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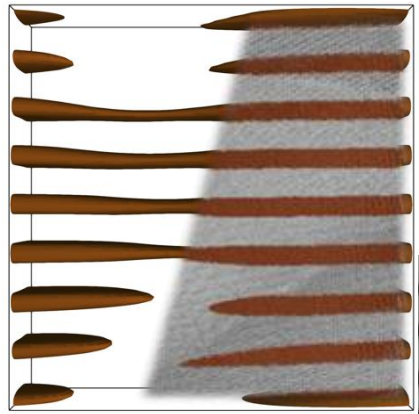
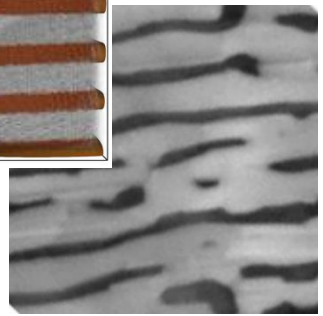
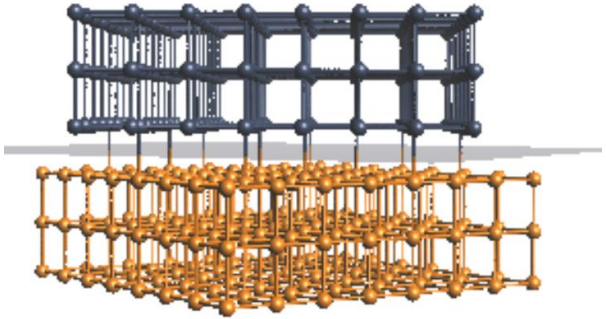
Modeling Interfaces and Microstructures with *MedeA*

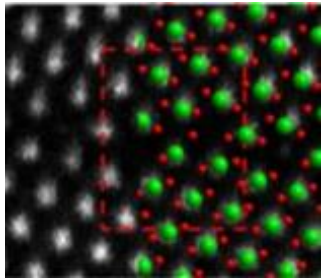
Mikael Christensen and Leonid Kahle

MDI Webinar









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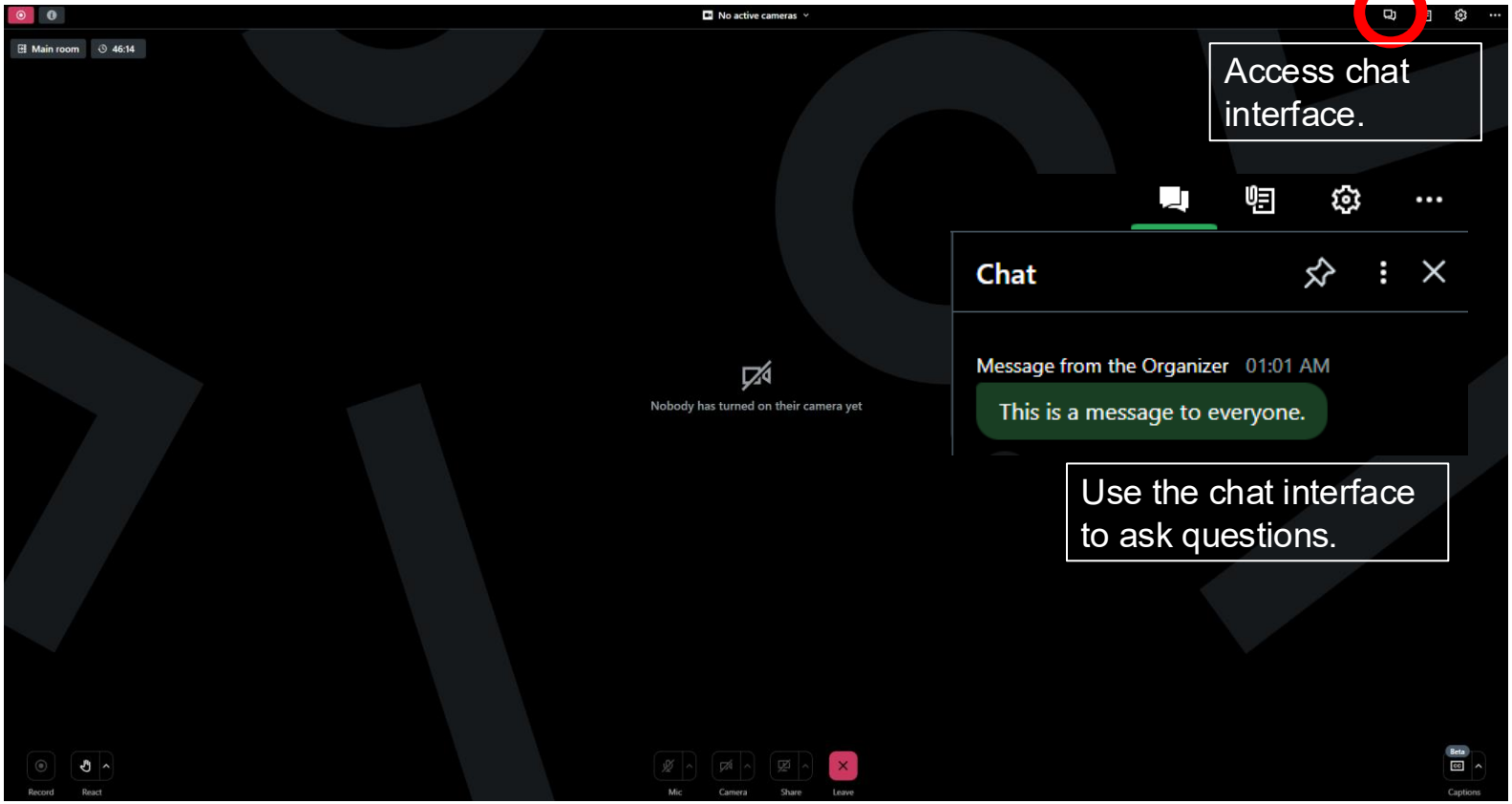

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Webinar Speakers

Katherine Hollingsworth ***Dr. Mikael Christensen*** ***Dr. Leonid Kahle***

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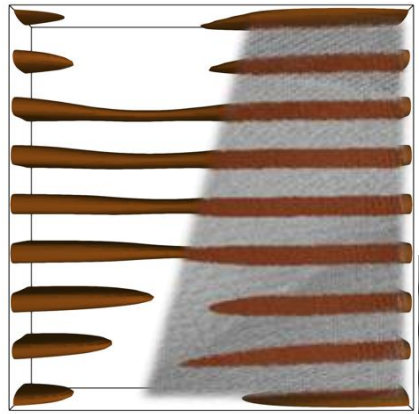
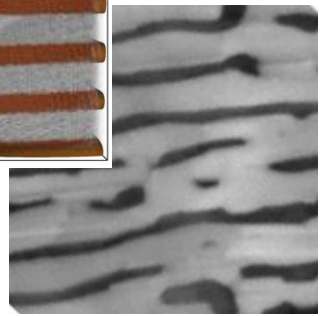
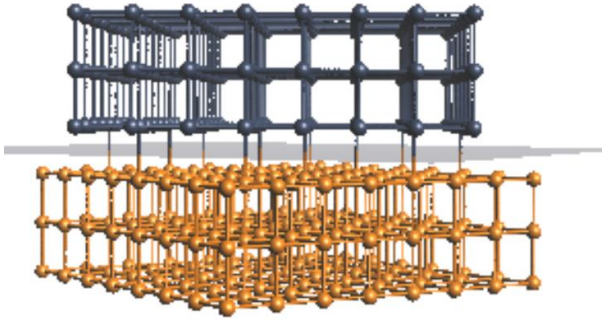
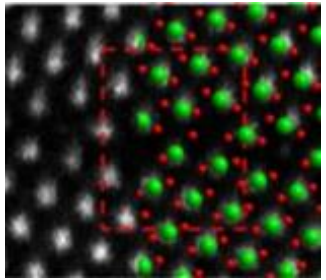
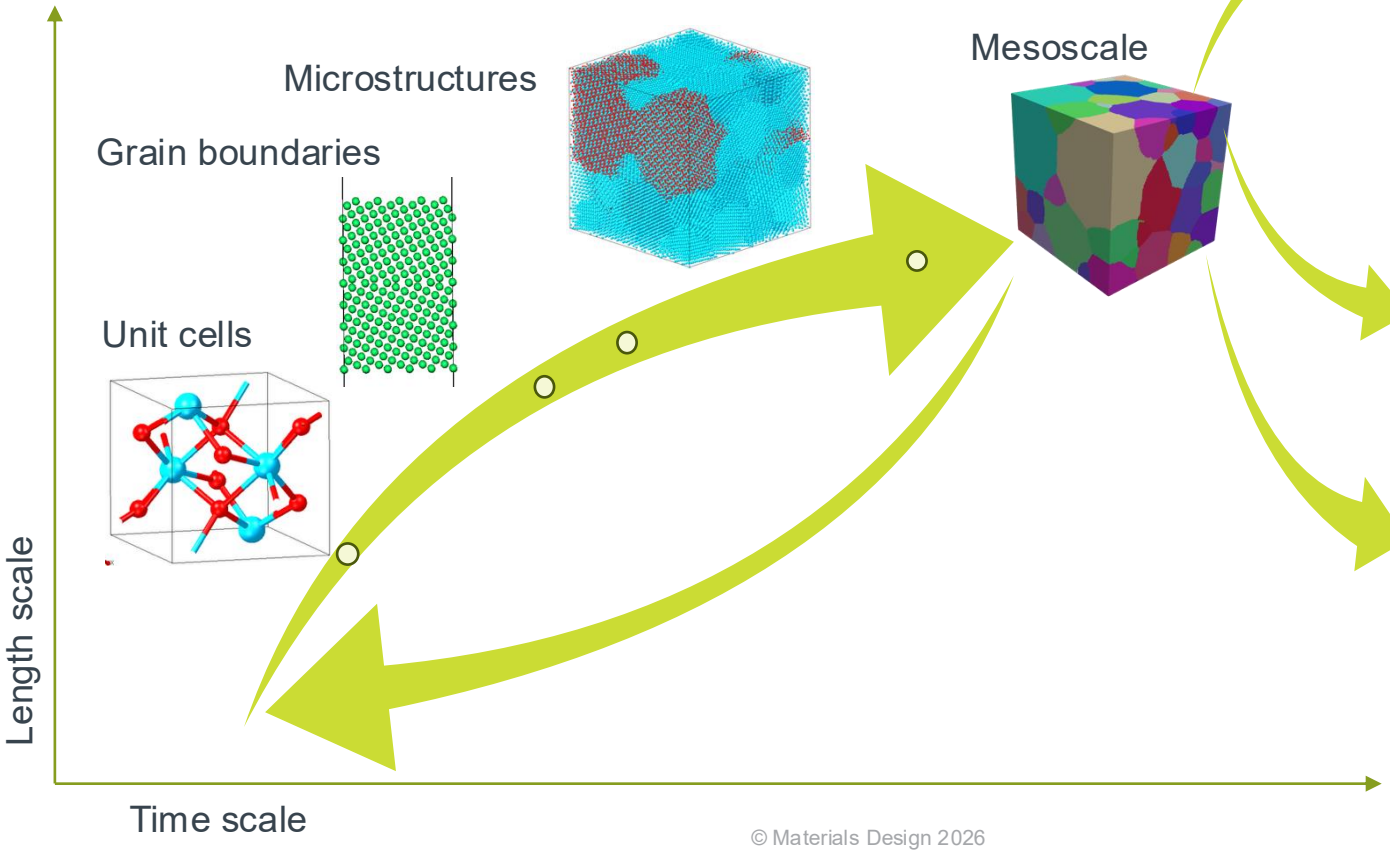


