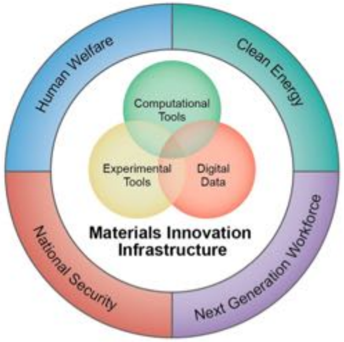
PRISMS Center

Center for PRedictive Integrated Structural Materials Science

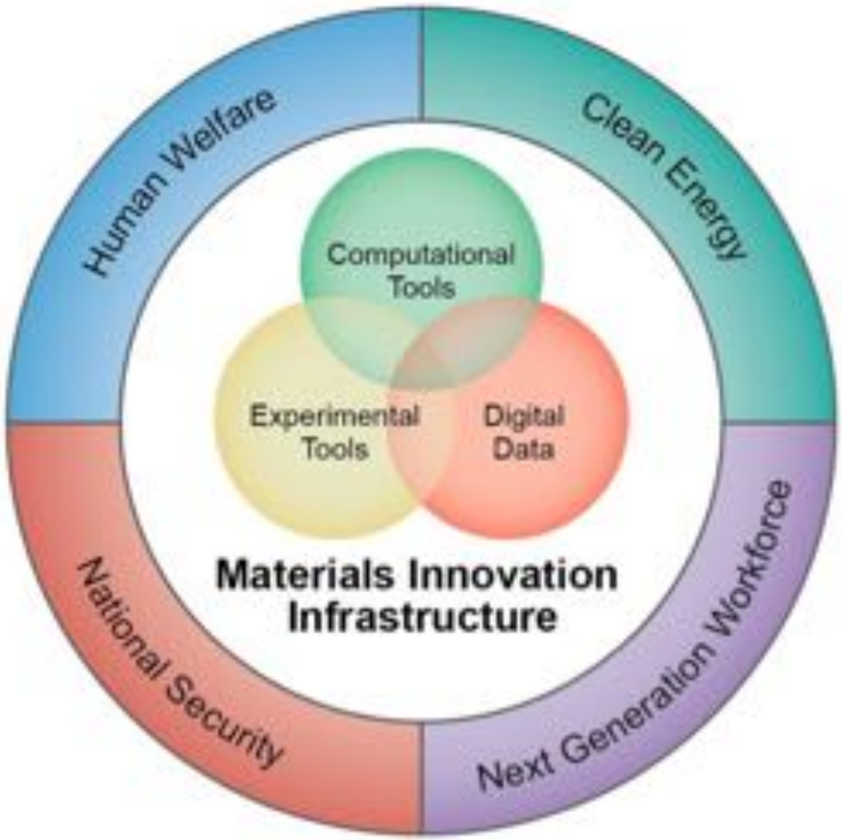
A DOE Software Innovation Center for the Structural Metals Community



2016 ICME Short Course

Website: prisms-center.org

Materials Genome Initiative



. . . This initiative offers a unique opportunity for the United States to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost.

President Barack Obama, 24 June 2011
Announcing the *Materials Genome Initiative*

"(In this context) genome connotes a fundamental building block toward a larger purpose" NSTC MGI White Paper, 2011

PRISMS Center Members

U.S. DEPARTMENT OF ENERGY | O S

UCSB

UNIVERSITY OF MICHIGAN

Center for PRedictive Integrated Structural Materials Science

PRISMS

PRISMS Center – Faculty and Staff

Faculty

- John Allison, Center Director
- Samantha Daly (ME)
- Krishna Garikipati (ME)
- Vikram Gavini (ME)
- Margaret Hedstrom (SI)
- H. V. Jagadish (CSE)
- J. Wayne Jones (MSE)
- Emmanuelle Marquis (MSE)
- Amit Misra (MSE)
- Veera Sundararaghavan (Aero)
- Katsuyo Thornton (MSE)
- Anton Van der Ven - UCSB

Staff

- Steve DeWitt
- Brian Puchala
- Shiva Rudraraju
- Sravya Tamma
- Glenn Tarcea













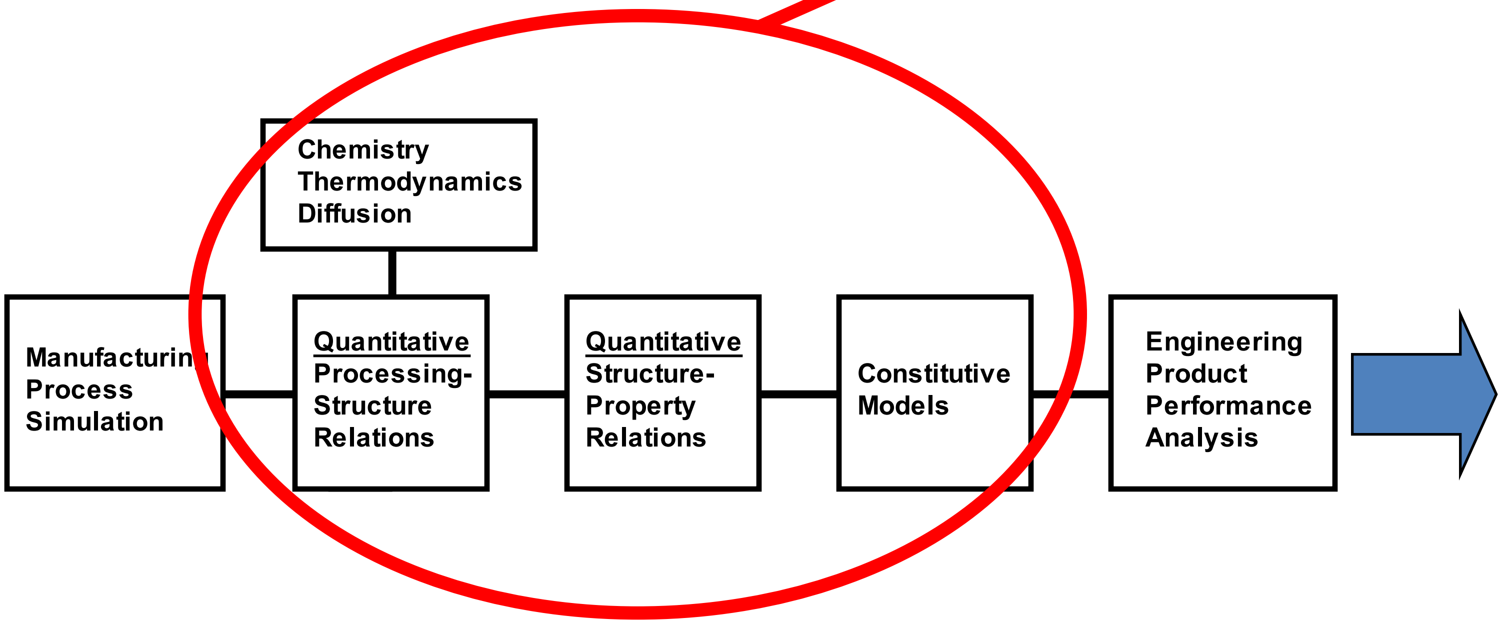




PRISMS Center – Vision of Success

Provide the capability for rapid insertion of the latest science into the engineering process

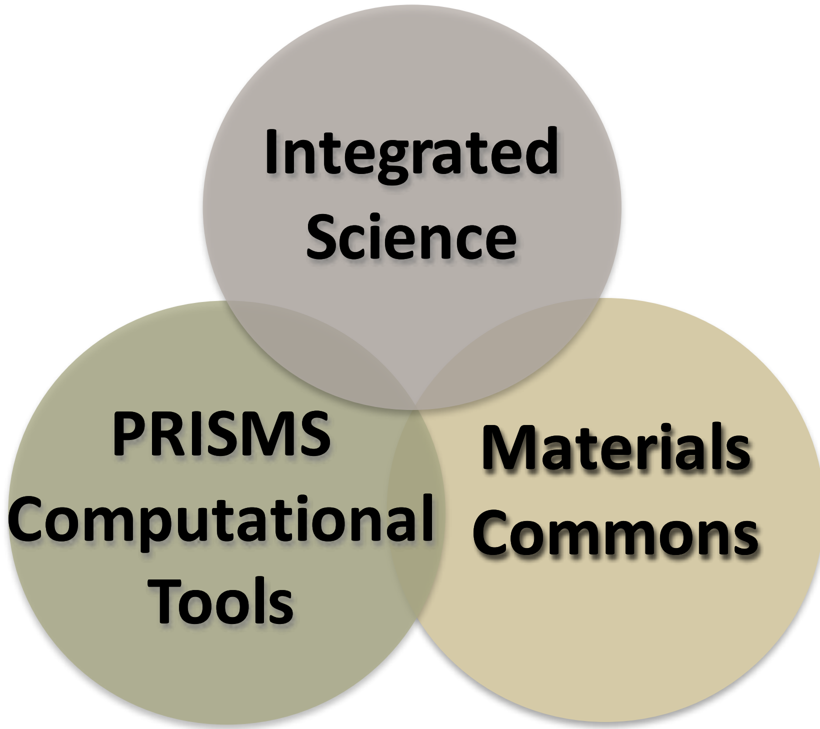
PRISMS – extensible scientific core for ICME for structural metals



- Process & product optimization
- Innovation

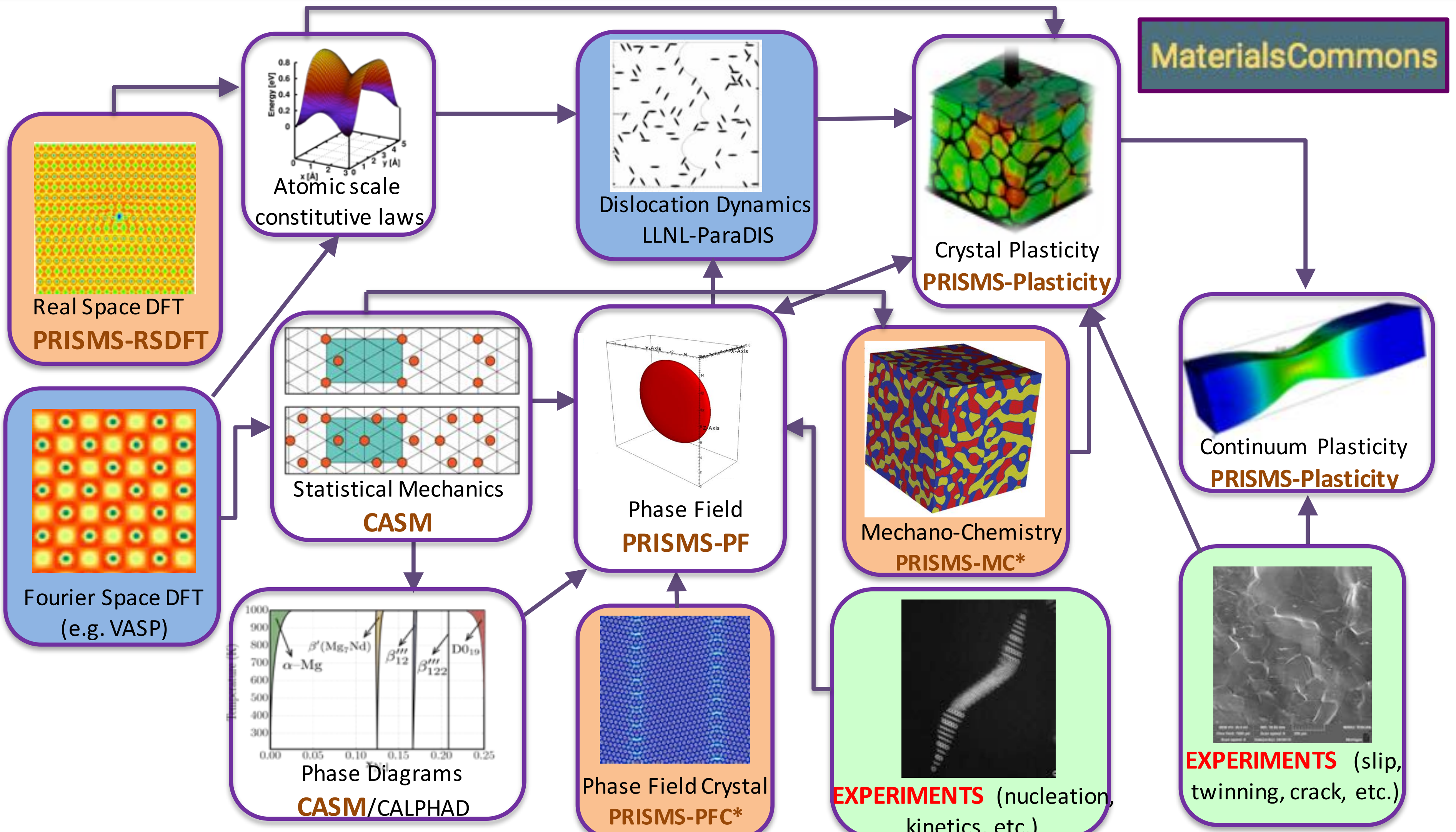
PRISMS Center – Our Goal

Establish a unique scientific platform that will enable accelerated predictive materials science



PRISMS Center Integrated Framework

Enabling accelerated predictive materials science



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Center for PRedictive Integrated Structural Materials Science

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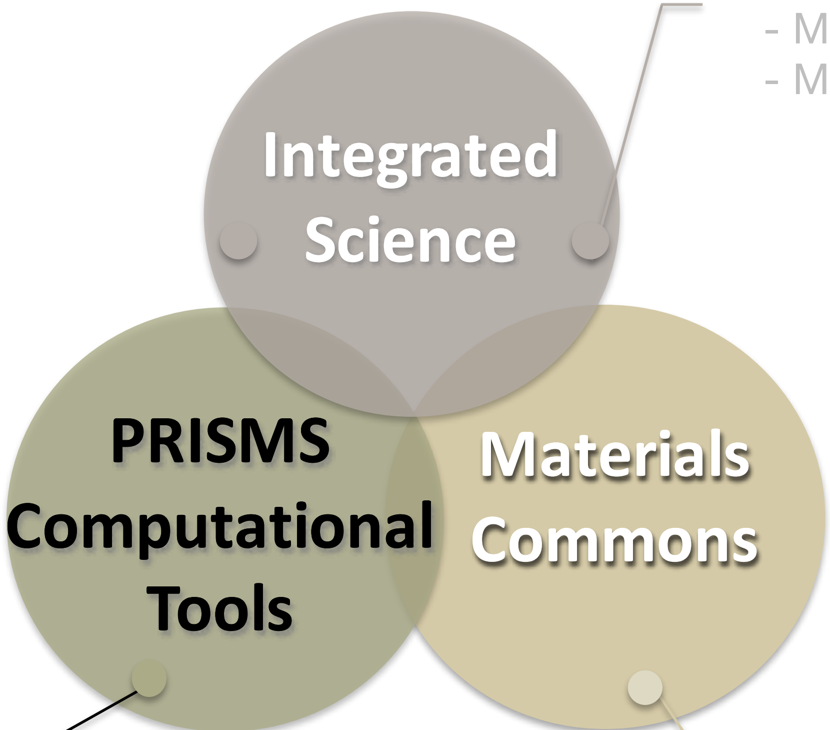
PRISMS Center

Enabling accelerated predictive materials science.

- Open Source
- Integrated Hierarchical Multi-Scale
- Scalable, Extensible
- Advanced Methods



- Use Cases (Magnesium Alloys)
  - Microstructural Evolution
  - Mechanical Behavior

- Collaboration & Community
- Experimental & Simulation Information
- Seamless, Continuous
- Workflow
- Provenance Tracking
- Accelerate model building and validation

PRISMS Integrated Computational Software

- Github based release management
- Documentation: README's, Doxygen files, user manuals and formulation details
- Unit tests
- Open Source License: LGPL
- User Support: Mailing lists, workshops, etc.

