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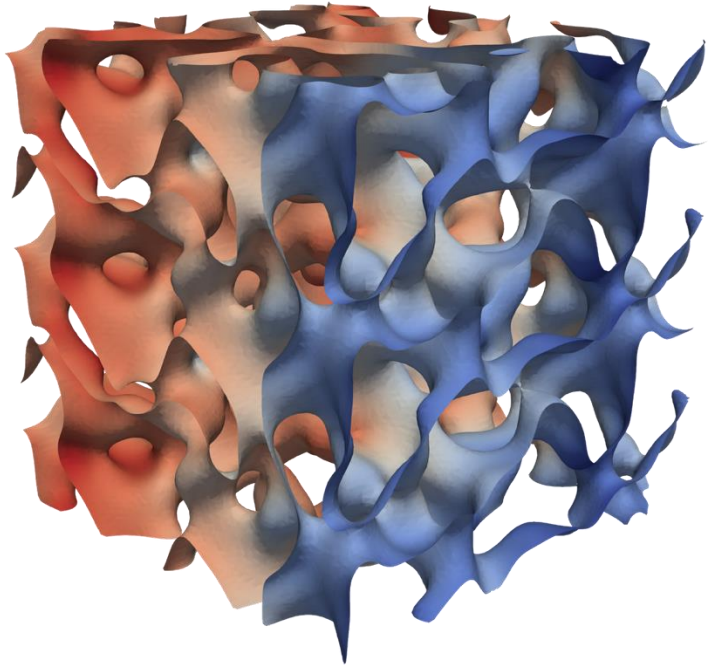
Accessing the Mesoscale with Phase-field Modeling



by Michele Kotiuga, Kyle Starkey, Leonid Kahle

18-21 November 2025

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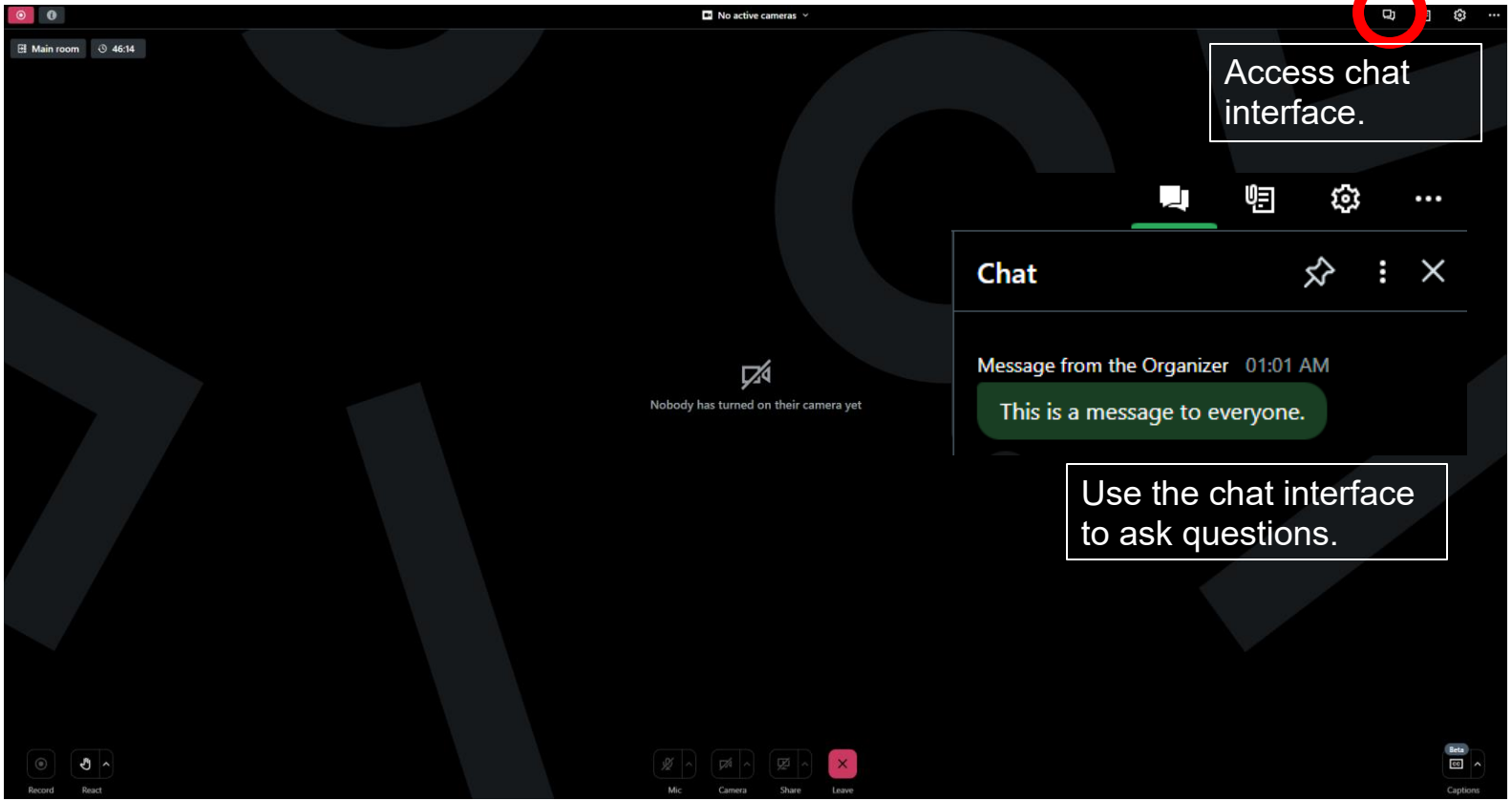

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Webinar Speakers

Katherine Hollingsworth ***Dr. Kyle Starkey*** ***Dr. Michele Kotiuga*** ***Dr. Leonid Kahle***

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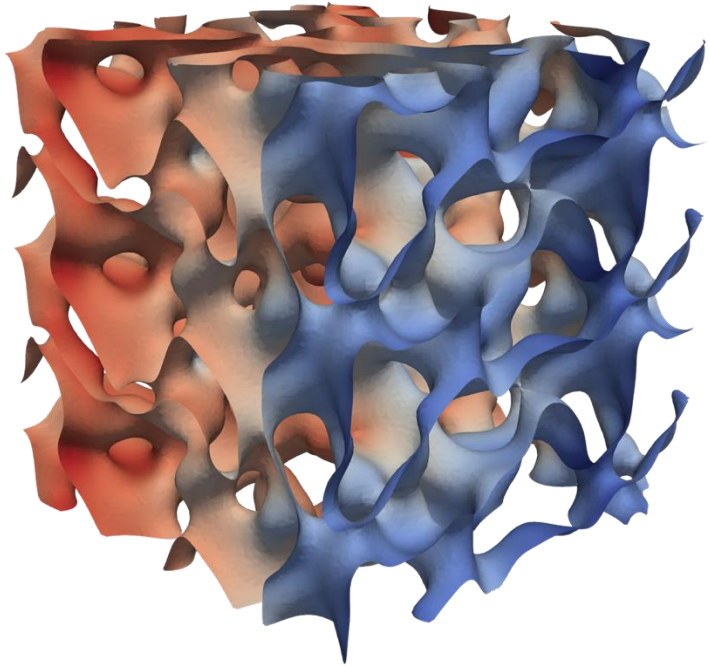
Accessing the Mesoscale with Phase-field Modeling



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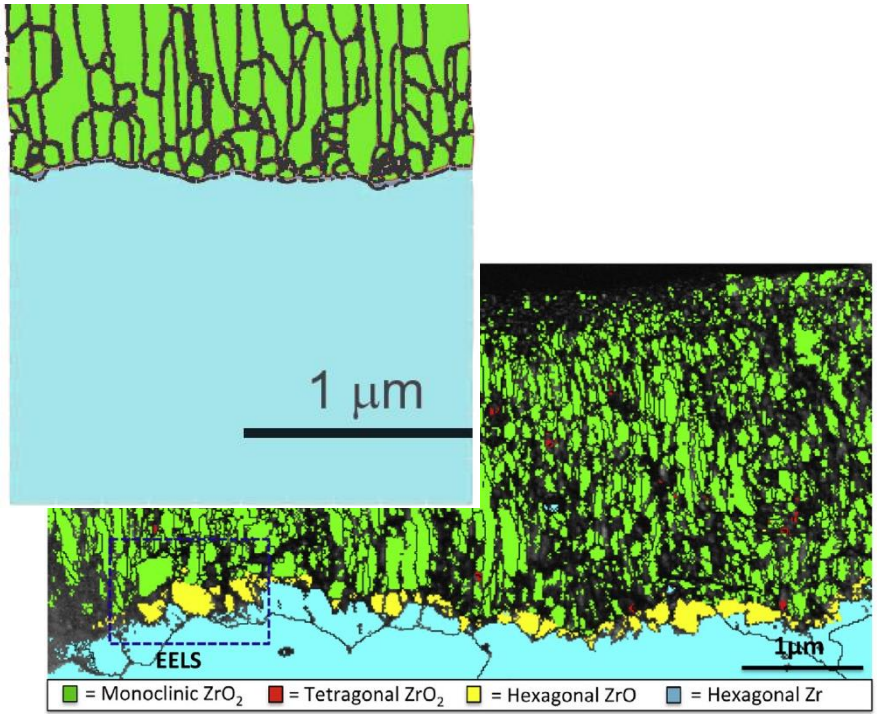
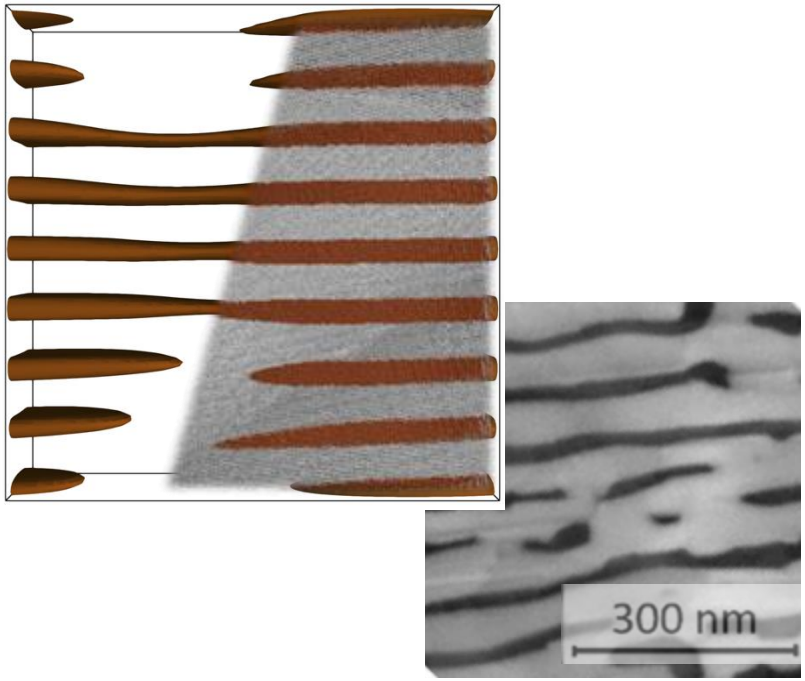
MedeA PhaseField elucidates the microstructure!