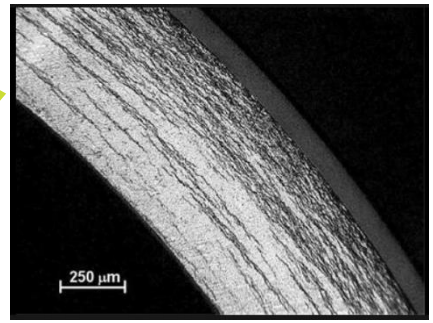


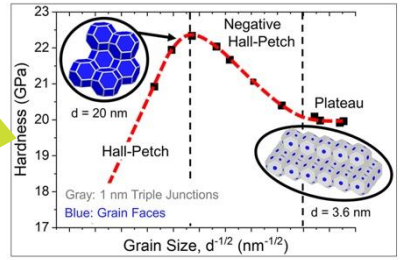


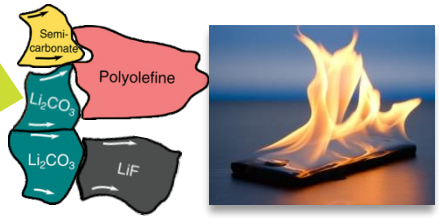


Bridging time and length scales









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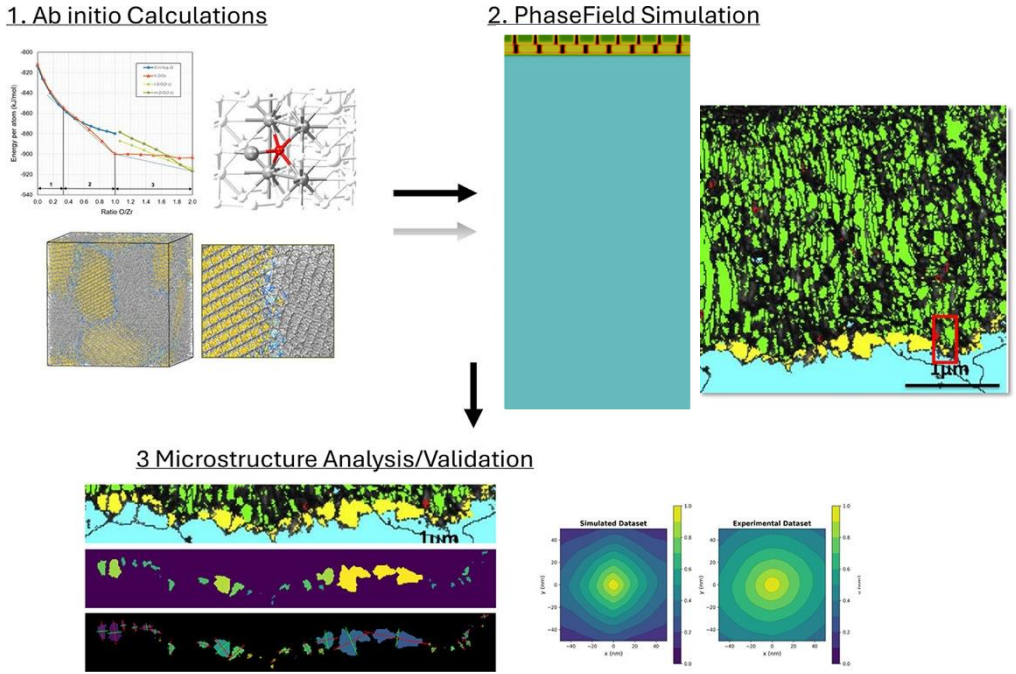
Microstructure of ZrO_2 Corrosion Film

Understanding Zr corrosion important for HPU pickup in Zr cladding in PWR.

1. Ab initio calculations of material properties
2. Phase field simulations reproduce experimental microstructures[1] in a few hours (vs 360-day exp.)
3. Obtain very good agreement with respect to experiment[2]



[1] Hu et al., *Micron* **69**, 35 (2015)
[2] Starkey et al, *JNM* **625**, 156521 (2026)

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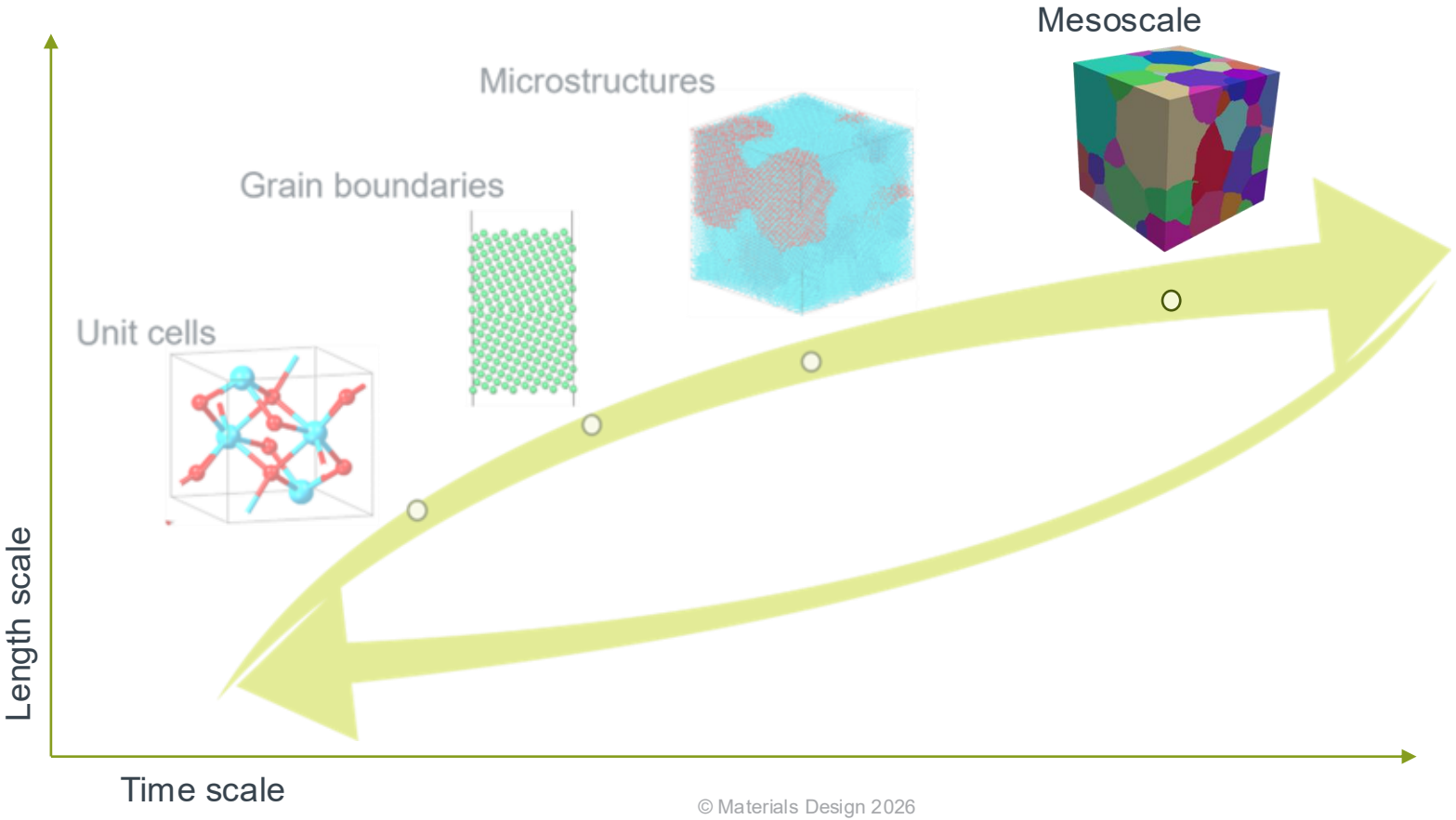
Bridging time and length scales



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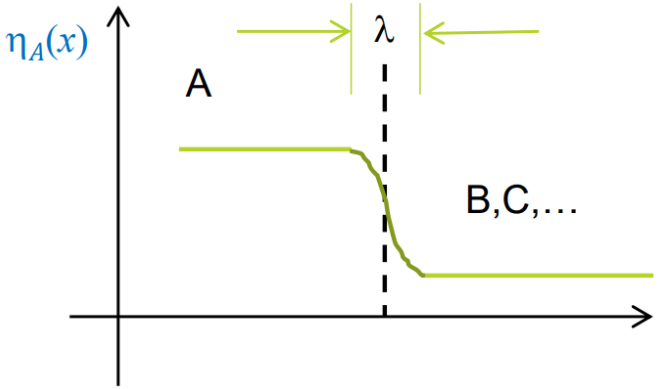
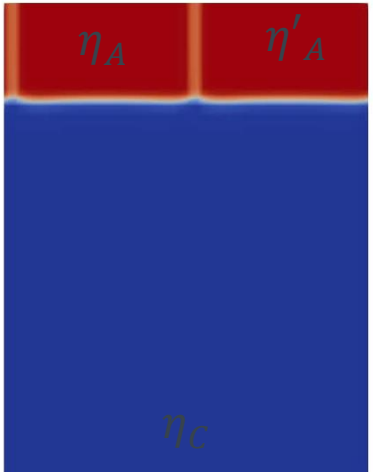
The phase-field method

To move up length and time scales, we coarse-grain atom positions and move to a continuum approach where phases are represented as fields

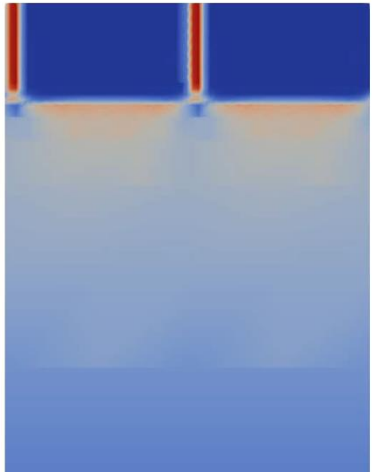
$$\eta_A = \begin{cases} 1 & \text{Phase A} \\ 0 & \text{other phases} \end{cases}$$



