Multiscale Modeling in Materials Science

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MPIE research focus: multiscale modeling in the CPTS

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Zeitalter tragen die Namen von Materialien
70% of all **industrial innovations** are associated with progress in **materials science**

**Complex Materials** occupy key roles (energy, transportation, health, safety, infrastructure)

Materials-related industries account for 46% of all EU manufacturing value and 11% of the EU’s total domestic product

3.5 billion € per day in the EU

**World Trade Organisation**

**Mission:** Understanding and designing complex materials from first principles
Scientific mission: complex materials in real environments

Multiple phenomena
Interactions
multiple scales
Multiscale Modeling and Experimentation

- Length [m]
  - $10^0$
  - $10^{-3}$
  - $10^{-6}$
  - $10^{-9}$
  - $10^{-12}$

- Time [s]
  - $10^{-15}$
  - $10^{-9}$
  - $10^{-3}$
  - $10^3$

- Phases, crystals
- Kinetics of defects
- Structure of defects
- Structure of matter
- Boundary conditions
Multiscale Modeling and Experimentation

Length [m]

- $10^0$
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- $10^{-12}$

Structure of defects

Structure of matter

Kinetics of defects

Phases, crystals

Boundary conditions

Time [s]

$10^{-15}$ $10^{-9}$ $10^{-3}$ $10^3$
Multiscale crystal plasticity FEM

PDE solver:

FEM
MC
FFT
CA
LBM
Multiscale crystal plasticity FEM

- External boundary conditions
- Mesh
- Elastic tensor
- Phase fractions
- Defect dynamics
- Crystal kinematics
- Orientation
- Homogenization

FEM
FFT
CA
LBM

\[ \dot{\gamma} = \frac{d\gamma}{dt} = \rho_m b v \]

\[ L_p = \sum_{\alpha=1}^{12} \dot{\gamma}_\alpha \vec{b}_\alpha \otimes \vec{n}_\alpha \]
Towards the limits of strength: cold-drawn pearlitic steel

- Ferrite (~50 ppm C)
- Cementite (25 at.% C)
Towards the limits of strength: cold-drawn pearlitic steel

Ferrite (~50 ppm C)  Cementite (25 at.% C)

C iso-concentration (7 at.%)  (ε = 2)

Deformation-driven cementite dissolution - oversaturated ferrite
Towards the limits of strength: cold-drawn pearlitic steel

C iso-concentration (7 at.%)
New materials for key technologies: Aero-space
New materials for key technologies: Aero-space
Complex Ni-based superalloy (ERBO, CMSX-4) 56 at.% Al, Re, W, Ni iso
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Complex Ni-based superalloy (ERBO, CMSX-4)

Al  Re  W  Ni-iso (56 at.%)
Change of microstructure
Exoskeleton component of more than 90% of all species ... adaptive material ➔ candidate for bio-inspired material
## Hierarchical stiffness modeling

<table>
<thead>
<tr>
<th>Scale</th>
<th>0.1 nm – 10 nm</th>
<th>10 nm – 100 nm</th>
<th>100 nm – 10 μm</th>
<th>10 μm – 1 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Hierarchical structure unit</strong></td>
<td>α-chitin (H-bonded anti-parallel N-acetyl-glucosamine molecular chains)</td>
<td>Mineralized chitin-protein nanofibrils in a planar array</td>
<td>Twisted plywood stack of mineralized chitin-protein planes without pore canals</td>
<td>Twisted plywood stack of mineralized chitin-protein planes with pore canals</td>
</tr>
<tr>
<td><strong>Experimental method</strong></td>
<td>Transmission electron microscope</td>
<td>Field emission scanning electron microscope</td>
<td>Field emission scanning electron microscope</td>
<td>Field emission scanning electron microscope</td>
</tr>
<tr>
<td><strong>Microstructure</strong></td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
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<tr>
<td><strong>Schematic</strong></td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
<td><img src="image7.png" alt="Image" /></td>
<td><img src="image8.png" alt="Image" /></td>
</tr>
<tr>
<td><strong>Simulation method</strong></td>
<td>Ab initio; density functional theory</td>
<td>Mori-Tanaka scheme (chitin-protein fiber); Torquato 3-point scheme (mineral-protein matrix)</td>
<td>Voigt estimate, tensor rotation</td>
<td>Torquato 3-point homogenization</td>
</tr>
<tr>
<td><strong>Elastic behavior, 3D map of Young’s modulus [GPa]</strong></td>
<td><img src="image9.png" alt="Image" /></td>
<td><img src="image10.png" alt="Image" /></td>
<td><img src="image11.png" alt="Image" /></td>
<td><img src="image12.png" alt="Image" /></td>
</tr>
<tr>
<td><strong>a,b-axis:</strong> basal directions of chitin cell</td>
<td><img src="image13.png" alt="Image" /></td>
<td><img src="image14.png" alt="Image" /></td>
<td><img src="image15.png" alt="Image" /></td>
<td><img src="image16.png" alt="Image" /></td>
</tr>
<tr>
<td><strong>c-axis:</strong> longitudinal axis of molecule</td>
<td><img src="image17.png" alt="Image" /></td>
<td><img src="image18.png" alt="Image" /></td>
<td><img src="image19.png" alt="Image" /></td>
<td><img src="image20.png" alt="Image" /></td>
</tr>
</tbody>
</table>
BCC Ti alloys as biomaterials (implants)

- Strategy for lower elastic stiffness:
  - β-Ti (BCC: Ti-Nb, Ti-Mo, Ti-V,...)
  - Bio-compatible alloy elements

20-25 GPa

20-25 GPa

Ti-Nb

5 GPa
Elastic properties: Ti-Nb system

Young’s modulus surface plots

Ti-18.75at.%Nb

$A_z = 3.210$

Ti-25at.%Nb

$A_z = 2.418$

Ti-31.25at.%Nb

$A_z = 1.058$

Pure Nb

$A_z = 0.5027$

$A_z = 2 \frac{C_{44}}{(C_{11} - C_{12})}$

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Elastic properties: Ti-Nb system

Young's modulus surface plots

- Ti: 115 GPa
- Ti-35wt.%Nb: 59.9 GPa

\[ A_z = \frac{2 C_{44}}{C_{11} - C_{12}} \]
Successfully dealing with:
Complexity, multiple scales, interaction with experiments

Grand challenges / quo vadis:
Massive parallelization of PDE models
Exchange-correlation functions in DFT
Inverse models
Time scale bridging
Scale hoping
More physics into continuum theory
Systematics of coarse graining: Renormalization group theory
The Düsseldorf Max-Planck Team

Thank you for the attention