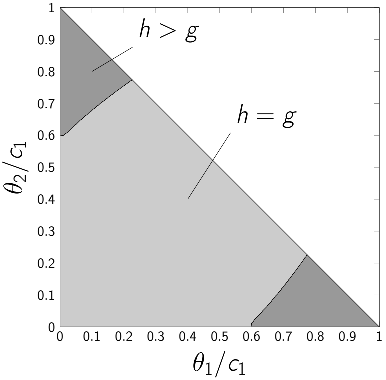
$(\theta_1, \theta_2) = t(\cos\alpha, \sin\alpha)$, $\alpha = \frac{\pi}{20}$



Lower bound on the mixing energy $(c_1 = 0.2)$

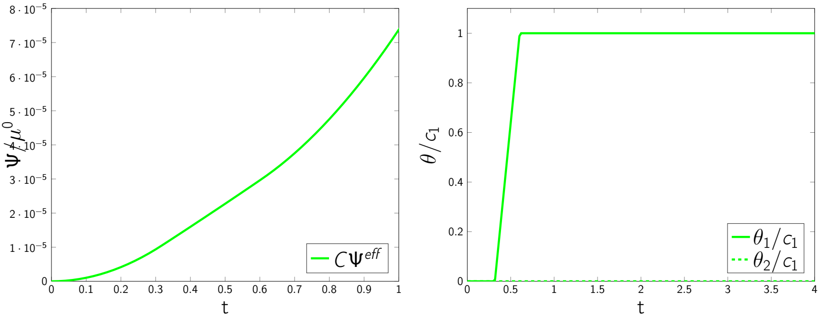
$$(\theta_1, \theta_2) = t(\cos\alpha, \sin\alpha) \ , \ \alpha = \frac{\pi}{20}$$





Lower bound Ψ_{-}^{eff} on the effective energy

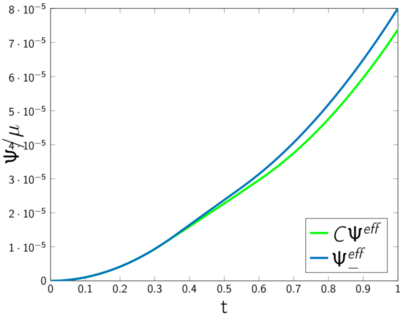
$$\Psi_{-}^{eff}(\bar{\varepsilon}) = \inf_{(\theta_1,\theta_2)} \frac{1}{2}(\bar{\varepsilon} - \sum_{i=1}^{2} \theta_i \boldsymbol{\varepsilon_i^{tr}}) : \boldsymbol{L} : (\bar{\varepsilon} - \sum_{i=1}^{2} \theta_i \boldsymbol{\varepsilon_i^{tr}}) + \lambda_T \sum_{i=1}^{2} \theta_i + h(\theta_1, \theta_2)$$

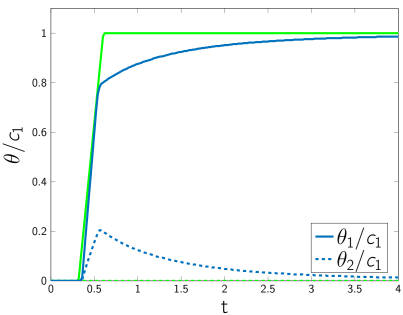


$$\bar{\varepsilon} = t(0.8\boldsymbol{\varepsilon_1^{tr}} + 0.2\boldsymbol{\varepsilon_2^{tr}}),\ \eta = 0.01,\ \lambda_T/\mu = 2.67\,10^{-4}$$

Lower bound Ψ_-^{eff} on the effective energy

$$\Psi_-^{eff}(\bar{\varepsilon}) = \inf_{(\theta_1,\theta_2)} \frac{1}{2}(\bar{\varepsilon} - \sum_{i=1}^{2} \theta_i \varepsilon_i^{tr}) : \boldsymbol{L} : (\bar{\varepsilon} - \sum_{i=1}^{2} \theta_i \varepsilon_i^{tr}) + \lambda_T \sum_{i=1}^{2} \theta_i + h(\theta_1, \theta_2)$$





$$\bar{\varepsilon} = t(0.8\varepsilon_1^{tr} + 0.2\varepsilon_2^{tr}),\ \eta = 0.01,\ \lambda_T/\mu = 2.67\,10^{-4}$$