Order parameters



Flux



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

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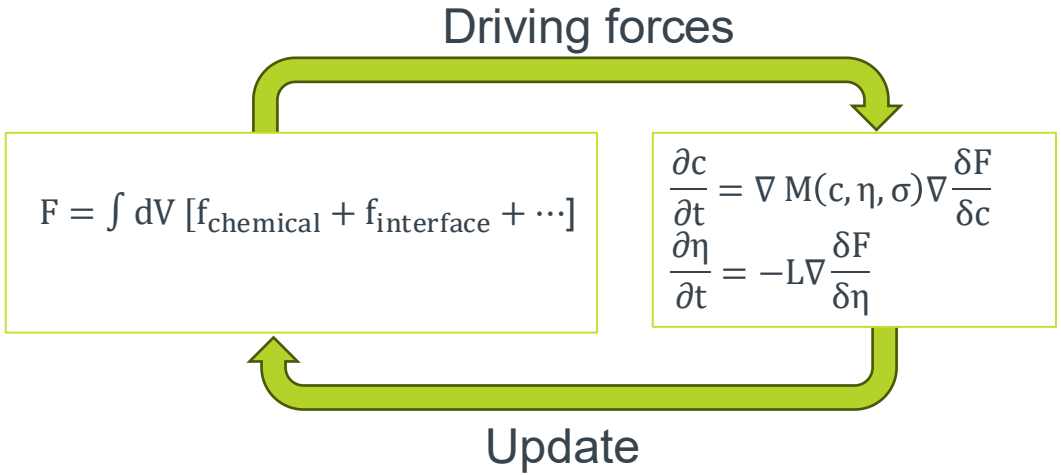
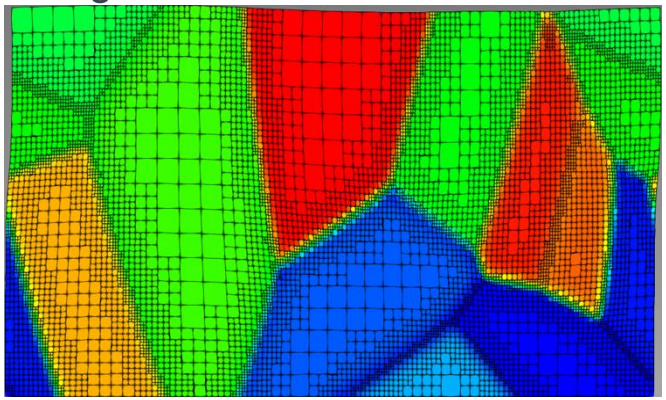
Solving the phase-field equations

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



Implementation of the
Cahn-Hilliard & Allen-Cahn equations

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



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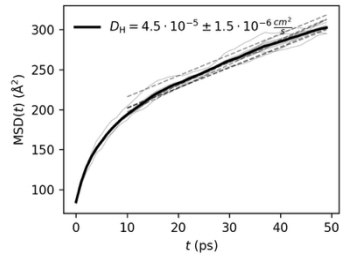
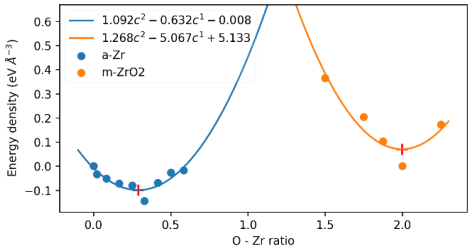
Predicting microstructures evolution

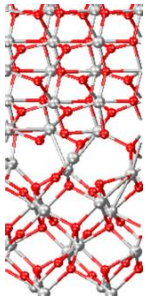
Diffusion (bulk & GB)



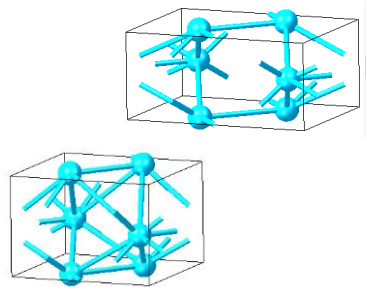
Free energy



Interfaces



Elastic energy



- Cracking
- Nucleation
- Reactions
- Temperature

Phase-field equations

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

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

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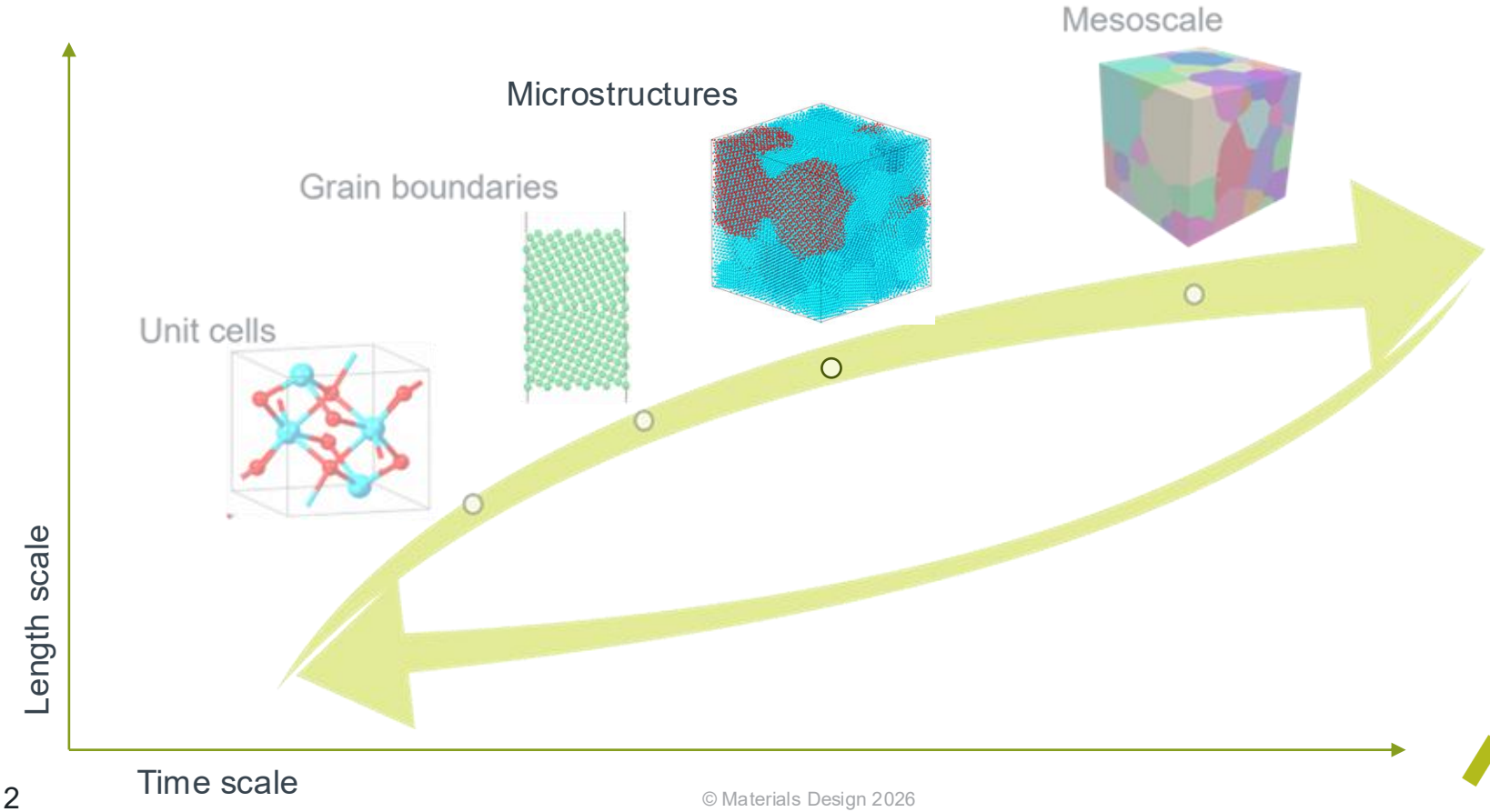
Bridging time and length scales



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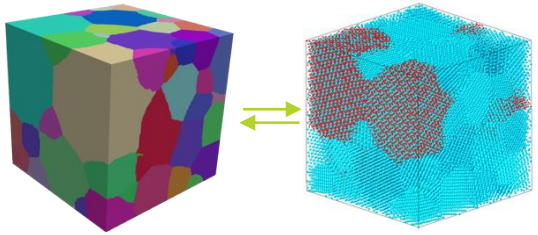
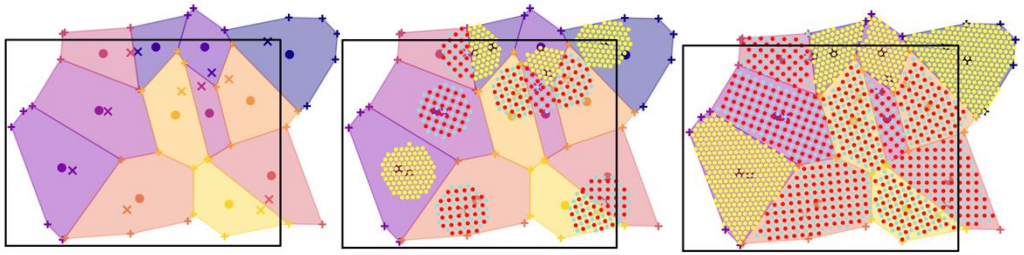
Building atomic microstructures



1) Generate atomic microstructures *via* "Seed & Growth" algorithm:

- Define seed points where "crystal growth" initiates.
- Grow crystals from seed point until other grains are met.
- Constrain interatomic distance or phase stoichiometry.

2) Populate existing microstructure definition with atoms



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The *MedeA* Microstructure Builder

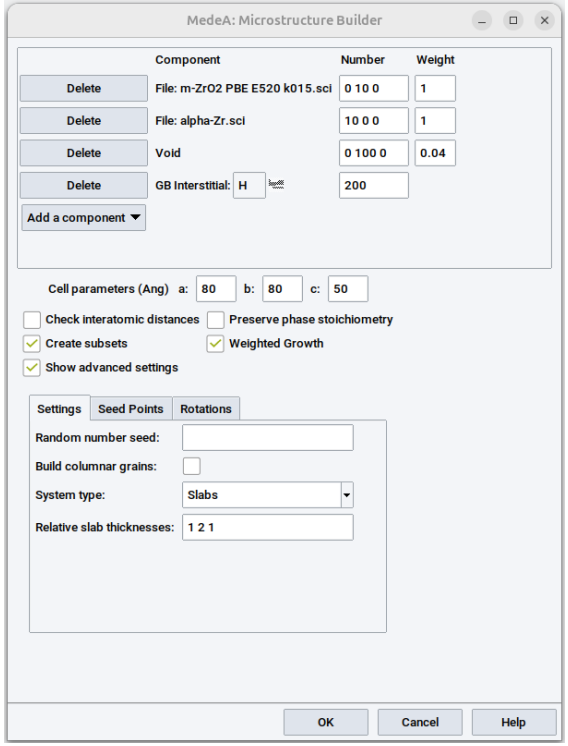
Select components:
- Phases and number of grains
- Growth speed (*via* weight)
- Voids (empty space)
- GB interstitial atoms