Columnar structure in corrosion layer



Hu et al., Micron **69**, 35 (2015)

Lamellar structure in spinodal decomposition



Kwon et al., J Mater Sci **54**, 9168 (2019)

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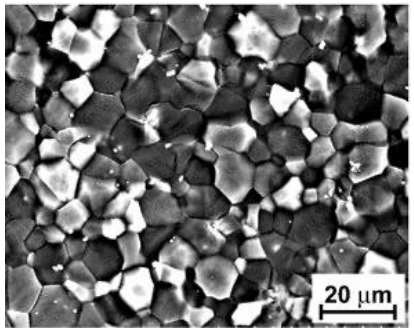
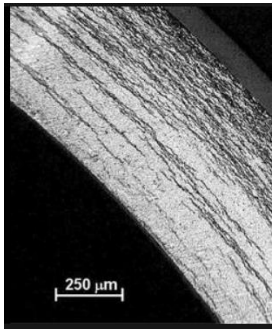
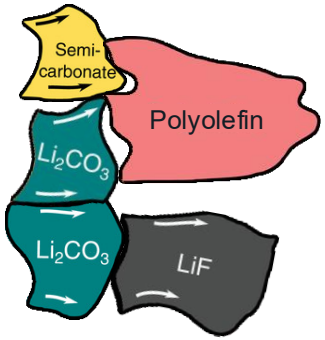
Why study materials' microstructure?

Material behavior is often determined at micrometers scale over seconds/years:

- Grain morphology/distribution when crystallizing alloys from melt
- Hydride formation in metals and resulting component degradation
- Buildup of solid-electrolyte interphases and effect on battery performance
- Corrosion and cracking of metals and resulting surface passivation or cracking







- **Bulk diffusion** • **Phase stability** • **Grain nucleation** • **Elastic deformation** • **Cracking**
- **Electrochemistry** • **Electrostatics** • **Porosity** • **Grain boundary diffusion**

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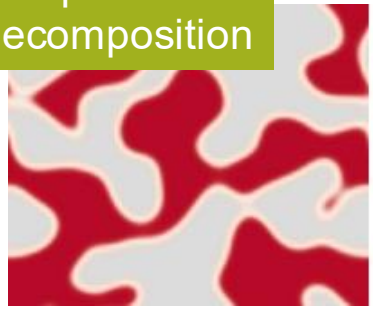
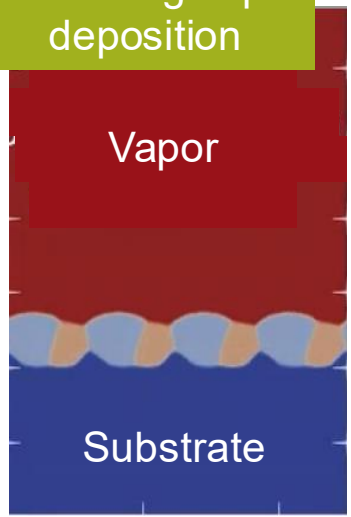
Today's agenda

MedeA PhaseField: the machinery under the hood

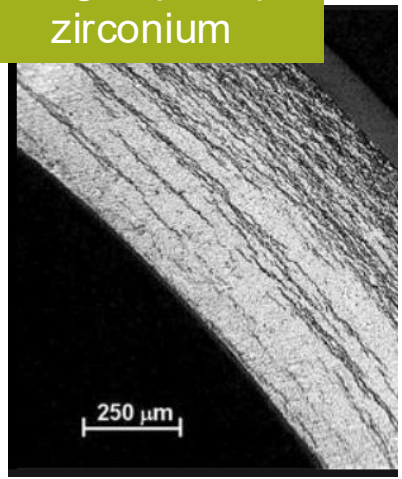
Spinodal decomposition



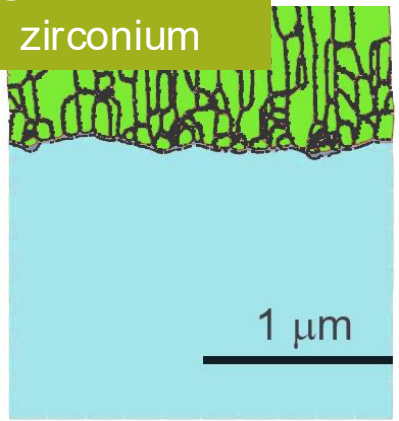
Simulating vapor deposition



Hydrogen pickup in zirconium



Corrosion of zirconium



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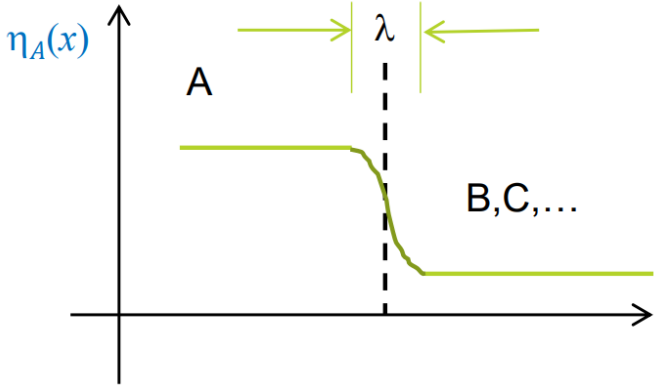
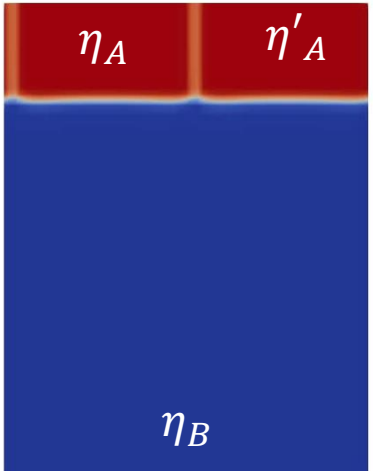
The phase-field method

A continuum approach where **phases** are represented as **fields**
– no explicit atoms or particles

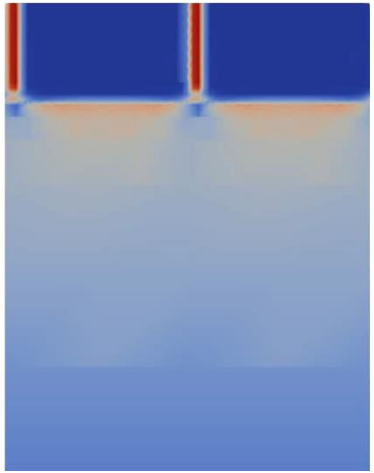
$$\eta_A = \begin{cases} 1 & \text{Phase A} \\ 0 & \text{other phases} \end{cases}$$



Order parameters



Flux



Order parameters (η) are used to delineate different **phases**/grains → Phase field

Concentration and stresses are also represented as fields

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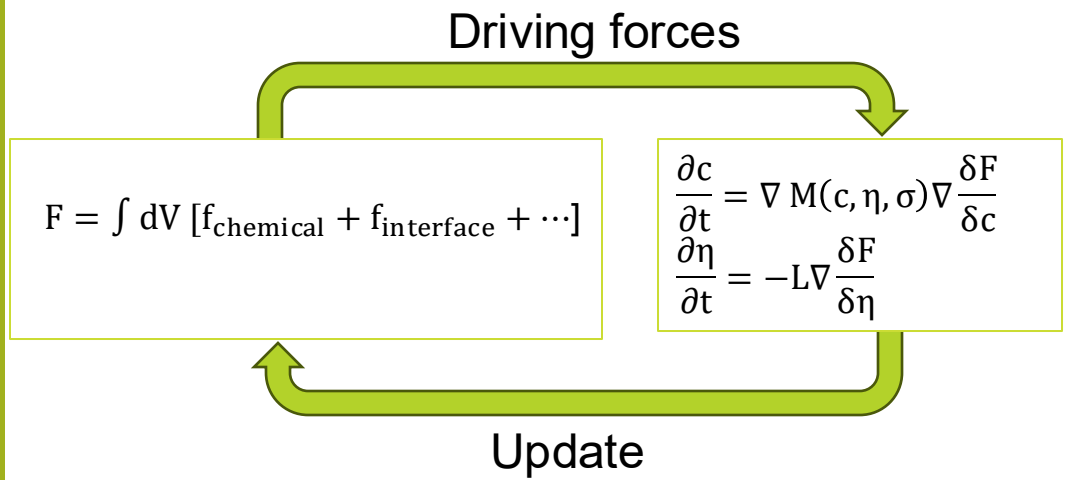
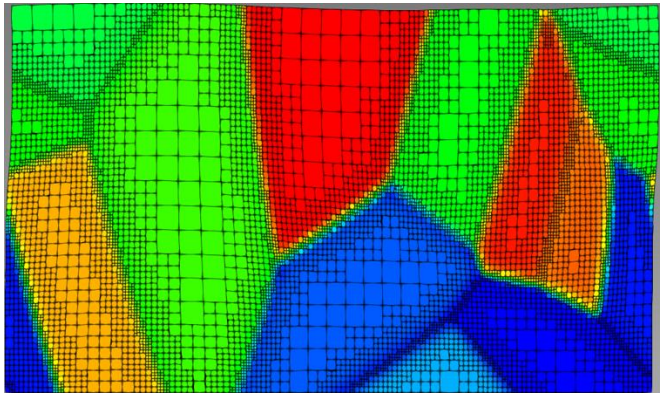
Solving the phase-field equations

The energy becomes a functional of the order parameters η, concentration c, stress σ, etc.

We solve the phase-field equations on an adaptive 2D or 3D mesh using Finite Elements:





Implementation of the
Cahn-Hilliard & Allen-Cahn equations

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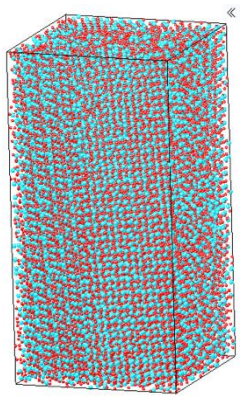
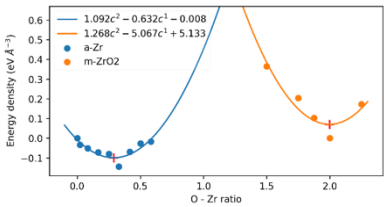
Physics included in model