Computational aspects

$$\Psi^{eff}(\bar{\varepsilon}) \geq \inf_{\bar{\boldsymbol{\theta}} \in \mathcal{T}^{eff}} C\Psi^{eff}(\bar{\varepsilon}, \bar{\boldsymbol{\theta}}) + g(\bar{\boldsymbol{\theta}})$$

with

$$g(\bar{\boldsymbol{\theta}}) = \sup_{\boldsymbol{K} \in \mathcal{C}} \frac{1}{4} \sum_{r,s,i,j} \bar{\theta}_i^r \bar{\theta}_j^s (\varepsilon_i^r - \varepsilon_j^s) : \boldsymbol{M}^0(\boldsymbol{K}) : (\varepsilon_i^r - \varepsilon_j^s)$$

$$\mathcal{C} = \{\boldsymbol{K}(\boldsymbol{a}) : \boldsymbol{a} \succeq 0, \boldsymbol{L} - \boldsymbol{K}(\boldsymbol{a}) \succ 0\}$$

- Nested optimization problems
- Except in special cases, a numerical optimization algorithm is necessary (a descend algorithm, for instance).
- The practical performance of such algorithms is conditioned by the choice of an initial guess.

Example : CuAlNi polycrystal

ε_1^0	ε_2^0	ε_3^0
$\begin{pmatrix} \alpha & 0 & \delta \\ 0 & \beta & 0 \\ \delta & 0 & \alpha \end{pmatrix}$	$\begin{pmatrix} \alpha & 0 & -\delta \\ 0 & \beta & 0 \\ -\delta & 0 & \alpha \end{pmatrix}$	$\begin{pmatrix} \alpha & \delta & 0 \\ \delta & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix}$
ε_4^0	ε_5^0	ε_6^0
$\begin{pmatrix} \alpha & -\delta & 0 \\ -\delta & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix}$	$\begin{pmatrix} \beta & 0 & 0 \\ 0 & \alpha & \delta \\ 0 & \delta & \alpha \end{pmatrix}$	$\begin{pmatrix} \beta & 0 & 0 \\ 0 & \alpha & -\delta \\ 0 & -\delta & \alpha \end{pmatrix}$

$\alpha = 0.0425$, $\beta = -0.0822$, $\delta = 0.0194$

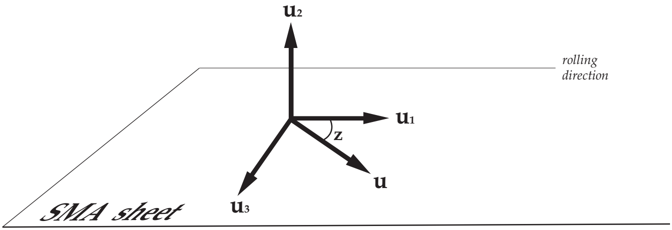
Example : CuAlNi polycrystal

CuAlNi (orthorombic martensite) with 2 crystalline orientations defined by the rotations

$$\boldsymbol{R}^1 = \begin{pmatrix} 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & -1 & 0 \end{pmatrix}, \ \boldsymbol{R}^2 = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -1/\sqrt{6} & 1/\sqrt{6} & \sqrt{2/3} \\ 1/\sqrt{3} & -1/\sqrt{3} & 1/\sqrt{3} \end{pmatrix}$$