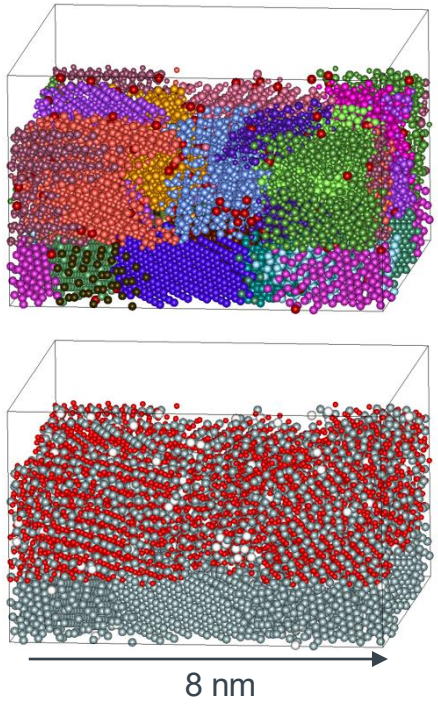
Set growth parameters:
- Stoichiometric growth
- Interatomic distances at GB

Advanced settings:
- Seed point coordinates
- Grain rotations (Euler or *hkl*)
- Interatomic distance thresholds
- Columnar & slab geometries

Output options:
- Analysis of grains & interfaces

Green: New feature in MedeA 3.12





A slab microstructure of ZrO2 grains on top of α-Zr grains

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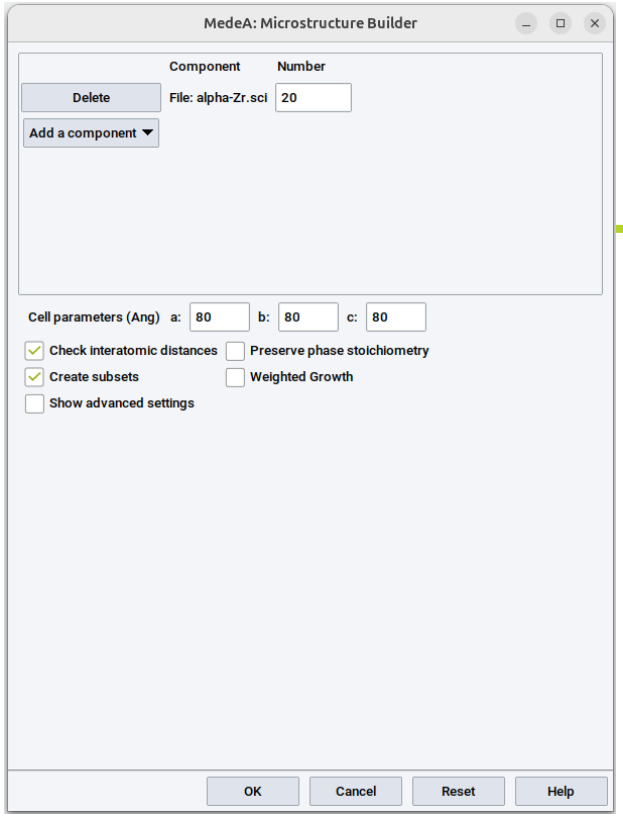
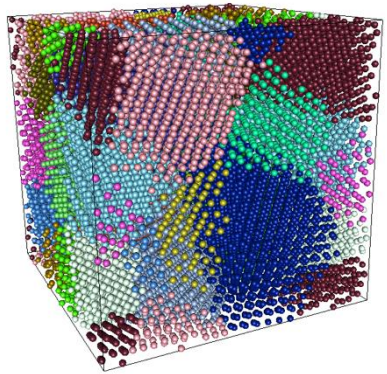
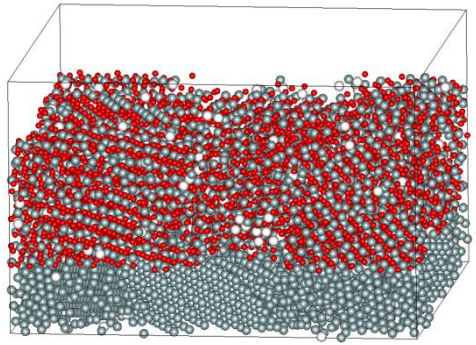
Demonstration in MedeA







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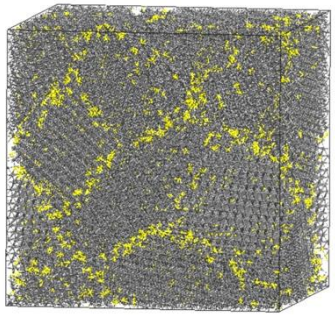
Atomic microstructures to compute interface energies

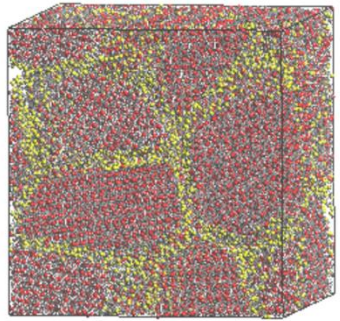
Can we calculate average interface energies in α-Zr/h-ZrO system?

1) Build several polycrystalline models (α-Zr, h-ZrO, mixed)
2) Relax structures using MD simulations (NPT) followed by atomic relaxations
3) Interface energy = $\frac{Energy\ grains - Energy\ bulk}{Interface\ area}$

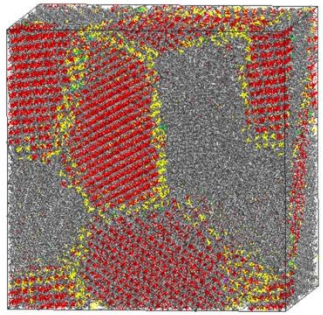


α-Zr (γ = 0.50 J/m^2)

DFT, 8 CSL GBs
γ = 0.51 J/m^2
Plowman and Race, JNM 568, 153853 (2022)



h-ZrO (γ = 1.80 J/m^2)



α-Zr and h-ZrO (γ = 1.39 J/m^2)

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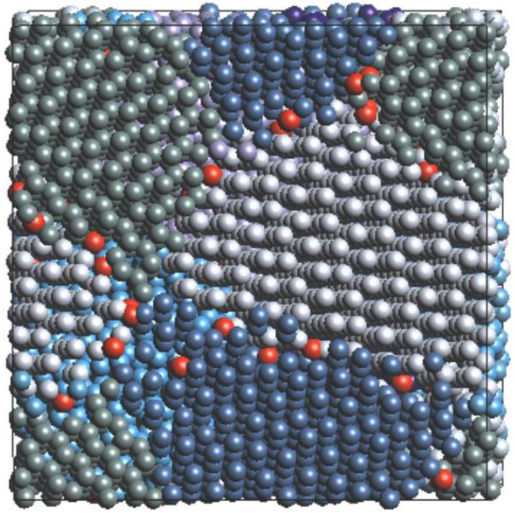
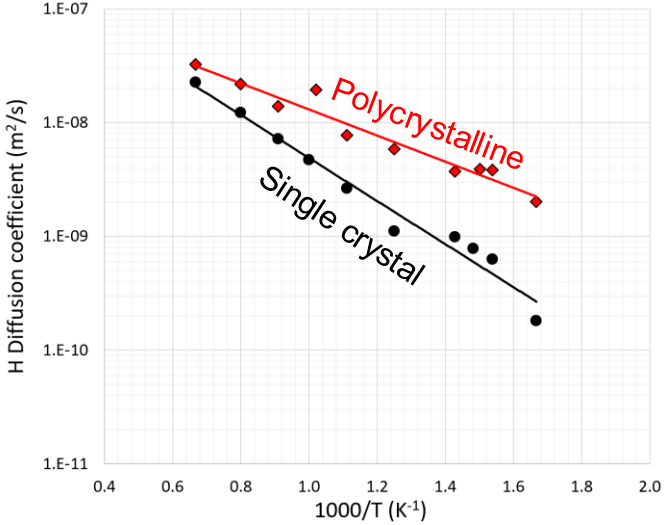
H grain boundary diffusion in Zr

Polycrystalline model of Zr with atoms in GBs can be built directly in the Microstructure Builder



H diffusion as function of T in polycrystalline or single crystal model



Faster diffusion in polycrystal than in single crystal

1) Build 2 models:
    1) Polycrystalline
    2) Single crystal – no GBs
2) Populate with H and compute diffusion coefficient
3) Diffusion of H is enhanced when GBs are present

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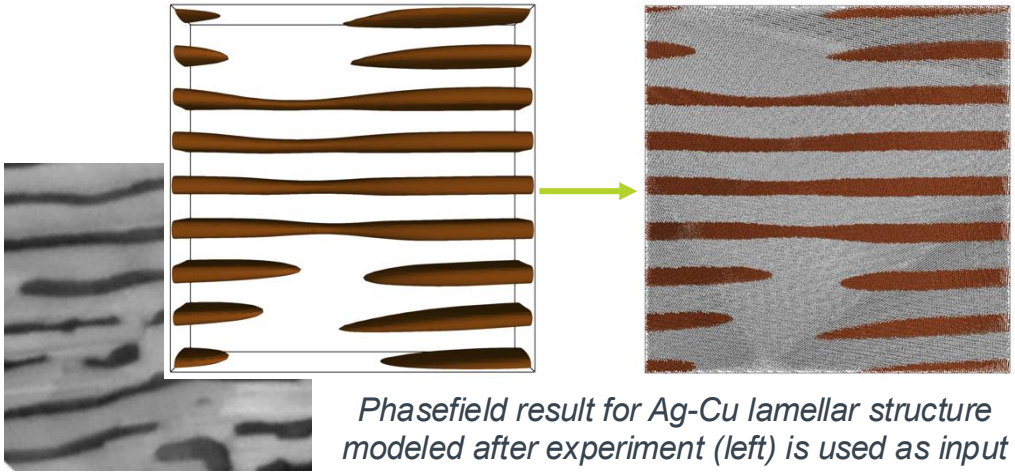
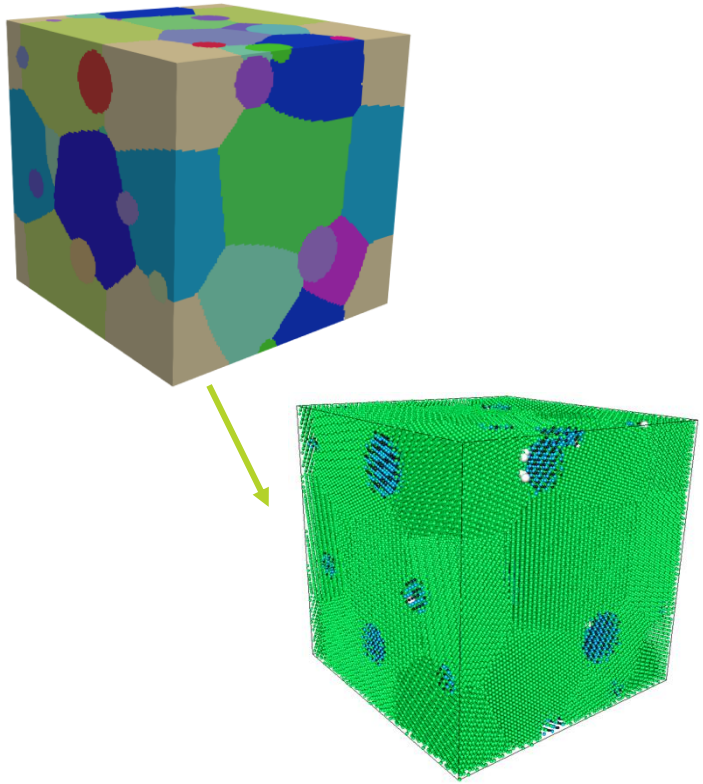
New capabilities

