Modeling of polycrystalline materials using a two-scale FE-FFT-based simulation approach

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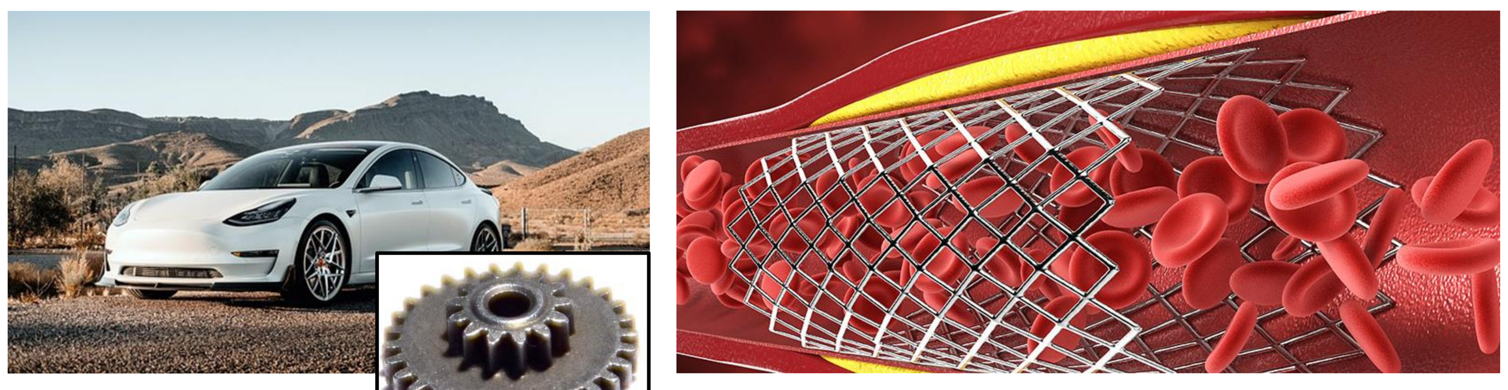
Motivation

Polycrystalline materials used in engineering applications



Automotive industry Medical applications

Desired material properties

- High strength
- Long durability
- Light weight
- Wear resistance

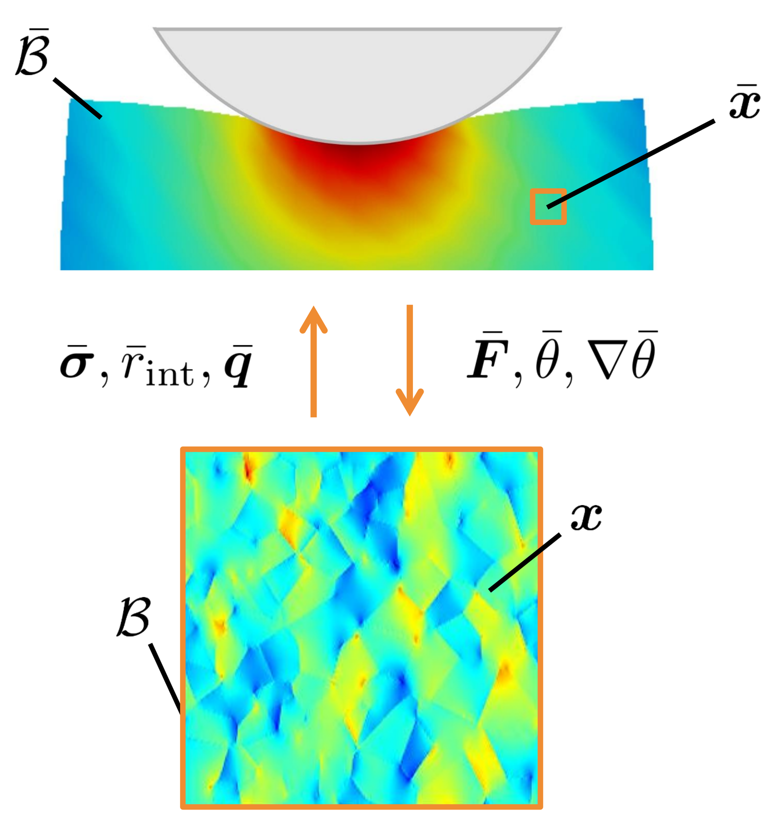
Development of optimized components

- Reduced material consumption
- Targeted adjustment of functional properties

- Prediction of material behavior using a two-scale thermo-mechanically coupled FE-FFT-based simulation approach

Two-scale FE-FFT-based simulation

Homogeneous macroscale



Heterogeneous microscale

$\bar{(\bullet)}$:	Macroscopic quantity
$(\bullet)$:	Microscopic quantity
$\boldsymbol{x}$:	Position vector
$\boldsymbol{F}$:	Deformation gradient
$\boldsymbol{\sigma}$:	Cauchy stress
θ :	Temperature
$\nabla\theta$:	Temperature gradient
r_{int} :	Internal heat sources
$\boldsymbol{q}$:	Heat flux

