Bounds and estimates on the effective energy of shape memory alloys

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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.

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

$$\Psi^0(arepsilon) = \min_{1 \leq i \leq k} \Psi^0_i(arepsilon)$$

where

$$\Psi_i^0(arepsilon) = rac{1}{2}(arepsilon-arepsilon_i^0): oldsymbol{L}^0: (arepsilon-arepsilon_i^0) + w_i^0$$

represents the free energy of phase *i*.

- The mesoscopic free energy of the reference single crystal is the relaxation (or quasi-convexification) of Ψ⁰
- 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.

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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

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

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Mesoscopic free energy

Following Kohn(1991), we have

$$Q\Psi^0(ar{arepsilon}) = \inf_{oldsymbol{ heta}\in\mathcal{T}} Q\Psi^0(ar{arepsilon},oldsymbol{ heta}) \, .$$

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

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

The first infimum is taken over characteristic functions χ_i compatible with volume fractions θ . Such functions satisfy

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

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

For arbitrary comparison potential U(ε) and polarization τ, introduce the Legendre transform :

$$(\Psi^0_i - \mathsf{U})_*(au) = \sup_{arepsilon} arepsilon: au - \Psi^0_i(arepsilon) + \mathsf{U}(arepsilon)$$

From that definition, we obtain

$$\sum_{i=1}^k \chi_i({m x}) \Psi^0_i(arepsilon) \geq arepsilon: {m au} - \sum_{i=1}^k \chi_i({m x}) (\Psi^0_i - {m U})_*({m au}) + {m U}(arepsilon)$$

• Taking 'inf $_{\chi_i}$ inf $_{\varepsilon \in \mathcal{K}(\overline{\varepsilon})} \int_{\Omega}$ ' yields

$$Q\Psi^0(ar{arepsilon},oldsymbol{ heta}) \geq ar{arepsilon}: oldsymbol{ au} - \sum_{i=1}^k heta_i (\Psi^0_i - {\sf U})_*(oldsymbol{ au}) + \inf_{oldsymbol{arepsilon}\in\mathcal{K}(ar{arepsilon})} rac{1}{|\Omega|} \int_\Omega {\sf U}(oldsymbol{arepsilon}) \, doldsymbol{x}$$

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Choice of comparison potential U

$$Q\Psi^0(ar{arepsilon},oldsymbol{ heta}) \geq ar{arepsilon}: oldsymbol{ au} - \sum_{i=1}^k heta_i (\Psi^0_i - {\sf U})_*(oldsymbol{ au}) + \inf_{oldsymbol{arepsilon}\in\mathcal{K}(ar{arepsilon})} rac{1}{|\Omega|} \int_\Omega {\sf U}(arepsilon) \, doldsymbol{x}$$

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

$$Q\Psi^0(ar{arepsilon}) \geq \inf_{oldsymbol{ heta}\in\mathcal{T}} C\Psi^0(ar{arepsilon},oldsymbol{ heta})$$

with

$$C\Psi^0(ar{arepsilon},oldsymbol{ heta}) = rac{1}{2}(ar{arepsilon}-arepsilon^0(oldsymbol{ heta})):L^0:(ar{arepsilon}-arepsilon^0(oldsymbol{ heta}))+\sum_{i=1}^k heta_iw_i^0$$

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

Choice of comparison potential U

$$Q\Psi^0(ar{arepsilon},oldsymbol{ heta}) \geq ar{arepsilon}:oldsymbol{ au} - \sum_{i=1}^k heta_i (\Psi^0_i - {f U})_*(oldsymbol{ au}) + \inf_{oldsymbol{arepsilon}\in\mathcal{K}(ar{arepsilon})} rac{1}{|\Omega|} \int_\Omega {f U}(oldsymbol{arepsilon}) \, doldsymbol{x}$$

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

$$\blacktriangleright L^0 - K \succ 0$$

$$ar{oldsymbol{arepsilon}}:oldsymbol{\mathcal{K}}:oldsymbol{arepsilon}\leqrac{1}{|\Omega|}\int_{\Omega}oldsymbol{arepsilon}:oldsymbol{\mathcal{K}}:oldsymbol{arepsilon}\,doldsymbol{x}\;\;orallar{oldsymbol{arepsilon}}$$

