LA-UR- 11-06618

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Title: LDRD DR APPRAISAL
PROJECT OVERVIEW: Innovative and validated submicron to meso-scale modeling of the evolution of interface structure and properties under extreme strains

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Team: K. Barros, C.Bronkhorst, J. Carpenter, H. Chu, R. Dickerson, W. Han, B. Hansen, K. Kang, T. Lookman, N.A. Mara, J. Mayeur, R. McCabe, H. Mourad, S.Sintay, S. Vogel, J. Wang, S. Zheng

Intended for: DDI Worshop
Los Alamos, New Mexico USA

November 14-16, 2011

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Abstract
Irene Beyerlein

The goal of this work is to determine the class of bi-metal interfaces that will create composite materials with extraordinary failure resistance under extreme mechanical strains. The evolution of bi-metal interface properties were studied in Cu-Nb multi-layered composites synthesized using a severe plastic deformation (SPD) technique called accumulative roll bonding (ARB). EBSD and TEM analyses strongly suggest that most interfaces in nanolayered ARB material are {112}fcc//{112}bcc with a Kurdjumov-Sachs orientation relationship. Atomistic simulation, dislocation theory, and polycrystal plasticity modeling are employed to determine the structural aspects that make this interface stable under SPD and its role in governing slip and twinning activity.

LDRD DR Appraisal
Nov. 15, 2012

Project Overview: Innovative and validated submicron to meso-scale modeling of the evolution of interface structure and properties under extreme strains

Irene J. Beyerlein (PI)

DR TEAM

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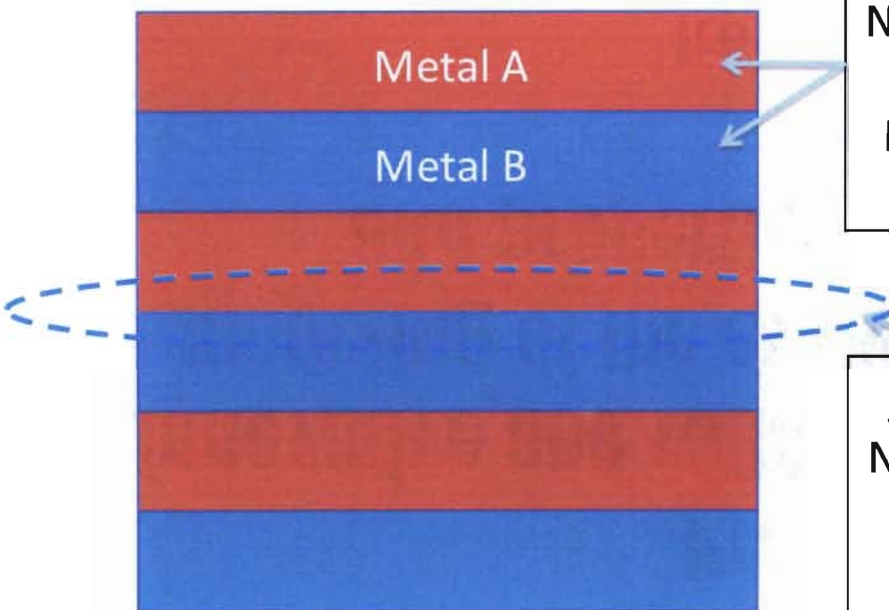
Interface-driven material behavior

Constituent-dominated behavior → **Interface-dominated behavior**



<u>Phases</u>
Nucleation
Storage
Recovery
Blocking

<u>Interface</u>
Nucleation
Storage
Recovery
Blocking

Low density of interfaces

High density of interfaces

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Hypothesis and Goal

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1-2 microns

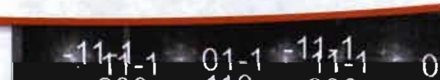
Bulk Dislocation density

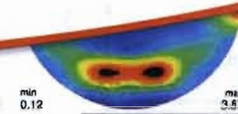
1 micron to 500 nm

Substructure

500 nm to 50 nm

MICRON GAP





Interface Dominance

To pioneer an innovative Meso (nm to micron) Multi-Scale (M^2S) model for synthesizing interface-dominant materials with the interfacial properties we want

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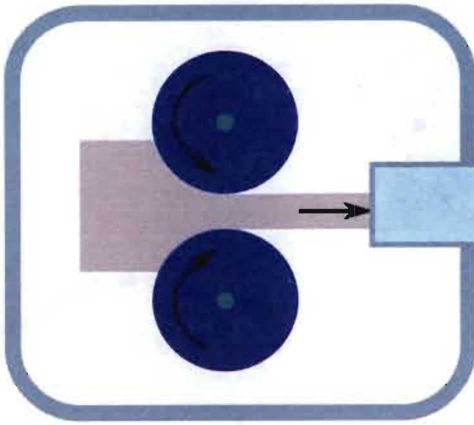
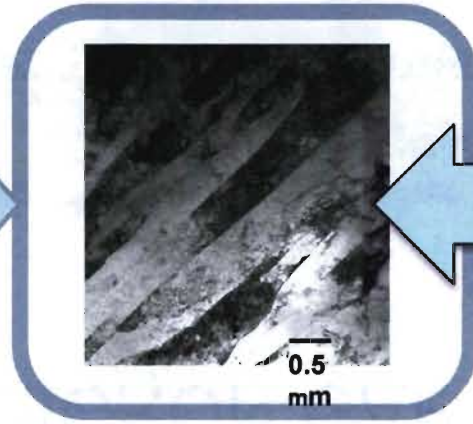
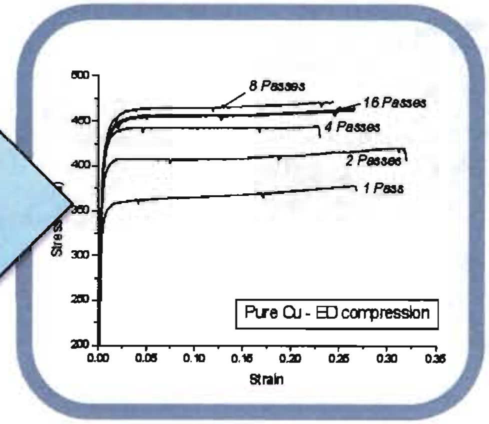
Process Aware Performance