Numerical methods [1,2,3]

- Finite element (FE) method on macroscale
- Fast Fourier transform (FFT)-based simulation technique on microscale

Microscopic FFT-based solution approach

Governing equations in Fourier space

- Mechanical boundary value problem

$$\hat{\boldsymbol{F}}(\boldsymbol{\xi}) = \begin{cases} -\hat{\boldsymbol{\Gamma}}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}) & \text{for } \boldsymbol{\xi} \neq \boldsymbol{0} \\ \bar{\boldsymbol{F}} & \text{for } \boldsymbol{\xi} = \boldsymbol{0} \end{cases}$$

- Thermal boundary value problem

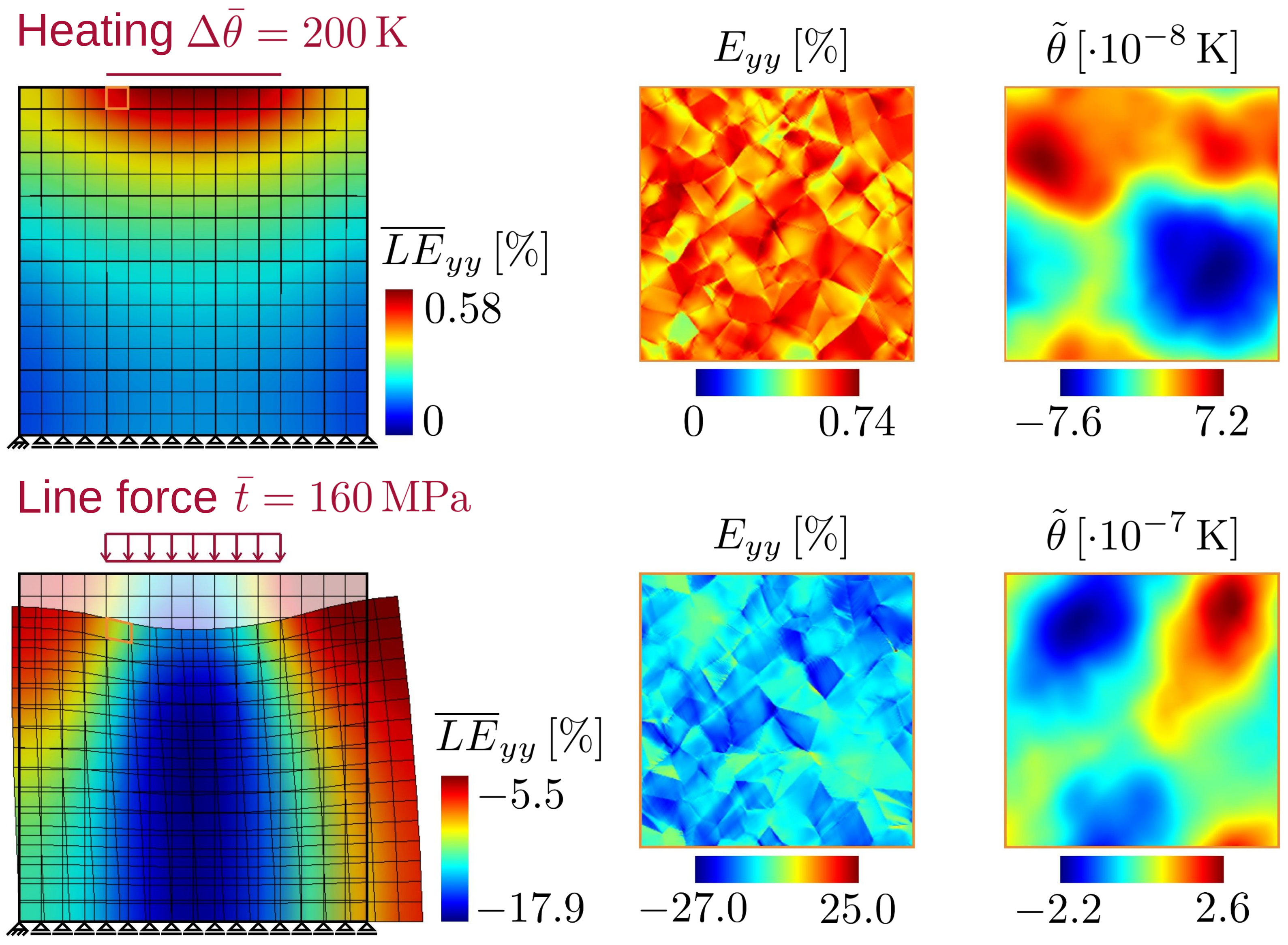
$$\nabla\hat{\theta}(\boldsymbol{\xi}) = \begin{cases} \dfrac{\hat{r}_{\text{int}}(\boldsymbol{\xi})}{\kappa\,\boldsymbol{\xi}\cdot\boldsymbol{\xi}}\boldsymbol{\xi} & \text{for } \boldsymbol{\xi} \neq \boldsymbol{0} \\ \nabla\bar{\theta} & \text{for } \boldsymbol{\xi} = \boldsymbol{0} \end{cases}$$