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A lower bound on $Q\Psi^0(ar{arepsilon}, heta)$

After some manipulation, we find :

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$$Q\Psi^0(ar{arepsilon},oldsymbol{ heta})\geq rac{1}{2}ar{arepsilon}:oldsymbol{{K}}:ar{arepsilon}+ar{arepsilon}:oldsymbol{ au}+ar{arepsilon}^r(oldsymbol{ heta};oldsymbol{{K}},oldsymbol{ au})$$

where

$$egin{aligned} & \mathcal{F}^r(m{ heta};m{K},m{ au}) \geq & -rac{1}{2}m{ au}:(m{L}^0-m{K})^{-1}:m{ au}+\sum_{i=1}^k heta_iw_i^0 \ & & -m{ au}:(m{L}^0-m{K})^{-1}:m{L}^0:m{arepsilon^0}(m{ heta})+rac{1}{2}\sum_{i=1}^k heta_im{arepsilon}_i^0:m{M}^0(m{K}):m{arepsilon}_i^0 \end{aligned}$$

(quadratic in au)

and

$$arepsilon^0(oldsymbol{ heta}) = \sum_{i=1}^{\kappa} heta_i arepsilon_i^0 \ , \ oldsymbol{M}^0(oldsymbol{K}) = oldsymbol{L}^0 - oldsymbol{L}^0 : (oldsymbol{L}^0 - oldsymbol{K})^{-1} : oldsymbol{L}^0$$

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A lower bound on $Q\Psi^0$

Optimizing with respect to au yields

$$Q\Psi^0(ar{arepsilon}) \geq \inf_{oldsymbol{ heta}\in\mathcal{T}} \{C\Psi^0(ar{arepsilon},oldsymbol{ heta}) + g(oldsymbol{ heta})\}$$

where

$$g(oldsymbol{ heta}) = rac{1}{2}\sum_{i,j=1}^k heta_i heta_j (oldsymbol{arepsilon}_i^0 - oldsymbol{arepsilon}_j^0) : oldsymbol{M}^0(oldsymbol{K}) : (oldsymbol{arepsilon}_i^0 - oldsymbol{arepsilon}_j^0)$$

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A family of quasiconvex tensors K

Let ε^* be the adjugate of ε , i.e :

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

Define K(a) by

$$rac{1}{2}oldsymbol{arepsilon}:oldsymbol{arepsilon}=-oldsymbol{a}:oldsymbol{arepsilon}^*$$

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

Using that family of tensors, we obtain

$$g(m{ heta}) = \sup_{m{m{K}}\in\mathcal{C}}rac{1}{4}\sum_{i,j} heta_i heta_j(m{arepsilon}_i^0-m{arepsilon}_j^0):m{M}^0(m{K}):(m{arepsilon}_i^0-m{arepsilon}_j^0)$$

with

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

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Summary

$$Q\Psi^0(ar{arepsilon}) \geq \inf_{oldsymbol{ heta}\in\mathcal{T}} \{C\Psi^0(ar{arepsilon},oldsymbol{ heta}) + g(oldsymbol{ heta})\}$$

with

$$g(oldsymbol{ heta}) = \sup_{oldsymbol{K}\in\mathcal{C}}rac{1}{4}\sum_{i,j} heta_i heta_j(arepsilon_i^0-arepsilon_j^0):oldsymbol{M}^0(oldsymbol{K}):(arepsilon_i^0-arepsilon_j^0)$$

and

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

- 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.

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Polycrystal : lower bound on the energy

Simple examples

Computational aspects

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Image: A matrix

Polycrystal

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

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

The macroscopic (or effective) energy of the polycrystal is

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

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

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

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

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

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

$$Q\Psi^r(arepsilon(oldsymbol{x})) = \inf_{oldsymbol{ heta}\in\mathcal{T}} Q\Psi(arepsilon(oldsymbol{x}),oldsymbol{ heta}) \geq \inf_{oldsymbol{ heta}\in\mathcal{T}} Q\Psi^r_-(arepsilon(oldsymbol{x}),oldsymbol{ heta})$$

where

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

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Step 1 - Pointwise lower bound on $Q\Psi'(\varepsilon(\mathbf{x}))$