Fabrication Process

Microstructure

Property

Performance

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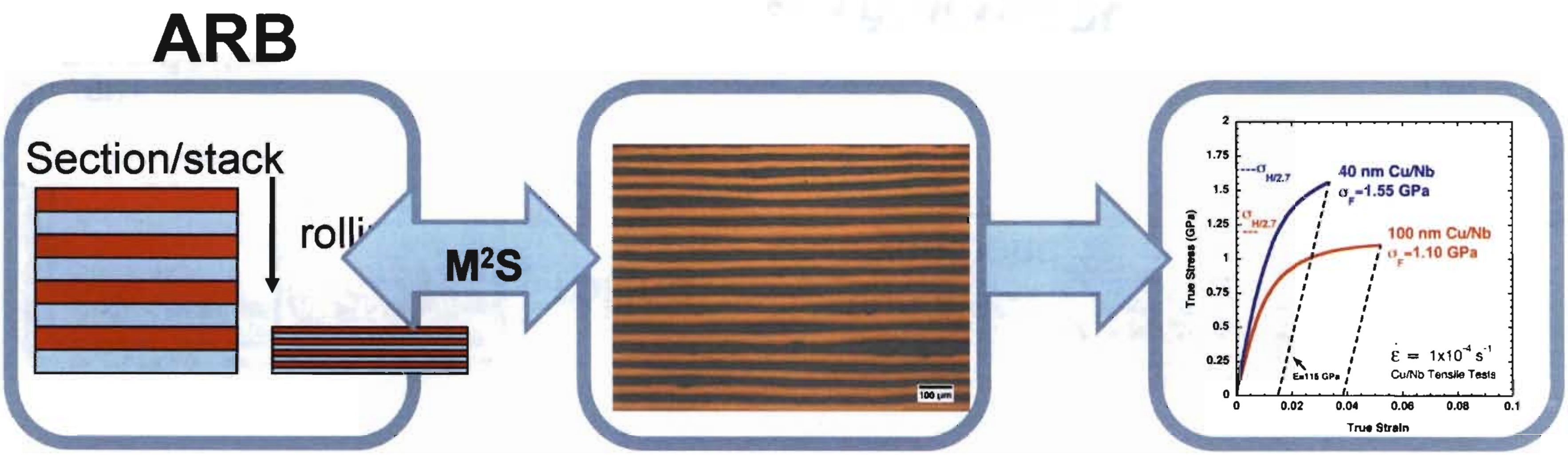
Process Aware Performance for interface-dominated materials



Fabrication Process

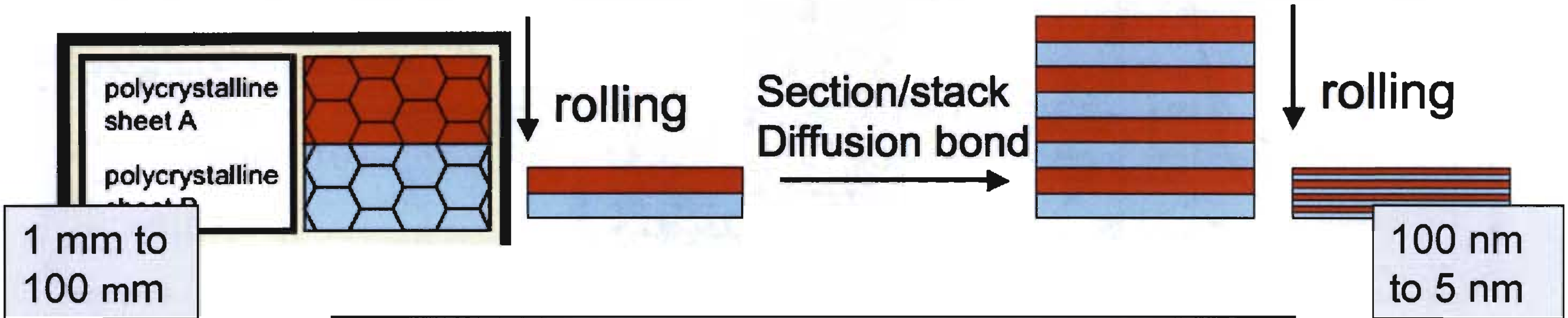
Interface-dominated structure

Interface-dominated property

Model method for synthesizing interface dominant materials

Accumulative Roll Bonding (ARB):

Achieving extreme strains beyond those possible with conventional rolling



ARB serves several purposes:

- *Synthesis of bulk layered material*
- *Controllable strain*
- *Controllable layer thickness*
- *Model architecture*
- *One primary interface plane*
- *Relevant thermomechanical process*