Based on *deal.ii* open source FEM framework

PRISMS Software Development

- PRISMS-IntegrationTools
- CASM (Statistical Mechanics)
- PRISMS-PF (Phase Field)
- PRISMS-Plasticity (Crystal & Continuum)
- PRISMS-RSDFT (Real Space DFT)
- Phase Field Crystal*
- Mechano-Chem *

Released Codes!!

*Internal research codes

PRISMS Integrated Computational Software

PRISMS Software Development

- PRISMS-IntegrationTools
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- PRISMS-RSDFT (Real Space DFT)
- Phase Field Crystal*
- Mechano-Chem *

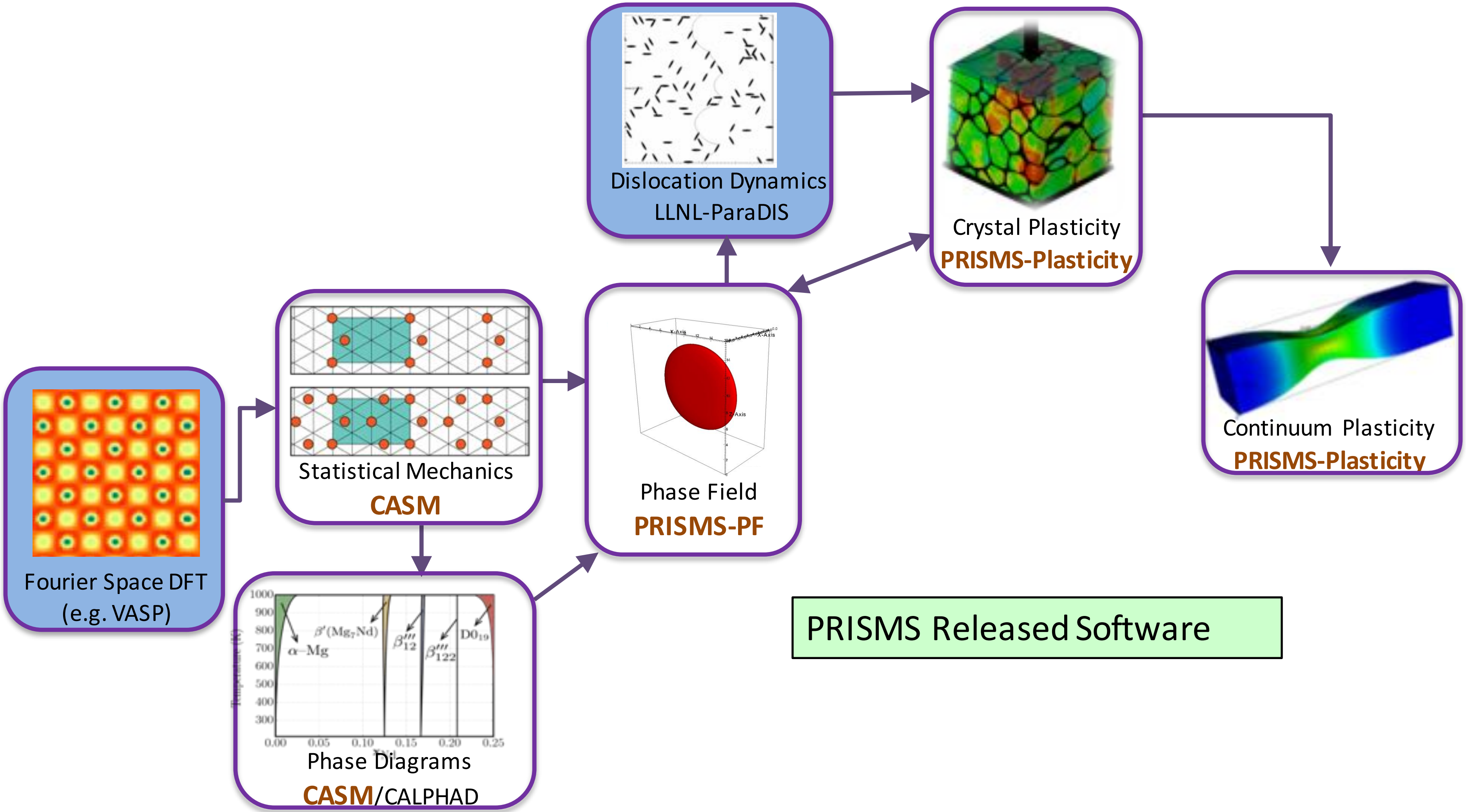
*Internal research codes

Based on *deal.ii* open source FEM framework

PRISMS Computational Method Talks at TMS

- Anton Van der Ven
  "CASM"
  Monday 10:10 am
- Vikram Gavini
  "RSDFT"
  Tuesday 8:30am
  Room 209A
- Jason Luce
  "Phase Field Crystal"
  Tuesday 3:10pm
  Room 209A

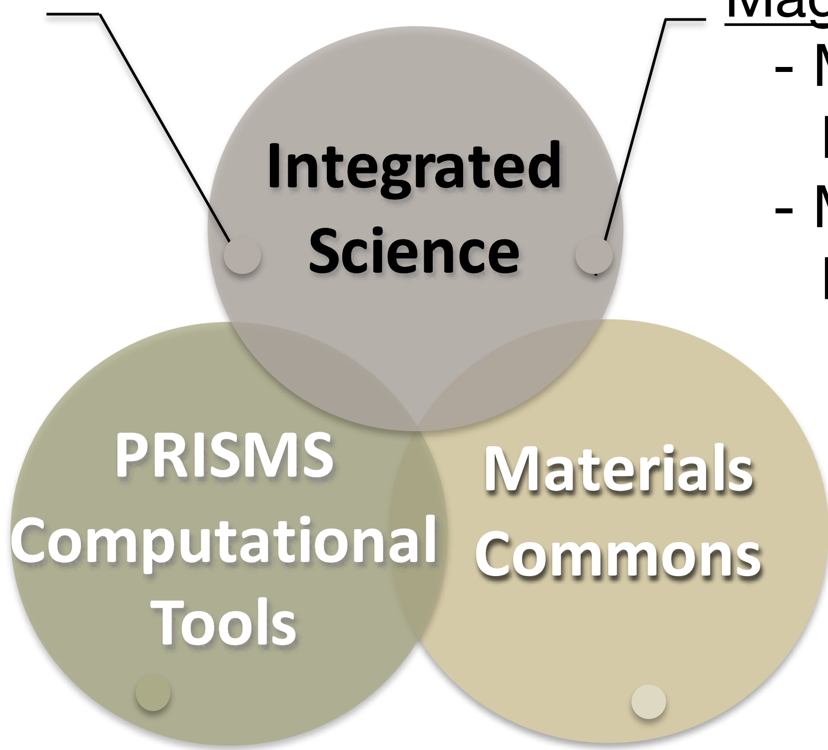
PRISMS Center Integrated Software: Released Codes



PRISMS Center

Enabling accelerated predictive materials science.

- Linking Experiments & Simulations
- Advanced Quantitative Experiments
- Collaborative Community



- Use Cases:
  <u>Magnesium Alloys</u>
  - Microstructural Evolution
  - Mechanical Behavior

Magnesium Alloys as a PRISMS Demonstrator

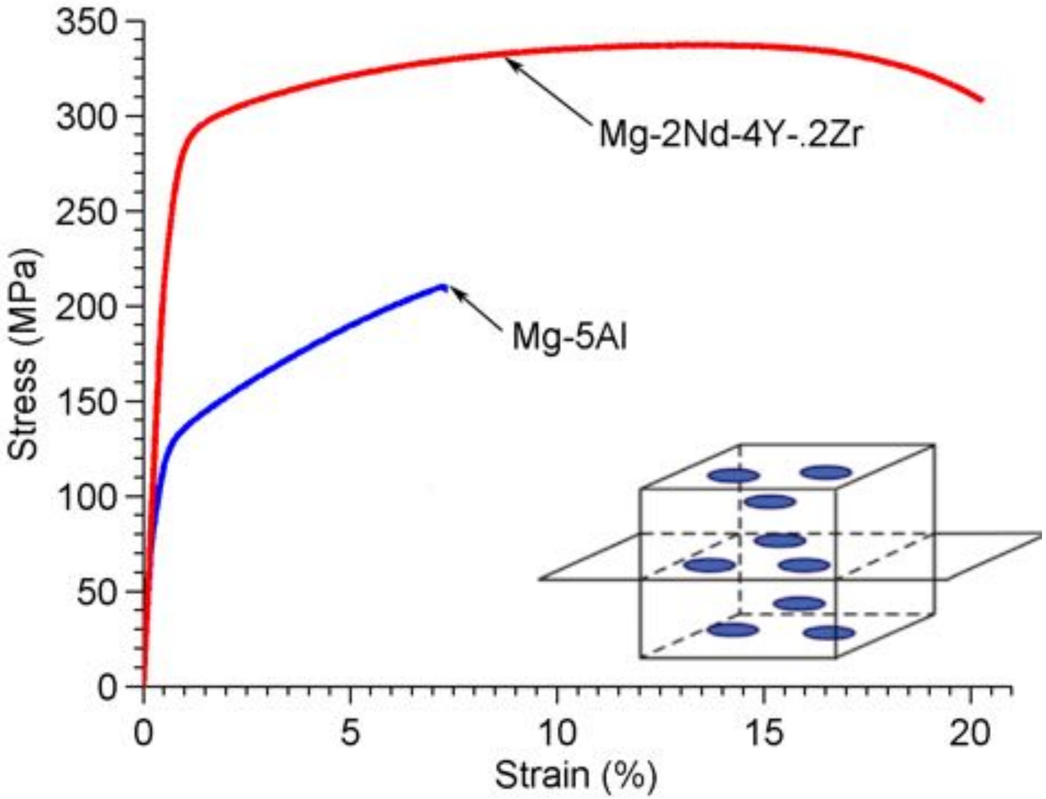
- Magnesium alloys are an important material choice for lightweighting vehicles, saving fuel and reducing emissions.
- To expand the application space, property improvements are required.
- Magnesium alloy development is at a very immature stage
- Magnesium alloys represent an important opportunity for demonstrating the PRISMS framework & capability

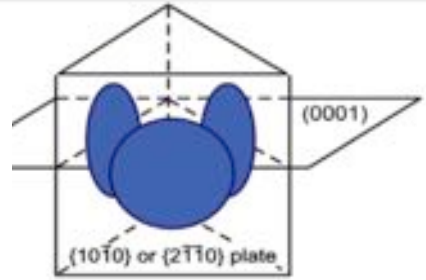
Magnesium Alloy Development Needs

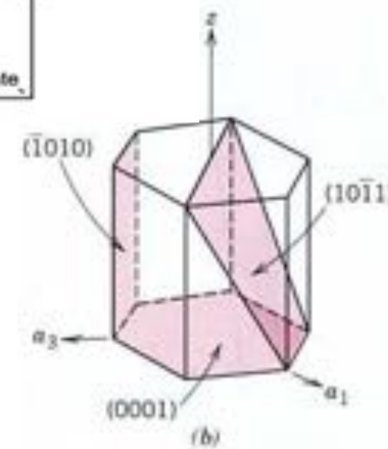
- <u>Strength</u>
- <u>Fatigue</u>
- Ductility
- Corrosion
- Creep
- Affordability

We can't do it all within The PRISMS Center – so we need to have an extensible capability and a community of collaborators to extend it.

Mg-Rare Earth alloys are unusually strong



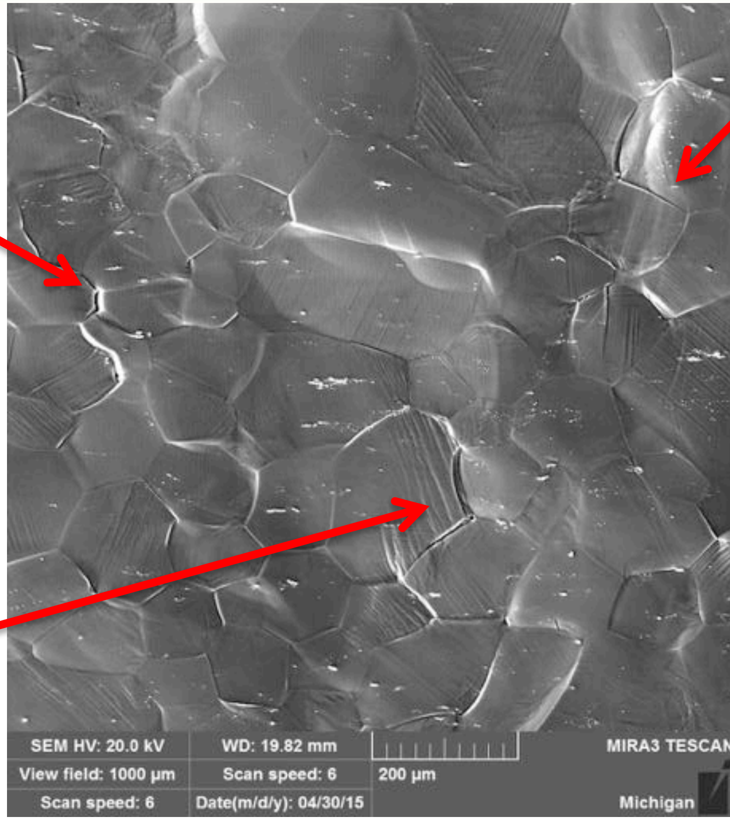




Precipitates oriented perpendicular to the basal plane are more likely to block dislocations gliding on basal planes

- Why do Mg-RE alloys have precipitates oriented in this special way?
- Are there other alloying approaches that might behave in similar ways?
- Can we predict precipitate effects on properties to optimize alloys & processes?