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

$$Q\Psi^r(arepsilon(oldsymbol{x})) = \inf_{oldsymbol{ heta}\in\mathcal{T}} Q\Psi(arepsilon(oldsymbol{x}),oldsymbol{ heta}) \geq \inf_{oldsymbol{ heta}\in\mathcal{T}} Q\Psi^r_-(arepsilon(oldsymbol{x}),oldsymbol{ heta})$$

where

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

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

$$\inf_{oldsymbol{ heta}\in\mathcal{T}} Q \Psi^r_-(arepsilon(oldsymbol{x}),oldsymbol{ heta}) = Q \Psi^r_-(arepsilon(oldsymbol{x}),oldsymbol{\Theta}^r(oldsymbol{x}))$$

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Step 1 - Pointwise lower bound on $Q\Psi'(\varepsilon(\mathbf{x}))$

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

$$Q\Psi^r(arepsilon(oldsymbol{x})) = \inf_{oldsymbol{ heta}\in\mathcal{T}} Q\Psi(arepsilon(oldsymbol{x}),oldsymbol{ heta}) \geq \inf_{oldsymbol{ heta}\in\mathcal{T}} Q\Psi^r_-(arepsilon(oldsymbol{x}),oldsymbol{ heta})$$

where

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

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

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

Hence

$$Q\Psi^r(arepsilon(m{x}))\geq \sup_{m{K}\in\mathcal{C}}\sup_{m{ au}}rac{1}{2}arepsilon(m{x}):m{K}:arepsilon(m{x})+arepsilon(m{x}):m{ au}+m{F}^r(m{\Theta}^r(m{x});m{K},m{ au})$$

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

• Consider a piecewise constant function au(x) :

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

We have

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

where

$$ar{\Theta}^r = rac{1}{|\Omega|} \int_{\Omega} \chi^r(oldsymbol{x}) \Theta^r(oldsymbol{x}) \, doldsymbol{x}, \quad c_r = rac{1}{|\Omega|} \int_{\Omega} \chi^r(oldsymbol{x}) \, doldsymbol{x}$$

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

$$\mathcal{T}^{eff} = \{ \bar{\boldsymbol{\theta}} \in \mathbb{R}^n_k | \bar{\theta}^r_i \ge 0; \sum_{i=1}^{\kappa} \bar{\theta}^r_i = c^r \ \forall r \}$$

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Step 3 - Make the bound independent of arepsilon

Set

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

We have

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

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Step 3 - Make the bound independent of arepsilon

Set

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

We have

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

▶ Since $\bar{\Theta} \in \mathcal{T}^{\textit{eff}}$, we have

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

The RHS is independent of ε

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Summary

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

with

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

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

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

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Convex bound

Choice 1

$$K = 0$$
 and $\tau^r = \tau$ independent of r

• We have
$$W(ar{arepsilon}) = ar{arepsilon}$$
 : $oldsymbol{ au}$

• Optimizing with respect to au gives

$$\Psi^{eff}(ar{arepsilon}) \geq \inf_{ar{m{ heta}} \in \mathcal{T}^{eff}} \{ C \Psi^{eff}(ar{arepsilon},ar{m{ heta}}) \}$$

with

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

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Bound depending on one-point statistics

Choice 2

K quasiconvex and $au^r = au$ independent of r

► We have

$$W(ar{arepsilon}) \geq ar{arepsilon}:oldsymbol{ au} + rac{1}{2}ar{arepsilon}:oldsymbol{K}:ar{arepsilon}$$

• Optimizing with respect to au gives

$$\begin{split} \Psi^{eff}(\bar{\varepsilon},\bar{\theta}) \geq & \frac{1}{2}\bar{\varepsilon}:\boldsymbol{K}:\bar{\varepsilon} + \frac{1}{2}\boldsymbol{f}:\left(\sum_{r=1}^{n}c^{r}\left(\boldsymbol{L}^{r}-\boldsymbol{K}\right)^{-1}\right)^{-1}:\boldsymbol{f} \\ & +\sum_{r,i}\bar{\theta}_{i}^{r}w_{i}^{0} + \frac{1}{2}\sum_{r=1}^{n}\sum_{i=1}^{k}\bar{\theta}_{i}^{r}\varepsilon_{i}^{r}:\boldsymbol{M}^{r}(\boldsymbol{K}):\varepsilon_{i}^{r} \end{split}$$
with $\boldsymbol{f}=\bar{\varepsilon}-\sum_{r}(\boldsymbol{L}^{r}-\boldsymbol{K})^{-1}:\boldsymbol{L}^{r}:\varepsilon^{r}(\bar{\theta})$ and $\varepsilon^{r}(\bar{\theta})=\sum_{i}\bar{\theta}_{i}^{r}\varepsilon_{i}^{r}$