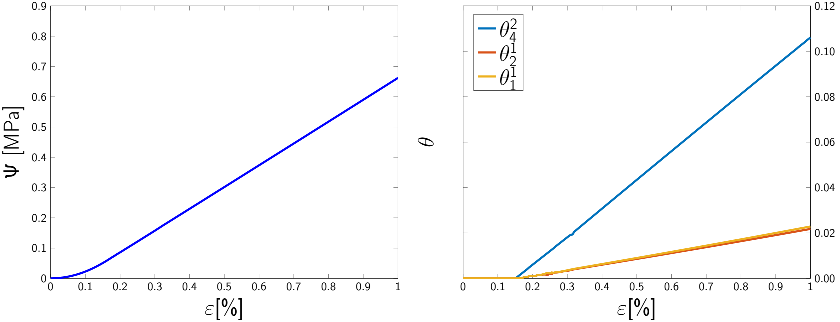
$$c_1 = 0.6, c_2 = 0.4$$

(Zhao-Beyer texture)



Uniaxial traction in a CuAlNi polycrystal

$$\varepsilon \mapsto \inf_{\substack{\bar{\boldsymbol{\varepsilon}} \\ \boldsymbol{n}\cdot\bar{\varepsilon}\cdot\boldsymbol{n}=\varepsilon}} \Psi_{-}^{eff}(\bar{\varepsilon}) \quad \text{with } \Psi_{-}^{eff}(\bar{\varepsilon}) = \inf_{\bar{\boldsymbol{\theta}}\in\mathcal{T}^{eff}} C\Psi^{eff}(\bar{\varepsilon}, \bar{\boldsymbol{\theta}}) + g(\bar{\boldsymbol{\theta}})$$



(the loading direction $\boldsymbol{n}$ makes a 5 deg angle with $\boldsymbol{u}_1$).

Uniaxial traction in a CuAlNi polycrystal

Values of $\boldsymbol{n}.\varepsilon_i^r.\boldsymbol{n}$

- Orientation 1 :

i	1	2	3	4	5	6
$\boldsymbol{n}.\varepsilon_i^1.\boldsymbol{n}$	0.0416	0.0415	0.0391	0.0459	−0.0813	−0.0813

- Orientation 2

i	1	2	3	4	5	6
$\boldsymbol{n}.\varepsilon_i^2.\boldsymbol{n}$	−0.0305	−0.0308	0.0234	0.0616	−0.0092	−0.0089

Upper bound on the effective energy

$$\psi^{eff}(\bar{\varepsilon}) = \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_\Omega \sum_{r=1}^{n} \chi^r(\boldsymbol{x}) Q\Psi^r(\varepsilon)\, d\boldsymbol{x}$$

- We have

$$Q\Psi^r(\varepsilon) = \inf_{\boldsymbol{\theta} \in \mathcal{T}} Q\Psi^r(\varepsilon, \boldsymbol{\theta})$$

  Hence, for any $\boldsymbol{\theta}(\boldsymbol{x}) \in \mathcal{T}$,

$$\psi^{eff}(\bar{\varepsilon}) \leq \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_\Omega \sum_{r=1}^{n} \chi^r(\boldsymbol{x}) Q\Psi^r(\bar{\varepsilon}, \boldsymbol{\theta}(\boldsymbol{x}))\, d\boldsymbol{x}$$

- Considering in particular a piecewise constant field $\boldsymbol{\theta}(\boldsymbol{x}) = \sum_{r=1}^{n} \chi^r(\boldsymbol{x}) \boldsymbol{\theta}_r$, we find

$$\psi^{eff}(\bar{\varepsilon}) \leq \inf_{\{\boldsymbol{\theta}_r\}} \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_\Omega \sum_{r=1}^{n} \chi^r(\boldsymbol{x}) Q\Psi^r(\bar{\varepsilon}, \boldsymbol{\theta}_r)\, d\boldsymbol{x}$$

Case of equal elastic moduli

- If austenite and martensite have the same elastic moduli, we have

$$Q\Psi^r(\bar{\varepsilon}, \boldsymbol{\theta}_r) = C\Psi^r(\bar{\varepsilon}, \theta_r) + f(\boldsymbol{\theta}_r)$$