Damage Mechanisms & Microstructures

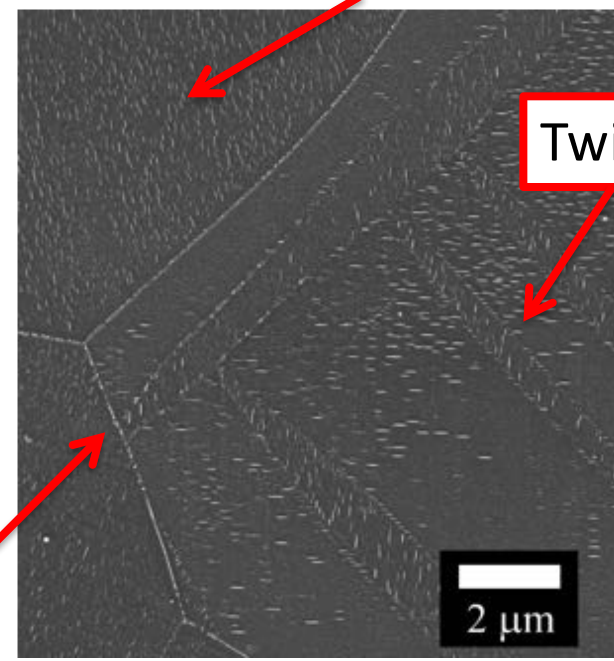


Grain Size & Texture

Cracks

Slip

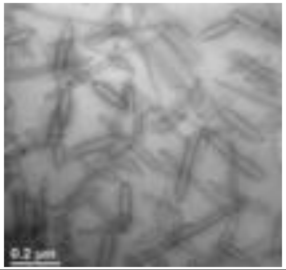
Fine precipitate Structures

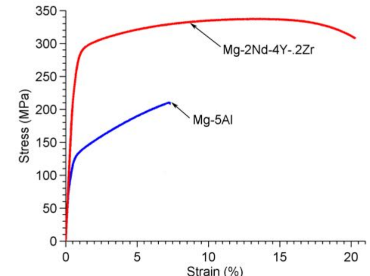


Twins

Grain boundary precipitates

PRISMS Use Case Integration



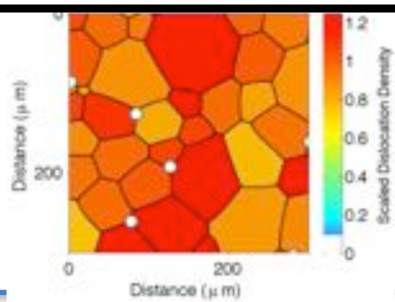


Precipitate Evolution → Tensile Behavior

Precipitate Evolution ↔ Recrystallization & Grain Growth

Recrystallization & Grain Growth → Tensile Behavior

Fatigue Behavior



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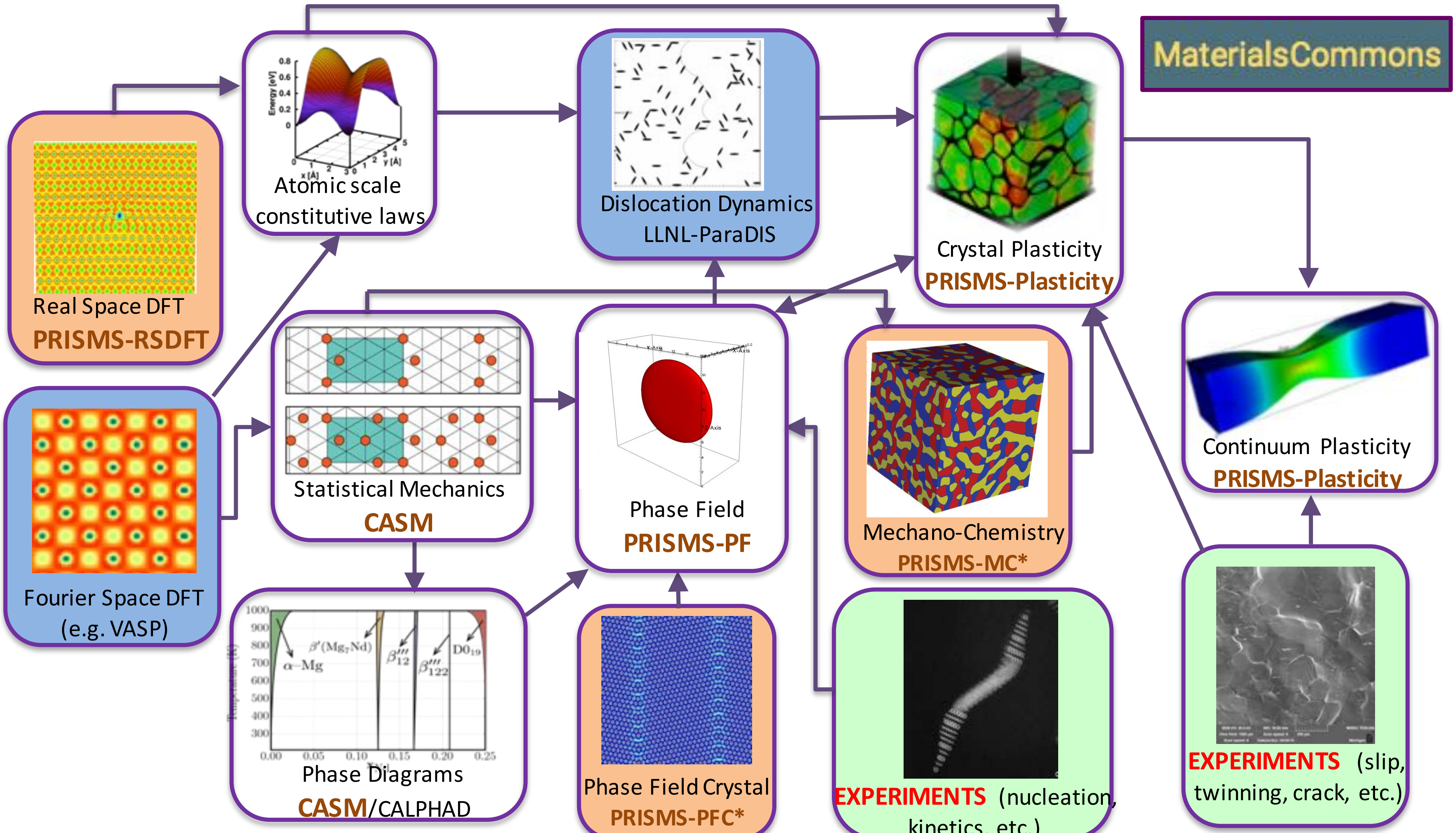
PRISMS Center Integrated Framework

Enabling accelerated predictive materials science



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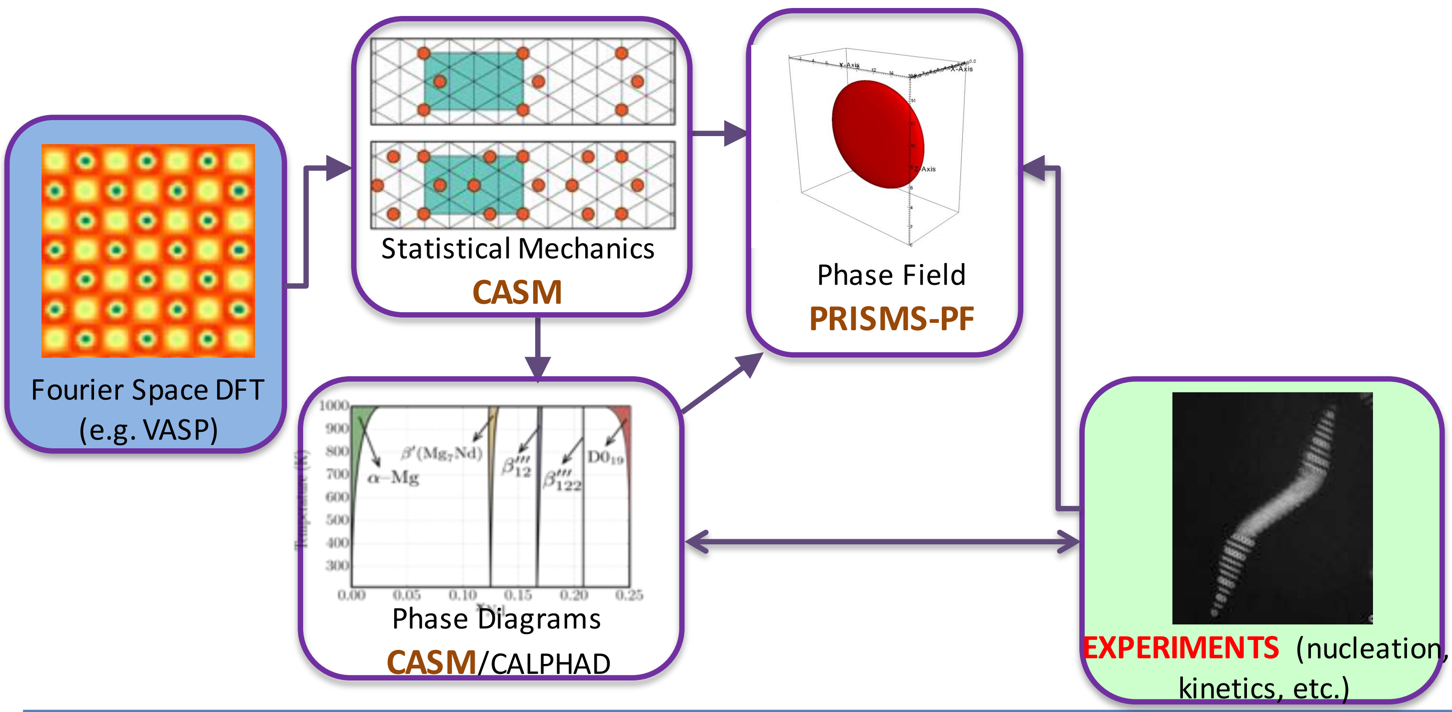
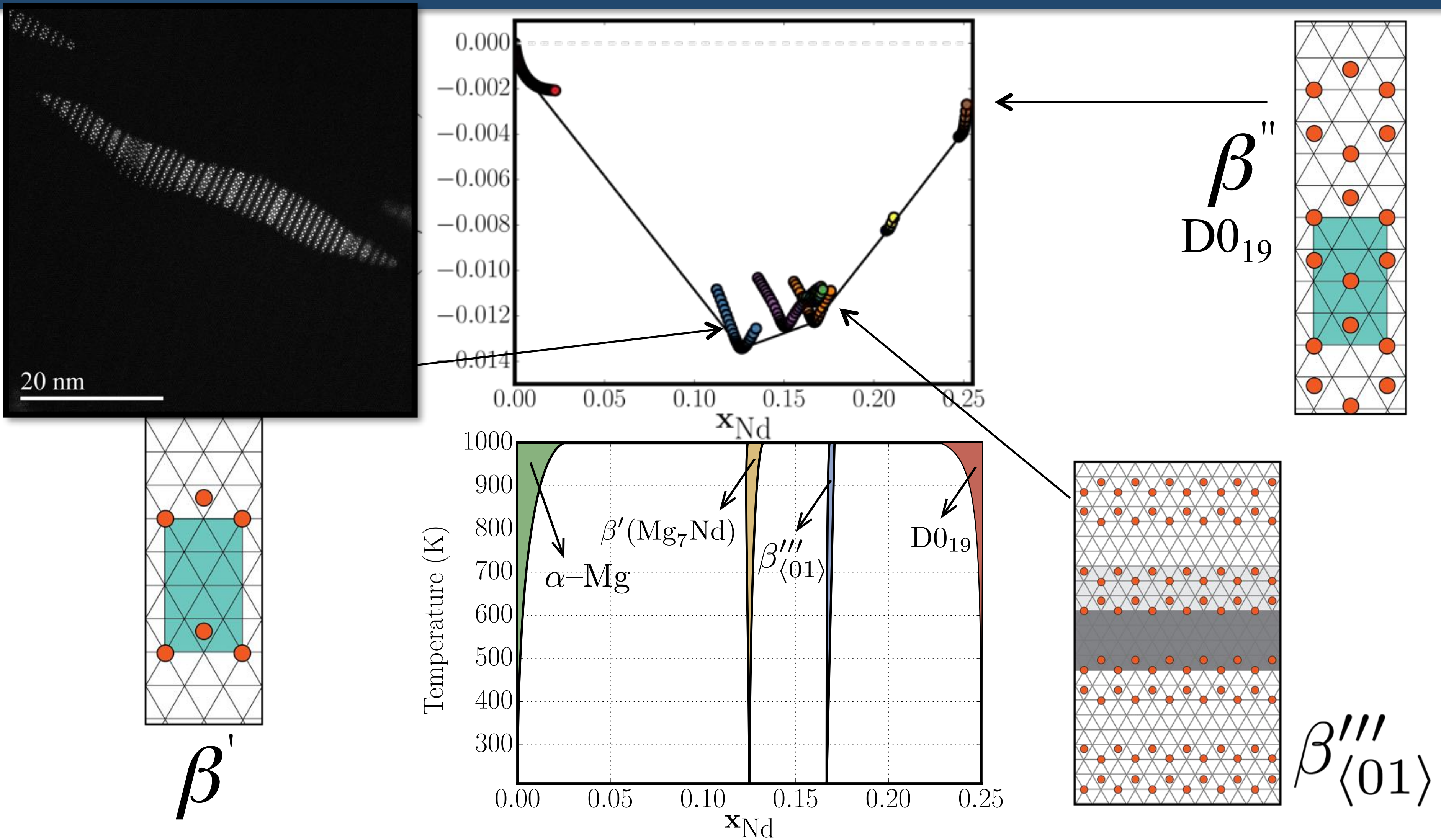
PRISMS Center Integrated Framework
Precipitate Evolution Use Case

MaterialsCommons



Calculated metastable hcp phase diagram

Integrating Experiments – Simulation - Theory



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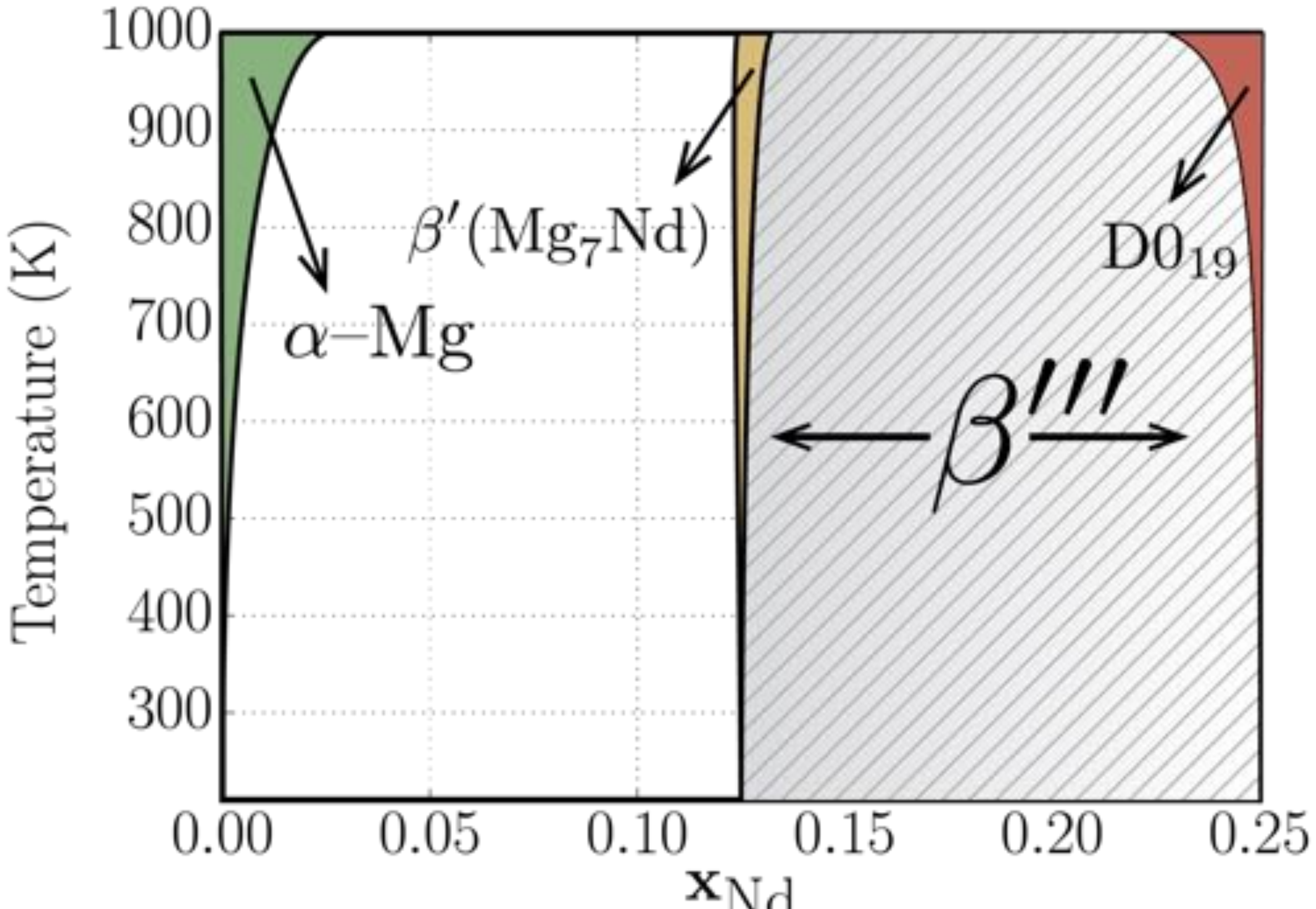
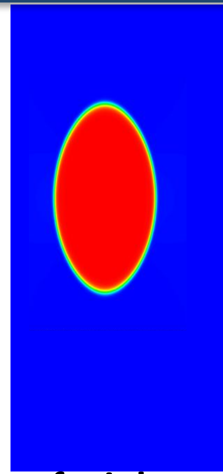
β''' and the metastable phase diagram



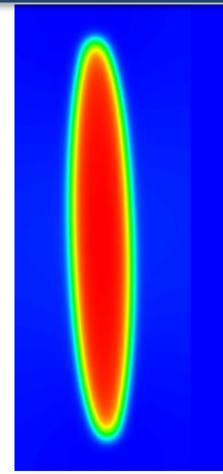
Natarajan, Solomon, Puchala, Marquis, Van der Ven, Acta Mat 2016