Bound depending on one-point statistics

Choice 2

- **K** quasiconvex and $\tau^r = \tau$ independent of r
- Case of equal elastic moduli $L_1 = \cdots = L_n (= L_0)$:

$$\Psi^{eff}(ar{arepsilon}) \geq \inf_{ar{m{ heta}}\in\mathcal{T}^{eff}} C \Psi^{eff}(ar{arepsilon},ar{m{ heta}}) + g(ar{m{ heta}})$$

with

$$\begin{aligned}
\mathcal{L}\Psi^{eff}(\bar{\varepsilon},\bar{\theta}) &= \frac{1}{2}(\bar{\varepsilon} - \sum_{r,i} \bar{\theta}_{i}^{r} \varepsilon_{i}^{r}) : \mathcal{L}^{0} : (\bar{\varepsilon} - \sum_{r,i} \bar{\theta}_{i}^{r} \varepsilon_{i}^{r}) + \sum_{r,i} \bar{\theta}_{i}^{r} w_{i}^{0} \\
g(\bar{\theta}) &= \frac{1}{4} \sum_{r,i} \bar{\theta}_{i}^{r} \bar{\theta}_{j}^{s}(\varepsilon_{i}^{r} - \varepsilon_{j}^{s}) : \mathcal{M}^{0}(\mathcal{K}) : (\varepsilon_{i}^{r} - \varepsilon_{j}^{s}) &= 0 \\
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\end{aligned}$$

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Bound depending on two-point statistics

Choice 3

$$\textbf{\textit{K}}=\tilde{\textbf{\textit{L}}}+\tilde{\textbf{\textit{K}}}$$
 with $\tilde{\textbf{\textit{K}}}$ quasiconvex and $\tilde{\textbf{\textit{L}}}>0$

We have

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

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Bound depending on two-point statistics

Choice 3

$$\textbf{\textit{K}}=\tilde{\textbf{\textit{L}}}+\tilde{\textbf{\textit{K}}}$$
 with $\tilde{\textbf{\textit{K}}}$ quasiconvex and $\tilde{\textbf{\textit{L}}}>0$

We have

$$W(ar{arepsilon}) \geq (1/2)ar{arepsilon}:ar{oldsymbol{\mathcal{K}}}:ar{arepsilon}+ ilde{W}(ar{arepsilon})$$

where

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

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Bound depending on two-point statistics

Choice 3

$$\textbf{\textit{K}}=\tilde{\textbf{\textit{L}}}+\tilde{\textbf{\textit{K}}}$$
 with $\tilde{\textbf{\textit{K}}}$ quasiconvex and $\tilde{\textbf{\textit{L}}}>0$

We have

$$W(ar{arepsilon}) \geq (1/2)ar{arepsilon}:ar{oldsymbol{\mathcal{K}}}:ar{arepsilon}+ ilde{W}(ar{arepsilon})$$

$$ilde{W}(ar{arepsilon}) = rac{1}{2}ar{arepsilon}: ar{oldsymbol{\mathcal{L}}}:ar{arepsilon} + \sum_r c^r oldsymbol{ au}^r: ar{arepsilon} - rac{1}{2}\sum_{r,s} oldsymbol{ au}^r: oldsymbol{\mathcal{A}}^{rs}: oldsymbol{ au}^s$$

with

$$oldsymbol{A}^{rs} = rac{1}{|\Omega|} \int_{\Omega} \chi^r(oldsymbol{x}) (oldsymbol{\Gamma} \chi^s)(oldsymbol{x}) \, doldsymbol{x}$$

and Γ is a singular integral operator (related to Green functions) (Willis 1981). 25 'Martensitic polycrystals' Workshop