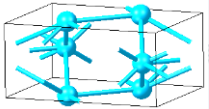
GB Diffusion

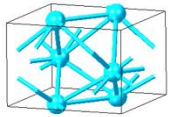


Bulk free energy

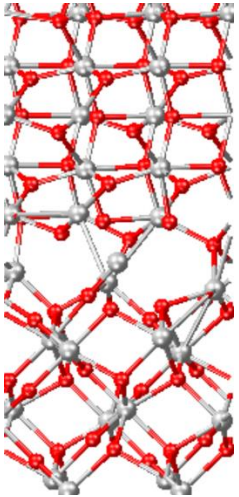


Elasticity

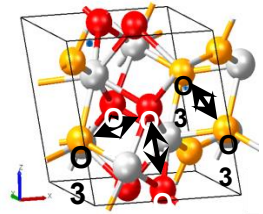




Interfaces



Bulk Diffusion



$$\frac{\partial c}{\partial t} = \nabla M(c, \eta, \sigma) \nabla \frac{\delta F}{\delta c}$$
$$\frac{\partial \eta}{\partial t} = -L \nabla \frac{\delta F}{\delta \eta}$$

$$F = \int dV \left[f_{chemical} + f_{elastic} + f_{interfacial} \right]$$

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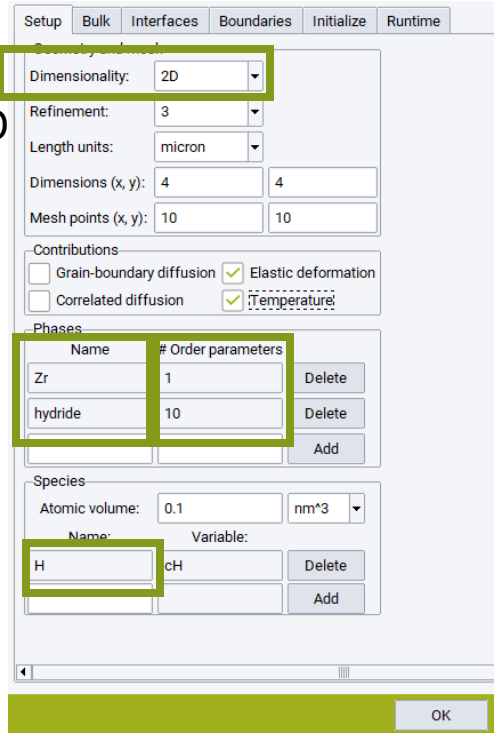
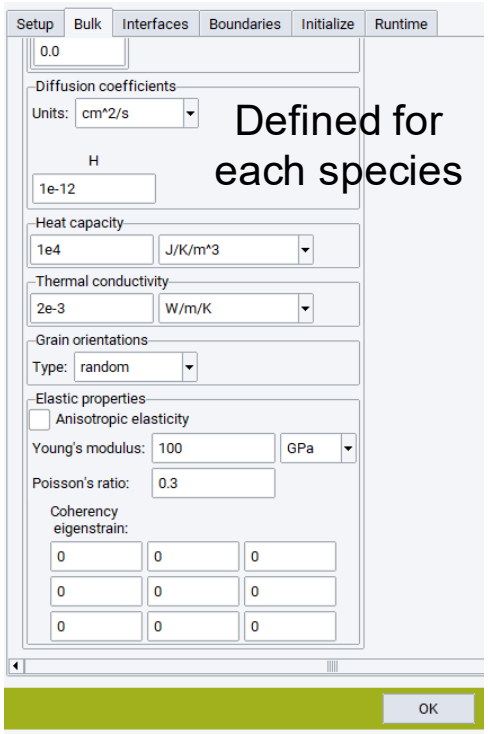
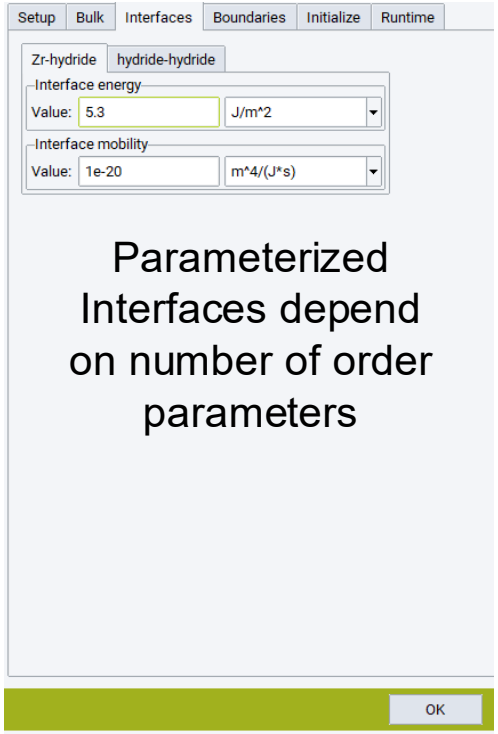
MedeA PhaseField interface

Select 2D or 3D





Defined for each species



Parameterized Interfaces depend on number of order parameters

Bulk parameters set for each phase

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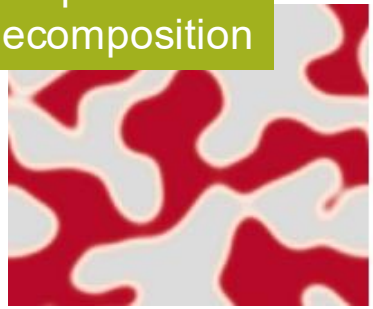
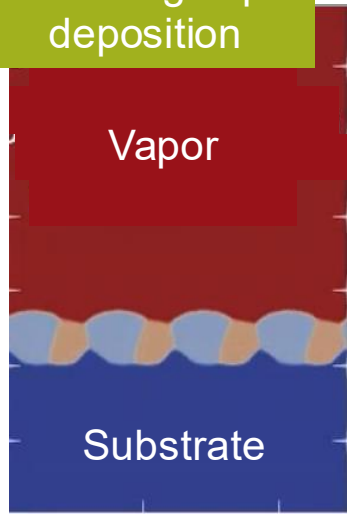
Today's agenda

MedeA PhaseField: the machinery under the hood

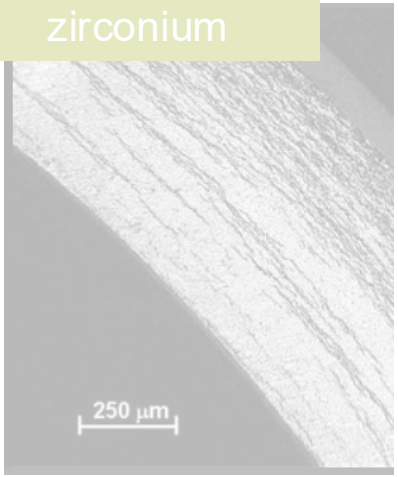
Spinodal decomposition



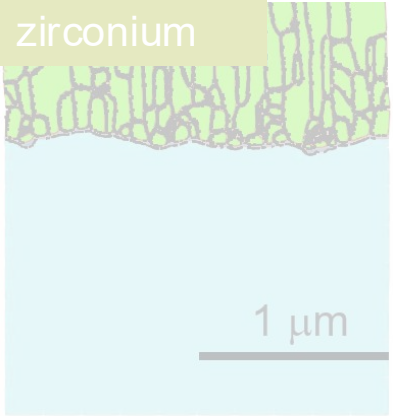
Simulating vapor deposition



Hydrogen pickup in zirconium



Corrosion of zirconium



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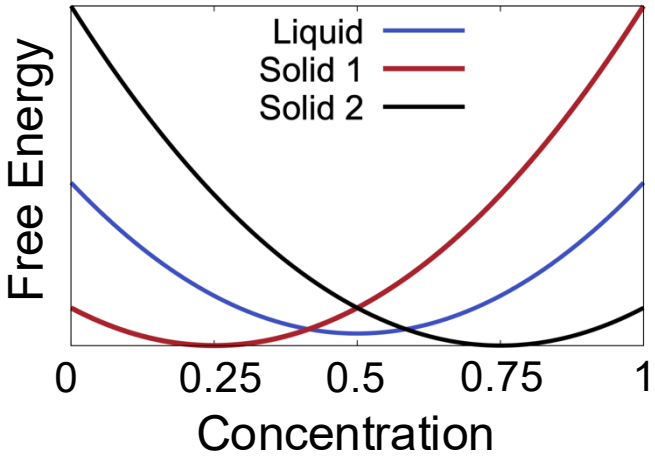
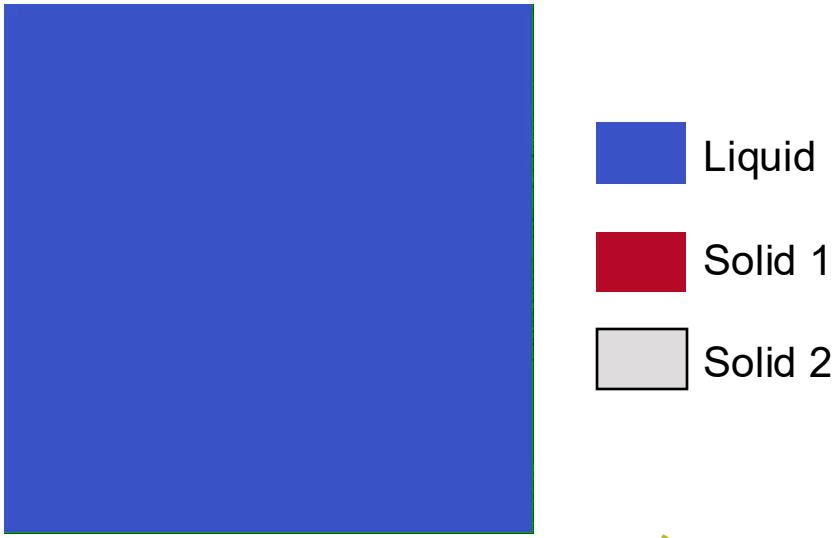
Spinodal decomposition with *MedeA PhaseField*

Liquid spontaneously separates into 2 phases caused by no thermodynamic barrier



Initialize a liquid with random perturbations:



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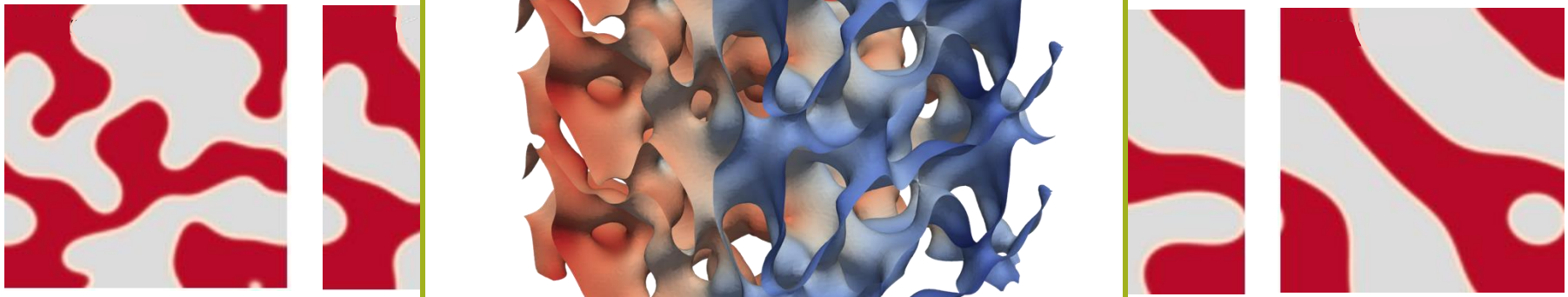
Smaller interface energy = More intricate microstructure

0.6 J/m^2 1 /m^2 3 J/m^2



Investigate and visualize 3D simulations as well!