It follows that

$$\Psi^{eff}(\bar{\varepsilon}) \leq \inf_{\{\boldsymbol{\theta}_r\}} W(\bar{\varepsilon}) + \sum_r c_r \left(f(\boldsymbol{\theta}_r) + \frac{1}{2}\sum_{i,j=1}^{k} \theta_i^r \theta_j^r \varepsilon_i^r : \boldsymbol{L}^r : \varepsilon_j^r + \sum_i w_i^0 \theta_i^r \right)$$

with

$$W(\bar{\varepsilon}) = \inf_{\varepsilon \in \mathcal{K}(\bar{\varepsilon})} \frac{1}{|\Omega|} \int_\Omega \sum_r \chi_r(\boldsymbol{x}) (\frac{1}{2}\varepsilon : \boldsymbol{L}^r : \varepsilon + \boldsymbol{\tau}_r : \varepsilon) d\boldsymbol{x}$$

and $\boldsymbol{\tau}_r = -\boldsymbol{L}^r : \sum_{i=1}^k \theta_i^r \varepsilon_i^r$.

- If $\boldsymbol{L}^1 = \cdots = \boldsymbol{L}^r$ $(= \boldsymbol{L}^0)$ then $W(\bar{\varepsilon}) = W(\bar{\varepsilon}, \boldsymbol{L}^0, \{\boldsymbol{\tau}_r\})$ can be calculated.

Texture with ellipsoidal symmetry

We obtain

$$\begin{aligned}\Psi^{eff}(\bar{\varepsilon}) \leq \quad & \inf_{\{\boldsymbol{\theta}_r\}} C\Psi^{eff}(\bar{\varepsilon}, \{c_r \boldsymbol{\theta}_r\}) + \sum_{r=1}^{n} c_r f(\boldsymbol{\theta}_r) \\ & + \frac{1}{2} \sum_{r=1}^{n} c_r \boldsymbol{\sigma}_r : (\boldsymbol{L}^{-1} - \boldsymbol{P}) : \boldsymbol{\sigma}_r - \frac{1}{2} \bar{\boldsymbol{\sigma}} : (\boldsymbol{L}^{-1} - \boldsymbol{P}) : \bar{\boldsymbol{\sigma}}\end{aligned}$$

where $\boldsymbol{\sigma}_r = \sum_{i=1}^{k} \theta_i^r \boldsymbol{L}^0 : \varepsilon_i^r$ and $\bar{\boldsymbol{\sigma}} = \sum_{r=1}^{n} c_r \boldsymbol{\sigma}_r$.

In general, the exact expression of the mixing energy f is not available.

- Replacing f with an upper bound gives an upper bound Ψ_+^{eff} on Ψ^{eff} (Hackl and Heinen, 2008)

Examples

- Minimal polycrystal
- Polycrystal with 2 martensitic variants in orientation 1

Example 1 : 'minimal' polycrystal

- 2 orientations (isotropically distributed)
  - Orientation 1 : austenite + 1 variant of martensite

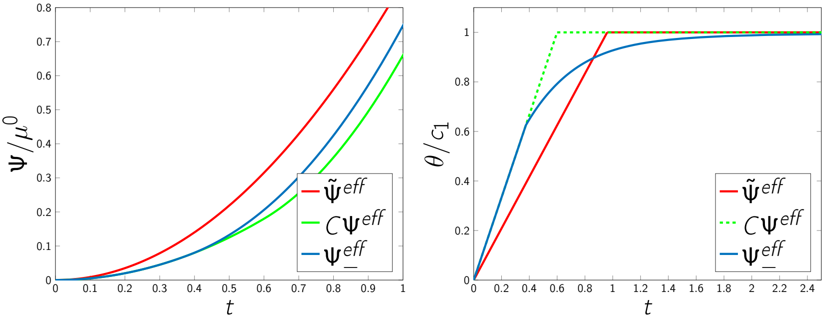
$$\operatorname{tr} \boldsymbol{\varepsilon}^{\boldsymbol{tr}} = 0$$

  - Orientation 2 : austenite only

- The elasticity tensor $\boldsymbol{L}^0$ is isotropic and incompressible ($\nu^0 \to 1/2$)