Case of equal elastic moduli

We obtain

$$\Psi^{eff}(ar{arepsilon}) \geq \inf_{ar{oldsymbol{ heta}} \in \mathcal{T}^{eff}} C \Psi^{eff}(ar{arepsilon},ar{oldsymbol{ heta}}) + h(ar{arepsilon},ar{oldsymbol{ heta}})$$

with

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

where $\pmb{K}= \pmb{ ilde{K}}+ \pmb{ ilde{L}}$ and $\{\pmb{ ilde{ au}}'\}$ is solution of

$$c^r (\mathcal{L}^0 - \mathcal{K})^{-1} : ilde{ au}^r + \sum_s \mathcal{A}^{rs} : ilde{ au}^s = c^r ar{arepsilon} - (\mathcal{L}^0 - \mathcal{K})^{-1} : \mathcal{L}^0 : arepsilon^r (ar{ heta})$$

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Case of ellipsoidal symmetry

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

$$oldsymbol{A}^{
m rs}=c^{
m r}(\delta_{
m rs}-c^{
m s})oldsymbol{P}(\widetilde{oldsymbol{L}})$$

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

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

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

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Lower bounds for polycrystals

[M.P., J.Mech.Phys.Solids, 2009]

Convex bound

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

Non convex bound, 1-point statistics

$$\Psi^{eff}(ar{m{arepsilon}}) \geq \inf_{ar{m{ heta}}\in\mathcal{T}^{eff}} C \Psi^{eff}(ar{m{arepsilon}},ar{m{ heta}}) + g(ar{m{ heta}})$$

Non convex bound, 2-point statistics

$$\Psi^{eff}(ar{arepsilon}) \geq \inf_{ar{m{ heta}} \in \mathcal{T}^{eff}} C \Psi^{eff}(ar{arepsilon},ar{m{ heta}}) + h(ar{m{ heta}})$$

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Lower bounds on the mixing energy

Bound depending on 1-point statistics

$$g(ar{m{ heta}}) = \sup_{m{m{K}}\in\mathcal{C}}rac{1}{4}\sum_{r,s,i,j}ar{m{ heta}}_j^rar{m{ heta}}_j^s(m{arepsilon}_i^r-m{arepsilon}_j^s):m{M}^0(m{K}):(m{arepsilon}_i^r-m{arepsilon}_j^s)$$

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

Bound depending on 2-point statistics

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

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

$$ilde{oldsymbol{\kappa}} \in \mathcal{C}, \quad ilde{oldsymbol{L}} \succ 0, \quad oldsymbol{L}^0 \succ ilde{oldsymbol{L}} + ilde{oldsymbol{\kappa}}$$

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Example 1 : 'minimal' polycrystal

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

 $\mathrm{tr}\, arepsilon^{tr} = 0$

- Orientation 2 : austenite only
- The elasticity tensor L^0 is isotropic and incompressible $(\nu^0 \rightarrow 1/2)$

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Lower bounds on the mixing energy

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

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

$$+2\mu_{0}^{2}\frac{c_{2}}{c_{1}}\theta^{2}\varepsilon^{tr} : (L^{0}-K+(L^{0}-K):P(\tilde{L}):(L^{0}-K))^{-1} : \varepsilon^{tr}\}$$

where $\pmb{K}= \pmb{ ilde{K}}+ \pmb{ ilde{L}}$

Optimization with respect to :

• Isotropic and incompressible elasticity tensors \tilde{L}

ightarrow 1 scalar parameter $ilde{\mu}$

• $\tilde{K} = K(a)$ with tensors a having the same eigenbasis as ε^{tr} \rightarrow 3 scalar parameters

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

It can be shown that the optimal value of a is

$$oldsymbol{a}=0$$
 (i.e. $ilde{oldsymbol{K}}=0$)

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

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

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



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

$$\Psi^{e\!f\!f}_{-}(\bar{\boldsymbol{\varepsilon}}) = \inf_{0 \leq \theta \leq c_1} \frac{1}{2} (\bar{\boldsymbol{\varepsilon}} - \theta \boldsymbol{\varepsilon}^{\boldsymbol{tr}}) : \boldsymbol{L}^0 : (\bar{\boldsymbol{\varepsilon}} - \theta \boldsymbol{\varepsilon}^{\boldsymbol{tr}}) + \lambda_T \theta + h(\theta)$$