You ca wing the
“ ial

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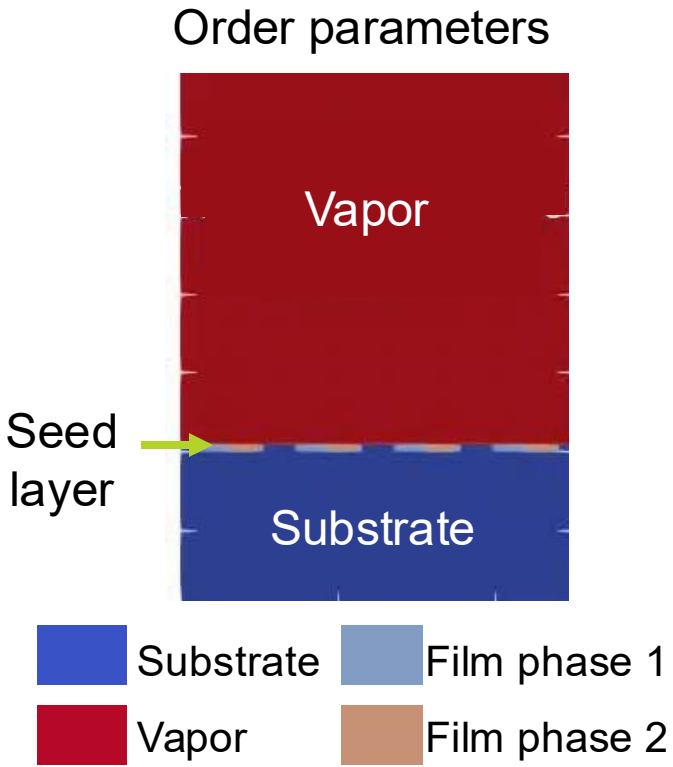
Vapor deposition: microstructures in a thin film



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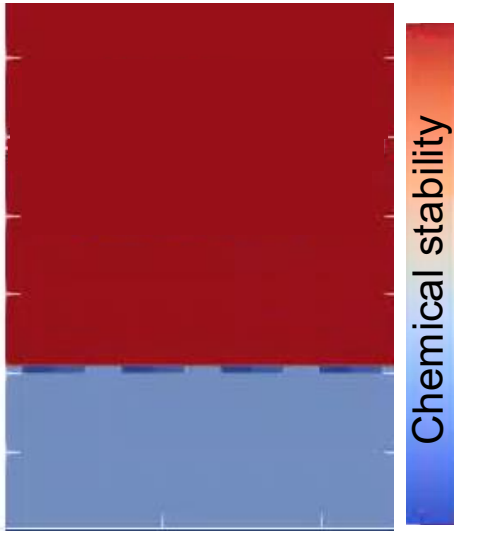
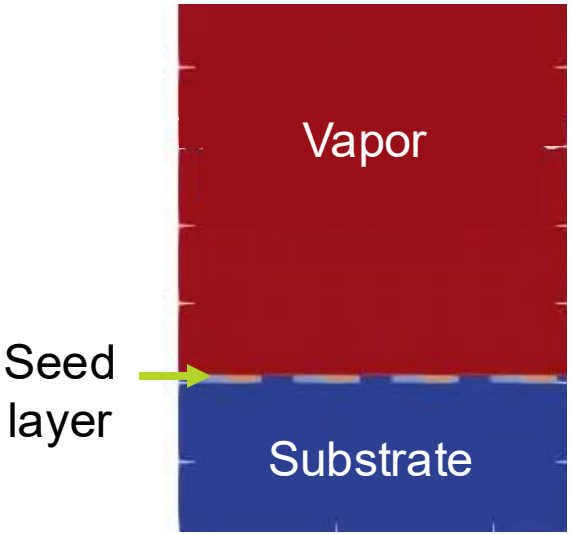
Vapor deposition: microstructures in a thin film

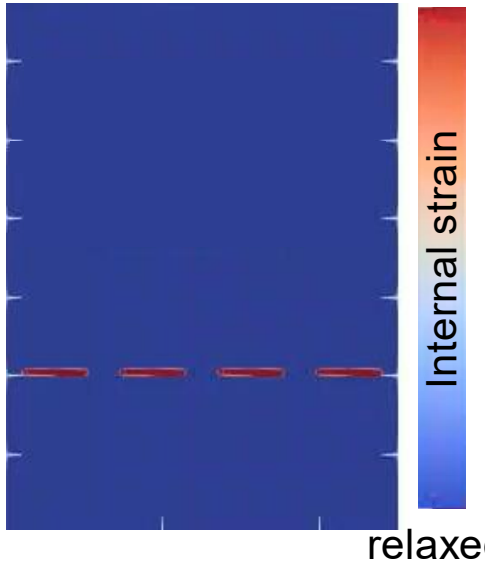
Chemical energy density



Order parameters



Elastic energy density



Substrate
Film phase 1
Vapor
Film phase 2

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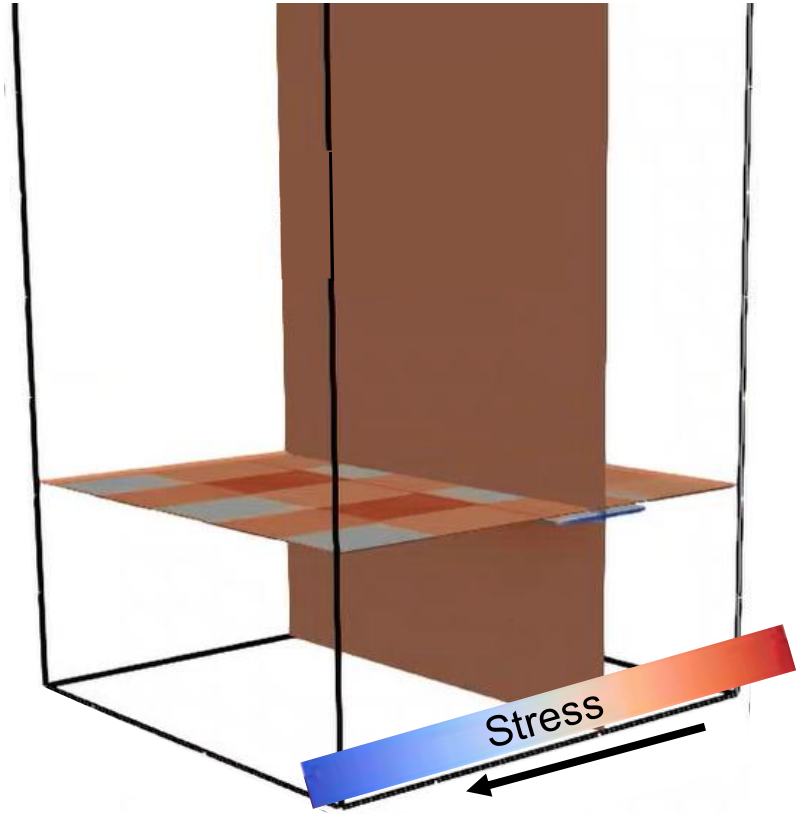
Vapor deposition: microstructures in a ***3D*** thin film



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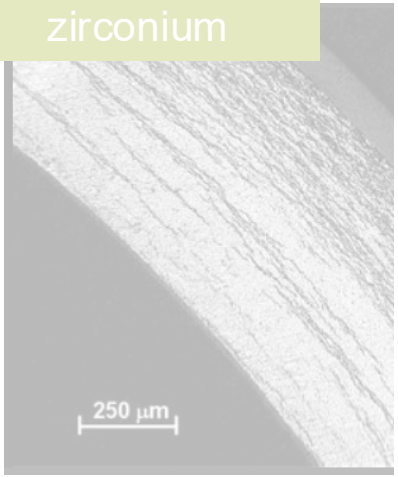
Today's agenda

MedeA PhaseField: the machinery under the hood

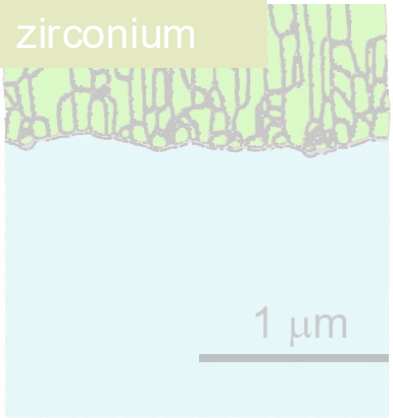
Spinodal decomposition

Simulating vapor deposition

Hydrogen pickup in zirconium



Corrosion of zirconium



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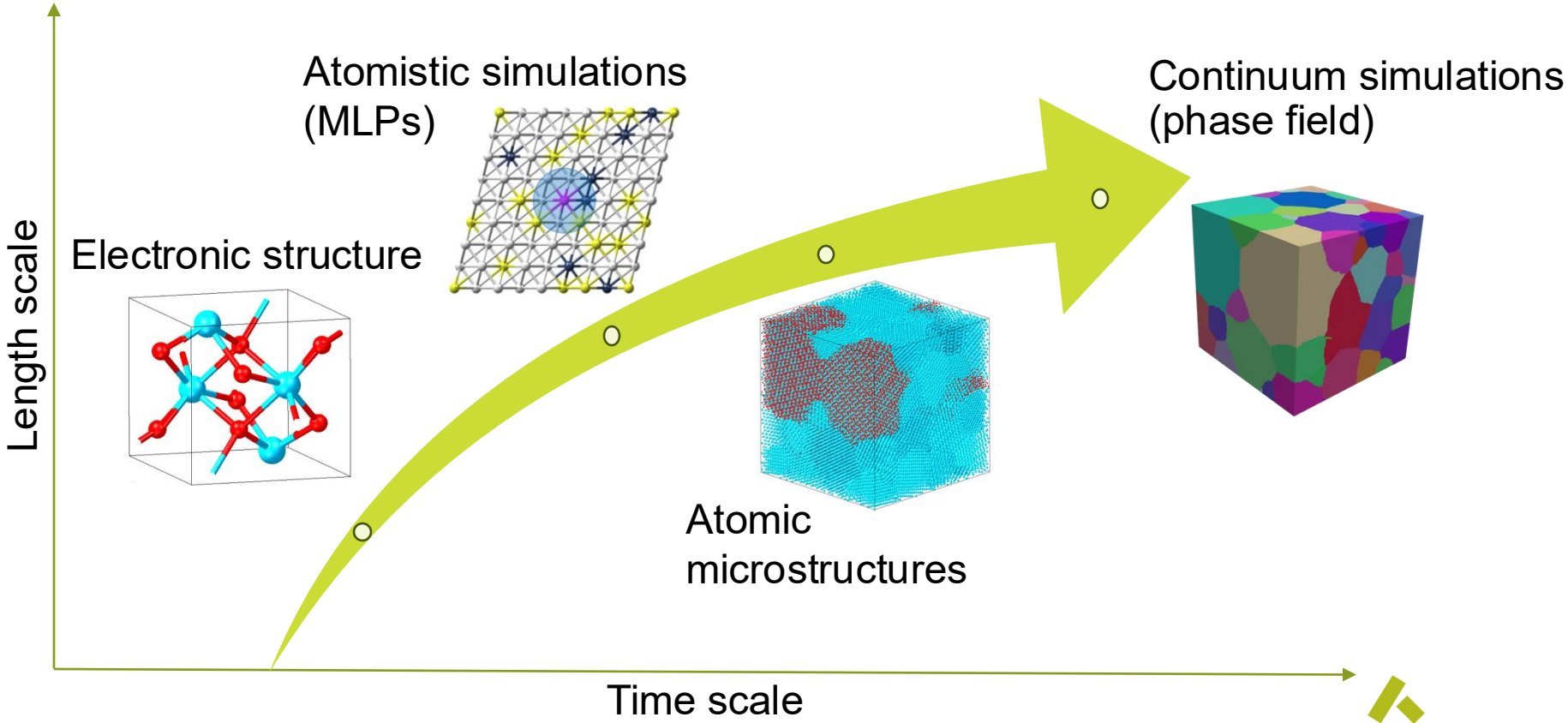
Multiscale modelling using the *MedeA* environment