Estimate $\tilde{\Psi}^{eff}$ of the effective energy $\quad \mathrm{Eig}\,\boldsymbol{\varepsilon}^{tr} = \frac{1}{2}\{-1,0,1\}$

$$\tilde{\Psi}^{eff}(\bar{\varepsilon}) = \inf_{0\le\theta\le c_1} \frac{1}{2}(\bar{\varepsilon} - \theta\boldsymbol{\varepsilon}^{tr}) : \boldsymbol{L} : (\bar{\varepsilon} - \theta\boldsymbol{\varepsilon}^{tr}) + \lambda_T\theta + \tilde{f}(\theta)$$

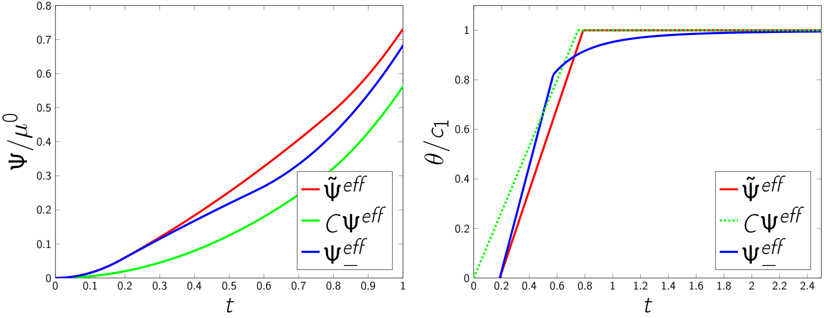


$$\bar{\varepsilon} = t\boldsymbol{\varepsilon}^{tr},\ \lambda_T = 0,\ c_1 = 0.6$$

- Complete transformation can be achieved.

Eig $\boldsymbol{\varepsilon}^{\boldsymbol{tr}} = \frac{1}{2}\{-1,-1,2\}$ Estimate of the effective energy

$$\tilde{\Psi}^{eff}(\bar{\varepsilon}) = \inf_{0\le\theta\le c_1} \frac{1}{2}(\bar{\varepsilon} - \theta\boldsymbol{\varepsilon}^{\boldsymbol{tr}}) : \boldsymbol{L}^0 : (\bar{\varepsilon} - \theta\boldsymbol{\varepsilon}^{\boldsymbol{tr}}) + \lambda_T\theta + \tilde{f}(\theta)$$



- Austenite-martensite compatibility has an influence on the onset of transformation

Example 2

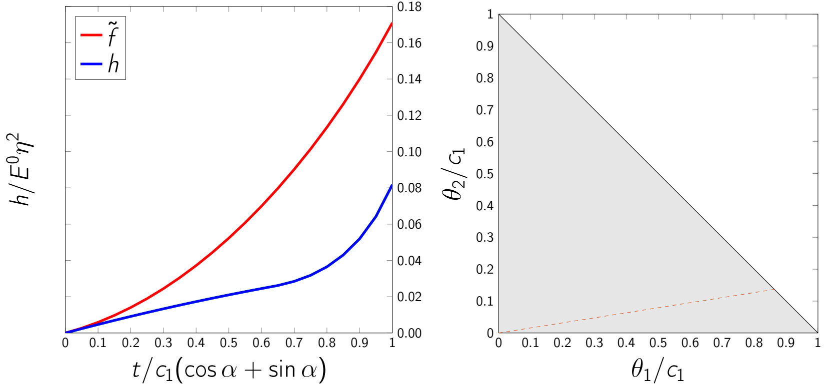
- 2 orientations (isotropically distributed)
  - Orientation 1 : austenite + 2 compatible variants of martensite

$$\boldsymbol{\varepsilon}_{\mathbf{1}}^{\boldsymbol{tr}} = \operatorname{diag} \eta(-1, -1, 2), \boldsymbol{\varepsilon}_{\mathbf{2}}^{\boldsymbol{tr}} = \operatorname{diag} \eta(2, -1, -1)$$

  - Orientation 2 : austenite only
- The elasticity tensor $\boldsymbol{L}$ is isotropic and incompressible.