1) Create microstructures from experiment or advanced pipelines *via* DREAM.3D code
2) Create atomic microstructure from phase field results



Phasefield result for Ag-Cu lamellar structure modeled after experiment (left) is used as input for atomic microstructure



DREAM.3D model TiC precipitates in bcc-Fe with H at the grain boundaries (top) is used to build atomic microstructure (bottom)

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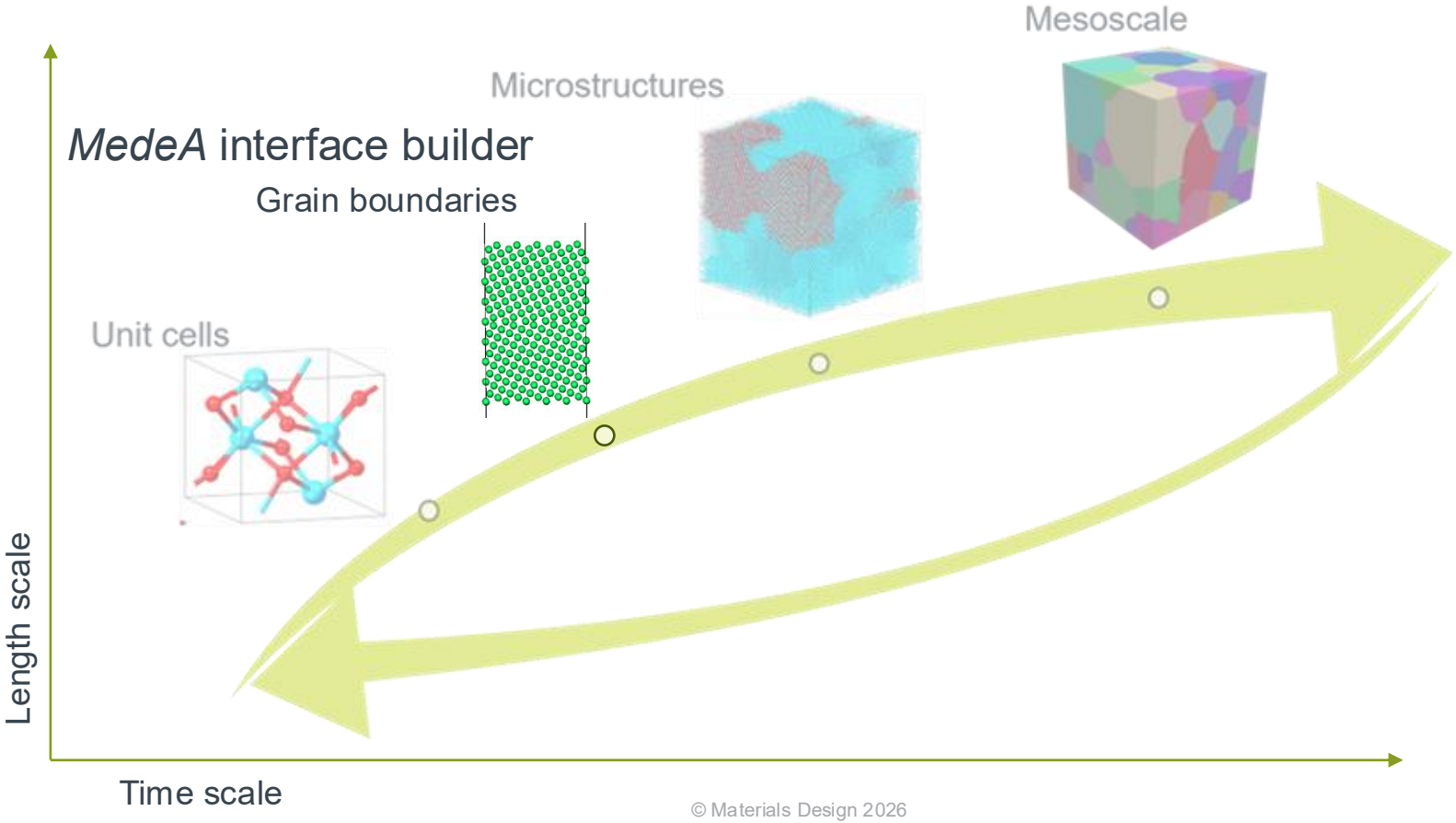
Bridging time and length scales



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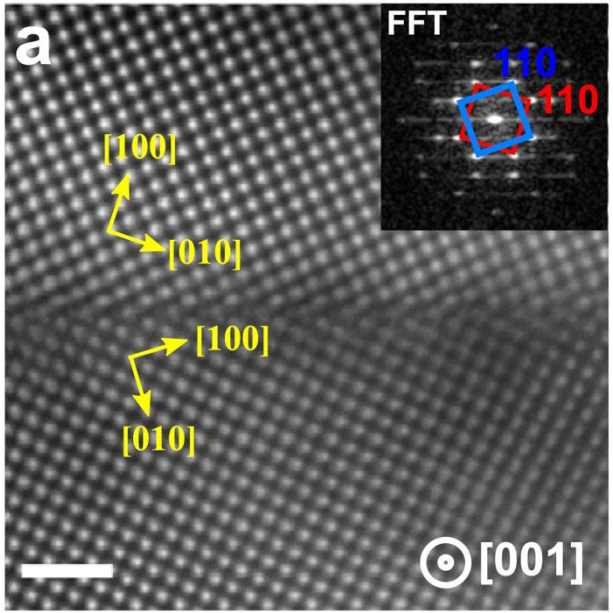
Experimental grain boundary: Σ5 (130)/[001] in Fe



Ahmadian *et al*. *Nat Commun* **12**, 6008 (2021).

How to build a model with *MedeA*?

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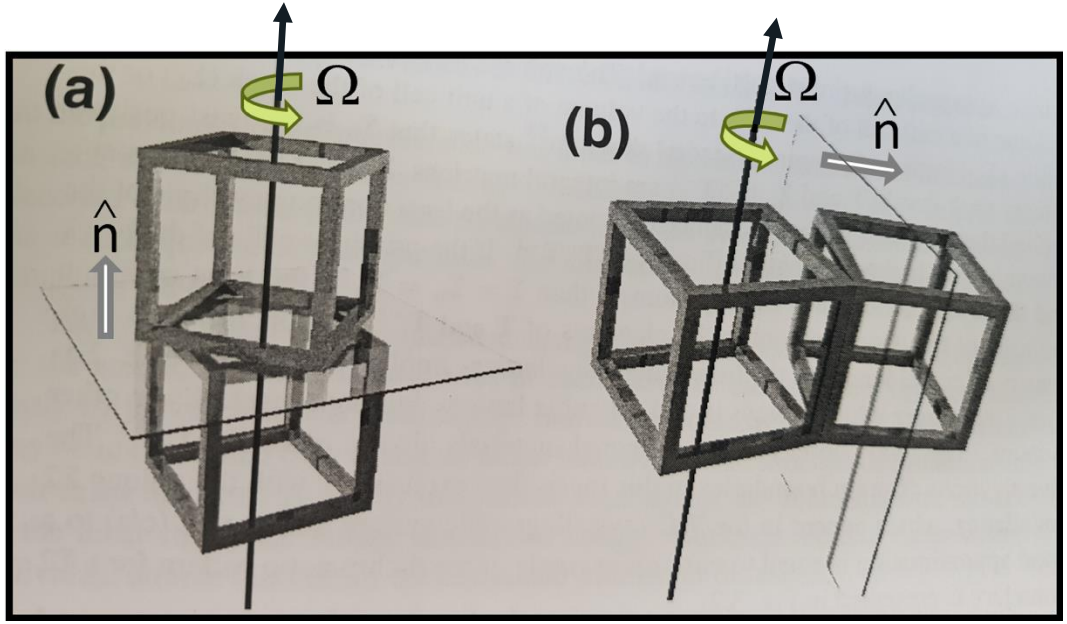
Grain boundary geometry

- Rotation axis
- Rotation angle Ω
- GB plane, normal $\hat{n}$
- GB type, Twist, Tilt
- CSL, Σ

Example: $\Sigma 5$ (130)/[001]



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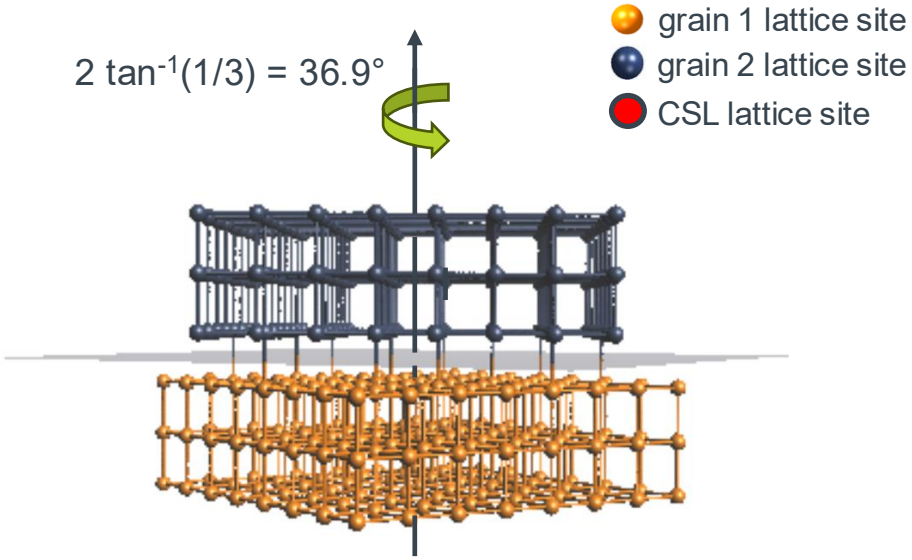
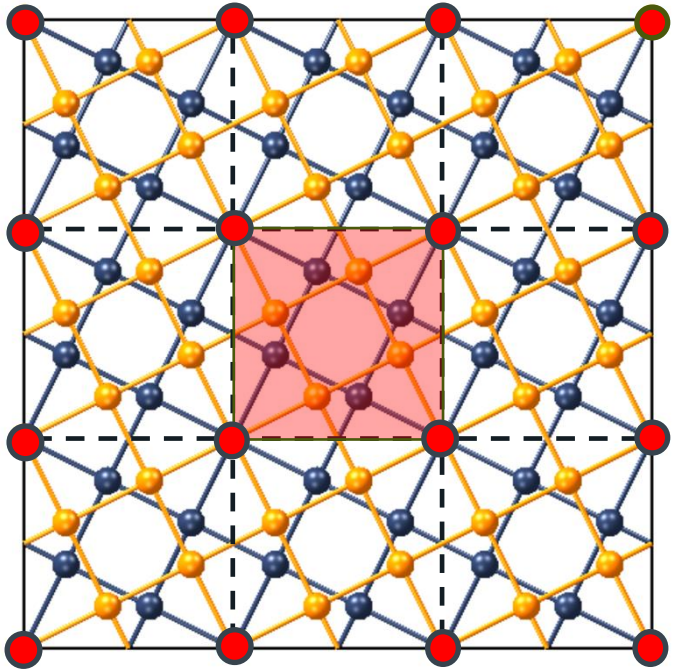
Coincidence site lattice

Example: Σ5 twist grain boundary





$$\Sigma = \frac{CSL\ unit\ cell\ volume}{Parent\ crystal's\ unit\ cell\ volume}$$

Σ = reciprocal density of coincident lattice points

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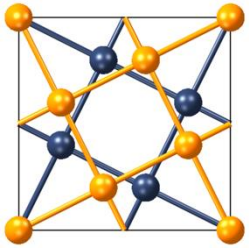
Building high-symmetry GBs

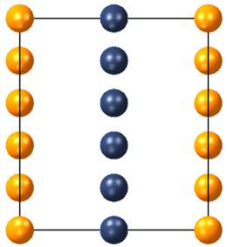
- The database files are structural templates with the irreducible part of the boundary structure (containing only the atomic information needed to construct boundary models with sizes specified by the user).