Using PRISMS-PF to study factors influencing β’ (β “’) precipitate morphology

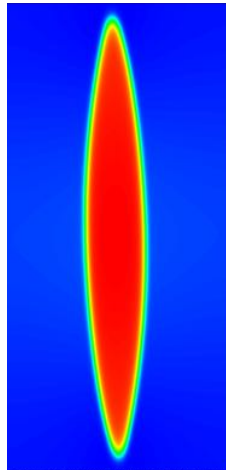
- 2D & 3D phase-field simulations of morphology



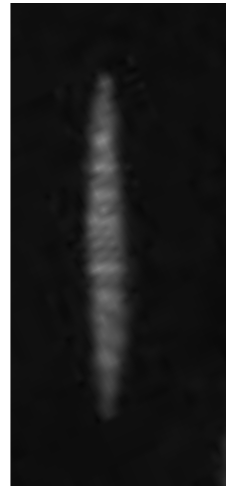
Interfacial energy anisotropy only



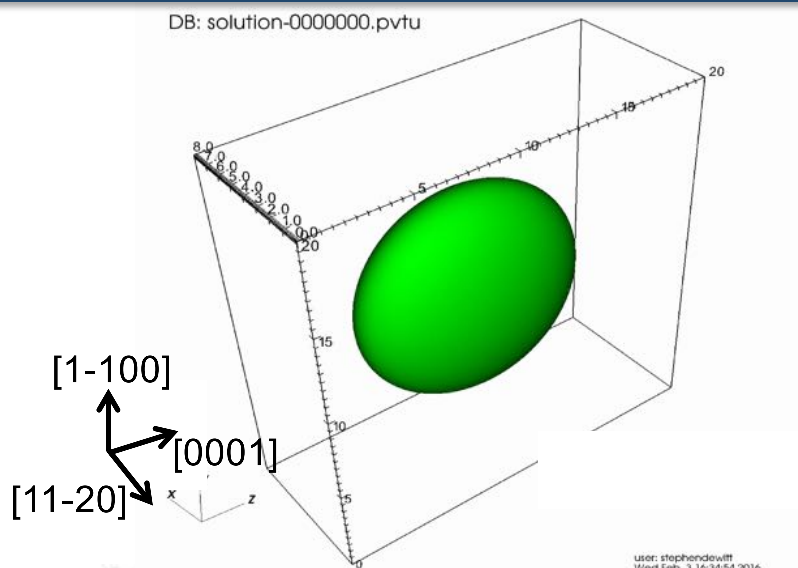
Elastic misfit strain only

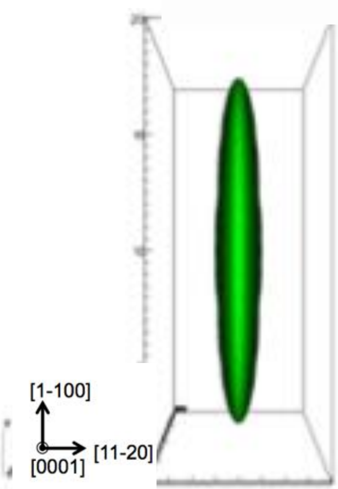


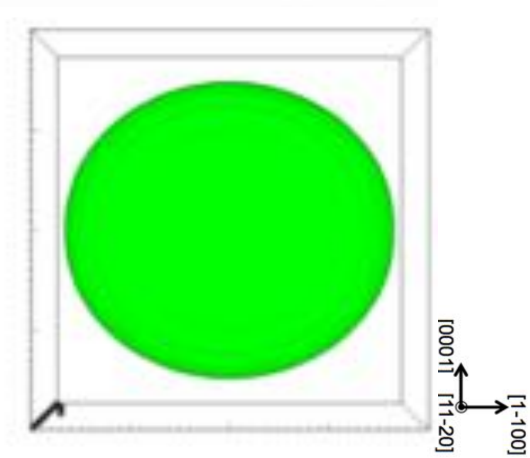
Interfacial energy anisotropy +Elastic misfit strain



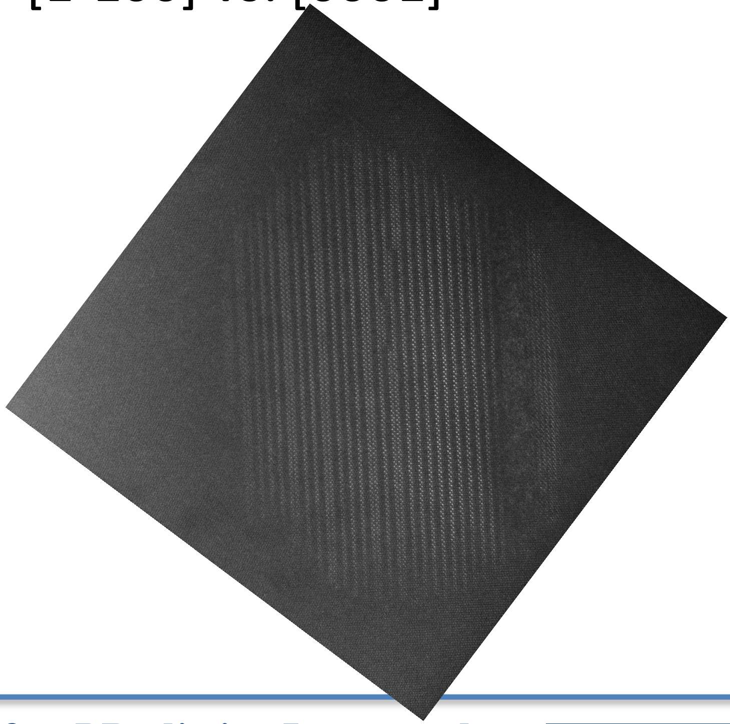
β’ (β’’’) Morphological Evolution







- 13% misfit along [11-20] causes the precipitate to flatten into a lenticular shape
- Interfacial energy anisotropy causes slight elongation along [1-100] vs. [0001]



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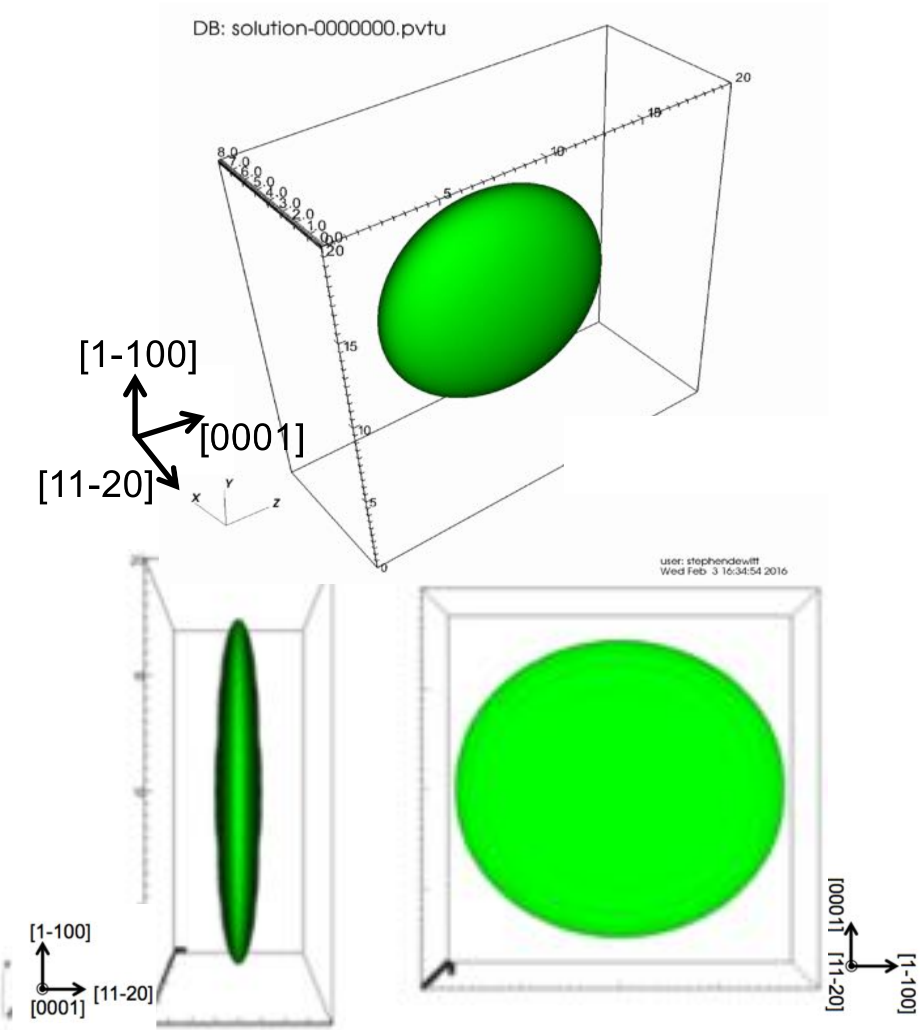

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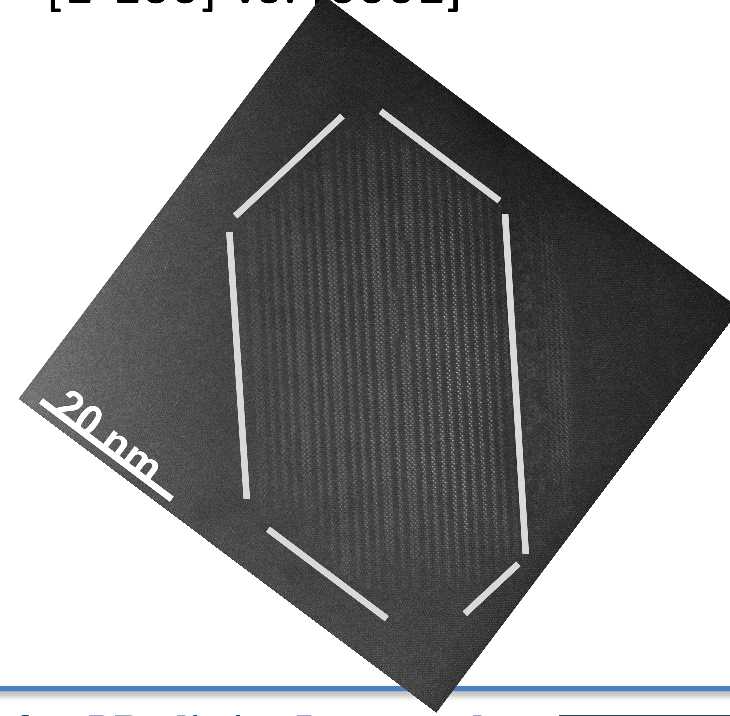
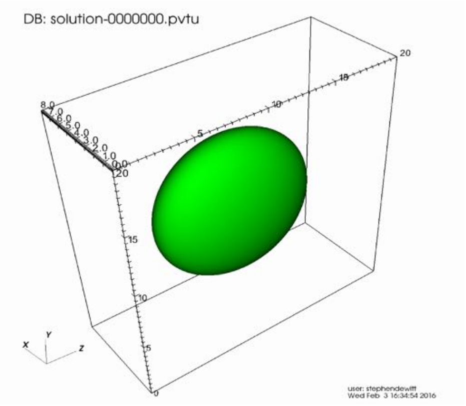
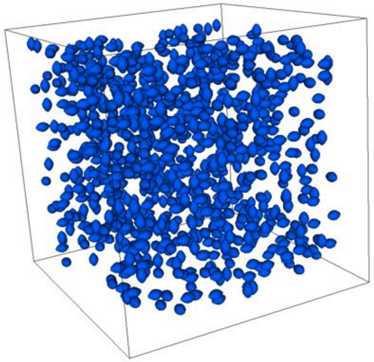


Using PRISMS-PF capabilities to simulate large precipitate populations

- Adding nucleation, anisotropic interfacial energy
- High precipitate density calculations ongoing



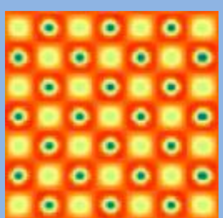


1000 Precipitates

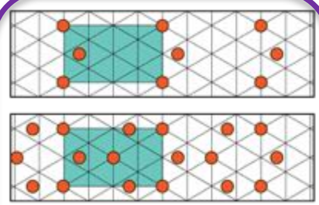
PRISMS Center Integrated Framework
Precipitate Evolution Use Case

PRISMS Precipitate Use Case TMS Talks:

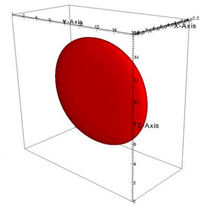
- Anton Van der Ven
  "CASM"
  Monday 10:10am
- Anidrudh Natarajan
  "Modeling precipitation in Mg-Nd"
  Tuesday 2:50pm
  Room 208B
- Ellen Solomon
  "Structure of beta''' in Mg-Nd"
  Tuesday 4:00pm
  Room 204



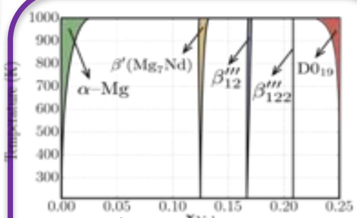
Fourier Space DFT
(e.g. VASP)



Statistical Mechanics
CASM



Phase Field
PRISMS-PF



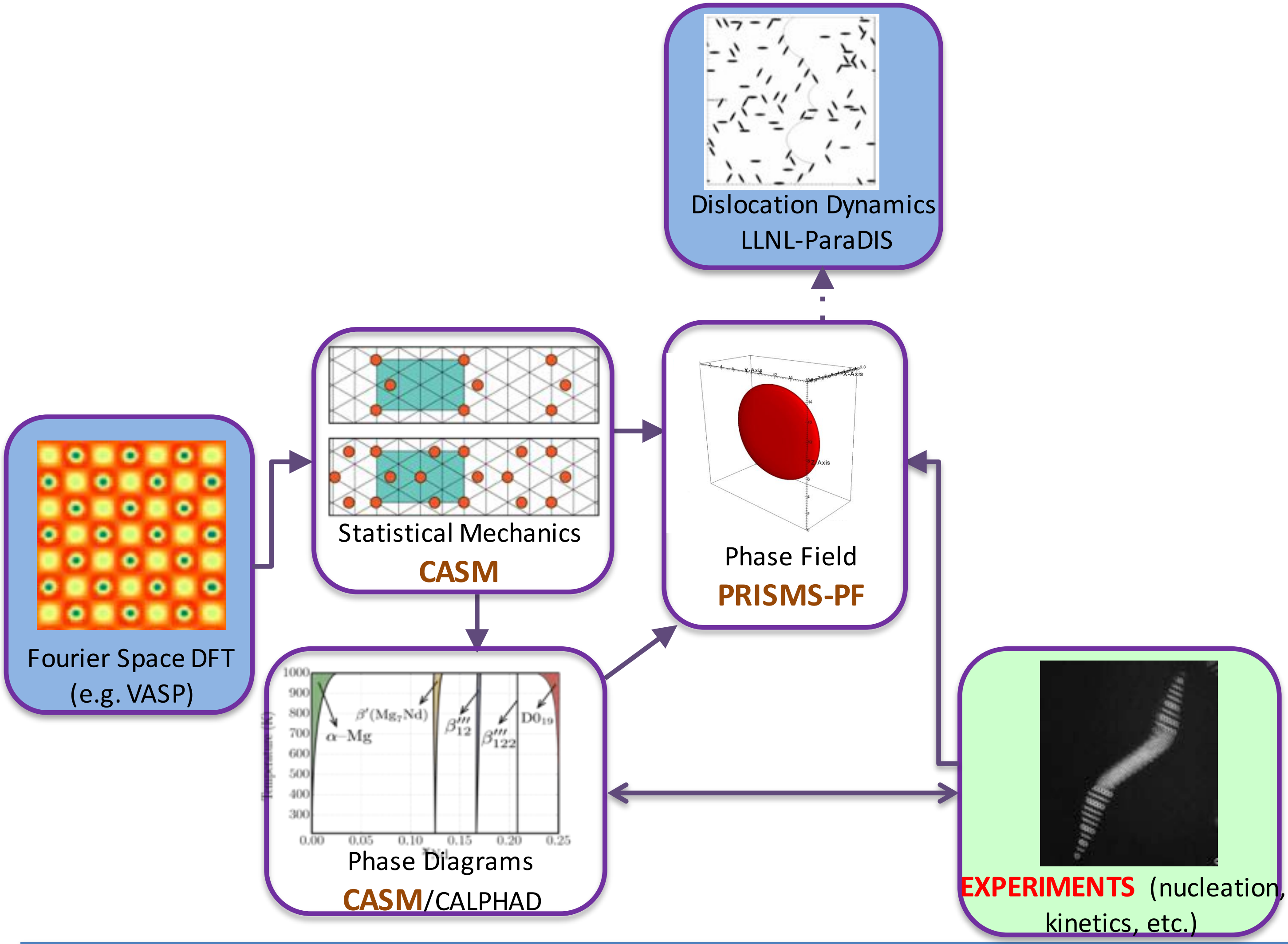
Phase Diagrams
CASM/CALPHAD

EXPERIMENTS (nucleation, kinetics, etc.)