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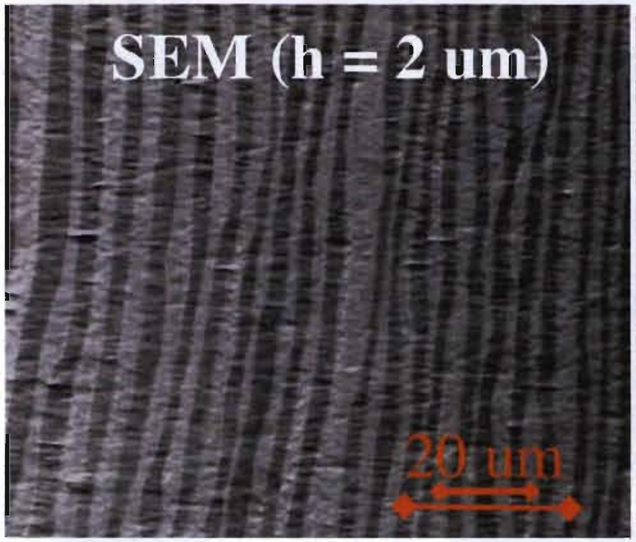
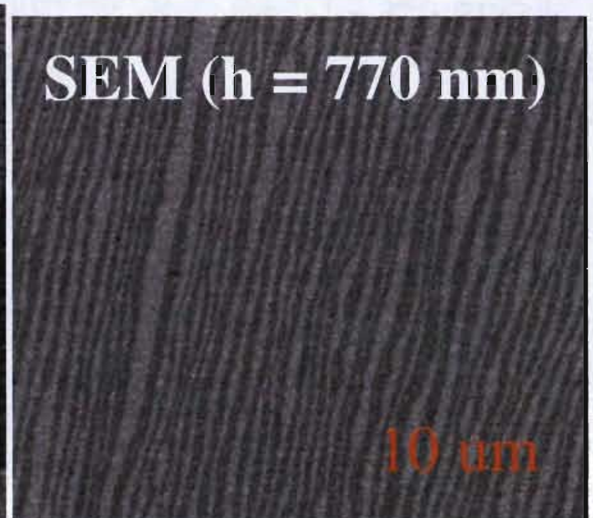
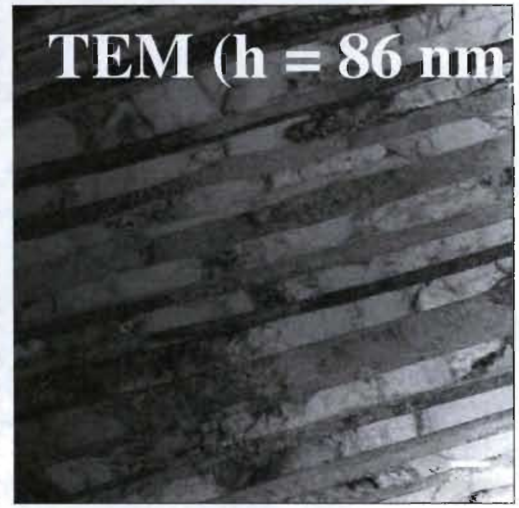
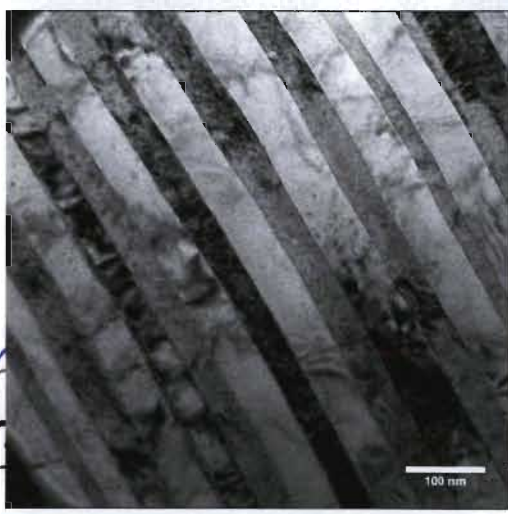
Cu/Nb ARB synthesis across length scales



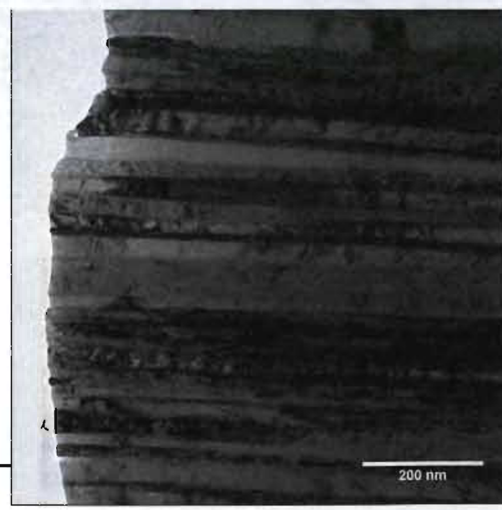




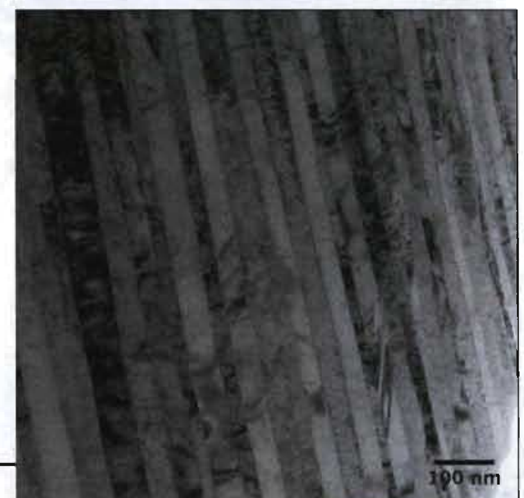
TEM (h = 48 nm)