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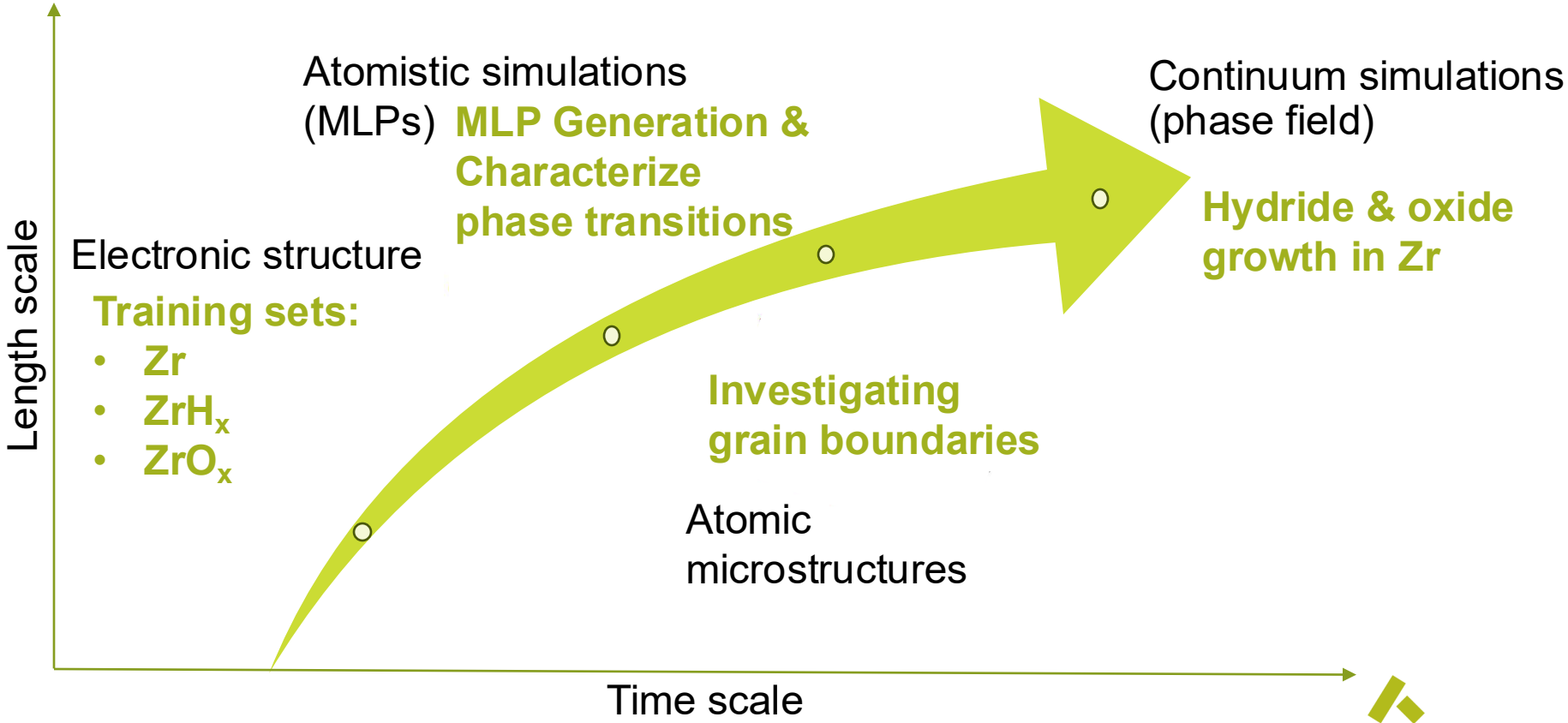
Multiscale modelling using the *MedeA* environment



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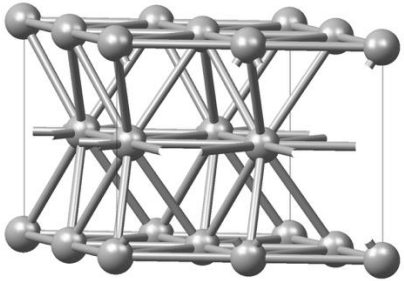
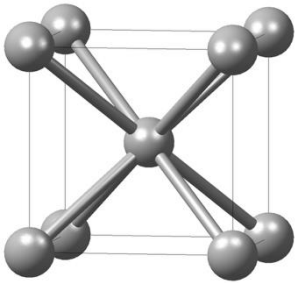
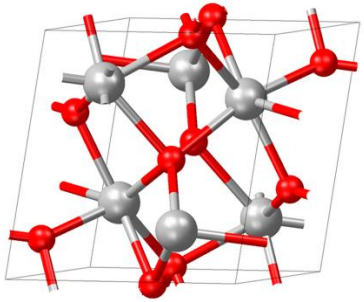
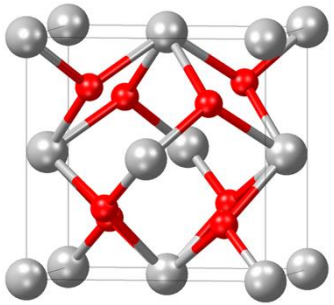
Generating a training set for Zr-O-H









Training set comprised of multiple phases of Zr, ZrH_x and ZrO_x including: strains, defects, ab initio molecular dynamics

~10,000 structures

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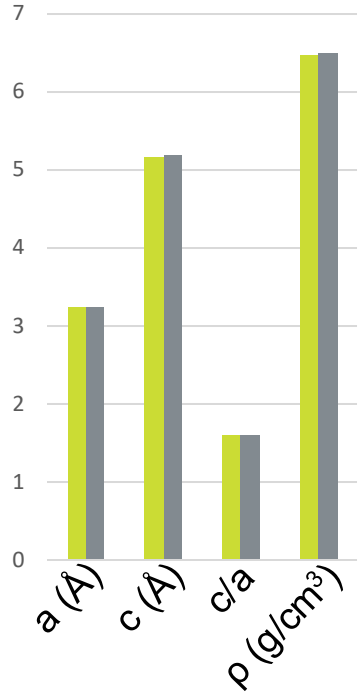
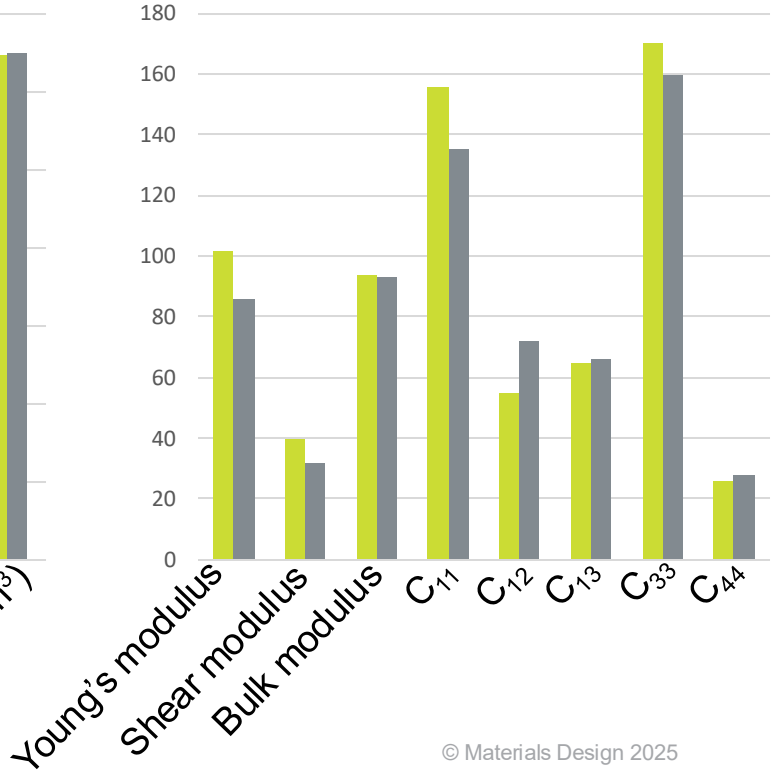
α-Zr: SNAP agreement with VASP training data

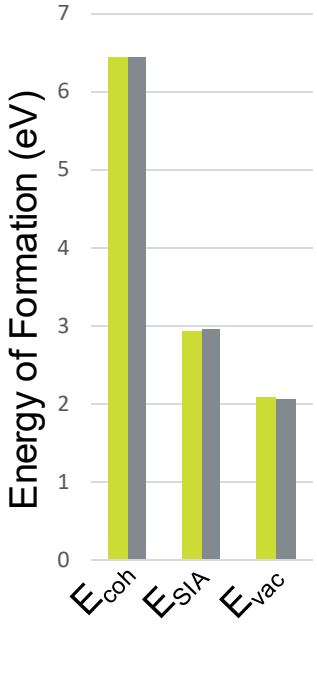
Structural properties

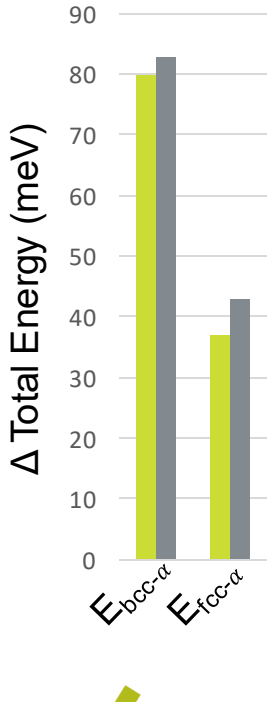


Elastic properties (GPa)



Energetics





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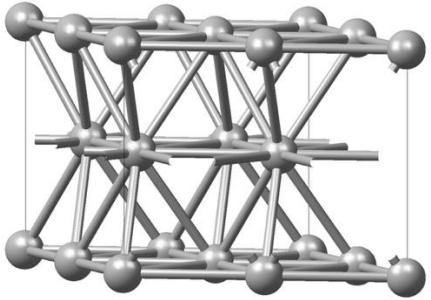
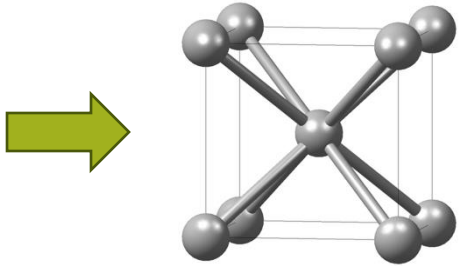
αZr-βZr: A Martensitic phase transition

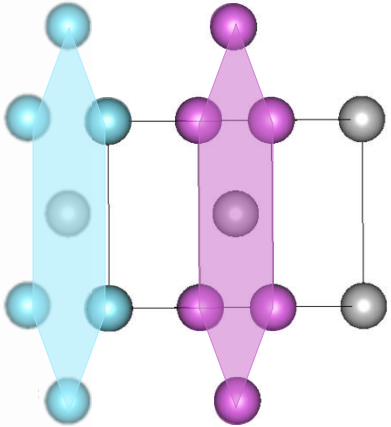
Low T: α-phase, hcp

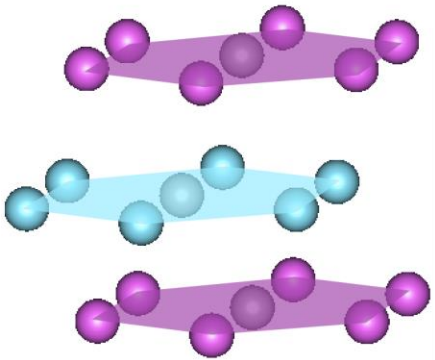
High T: β-phase, bcc





Consider the (110) plane

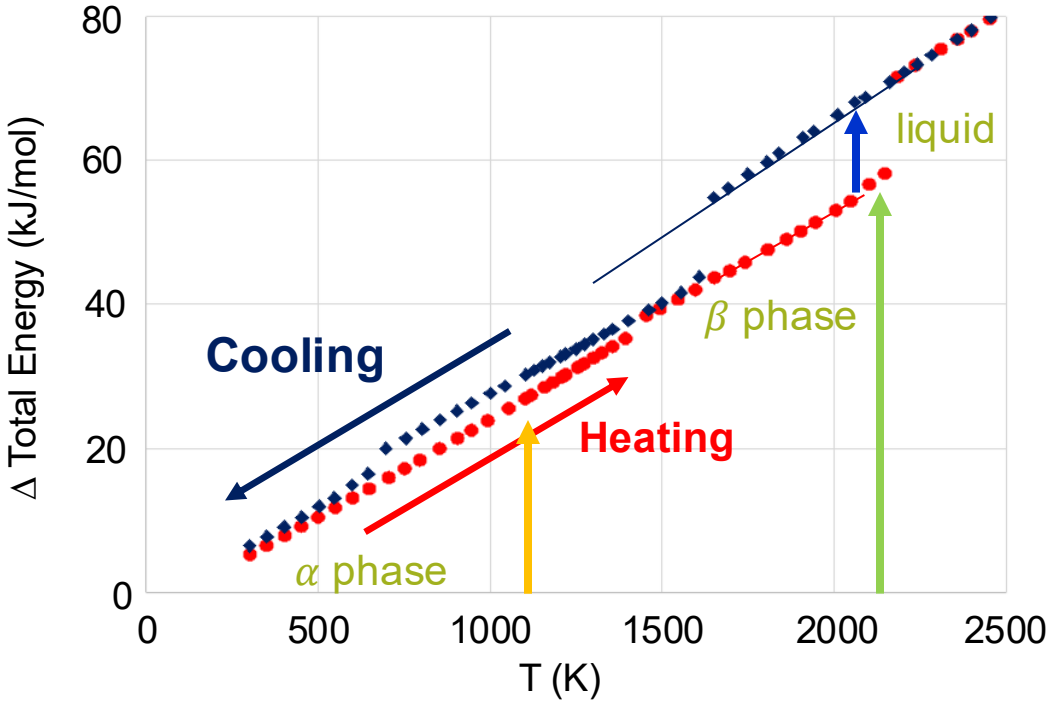




- Need a relative shift of the planes containing the hexagons
- In-plane shear to modify internal angles of hexagons

materials design

Zr: α-β phase transition & melting



Transition temperatures (exp):