PRISMS Center Integrated Framework

Precipitate Evolution Use Case

MaterialsCommons



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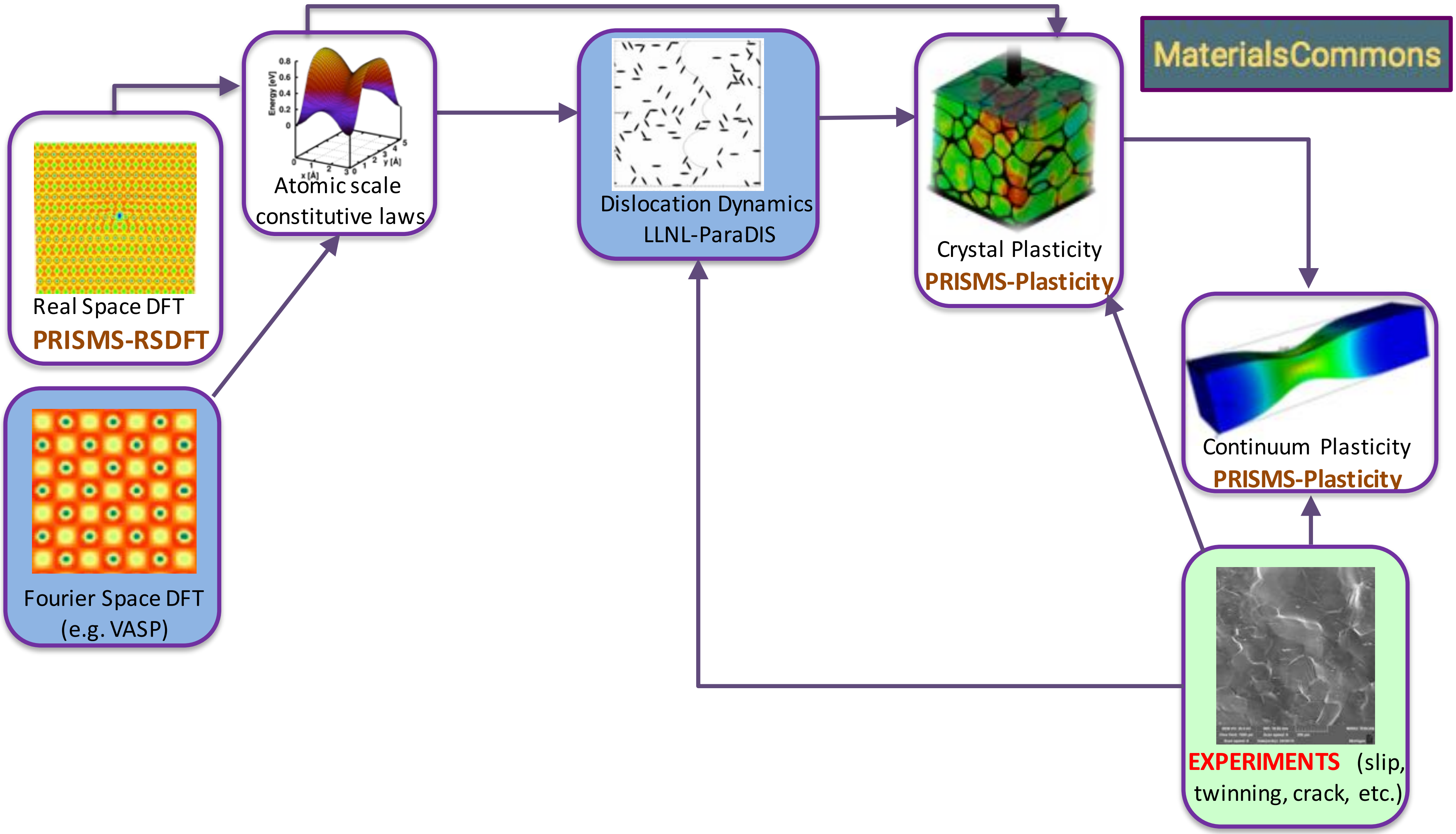
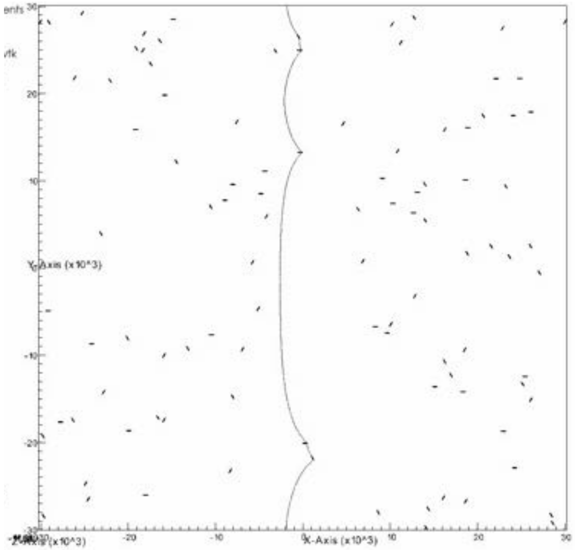
Tensile Behavior Use Case



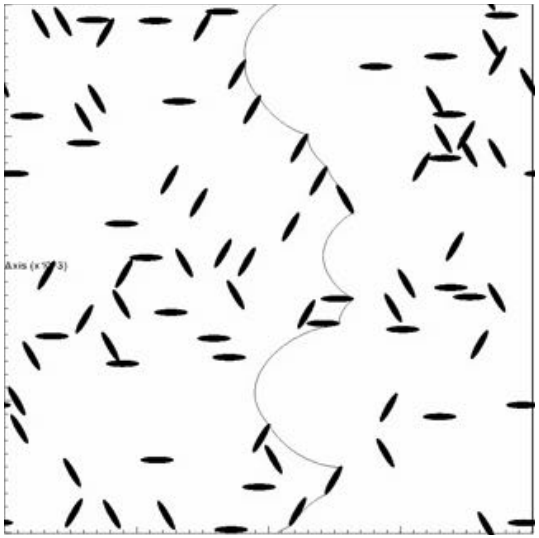
Simulating the influence of precipitates on critical resolved shear strength (CRSS)

Collaboration with LLNL: used pre-release version of PARADIS incorporating the mobility law for HCP materials, we modified the code to include precipitate strengthening.

- Simulate dislocation gliding on basal slip plane (using PARADIS)



10-hour Aged
CRSS = 3.5MPa



50-hour Aged
CRSS = 16MPa

Material: Mg-9Al-1Zn alloy
Aged at 168C

Predicted influence of statistical precipitate distributions on CRSS is ~40% higher than existing analytical models

Calculation of basal CRSS in AZ91

DFT Calculations

Peierls stress
0.7 MPa (Literature: Shen)

Solid Solution strengthening
4.6 MPa (Literature: Trinkle)

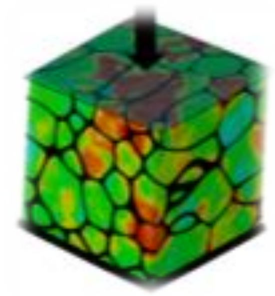
Experiments

Grain boundary strengthening
12 MPa (Literature: Caceres)

Dislocation Dynamics

Precipitate-Dislocation interactions
16.0 MPa (this work)

Slip system deformation resistance
33.3 MPa



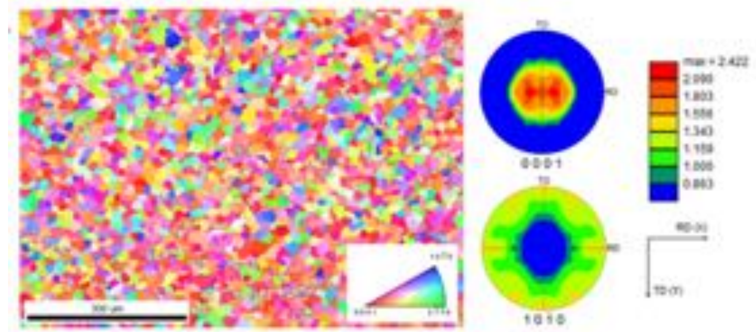
Experiment:
151 MPa/5 = **30.2 MPa**

Virtual tensile testing using PRISMS – Plasticity (CPFE)

Mode	τ_0^α (MPa)	h_0 (MPa)	τ_{sat} (MPa)	a
Basal <a>	22.5	30	63	1.1
Prism <a>	61.2	39	189	0.8
Pyram <a>	61.2	39	189	0.8
Pyram<c+a>	61.2	39	189	0.8

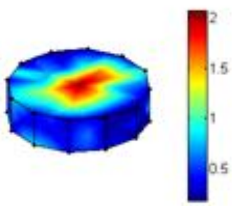
- Developed methods to instantiate statistically representative polycrystals from EBSD Maps
- PRISMS-Plasticity code parameters can be obtained from DFT/DD simulations and/or experiments

Mg-Nd-Y (WE43)



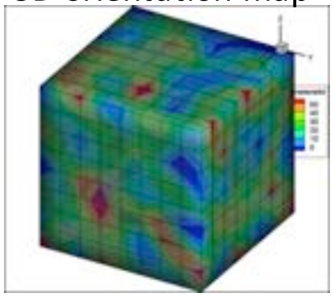
EBSD

Map to ODF

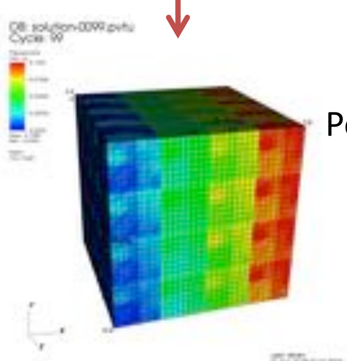


Sample RVE

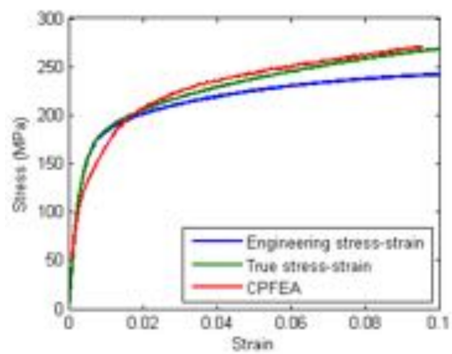
3D orientation map



CPFE tensile test



Postprocess



PRISMS-Plasticity (CPFE) is capable of simulating large microstructural sets

Elastic Moduli: (Flowers et al.)

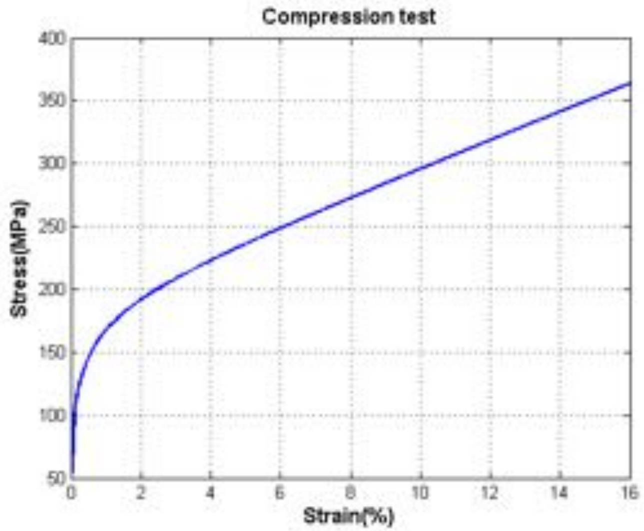
C_{11} = 153.97 GPa; C_{12} = 85.78GPa; C_{13} = 67.16 GPa;
C_{33}= 183.0 GPa; C_{44} = 46.27 GPa

Slip Resistance parameters: (Salem et al.)

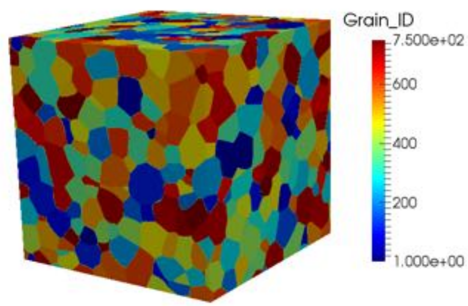
$\tau_{0\,(basal)}$ = 37 MPa; $\tau_{0\,(basal)}$ = 49 MPa; $\tau_{0\,(pyramidal)}$ = 197 MPa;
$\tau_{0\,(twin)}$ = 213 MPa; h_0=150 MPa; q=1.4

Hardening Rule:

$$\dot{\tau}_0^\alpha = \sum_{\beta}^{N} H^{\alpha\beta}\left|\dot{\gamma}_\beta\right| \qquad h^{\alpha\beta} = h_0^\beta(q + (1-q)\delta^{\alpha\beta})(1-\frac{\tau_0^\alpha}{\tau_{sat}})^a$$

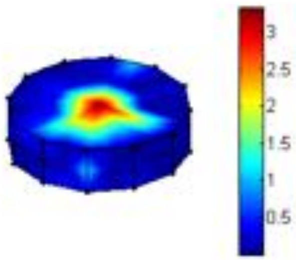


Initial Microstructure



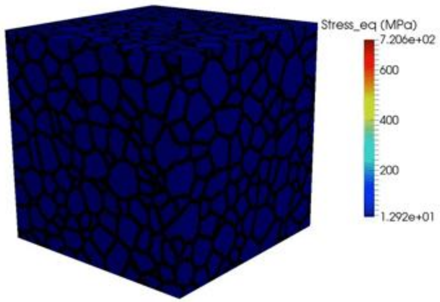
750 grains (600*600*600 μm)

Representative Texture ODF



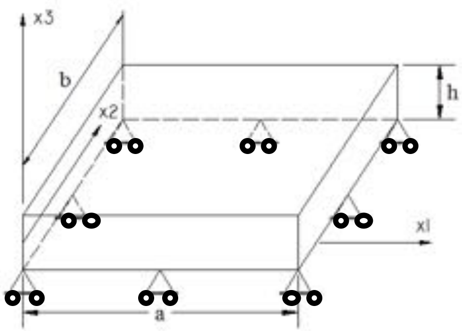
Weakly basal

CPFE simulation



(32*32*32 elements)=107811 DOF's
Computational cost ~ 96 CPU Hours
200 time steps (~1000 solve)

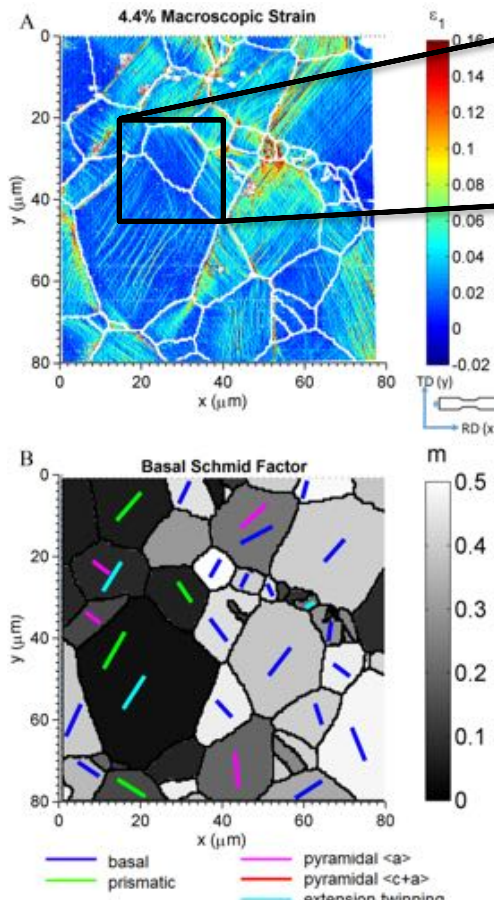
SEM-DIC validation of crystal plasticity predictions