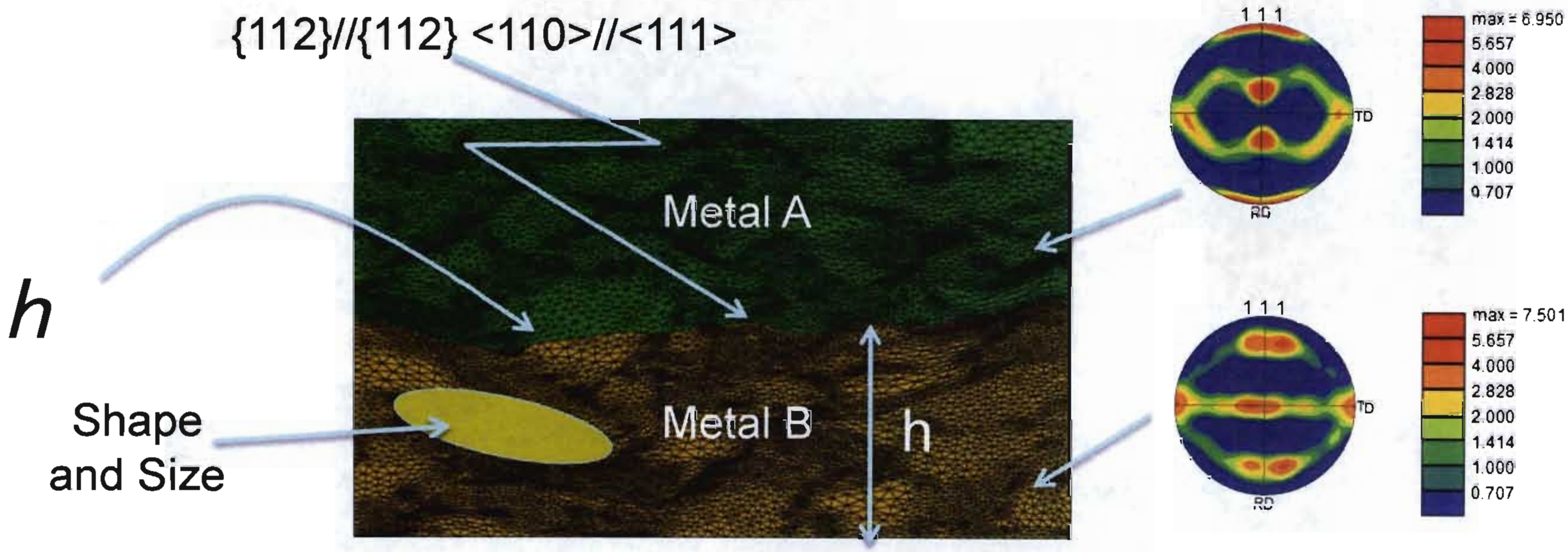
TEM (h = 18 nm)



TEM (h = 9 nm)



Deliverables



OUTPUT

- Texture evolution,
- Lattice dislocation density evolution
- Interfacial dislocation density evolution
- Interface crystallography
- Layer thickness
- Grain shape
- Internal stresses and strains

VALIDATION

- Texture evolution,
- Dislocation density in phases
- Defects in interface
- Interface crystallography
- Layer thickness
- Hardness
- Directional flow stress vs strain curves

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The M^2S model

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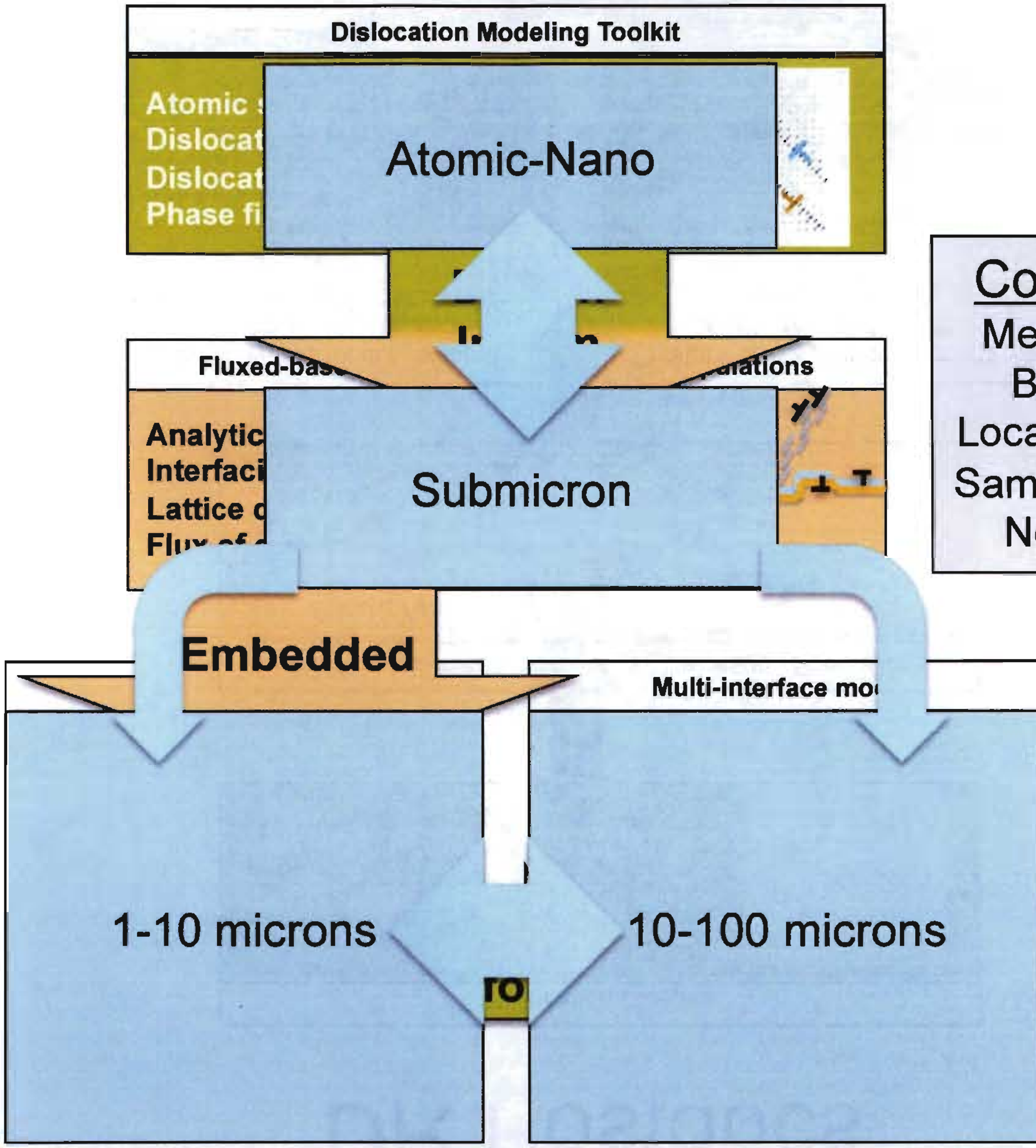