$\hat{(\bullet)}$:	Quantity in Fourier space
$\boldsymbol{\xi}$:	Fourier mode
$\boldsymbol{\Gamma}^0$:	Green's operator
κ :	Heat conductivity

Structural examples

Multi-physically coupled two-scale simulations

- Modeling the thermo-mechanically coupled material behavior of copper [4,5]

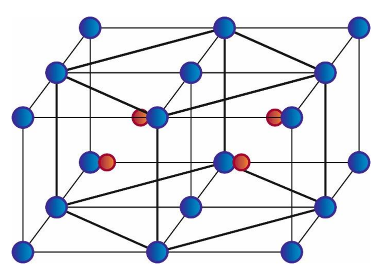


Heating Line force

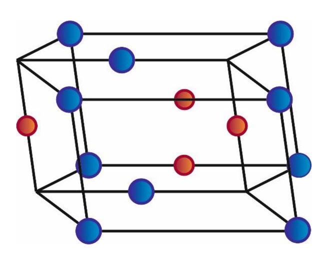
LE :	Logarithmic strain
E :	Green-Lagrange strain
$\tilde{\theta}$:	Fluctuating temperature field

Two-scale simulations of shape memory alloys

- Modeling stress-induced phase transformations between austenite and martensite [6,7]

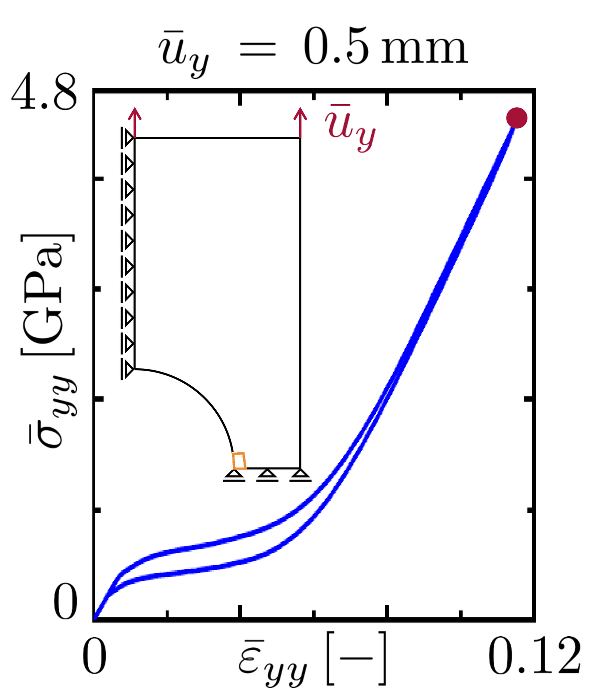


Austenitic lattice

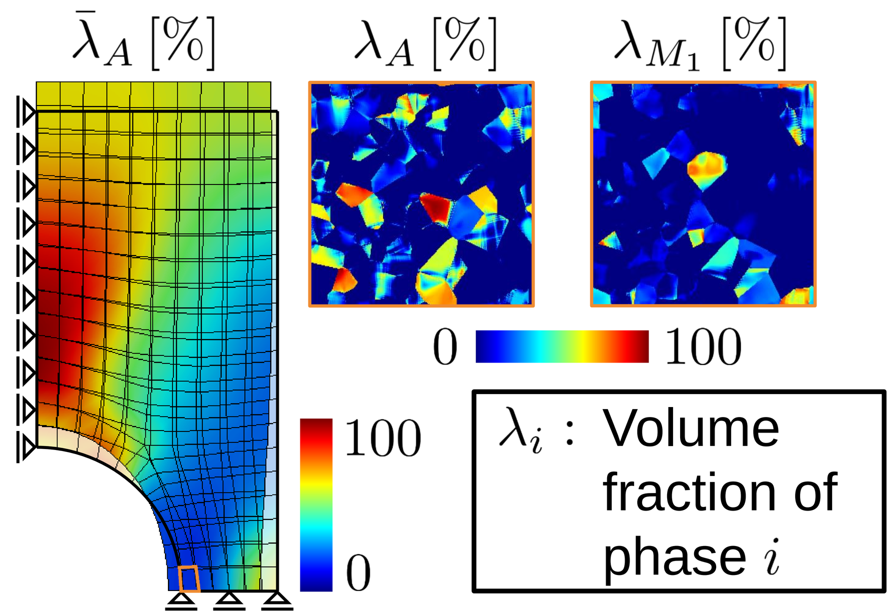


Martensitic lattice

- Pseudoelastic material behavior



- Martensitic phase transformation



λ_i : Volume fraction of phase i

Evolution of martensitic phase transformations over complete simulation time

References

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