- Digitize EBSD maps, extrude in 3D, perform PRISMS Crystal Plasticity simulation
- Displacement boundary conditions based on DIC

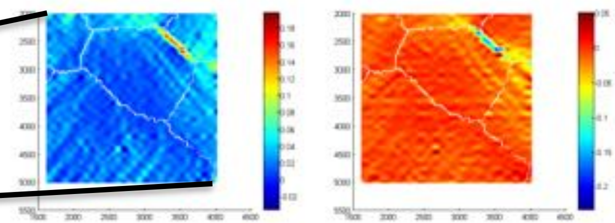
> Predicted slip activity and strain distribution compare well with experimental results

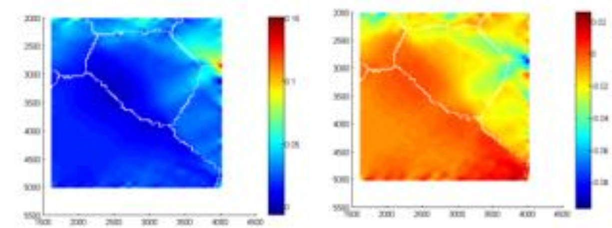
DIC



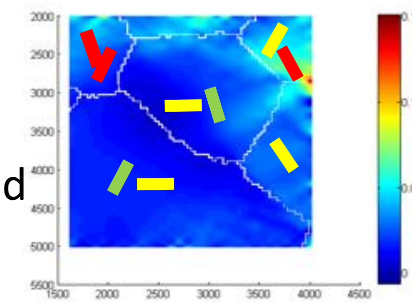
Measured Slip Activity

DIC





Predicted Slip Activity

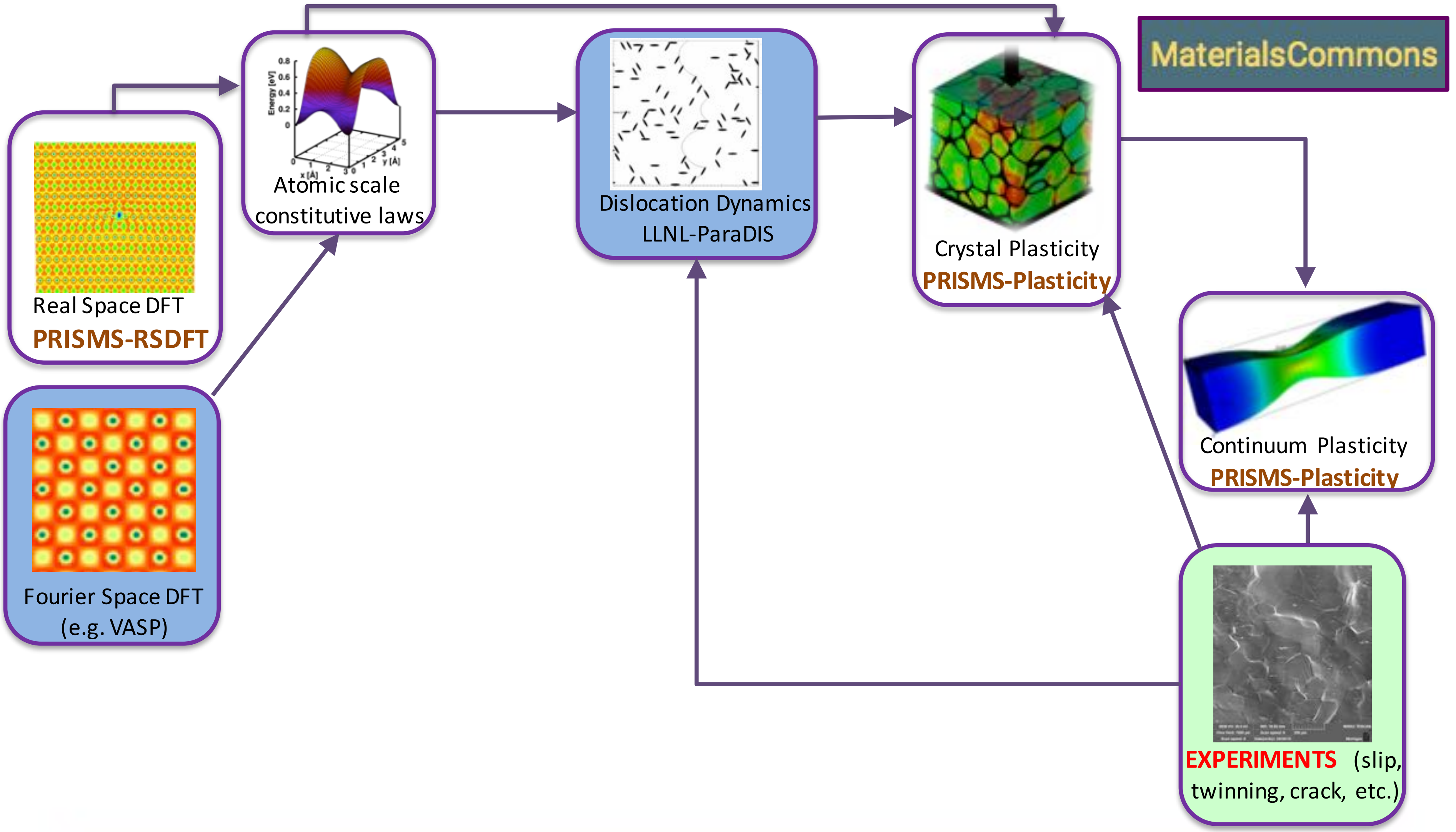


CPFEA Predictions

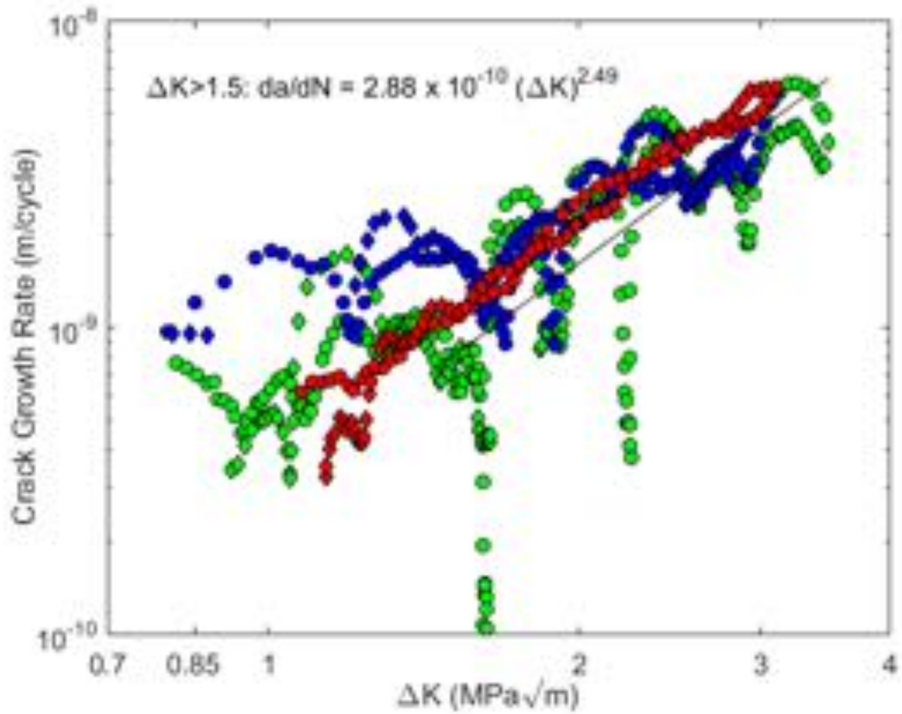
Basal
Prismatic
Pyramidal<a>

PRISMS Center Integrated Framework

Fatigue Behavior Use Case



Short Crack Growth Behavior – Microstructural Effects



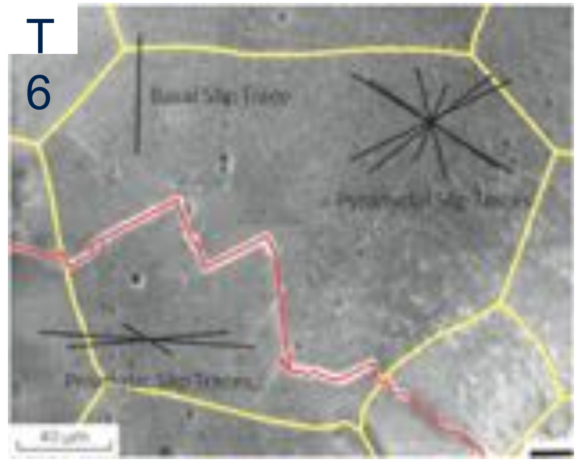
No significant influence of microstructure on average SFCG behavior

T5: Local microstructure had little effect on crack growth rates.

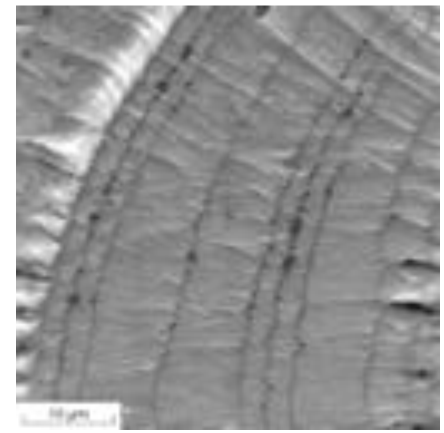
Underaged and T6: Strongly affected by local microstructure – growth rate curves show crack retardation and arrests.

Crack path analysis indicates a mix of cracking modes

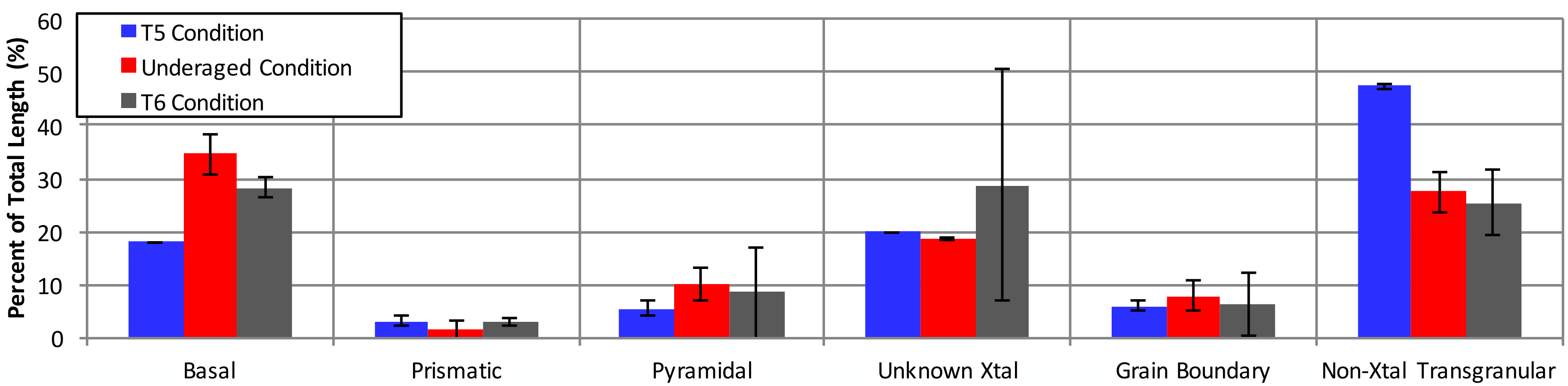
- High percentages of cracks along basal planes and non-crystallographic transgranular fracture
- Observation of "Micro-beach" marks allows quantification of local crack growth rates for use in FCG simulations



Crack Path Analysis

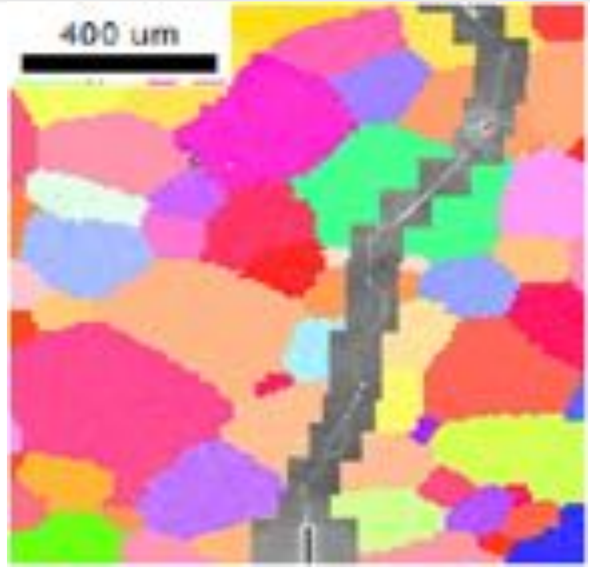


Micro-beach marks

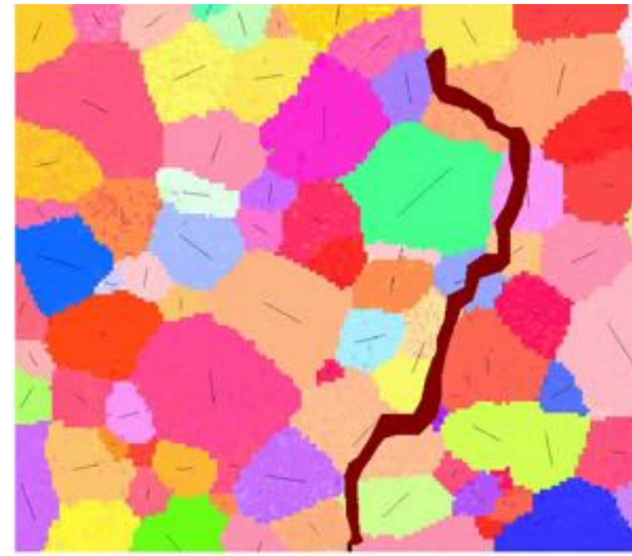


PRISMS-CPFE Fatigue Crack Path Prediction

- Crack paths simulated using PRISMS CE +VMM with cohesive traction law given by slip system CRSS and GB cohesive strength.
- The crack criteria is combination of CRSS and slip trace angle with max. principal stress plane.