- α-β transition: 1135 K
- melting: 2128 K

Latent heat of α-β transition:

- MLP: ΔH = 2.5 kJ/mol
- Exp.: ΔH = 4.0 kJ/mol

Heat of fusion:

- MLP: ΔH = 13 kJ/mol
- Exp.: ΔH = 14-17 kJ/mol

Specific heat:

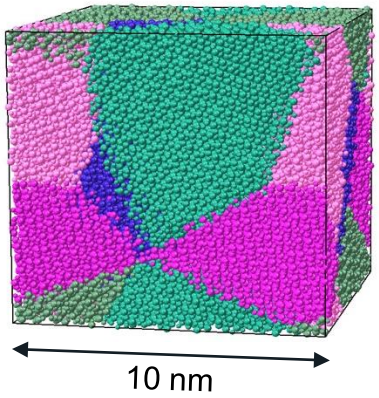
- MLP: c_p = 25-31 J/(mol·K)
- Exp.: c_p = 25-39 J/(mol·K)

Fisher & Renken, Phys. Rev. **135**, A482 (1964);
Chase, J. Phys. Chem. Ref. Data **9**, 1 (1998).

MLP capable of capturing multiple coordination environments!

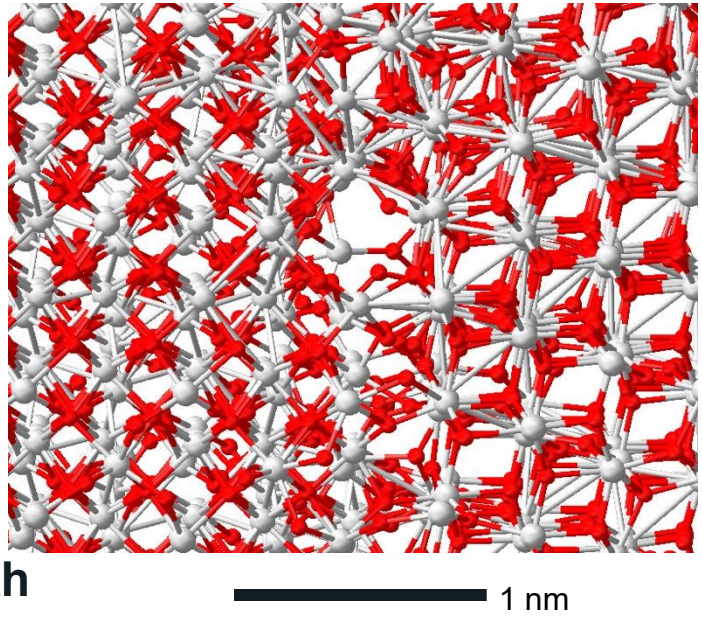
materials design

Grain boundary energy m-ZrO_2 || m-ZrO_2



Structure generated with *Microstructure builder*

Details of an oblique GB

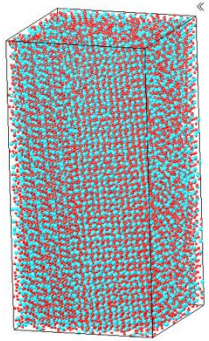


- Relaxed structures and energies are computed with a machine-learned potential trained on DFT data.
- Width of disordered region at GB: ~1 nm
- **Average GB energy: 2.6 J/m^2**

materials design

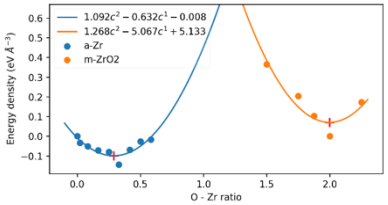
PhaseField parameterized via *ab initio*

GB Diffusion



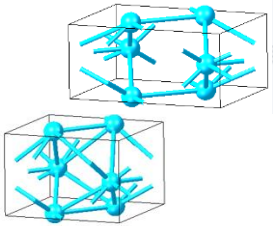
LAMMPS, KMC

Bulk free energy



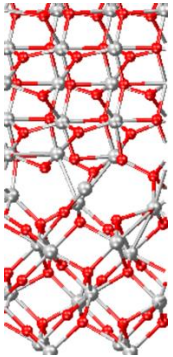
LAMMPS, UNCLE, Phonon

Elasticity



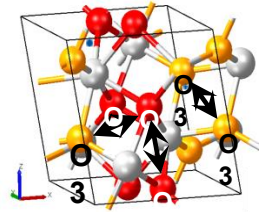
VASP, MT

Interfaces



LAMMPS, VASP, Interfaces, Microstructure Builder

Bulk Diffusion



LAMMPS, KMC

$$\frac{\partial c}{\partial t} = \nabla M(c,\eta,\sigma)\nabla\frac{\delta F}{\delta c}$$
$$\frac{\partial \eta}{\partial t} = -L\nabla\frac{\delta F}{\delta \eta}$$

$$F = \int dV\,[f_{chemical} + f_{elastic} + f_{interfacial}]$$

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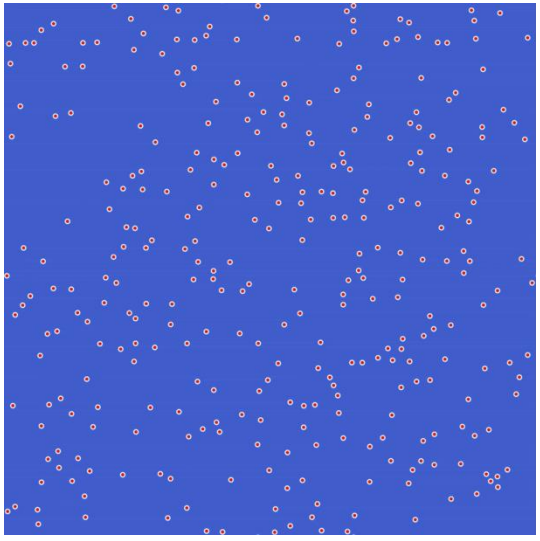
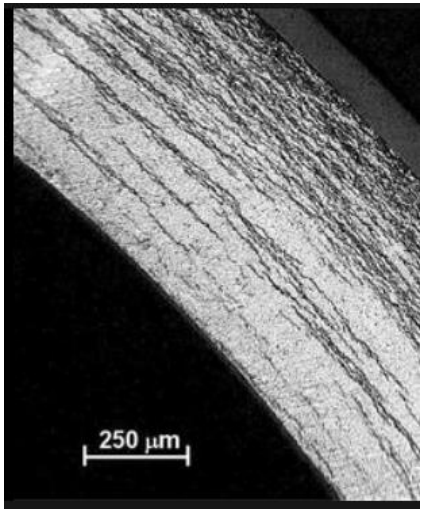
Hydride growth in zirconium

Calculated with *MedeA:*
Elastic constants;
Formation energy

From Literature:
Eigenstrain;
Diffusion;
Surface energy;
Interface mobility

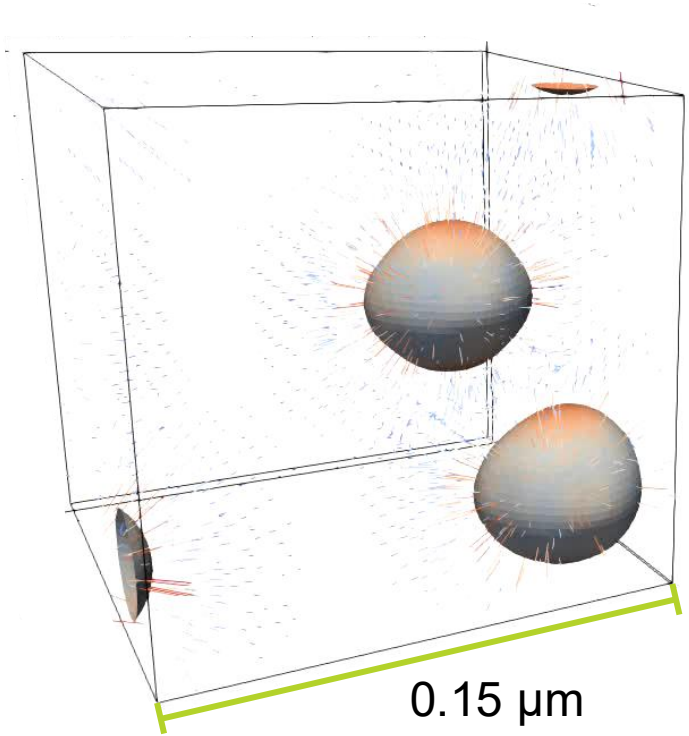




Zr and hydride phase evolution (for 0.07s at 600K)
shows effect of elastic anisotropy

materials design

Hydride growth in 3D zirconium



- Hydride needle evolution over 3 ms
- Arrows indicate hydrogen flux
- Hydrostatic stress colored on needle surface

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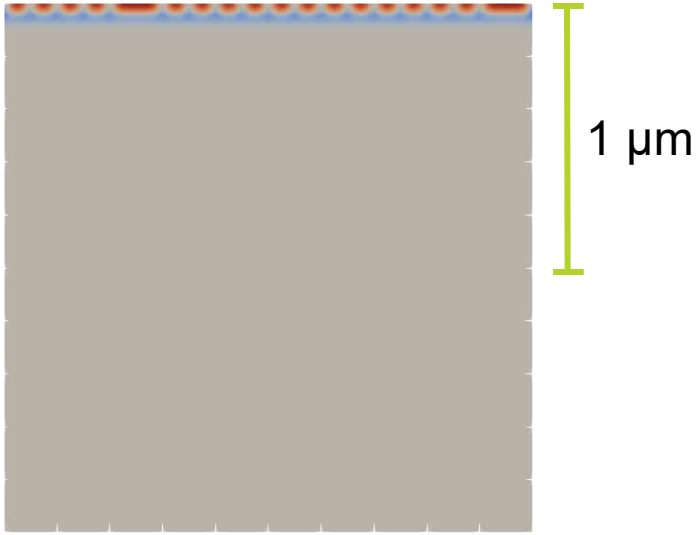
Oxide growth on zirconium