Common features

Metal Crystallography

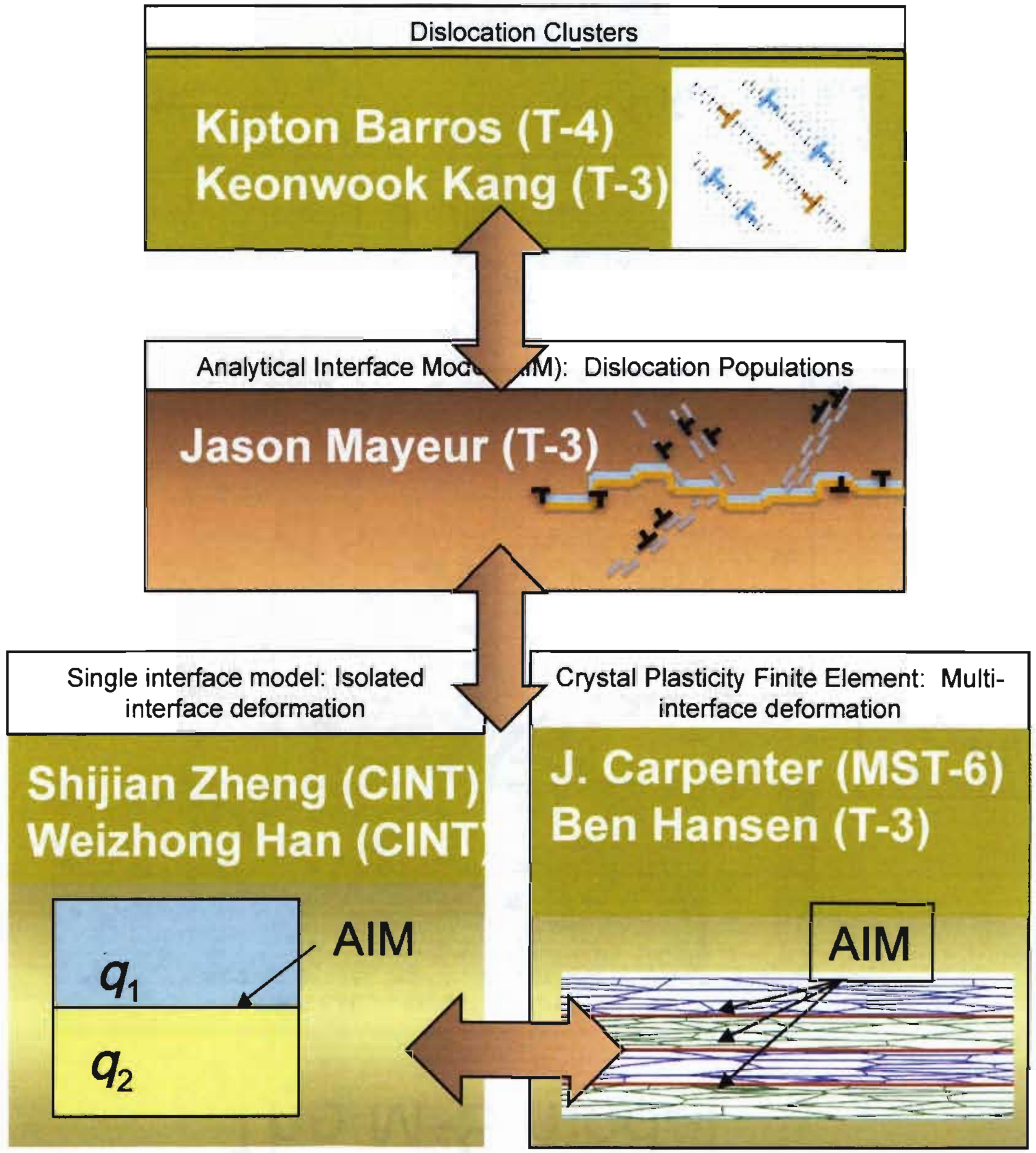
Bi-metal interfaces

Local Stress and Energy

Same defect populations

No homogenization

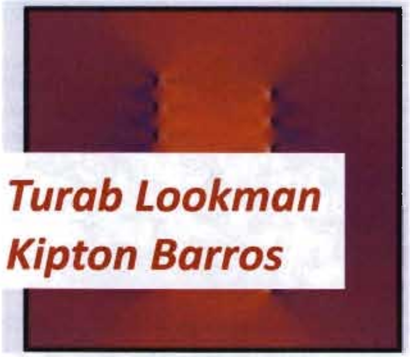
DR Postdocs



Dislocation Clusters
Kipton Barros (T-4)
Keonwook Kang (T-3)
Analytical Interface Mod…IM): Dislocation Populations
Jason Mayeur (T-3)
Single interface model: Isolated interface deformation
Crystal Plasticity Finite Element: Multi-interface deformation
Shijian Zheng (CINT)
Weizhong Han (CINT)
J. Carpenter (MST-6)
Ben Hansen (T-3)
AIM
q_1
q_2
AIM