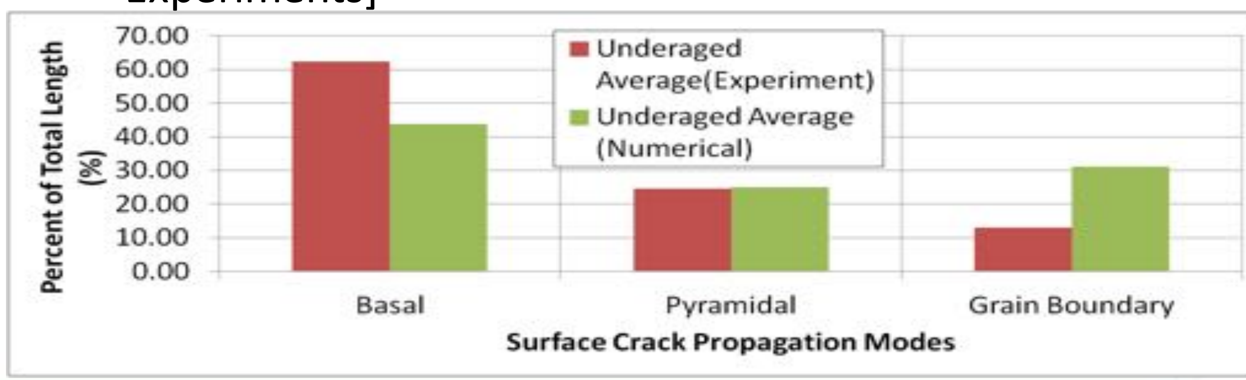
SEM crack path image on EBSD image [PRISMS Experiments]



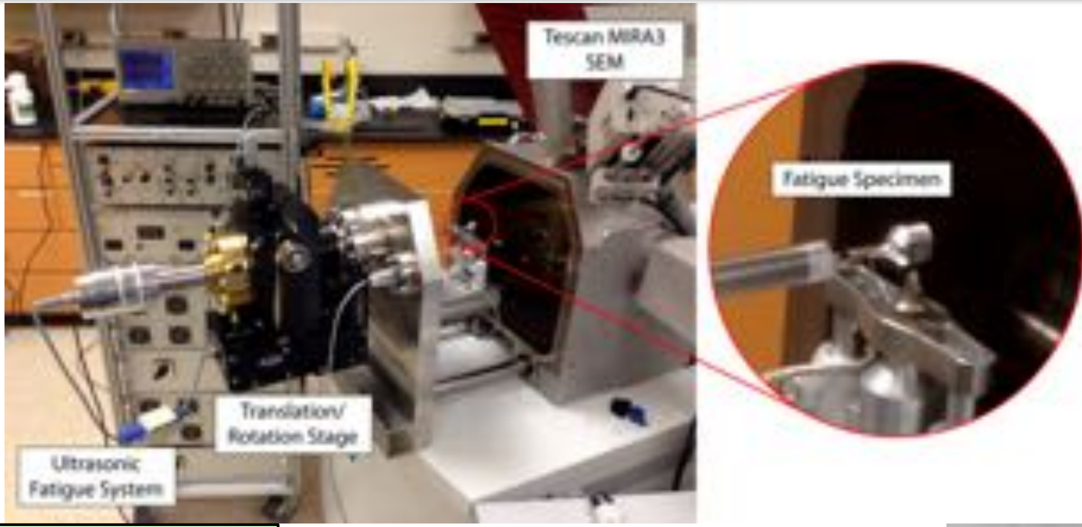
Numerical crack path (Basal trace of each grains are shown)

Preliminary results are directionally correct

Mode	τ_0^α (MPa)	h_0 (MPa)	τ_{sat} (MPa)
Basal <a>	20	30	56
Pyram <a>	54.4	39	168

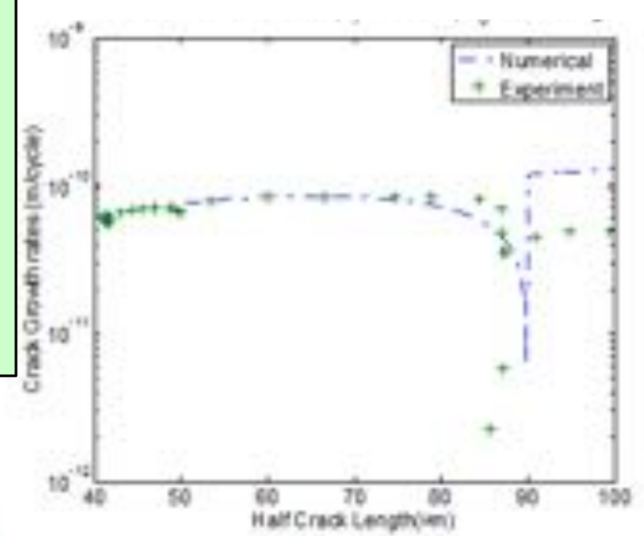


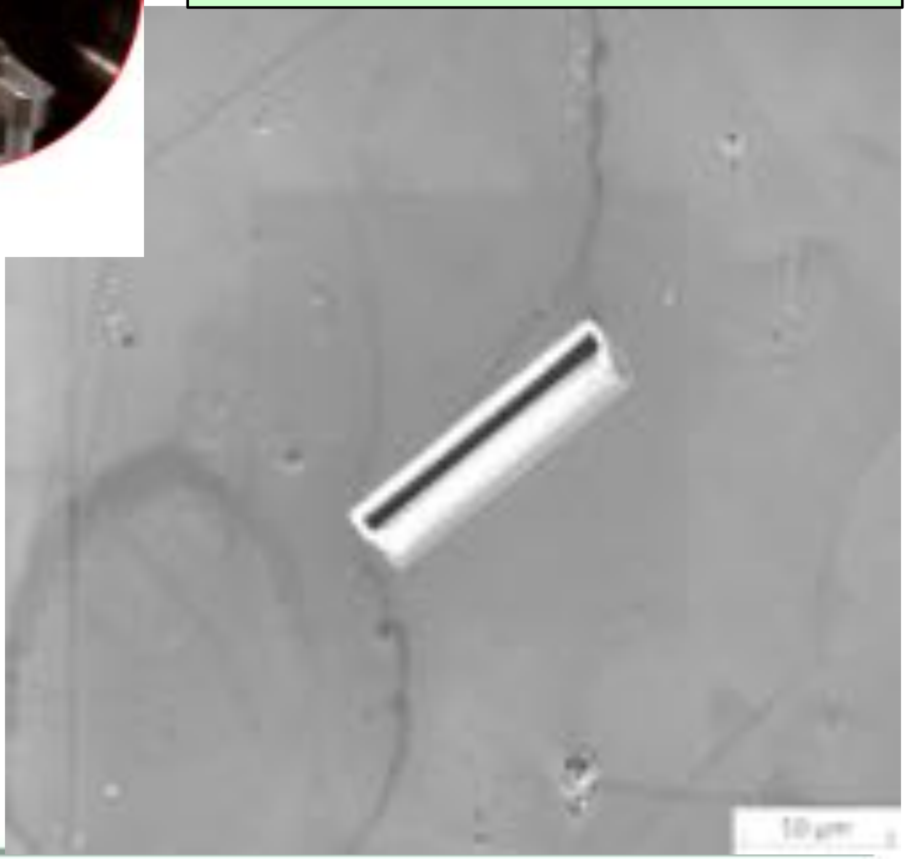
UFSEM: *in situ* ultrasonic fatigue short crack growth in SEM



- Use EBSD maps and FIB to select neighborhoods
- Grain boundaries cause reorientation of crack path

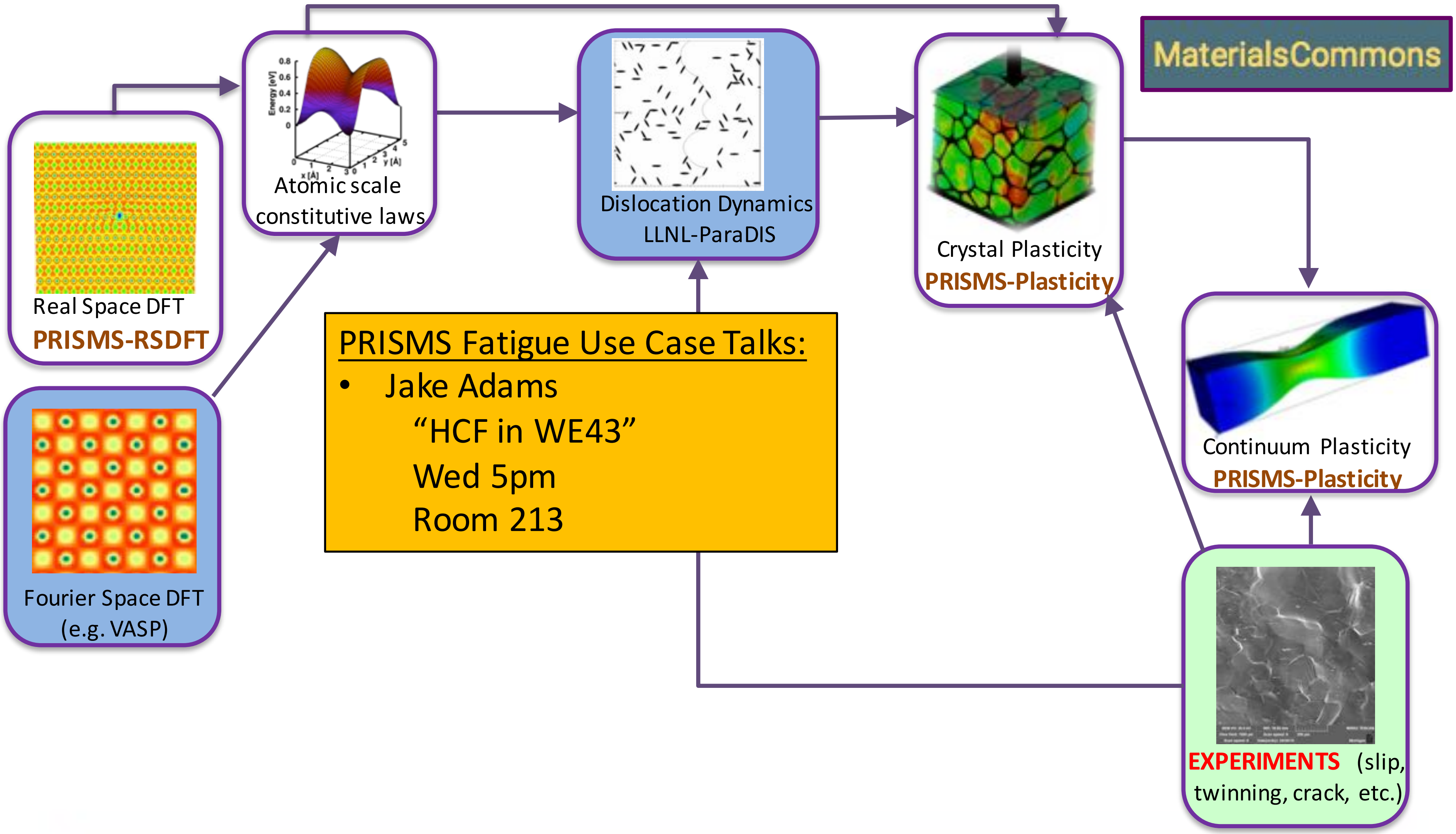
Comparison with simulations to predict local crack growth retardation





PRISMS Center Integrated Framework

Fatigue Behavior Use Case



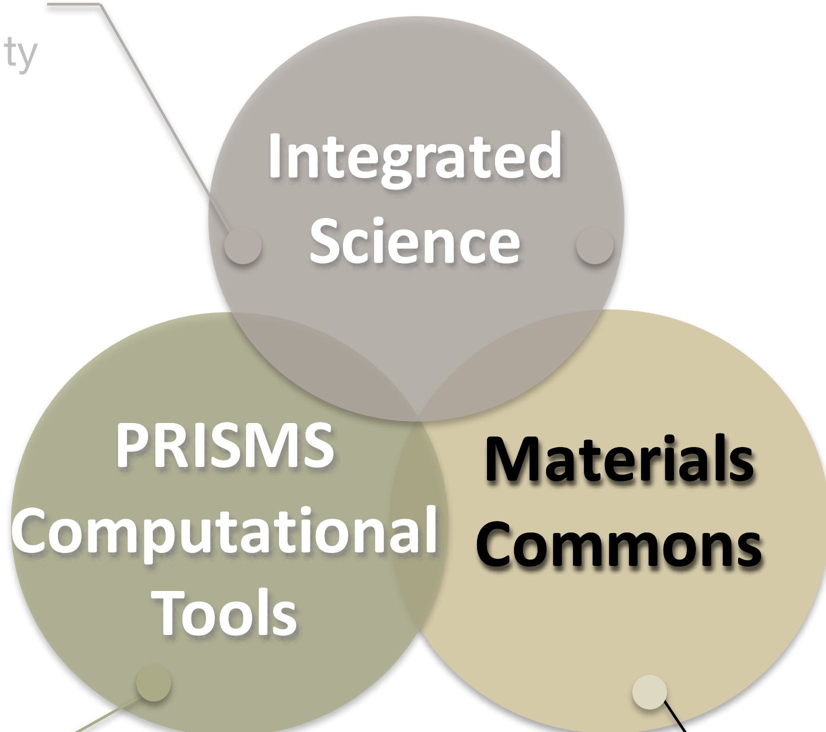
<u>PRISMS Fatigue Use Case Talks:</u>

- Jake Adams
  "HCF in WE43"
  Wed 5pm
  Room 213

PRISMS Center - Vision

Enable accelerated predictive materials science.

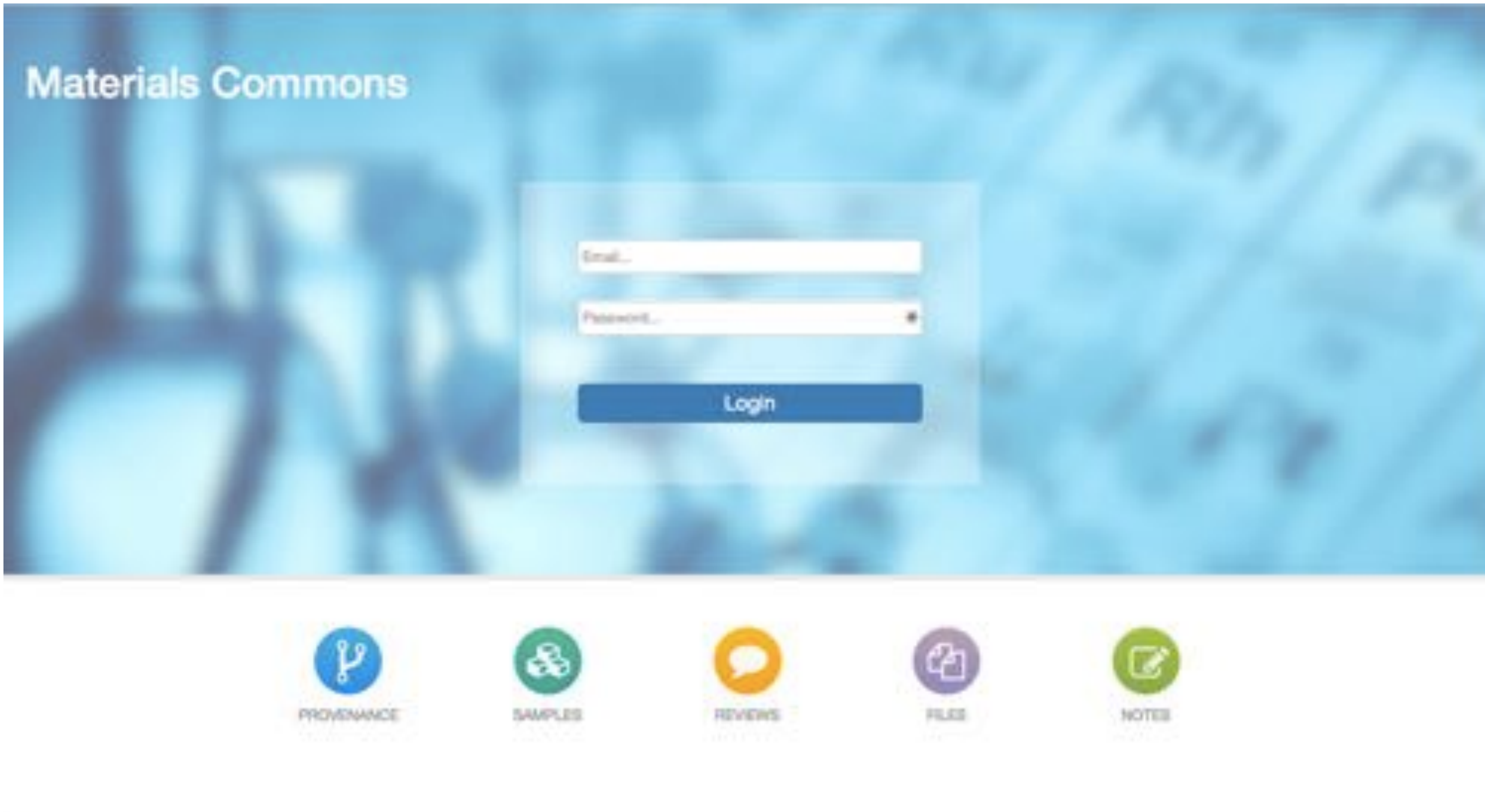
- Linking Experiments & Simulations
- Collaborative Community
- Advanced Quantitative Experiments