Example: Σ5 twist boundary in s.c. lattice

structure in database



View ∥ boundary normal



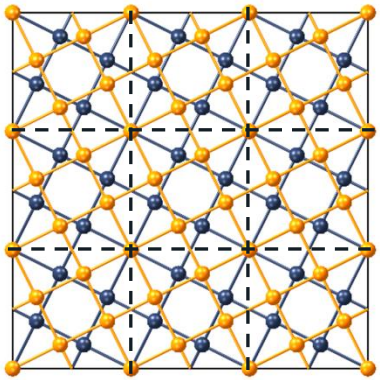
View ⊥ boundary normal

1 layer on each side of the interface

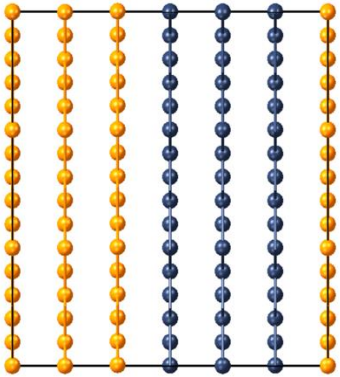
atom in grain 1

atom in grain 2

user specifies
3×3×3



View ∥ boundary normal



View ⊥ boundary normal

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Database of high-symmetry grain boundaries

Crystal structure	Atom types	Number of structures	Number of atoms
Simple cubic	Po	28	6 to 156
Body-centered cubic	V	28	12 to 156
Face-centered cubic	Ni	28	6 to 312
Fluorite	Ca,F	28	18 to 936
Rocksalt	Na,Cl	28	12 to 624
Zincblende (Sphalerite)	Zn,S	28	12 to 624
Hexagonal close-packed (ideal)	Co	13	28 to 248
Wurtzite	Zn,S	10	56 to 496
Nickeline	Ni,As	10	56 to 496

The database contains a total of 201 grain boundaries
146 tilt boundaries and 55 twist boundaries
Models constructed from cubic structures include $\Sigma 3$, $\Sigma 5$, $\Sigma 7$, $\Sigma 9$, $\Sigma 11$, $\Sigma 13$ boundaries
Models constructed from hexagonal close-packed structure include $\Sigma 3$, $\Sigma 5$, $\Sigma 13$ boundaries
Models constructed from Wurtzite and Nickeline structures include $\Sigma 5$, $\Sigma 13$ boundaries

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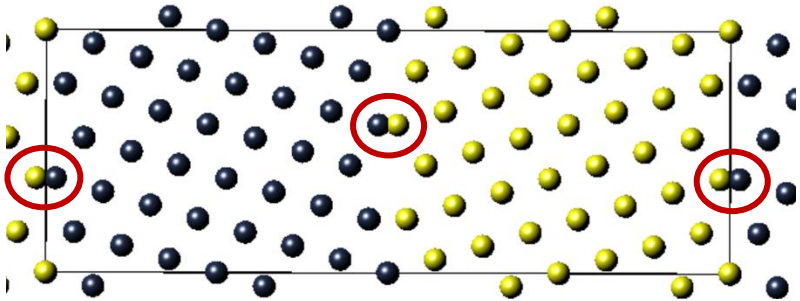
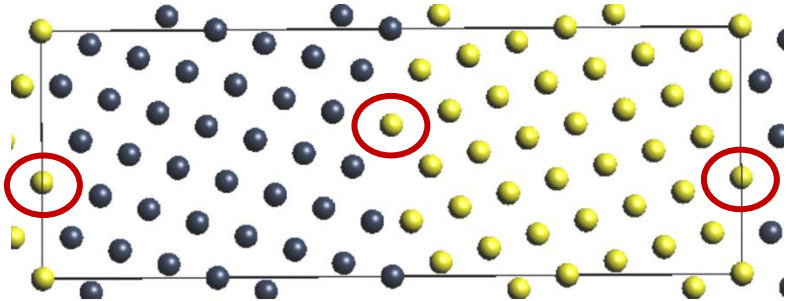
Removing short interatomic distances



Initial model with bad contacts



Final model without bad contacts

- Pairs of atoms in close proximity are replaced by single atoms in the center of the original pair.
- The stoichiometry of the model can be maintained when cleaning short distances.

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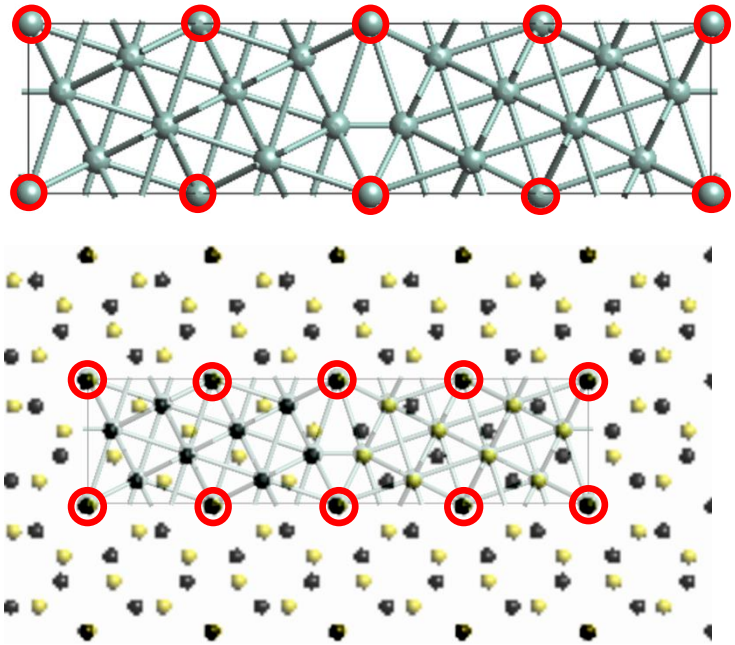
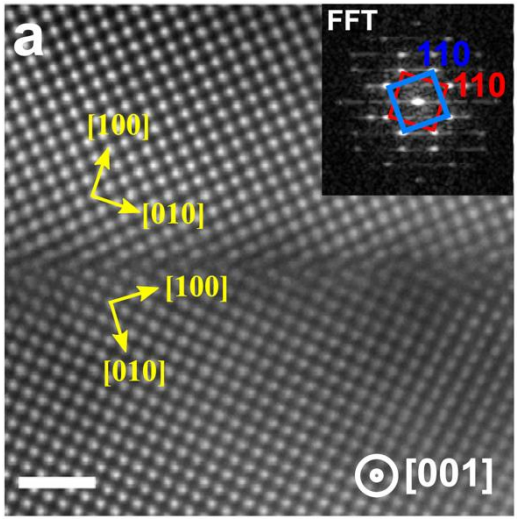
Example: Σ5 (130)/[001] in Fe



Σ5 (130)/[001] in iron (Fe 4 at.%Al)



Ahmadian *et al*. *Nat Commun* **12**, 6008 (2021).

- change element from V to Fe
- change lattice parameter from V to Fe (2.866 Å)
- set cell dimensions a, b, c (repetitions of template)

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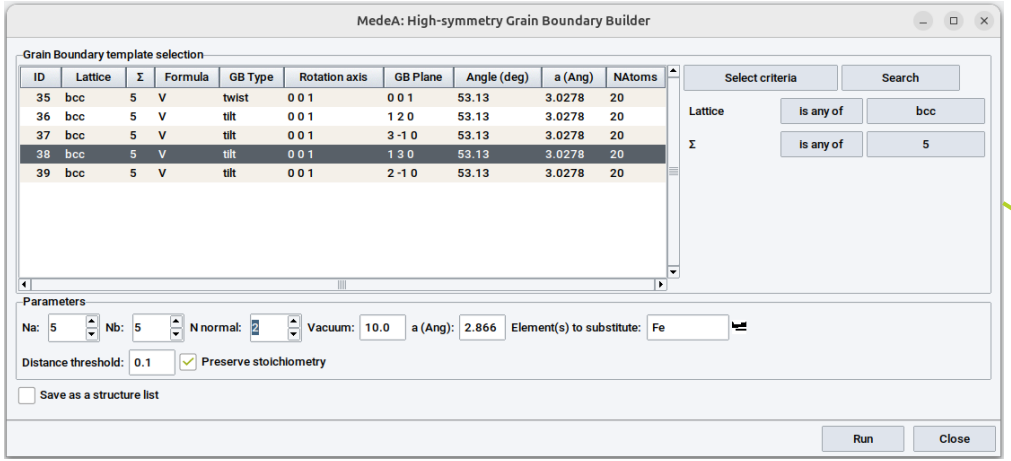
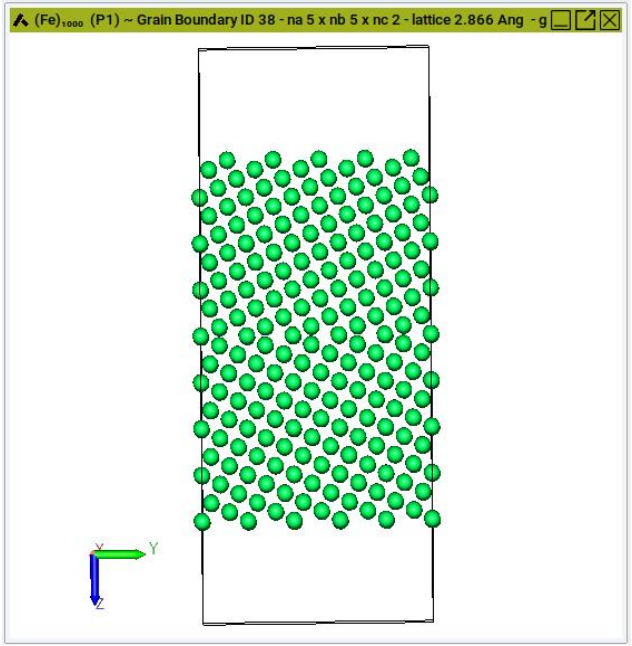
Demonstration in MedeA