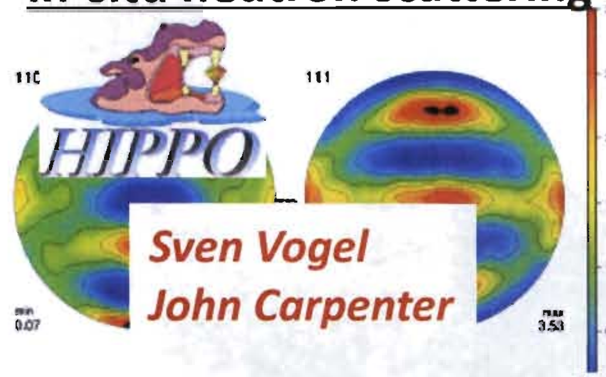
DR team personnel

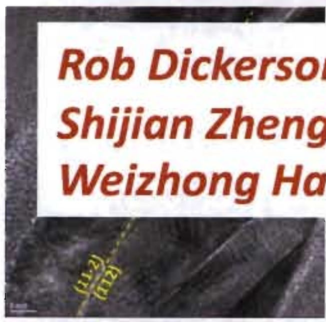
Phase field modeling



Nanomechanical Testing

In-situ neutron scattering

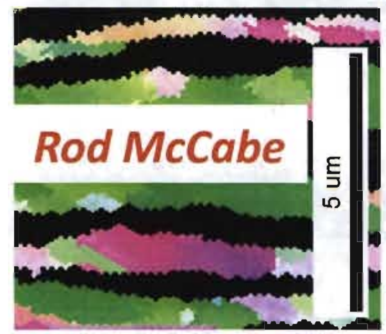




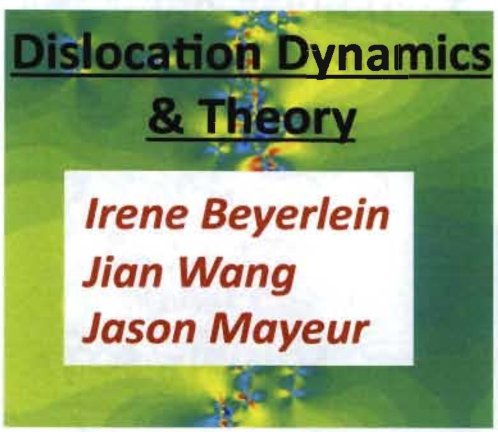
TEM
HR-TEM
In-situ TEM

Synthesis

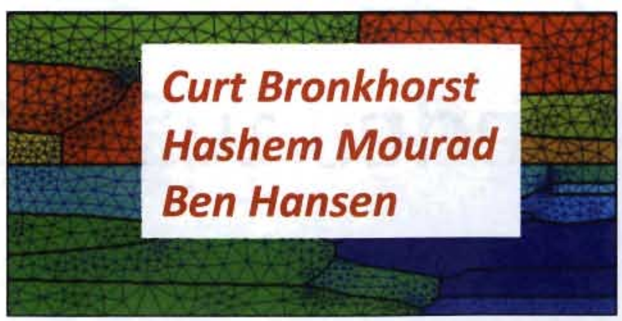
EBSD



Dislocation Dynamics & Theory



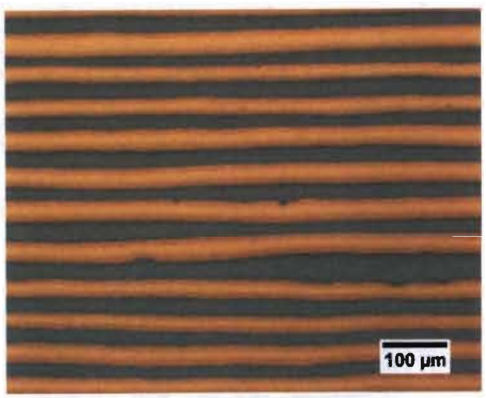
Crystal Plasticity Finite Element



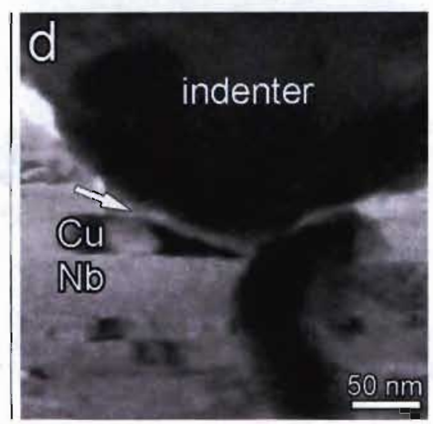
Microstructure Builder

Highlight capabilities

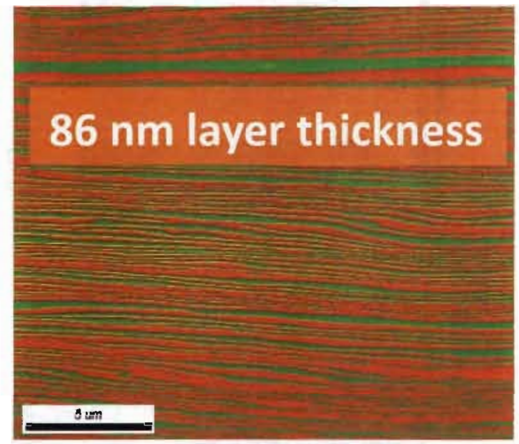
Bulk synthesis of two-phase interface dominant composites
Mara, LeDonne, Nizolek, Carpenter
Featured: Mara's talk



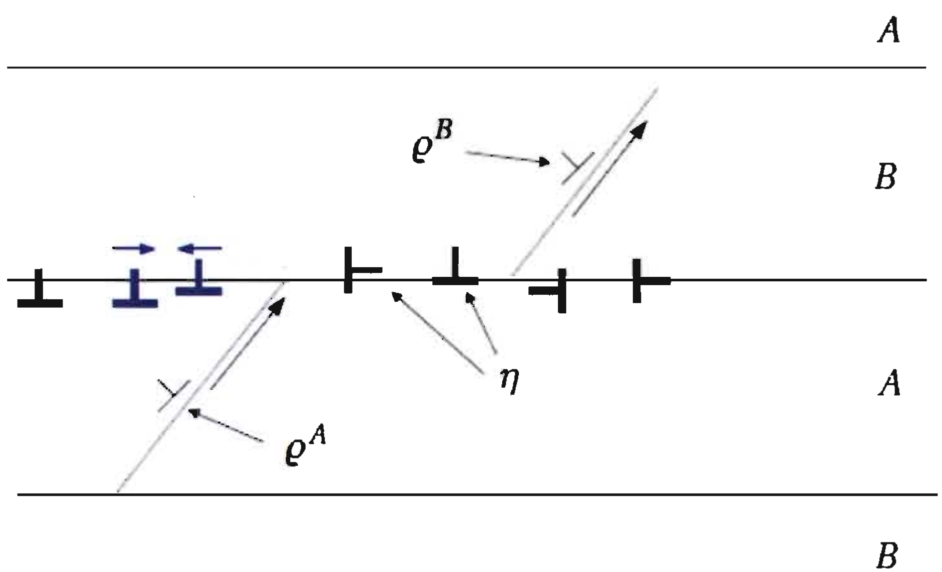
***In-situ* nano-indentation of two-phase metals**
Shijian Zheng
R. Dickerson
Featured: Zheng's poster



EBSD at fine length scales
Rod McCabe
Featured: McCabe's poster