Estimate $\tilde{f}$ of the mixing energy $(c_1 = 0.2)$

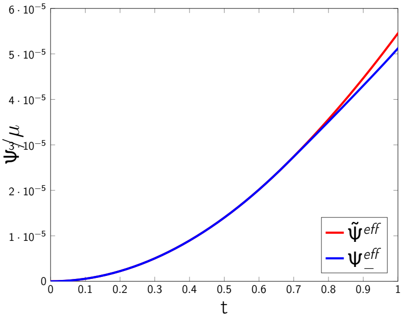
$(\theta_1, \theta_2) = t(\cos\alpha, \sin\alpha)$ $\alpha = \frac{\pi}{20}$

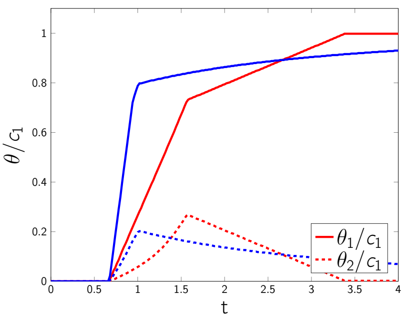


- The closed-form expression of $\tilde{f}$ is available

Estimate $\tilde{\Psi}^{eff}$ of the effective energy

$$\tilde{\Psi}^{eff}(\bar{\varepsilon}) = \inf_{(\theta_1,\theta_2)} \frac{1}{2}(\bar{\varepsilon} - \sum_{i=1}^{2} \theta_i \varepsilon_i^{tr}) : \boldsymbol{L}^0 : (\bar{\varepsilon} - \sum_{i=1}^{2} \theta_i \varepsilon_i^{tr}) + \lambda_T \sum_{i=1}^{2} \theta_i + \tilde{f}(\theta_1, \theta_2)$$





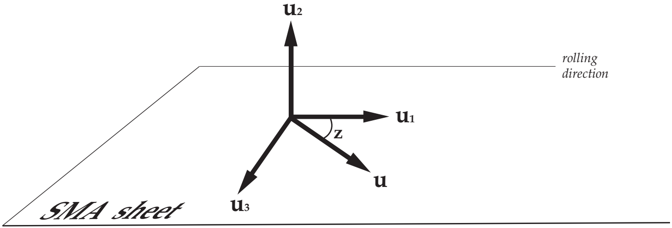
$$\bar{\varepsilon} = t(0.8\varepsilon_1^{tr} + 0.2\varepsilon_2^{tr}),\ \eta = 0.01,\ \lambda_T/\mu = 2.67\,10^{-4}$$

Example 3

CuAlNi (orthorombic martensite) with 2 crystalline orientations defined by the rotations

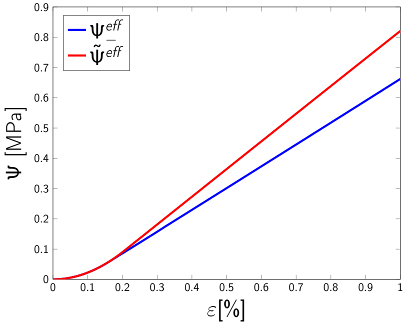
$$\boldsymbol{R}^1 = \begin{pmatrix} 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & -1 & 0 \end{pmatrix}, \quad \boldsymbol{R}^2 = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -1/\sqrt{6} & 1/\sqrt{6} & \sqrt{2/3} \\ 1/\sqrt{3} & -1/\sqrt{3} & 1/\sqrt{3} \end{pmatrix}$$

(Zhao-Beyer texture)



Traction in a CuAlNi polycrystal

$\varepsilon \mapsto \inf_{\bar{\boldsymbol{\varepsilon}}:\bar{\varepsilon}_{11}=\varepsilon} \tilde{\Psi}^{eff}(\bar{\boldsymbol{\varepsilon}})$



Concluding remarks

- Room for improvement
  - Choice of $\boldsymbol{K}$ and $\boldsymbol{L}$ in the calculation of the bounds
- Computational aspects :
  - speed up the calculation for the bound h (2-point statistics)
- Bounds and estimates :
  - study more complex polycrystals (NiTi)