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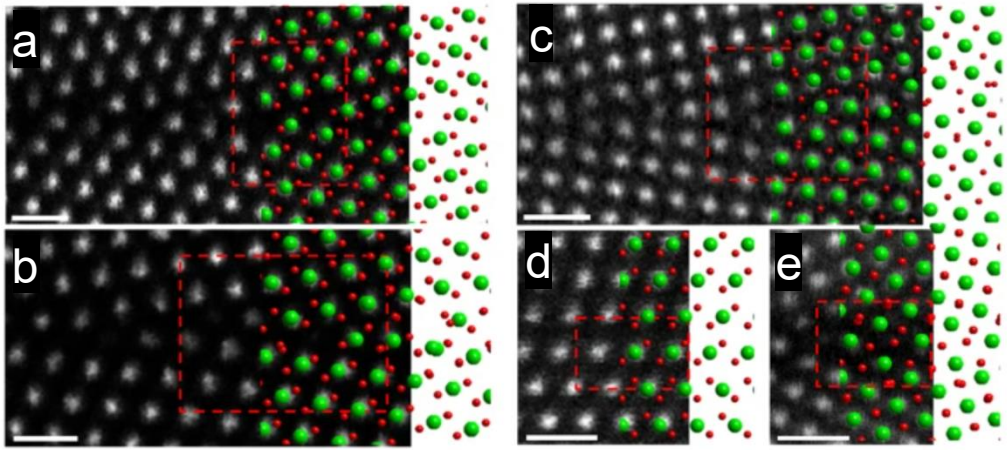
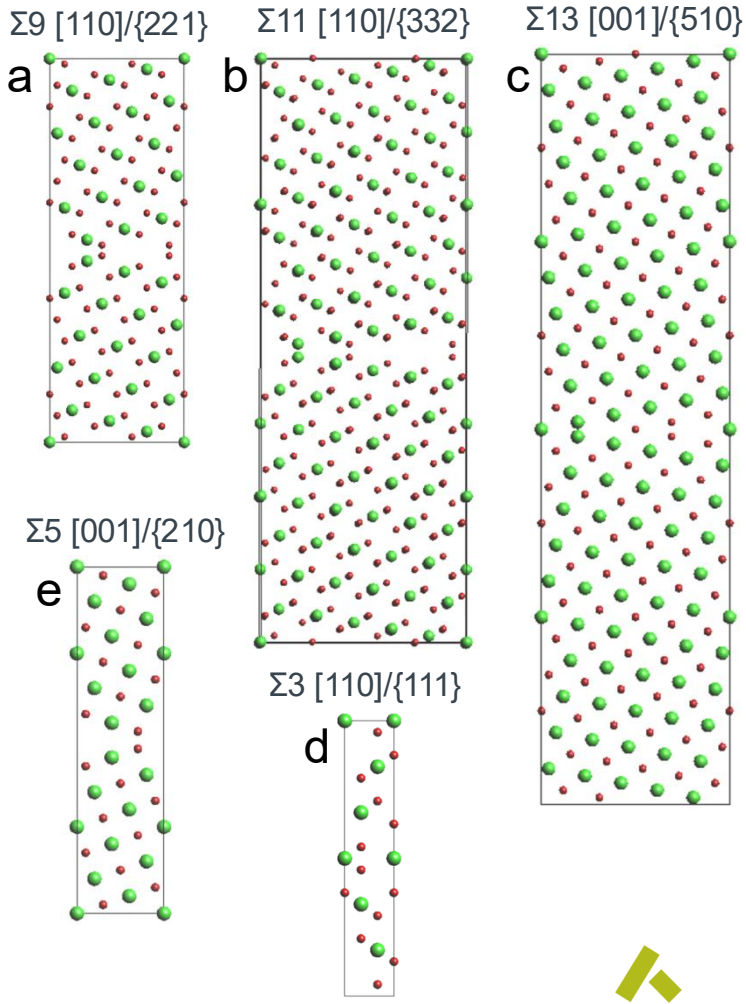
Example: CeO_2 grain boundaries

Feng, B. *et al. Sci Rep* **6**, 20288 (2016).

High angle annular dark field (HAADF) STEM



a) Σ9 [110]/{221}
b) Σ11 [110]/{332}
c) Σ13 [001]/{510}
d) Σ3 [110]/{111}
e) Σ5 [001]/{210}



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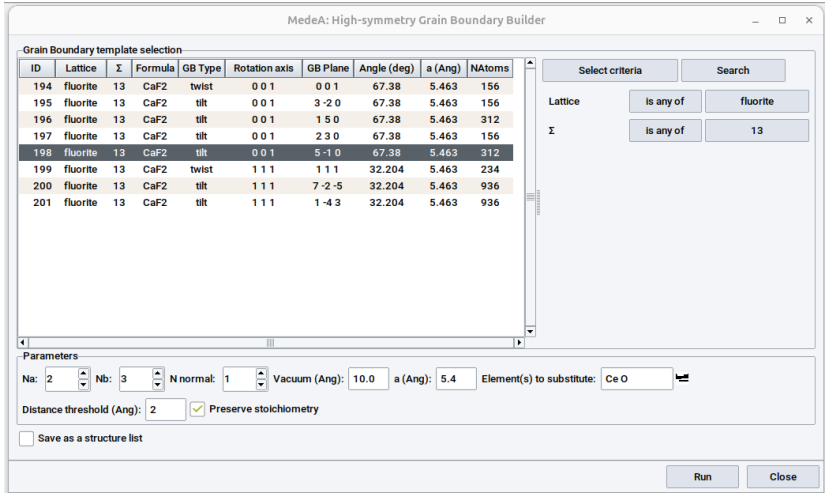
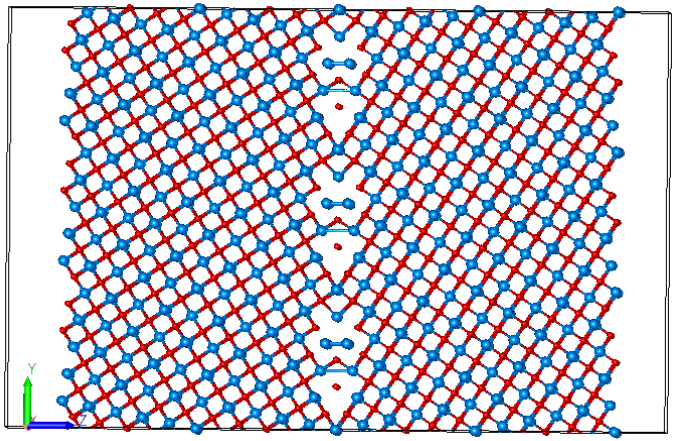
Demonstration in MedeA





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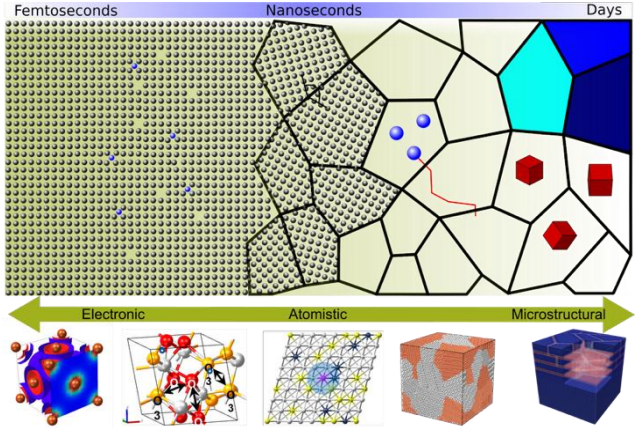
Summary



- Grain boundaries and microstructure are critical in determining many properties of materials.
- Microstructure models and phase field simulations form a bridge from the atomistic to the engineering scale.
- Generation of atomistic models of interfaces and complex microstructures has become easier – thanks to the *MedeA* high symmetry grain boundary database and the Microstructure Builder.

Datasheets:

1. Microstructure Builder
2. Interface Builder
3. Phase Field

Acknowledgements:

- Development: Pierre Caradec, Benoit Leblanc, Jason Aubry

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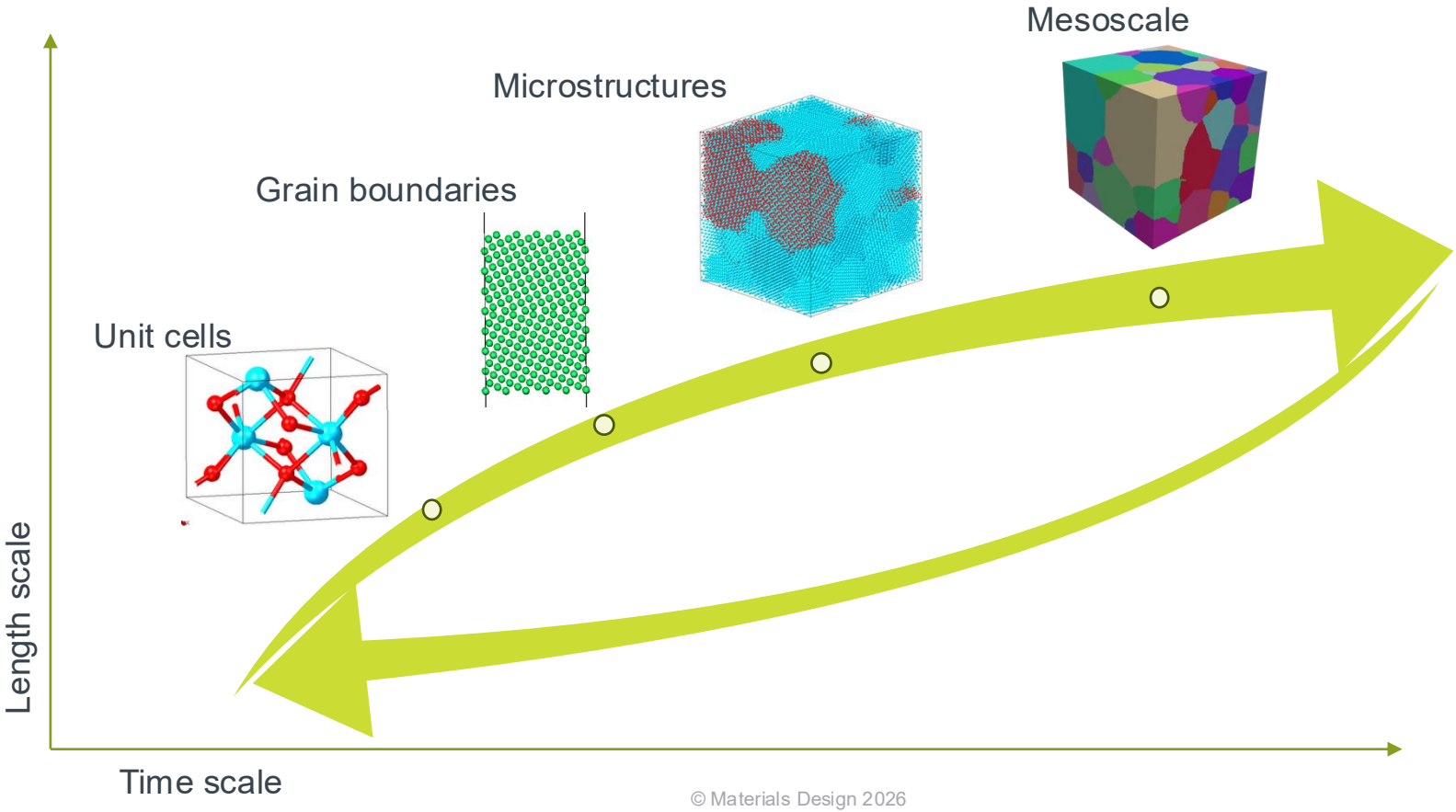
Bridging time and length scales



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Overview

1. Motivation
2. Building high-symmetry grain boundaries
3. Building complex microstructures
4. Real-world scientific applications

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Question and Answer Session

Mikael Christensen

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Benoit Minisini

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Leonid Kahle

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Datasheets, Tutorials, Documentation


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MedeA MLP

Efficient and Flexible Machine Learning Potential Support

At-a-Glance

MedeA® *MLP* (*Machine Learning Potential*) provides full *MedeA* support for LAMMPS based machine learning potential simulations, including the simulation of mechanical, vibrational, and transport properties combined with comprehensive *MedeA* based analysis of simulation results.