Analytical interface model: providing interface physics to the meso-scale



Rate equations for dislocation density evolution for a bi-metal composite

- Nucleation
- Annihilation
- Transmission
- Reflection
- Absorption

Analytical interface model: a fluxed-based approach

$$\dot{\rho} = \sum \Phi_r - \frac{1}{V} \oint_{\partial V} f \cdot a \, dA$$

Roters et al. 2010

Flux based expression for the evolution of dislocation densities

Formulation for two-phase composite

$$\frac{1}{V} \int_{\partial V} \boldsymbol{f} \cdot \mathbf{a} \, \mathrm{dA} \approx \frac{1}{V} \sum_{n} \left(j_{\mathrm{tran}}^{(n)} + j_{\mathrm{abs}}^{(n)} \right) \mathrm{A}^{(n)}$$

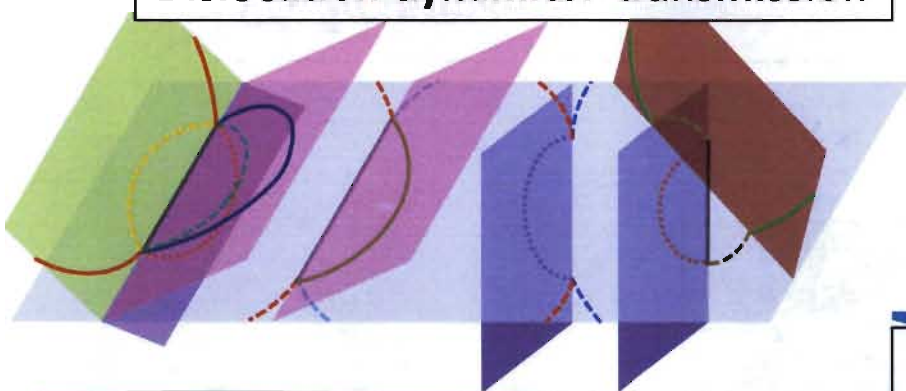
AIM: connection with interface physics

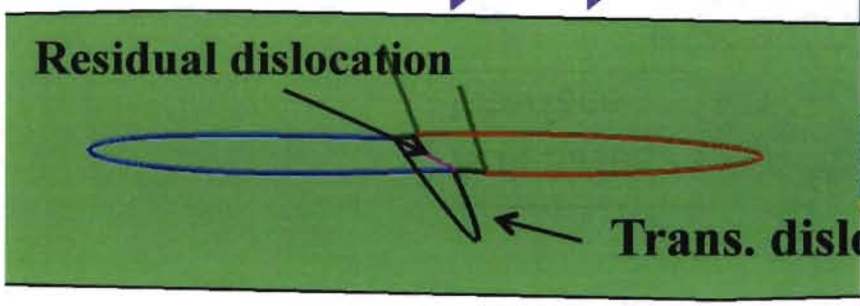
$$j_{\mathrm{tran}} = \sum_{\alpha} \sum_{\beta} \chi^{(\alpha,\beta)} \tilde{\boldsymbol{f}}^{(\alpha)} \cdot \mathbf{a}$$