Zr and Oxide phase evolution (40 days!)
shows a columnar microstructure

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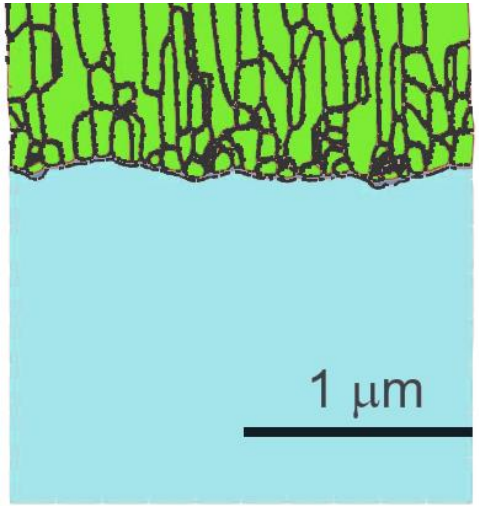
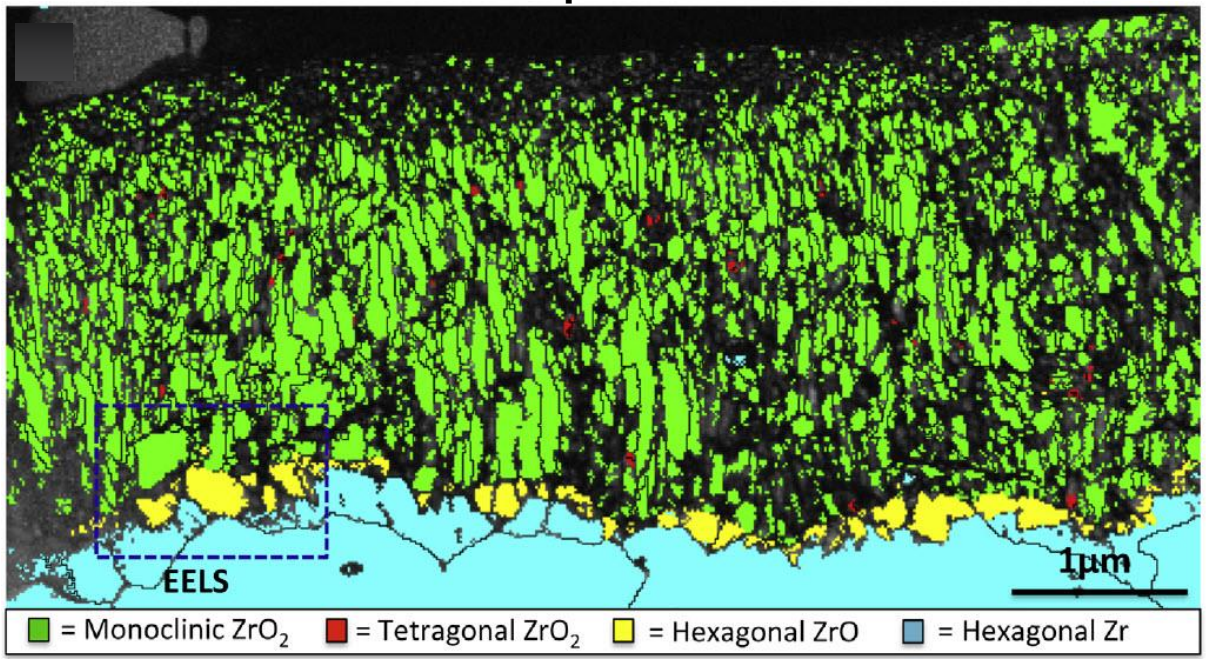
Microstructure of ZrO_2 Corrosion Film

Simulation
with *MedeA PhaseField*



40 simulated days
(2-3 days walltime)

Experiment



360 days

Hu et al., Micron **69**, 35 (2015)

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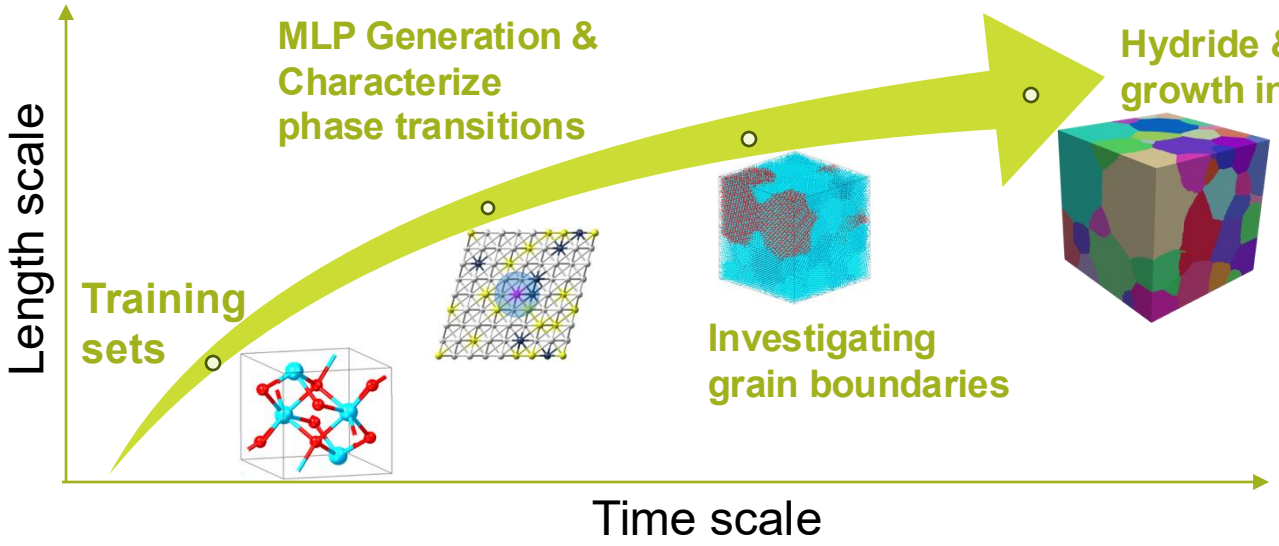
From atomistic to continuum modeling

- From electronic structure calculations (fs) to microstructure evolution (days)
- Captured microscale features of corrosion in Zr using a phase-field model parameterized by *ab initio* calculations & simulations using a trained MLP



Modules:

MedeA VASP
MedeA MLP/MLPG
MedeA LAMMPS
MedeA Microstructure Builder
MedeA PhaseField

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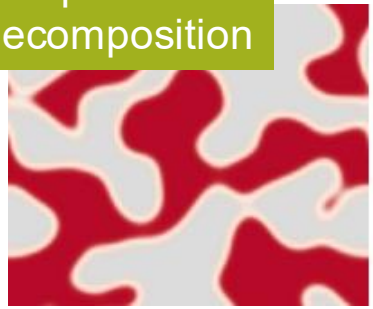
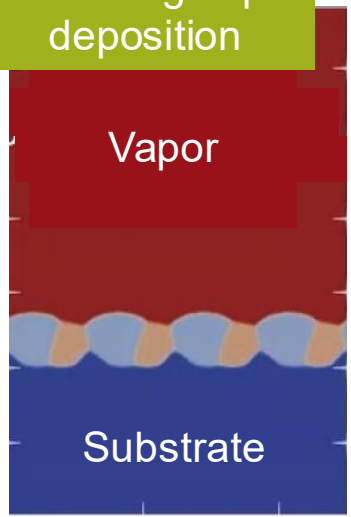
MedeA PhaseField: elucidating the mesoscale

MedeA PhaseField: the machinery under the hood

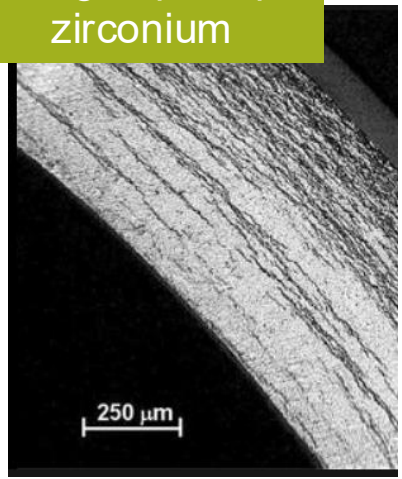
Spinodal decomposition



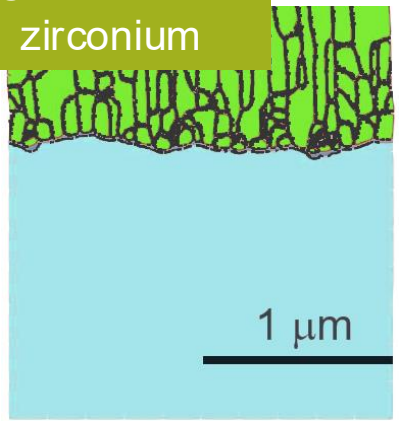
Simulating vapor deposition



Hydrogen pickup in zirconium



Corrosion of zirconium



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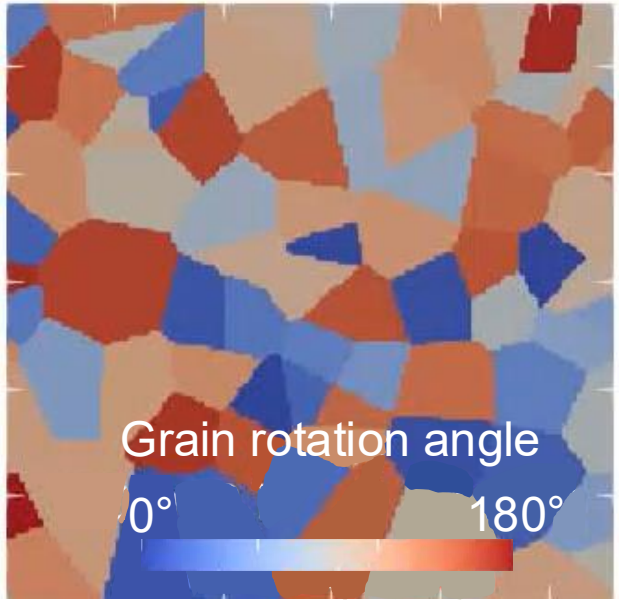
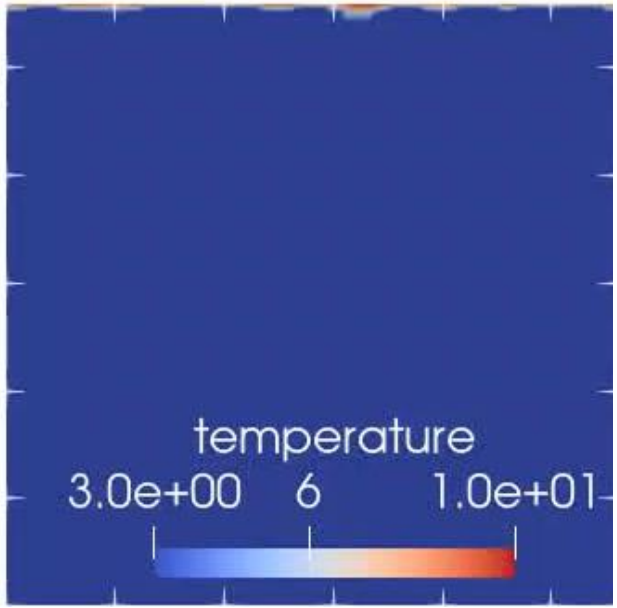
Coming soon: Temperature effects in *MedeA PhaseField*