Transformation hardening due to elastic interaction between grains

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

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

$$g(\theta) = h(\theta) = \frac{3}{8}\mu_0(1-\theta)\theta$$
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 $D = \sqrt{14c_1(c_2-\theta)\theta}$ and $P(D, c_2, \theta)$ is a polynomial

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



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

$$\Psi^{e\!f\!f}_{-}(\bar{\boldsymbol{\varepsilon}}) = \inf_{0 \leq \theta \leq c_1} \frac{1}{2} (\bar{\boldsymbol{\varepsilon}} - \theta \boldsymbol{\varepsilon}^{\boldsymbol{tr}}) : \boldsymbol{L}^0 : (\bar{\boldsymbol{\varepsilon}} - \theta \boldsymbol{\varepsilon}^{\boldsymbol{tr}}) + \lambda_T \theta + h(\theta)$$



The non compatibility has an influence on the onset of transformation

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Example 2

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

$$arepsilon_1^{tr} = \operatorname{diag} \eta(-1, -1, 2), arepsilon_2^{tr} = \operatorname{diag} \eta(2, -1, -1)$$

- Orientation 2 : austenite only
- The elasticity tensor L^0 is isotropic and incompressible.

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Image: A matrix and a matrix

Lower bounds on the mixing energy

$$g(\theta_1, \theta_2) = \sup \cdots$$
$$\tilde{K}$$
$$h(\theta_1, \theta_2) = \sup \tilde{K}$$
$$\tilde{K}, \tilde{L}$$

Optimization with respect to :

• Isotropic and incompressible elasticity tensors \tilde{L}

ightarrow 1 scalar parameter $ilde{\mu}$

•
$$\tilde{K} = K(a)$$
 with tensors *a* having the same eigenbasis as $\varepsilon_i^{tr} \rightarrow 3$ scalar parameters

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Lower bounds on the mixing energy

$$g(heta_1, heta_2) = \sup \cdots \ ilde{oldsymbol{\mathcal{K}}}$$

$$\rightarrow$$
 can be solved exactly

$$h(heta_1, heta_2) = \sup \cdots \\ ilde{oldsymbol{\mathcal{K}}}, ilde{oldsymbol{\mathcal{L}}}$$

 \rightarrow needs to be solved numerically

Optimization with respect to :

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

Lower bound on the mixing energy

$$(c_1 = 0.2)$$

$$(heta_1, heta_2)=t(\coslpha,\sinlpha)$$
 , $lpha=rac{\pi}{20}$



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

$$(heta_1, heta_2)=t(\coslpha,\sinlpha)$$
 , $lpha=rac{\pi}{20}$



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

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



Lower bound $\Psi_{-}^{e\!f\!f}$ on the effective energy

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



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Polycrystal : lower bound on the energy

Simple examples

Computational aspects

Upper bounds and estimates

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$$\Psi^{eff}(ar{arepsilon}) \geq \inf_{ar{m{ heta}}\in\mathcal{T}^{eff}} C \Psi^{eff}(ar{arepsilon},ar{m{ heta}}) + g(ar{m{ heta}})$$

with

$$g(\bar{\theta}) = \sup_{\boldsymbol{K} \in \mathcal{C}} \frac{1}{4} \sum_{r,s,i,j} \bar{\theta}_{i}^{r} \bar{\theta}_{j}^{s} (\varepsilon_{i}^{r} - \varepsilon_{j}^{s}) : \boldsymbol{M}^{0}(\boldsymbol{K}) : (\varepsilon_{i}^{r} - \varepsilon_{j}^{s})$$
$$\mathcal{C} = \{\boldsymbol{K}(\boldsymbol{a}) : \boldsymbol{a} \succeq 0, \boldsymbol{L} - \boldsymbol{K}(\boldsymbol{a}) \succ 0\}$$

- 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.