MedeA MLP includes a library of published machine learning potentials derived from the Spectral Neighbor Analysis Potential (SNAP)[2] formalism supported by LAMMPS.

MedeA LAMMPS based simulations using *MedeA MLP* typically show excellent agreement with first-principles methods for systems that are well represented by the training set employed in creating the machine learning potential.

Key Benefits

Productivity

- Extends *ab initio* simulation results to larger length and time scales through substantially reduced energy and force calculation times
- Efficient use of published machine learning potentials
- Automates the handling of files and data for efficient simulation

Access

- Supports the SNAP machine learning potential form
- Allows access to all *MedeA LAMMPS* simulation properties with machine learning potential accuracy
- Can be employed with the *Machine Learning Potential Generator* (*MedeA MLPG*) to access newly derived machine learning potentials
- Handles diverse atomic geometries including making and breaking of bonds

Machine learning methods allow rich first-principles datasets to be mined and employed in interpolation and inference. Such techniques are having a dramatic effect in many areas of science. In materials science, they allow researchers to obtain the accuracy and freedom from bias of *ab initio* methods at reasonable computational cost for substantial simulation times and system sizes.

'All science depends on past work. Machine Learning depends more than other science on previous work: it needs examples.'

Michael Levitt, Nobel Laureate.

Machine learning based methods for energy and force calculation have been used for a number of years. For example, Blank et al. in 1995 employed a neural net based methodology to probe the energetics of CO on the Ni(111) surface[3]. In recent years it has become increasingly clear that such approaches, employing novel descriptors and advanced machine learning techniques, can yield exceptionally accurate reproduction of quantum mechanical training data at substantially reduced computational cost[4].

MedeA MLP provides easy to use and efficient access to such methods. By making such machine learning potentials accessible for use with *MedeA LAMMPS*, *MedeA MLP* extends the range of *ab initio* methods to much larger length and time scales, while relying on first-principles results for

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.
[2] A. P. Thompson, L. P. Swiler, C. R. Trott, S. M. Foiles, and G. J. Tucker, *Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials*, J. Comp. Phys. **285**, 316 (2015)
[3] T. B. Blank, S. D. Brown, A. W. Calhoun, D. J. Doren, *Neural network models of potential energy surfaces*, J. Chem. Phys., **103**, 4129 (1995)
[4] J. Behler, and M. Parrinello, *Generalized neural-network representation of high-dimensional potential energy surfaces*, Phys. Rev. Lett. **98**, 146401 (2007)

Key Features

- Library of published machine learning potentials
- Full support for the SNAP description
- Enables LAMMPS MLP simulations in the *MedeA Environment*

Required Modules

MedeA Environment
MedeA LAMMPS

lated Modules

deA MT
deA Phonon
deA Diffusion
eA Surface Tension
eA Thermal Conductivity

Out More

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ecorded/Machine-Learning-Quantum%
mistry-Catalysts

Deng, R. Tran, H. Tang, I. H. Chu, S. P. Ong, *w field for molybdenum by machine learning data*, Phys. Rev. Mater. **1**, 043603 (2017)
Hu, C. Chen, Z. Deng, J. Luo, S. P. *-accurate spectral neighbor analysis potential Ni-Mo binary alloys and fcc metals*, Phys. 04 (2018)
A. Cusentino, B. D. Wirth, A. P. Thompson, *rial models for atomistic simulation*, Phys. 5 (2019)
X. Li, Z. Deng, Y. Chen, J. Behler, S. P. *and cost assessment of machine learning potentials*, J. Phys. Chem. A, **124**, 731
A. Wood, and A. P. Thompson, *Explicit ion of the Spectral Neighbor Analysis ally Complex Systems*, J. Phys. Chem.
H. Zheng, Y. Zuo, S. P. Ong, *Comechanisms in the NbMoTaW multi-*, npj Comput. Mater. **6**, 70 (2020)

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MedeA MLPG

Efficient Flexible Machine Learning Potential Generator

At-a-Glance

The *MedeA*® *MLPG* (Machine Learning Potential Generator) enables users to create their own machine learning potentials (or force-fields) from training-set data previously generated by quantum mechanical calculations. The resulting potentials allow users to perform simulations of systems substantially larger in size and for much larger simulation times than can be typically accessed using quantum mechanical methods while at the same time reflecting the high accuracy and validity of the latter.

In addition to managing selection of training and validation data, the *MedeA MLPG* allows you to generate machine learning potentials, using the Spectral Neighbor Analysis Potential (SNAP)[2] formalisms. The potentials created are ready for subsequent use with *MedeA* interface as well as VASP and LAMMPS, the *MedeA MLPG* thus provides efficient access to machine learning based simulation techniques.

Key Benefits

Productivity

- Automates the creation of machine learning potentials using the SNAP formalism
- Extends *ab initio* precision to larger length and time scales
- Manages training set data
- Full Ziegler-Biersack-Littmark (ZBL) potential support

Accuracy

- Yields machine learning descriptions based on the SNAP methods
- Provides access to all calculation details and information
- Provides machine learning potentials for use with all *MedeA LAMMPS* property calculation types

Machine learning potentials employ efficient descriptors of atomic environments combined with machine learning based correlative methods to describe the energetic behavior of atomic and molecular systems. The *MedeA MLPG* allows users to generate machine learning potentials by accurately reproducing supplied target first-principles data for a training set of structures.

Figure 1: The MedeA Machine Learning Potential Generator (MLPG) is integrated within the MedeA environment allowing straightforward use of first-principles information from VASP in the creation of MLPs.

The *MedeA MLPG* manages training-set data derived from first-principles calculations as the target to be reproduced by the MLP (machine learning potential). Configuration dependent energies, forces, and stresses can be considered in the fitting process. Using the SNAP approach the *MedeA MLPG* creates a machine learning potential by minimizing the deviations from the target energies, forces, and stresses calculated by quantum mechanical methods. While this process is guided by meaningful default parameters, the full flexibility of the underlying methods can be accessed by advanced settings. The *MedeA MLPG* has been developed as part of active research and development projects and is thoroughly validated.

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[2] A. P. Thompson, L. P. Swiler, C. R. Trott, S. M. Foiles, and G. J. Tucker, *Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials*, J. Comp. Phys. **285**, 316 (2015)

Technical Features

User Interface

- Selection of training and validation data
- Specification of terms for optimization
- Report and plot creation for analysis

Supported Target Data

Energies
Forces
Stress tensors

ey Features

Uses VASP derived DFT results
teractive selection and control
utomated results analysis
fficient handling of optimization

ired Modules

Environment
MLP
VASP
LAMMPS

Modules

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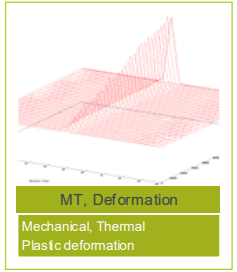
Highlighted *MedeA* Modules

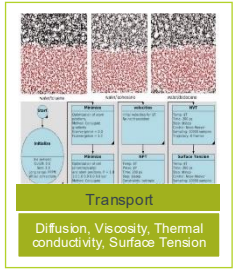
MedeA Environment: The *MedeA* software package is the leading environment for the atomistic simulation of materials. *MedeA* enables professional, day-to-day deployment of atomic-scale and nano-scale computations for materials engineering, materials optimization and materials discovery. In *MedeA*,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

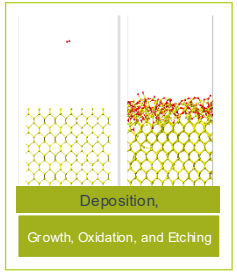
MedeA Interface Builder: Creates interfaces and grain boundaries using two different methods. The user can construct a high-symmetry Coincidence-Site Lattice (CSL) grain boundary by customizing template models. In addition, general interface models can be built from two surfaces, allowing for a certain degree of lattice mismatch between the layers. There is no restriction on the surface cells that you start with, they can be as complex or simple as needed.

The *MedeA Microstructure Builder:* creates microstructure models for atomistic simulations using a *Seed & Growth* algorithm with starting points either placed randomly or at user-specified coordinates within a supercell. Each such point is used as an origin to grow a crystalline grain by adding atoms from that seed point outwards, until a grain boundary is encountered.

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 years







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Problem Solving in the Golden Age of Computational Materials Science:

https://www.materialsdesign.com/webinars/recorded/problem-solving-in-the-golden-age-of-computational-materials-science

Accessing the Mesoscale with Phasefield Modeling

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Related *MedeA* Tutorials

An Introduction to PhaseField - Tungsten Oxidation,

Microstructure Builder

Interface Builder

Interface Construction of Al(111)/Graphene

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Question and Answer Session

Mikael Christensen

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Questions about Materials Design Webinars

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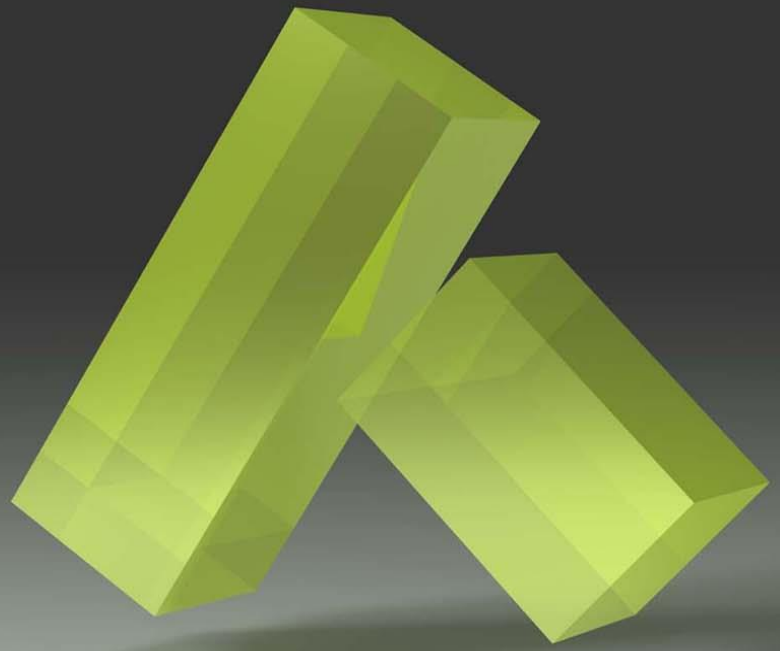

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Innovation by Simulation