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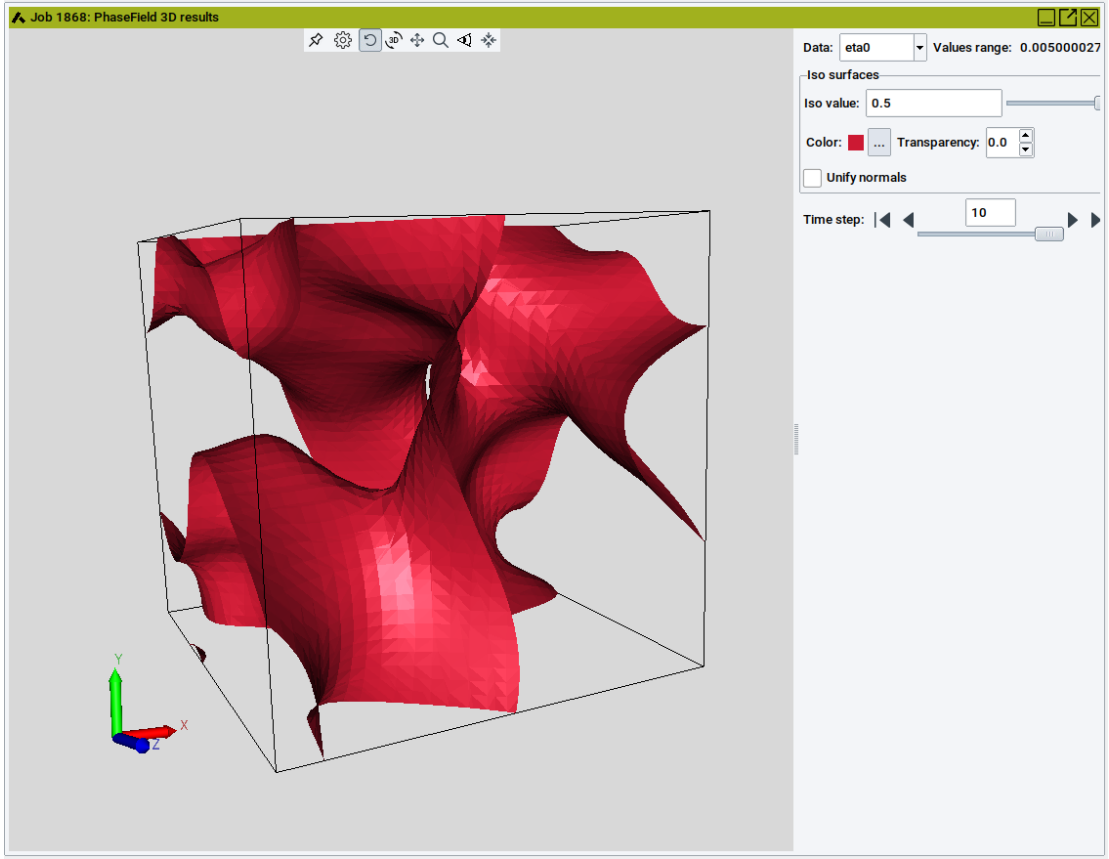
Coming soon: Interactive 3D plotting in *MedeA GUI*



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Acknowledgements

- Customers of Materials Design

- Science and technology partners, especially
  - Prof. Anter El-Azab (Purdue University): Phase-field modeling
  - Prof. Georg Kresse (University of Vienna and VASP GmbH)
  - Prof. Ralf Drautz (ICAMS, University of Bochum): MLP

- All colleagues at Materials Design, especially
  - Clint Geller, Benoit Leblanc for PhaseField development
  - Mikael Christensen, Volker Eyert, David Reith, Erich Wimmer for MLP generation and simulations

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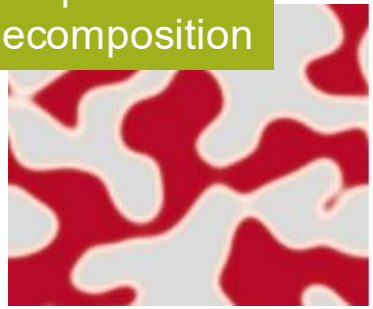
MedeA PhaseField: elucidating the mesoscale

MedeA PhaseField: the machinery under the hood

Spinodal decomposition



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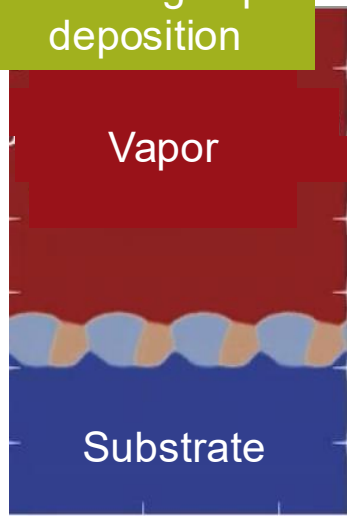
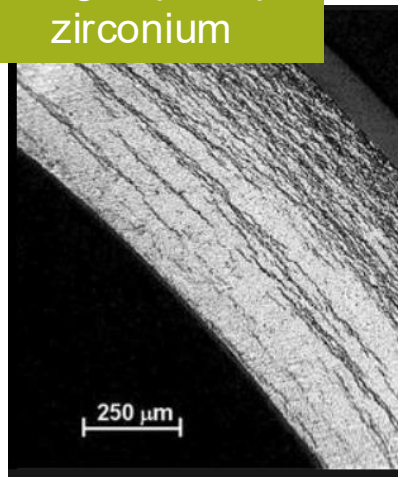
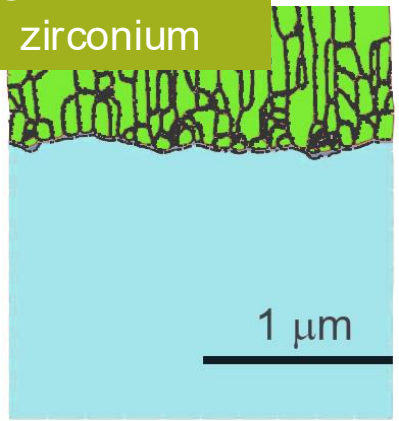


Hydrogen pickup in zirconium



Corrosion of zirconium



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Question and Answer Session

Leonid Kahle

Materials Design

Michele Kotiuga

Materials Design

Kyle Starkey

Materials Design

Highlighted *MedeA* Modules

MedeA PhaseField: Modeling the evolution of microstructures of metal alloys, oxides, ceramics, and organic materials, enabling the prediction of material properties and behaviors at scales of micrometers and days or year

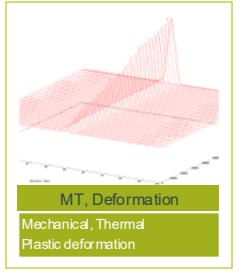
MedeA Environment: The *MedeA*[1] software package is the leading environment for the atomistic simulation of materials. *MedeA* enables professional, day-to-day deployment of atomic-scale and nano-scale computations for materials engineering, materials optimization and materials discovery. In *MedeA*, world-class simulation engines are integrated with elaborate property prediction modules, experimental databases, structure builders and analysis tools, all in one user-friendly environment

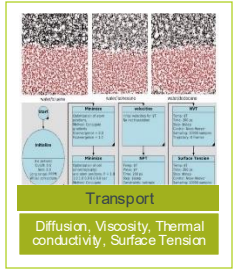
***MedeA* VASP:** Comprehensive access to the VASP Code via a graphical user interface (GUI) to set up, run and analyze multi-step VASP calculations

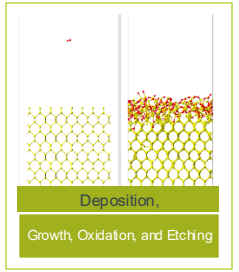
***MedeA* MLPG:** Fully integrated workflow from training-set generation (using *MedeA* HT) and MLP generation to MLP application using *MedeA* LAMMPS

***MedeA* HT:** Generation of large and consistent sets of computed data for input to machine learning procedures

***MedeA* LAMMPS:** Full access to the LAMMPS Code via a graphical user interface based on flowcharts to perform forcefield calculations using MLPs generated by *MedeA* MLPG







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Related *MedeA* Webinars

Predicting the Future of Materials – with Multiscale Modeling

https://www.materialsdesign.com/webinars/recorded/predicting-the-future-of-materials-%E2%80%93-with-multiscale-modeling

From the Femtoscale to Microstructures and Back: An Integrated Multiscale Approach

https://www.materialsdesign.com/webinars/recorded/from-the-femtoscale-to-the-mesoscale-and-back-an-integrated-multiscale-approach

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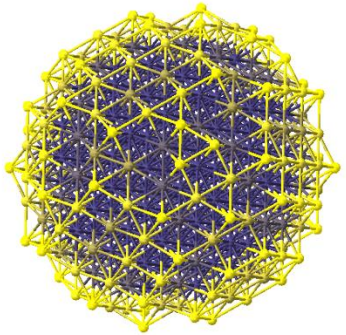
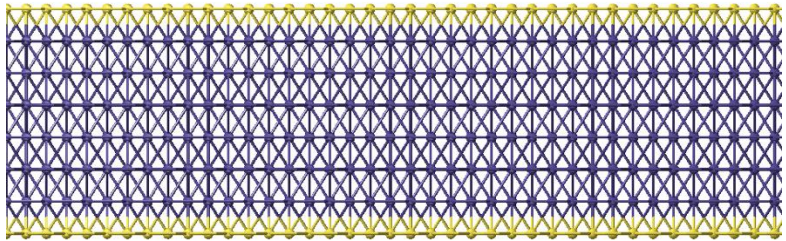


December Webinar Topic:

Machine-Learned Potentials in *MedeA*

Volker Eyert and Jörg-Rüdiger Hill, Materials Design



Question and Answer Session

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Materials Design

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Questions about Materials Design Webinars

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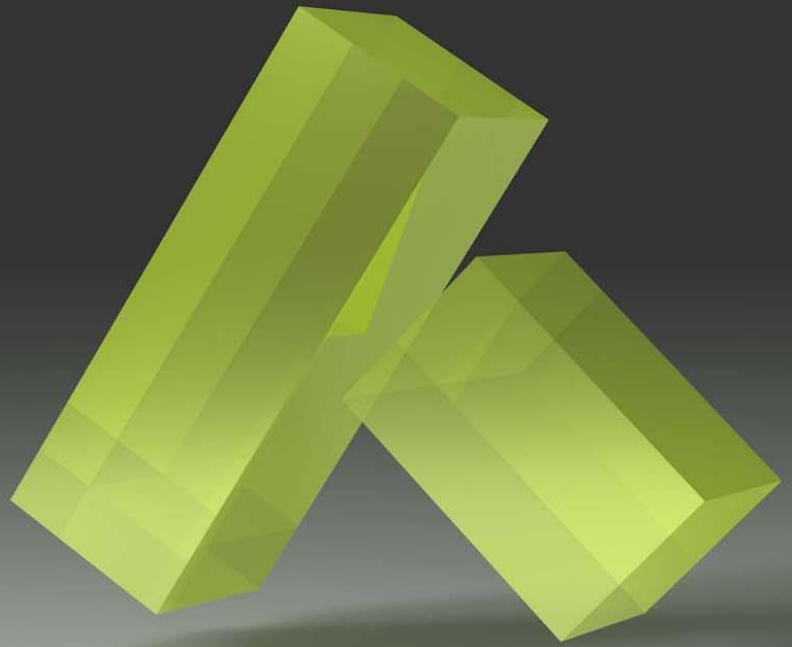

MedeA

Innovation by Simulation