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Example : CuAlNi polycrystal

ε_1^0	ε_2^0	ε_3^0
$\left(\begin{array}{ccc} \alpha & 0 & \delta \\ 0 & \beta & 0 \\ \delta & 0 & \alpha \end{array}\right)$	$\left(\begin{array}{ccc} \alpha & 0 & -\delta \\ 0 & \beta & 0 \\ -\delta & 0 & \alpha \end{array}\right)$	$\left(\begin{array}{ccc} \alpha & \delta & 0\\ \delta & \alpha & 0\\ 0 & 0 & \beta \end{array}\right)$
ε_4^0	ε_5^0	ε_6^0
$\left[\begin{array}{ccc} \alpha & -\delta & 0 \\ -\delta & \alpha & 0 \\ 0 & 0 & \beta \end{array}\right)$	$\left(\begin{array}{ccc} \beta & 0 & 0 \\ 0 & \alpha & \delta \\ 0 & \delta & \alpha \end{array}\right)$	$\left(\begin{array}{ccc}\beta & 0 & 0\\ 0 & \alpha & -\delta\\ 0 & -\delta & \alpha\end{array}\right)$

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

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Example : CuAlNi polycrystal

 CuAINi (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

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



(the loading direction n makes a 5 deg angle with u_1).

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Uniaxial traction in a CuAlNi polycrystal

Values of $\boldsymbol{n}.\boldsymbol{\varepsilon}_{i}^{r}.\boldsymbol{n}$

Orientation 1 :

i	1	2	3	4	5	6
$\mathbf{n} \cdot \boldsymbol{\varepsilon}_{i}^{1} \cdot \mathbf{n}$	0.0416	0.0415	0.0391	0.0459	-0.0813	-0.0813

Orientation 2

i	1	2	3	4	5	6
$\mathbf{n} \cdot \boldsymbol{\varepsilon}_{i}^{2} \cdot \mathbf{n}$	-0.0305	-0.0308	0.0234	0.0616	-0.0092	-0.0089

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Polycrystal : lower bound on the energy

Simple examples

Computational aspects

Upper bounds and estimates

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Image: A matrix

Upper bound on the effective energy

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

We have

$$Q\Psi^r(arepsilon) = \inf_{oldsymbol{ heta}\in\mathcal{T}} Q\Psi^r(arepsilon,oldsymbol{ heta})$$

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

$$\Psi^{eff}(ar{arepsilon}) \leq \inf_{arepsilon \in \mathcal{K}(ar{arepsilon})} rac{1}{|\Omega|} \int_\Omega \sum_{r=1}^n \chi^r(oldsymbol{x}) Q \Psi^r(ar{arepsilon}, oldsymbol{ heta}(oldsymbol{x}))) \, doldsymbol{x}$$

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

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

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Case of equal elastic moduli

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

$$Q\Psi^{r}(\bar{\varepsilon}, \theta_{r}) = C\Psi^{r}(\bar{\varepsilon}, \theta_{r}) + f(\theta_{r})$$

It follows that

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

with

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

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

▶ If $L^1 = \cdots = L^r$ (= L^0) then $W(\bar{\varepsilon}) = W(\bar{\varepsilon}, L^0, \{\tau_r\})$ can be calculated.

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Texture with ellipsoidal symmetry

We obtain

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

where
$$\boldsymbol{\sigma}_r = \sum_{i=1}^k \theta_i^r \boldsymbol{L}^0 : \boldsymbol{\varepsilon}_i^r$$
 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)

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

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Example 1 : 'minimal' polycrystal

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

 $\mathrm{tr}\, arepsilon^{tr} = 0$

- Orientation 2 : austenite only
- The elasticity tensor L^0 is isotropic and incompressible $(\nu^0 \rightarrow 1/2)$

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

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



Complete transformation can be achieved.

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

$$ilde{\Psi}^{eff}(ar{arepsilon}) = \inf_{0 \leq heta \leq c_1} rac{1}{2} (ar{arepsilon} - heta arepsilon^{tr}) : L^0 : (ar{arepsilon} - heta arepsilon^{tr}) + \lambda_{\mathcal{T}} heta + ilde{f}(heta)$$



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

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Example 2

2 orientations (isotropically distributed)

Orientation 1 : austenite + 2 compatible variants of martensite

$$\varepsilon_1^{tr} = \operatorname{diag} \eta(-1, -1, 2), \varepsilon_2^{tr} = \operatorname{diag} \eta(2, -1, -1)$$

- Orientation 2 : austenite only
- ► The elasticity tensor *L* is isotropic and incompressible.

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

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



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Example 3

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

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



Traction in a CuAlNi polycrystal

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



Concluding remarks

- Room for improvement
 - Choice of K and 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)