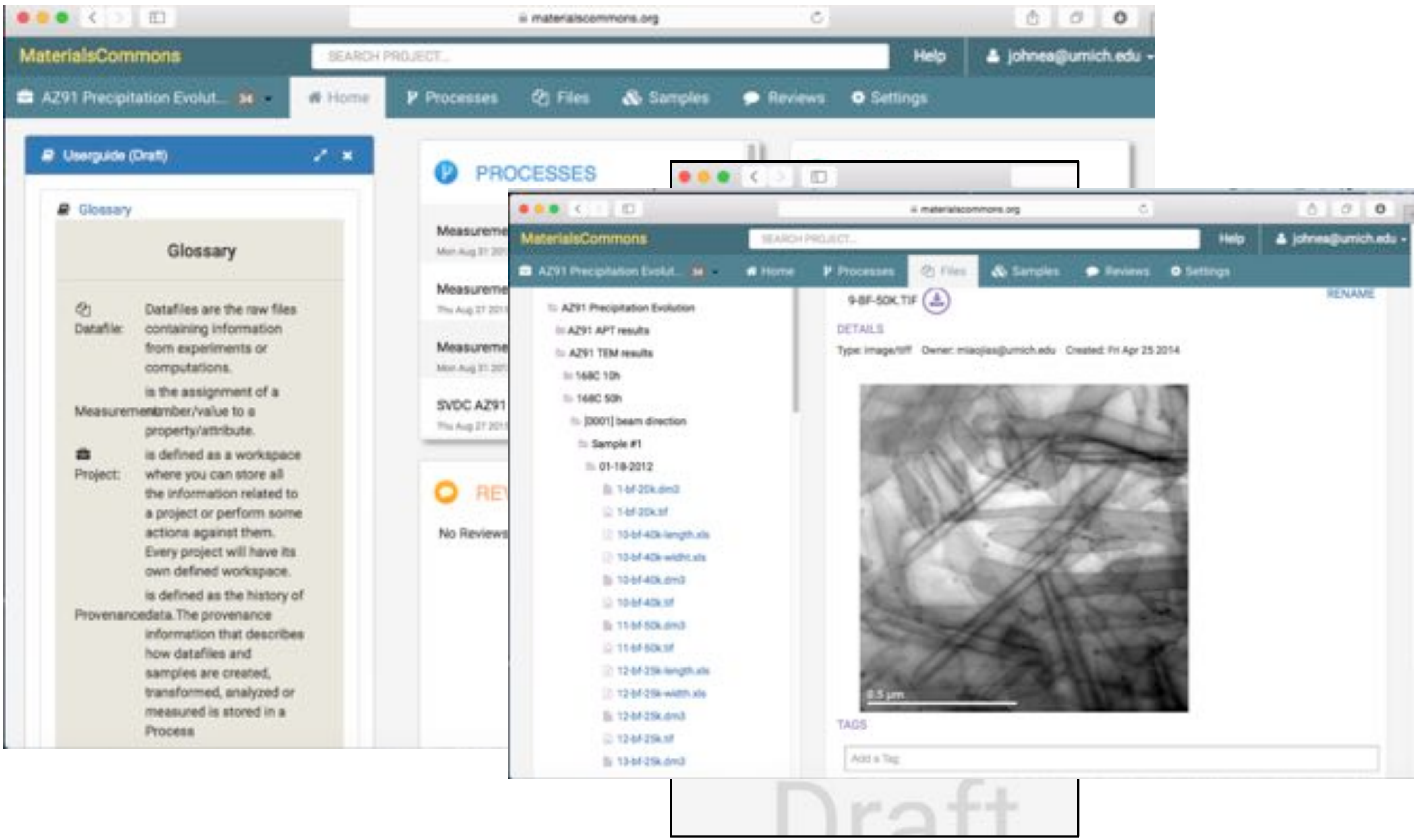
- Open Source
- Integrated Hierarchical Multi-Scale
- Computationally Efficient
- Extensible
- Advanced Methods

- Collaboration & Community
- Experimental & Simulation Information
- Seamless, Continuous Workflow
- Provenance Tracking
- Accelerate model building and validation

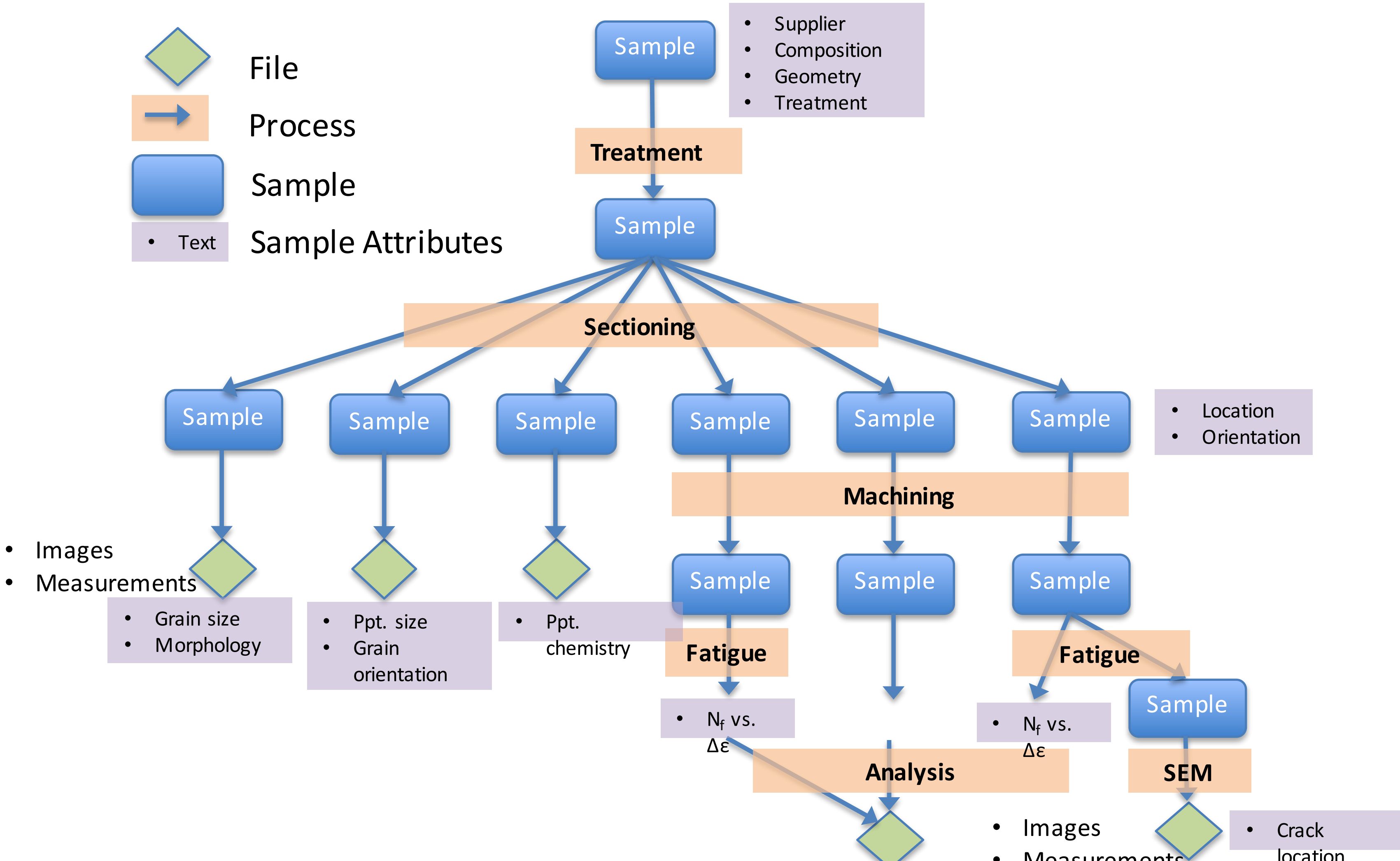
The Materials Commons
A unique collaborative environment



The Materials Commons User Interface



The Materials Commons Data Model



The Materials Commons
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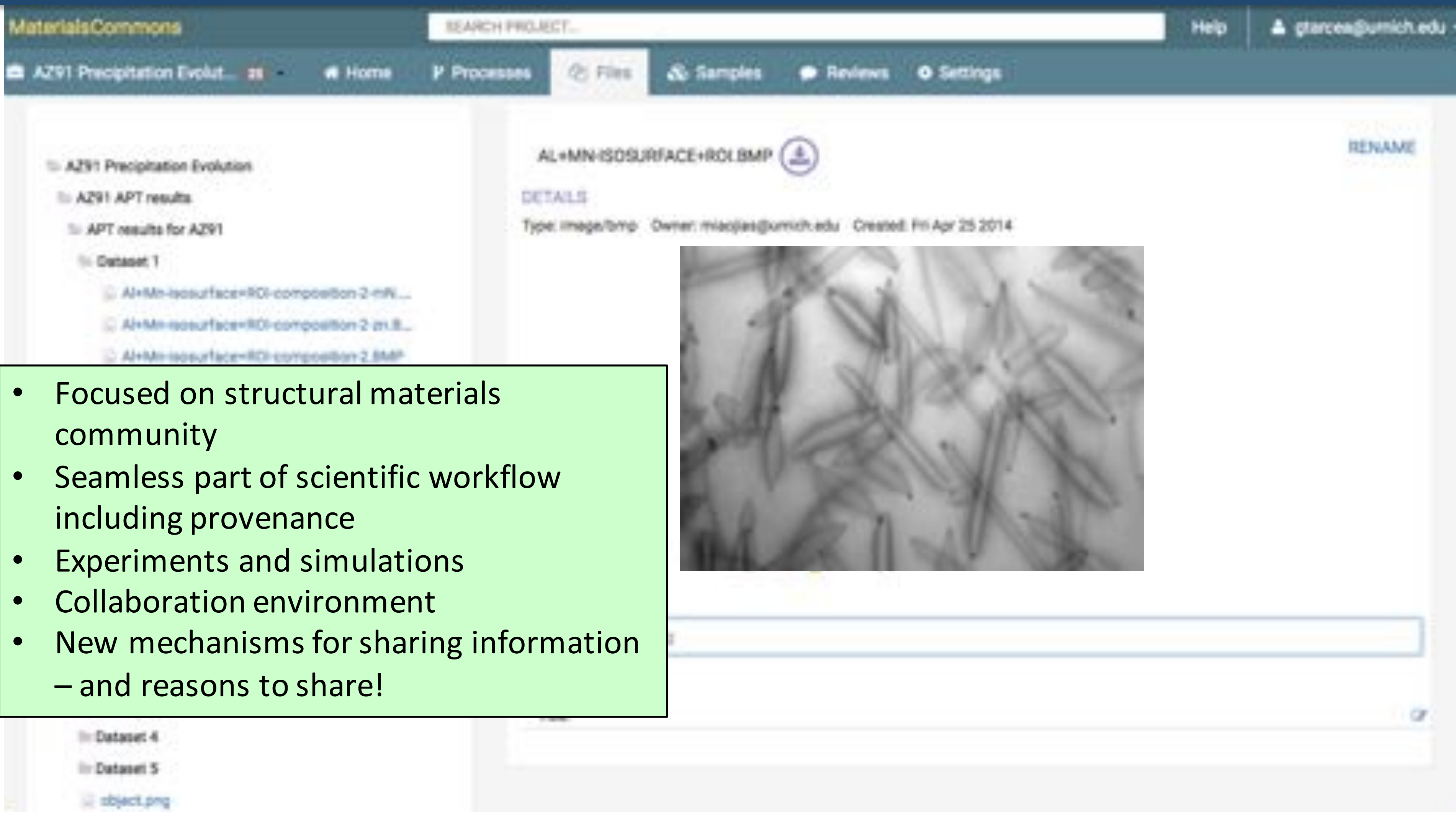
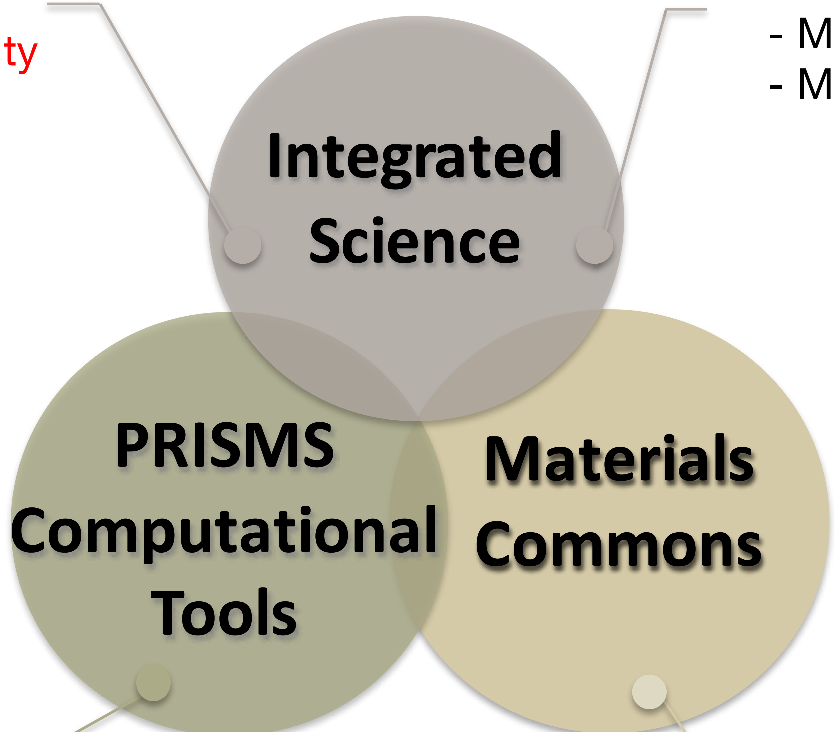


- Focused on structural materials community
- Seamless part of scientific workflow including provenance
- Experiments and simulations
- Collaboration environment
- New mechanisms for sharing information – and reasons to share!

PRISMS Center – Collaborative Community!

- Linking Experiments & Simulations
- Collaborative Community
- Advanced Quantitative Experiments

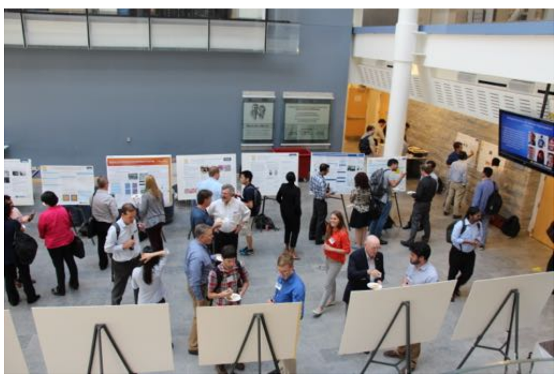
- Use Cases (Magnesium Alloys)
  - Microstructural Evolution
  - Mechanical Behavior



- Open Source
- Integrated Hierarchical Multi-Scale
- Computationally Efficient
- Extensible
- Advanced Methods

- Collaboration & Community
- Experimental & Simulation Information
- Seamless, Continuous
- Workflow
- Provenance Tracking
- Accelerate model building and validation

PRISMS Center Annual Workshop
Building the PRISMS Community



Next workshop: August 16-19, 2016

Website: prisms-center.org

The PRISMS Center
Summary

- The PRISMS Center is focused on providing new computational tools and a framework for the structural metals community and demonstrating on advanced Mg alloys.

- Working together we are making great progress and generating:
  - Exciting new science!
  - Software: Available now on GitHub
  - Information via Materials Commons: Stay Tuned

- We encourage you to use and co-develop these tools and join us at our next workshop Aug 16-19, 2016.

Thanks!

- Website: prisms-center.org
- Email: johnea@umich.edu

Thanks!

Website: prisms-center.org

My email: johnea@umich.edu