$$\chi^{(\alpha,\beta)} = m'' h(\tau, \eta)$$

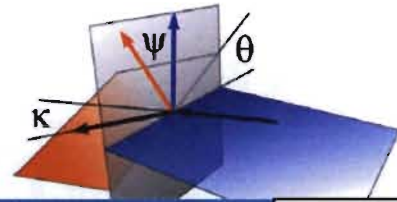
Analytical interface model: informed by lower-length scale physics

Dislocation dynamics: transmission



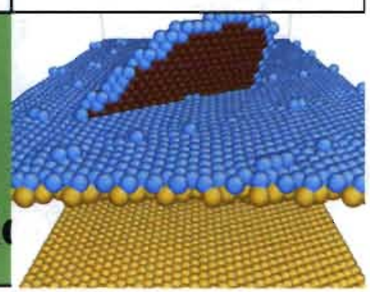


Crystal plasticity: transmission; residuals

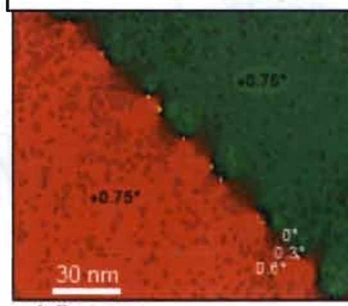


Phase field: Annihilation

MD: Nucleation

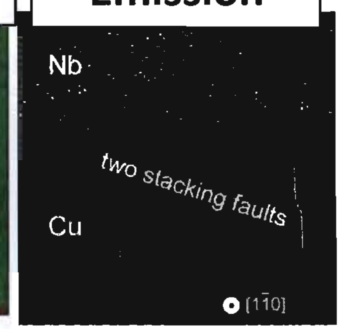


Rotation Map



rotation map

Emission



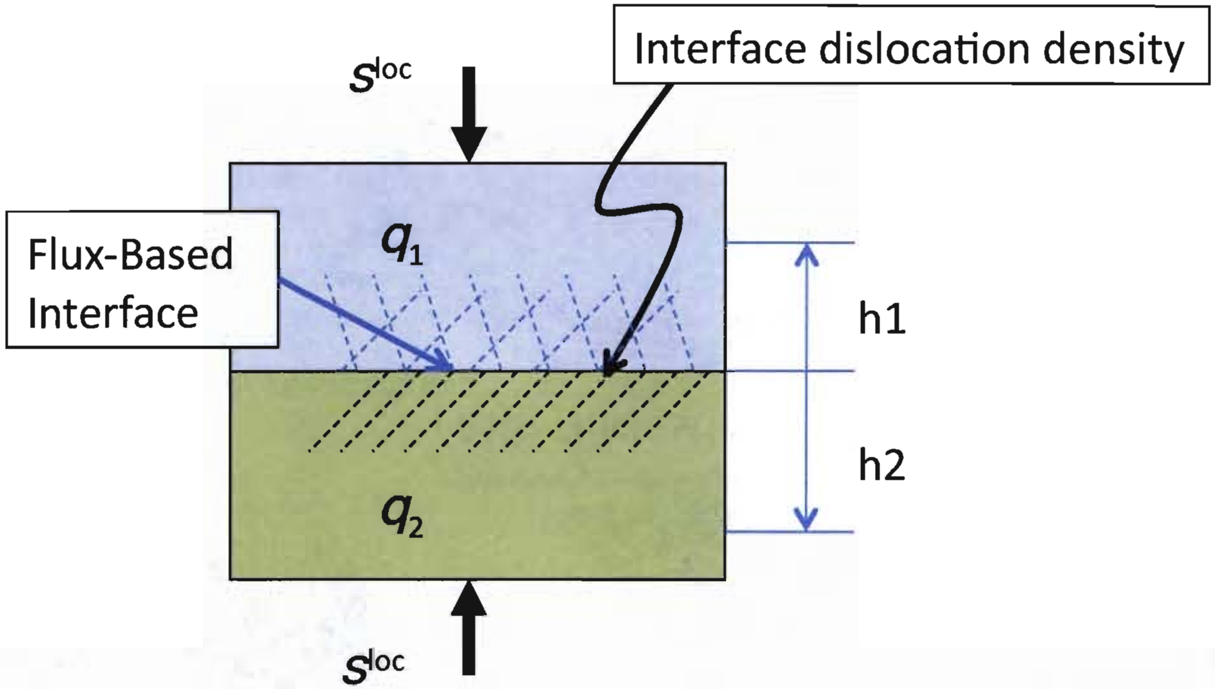
Residual dislocations left from transmissions across interface

Interface dislocations annihilated within the interface

$$\dot{\eta}^E = \underbrace{j_{\text{tran}}}_{\text{Residual}} - \phi^{EA}_{\text{rxn}} - \phi^{E}_{\text{ann}}$$

Emission from the interface

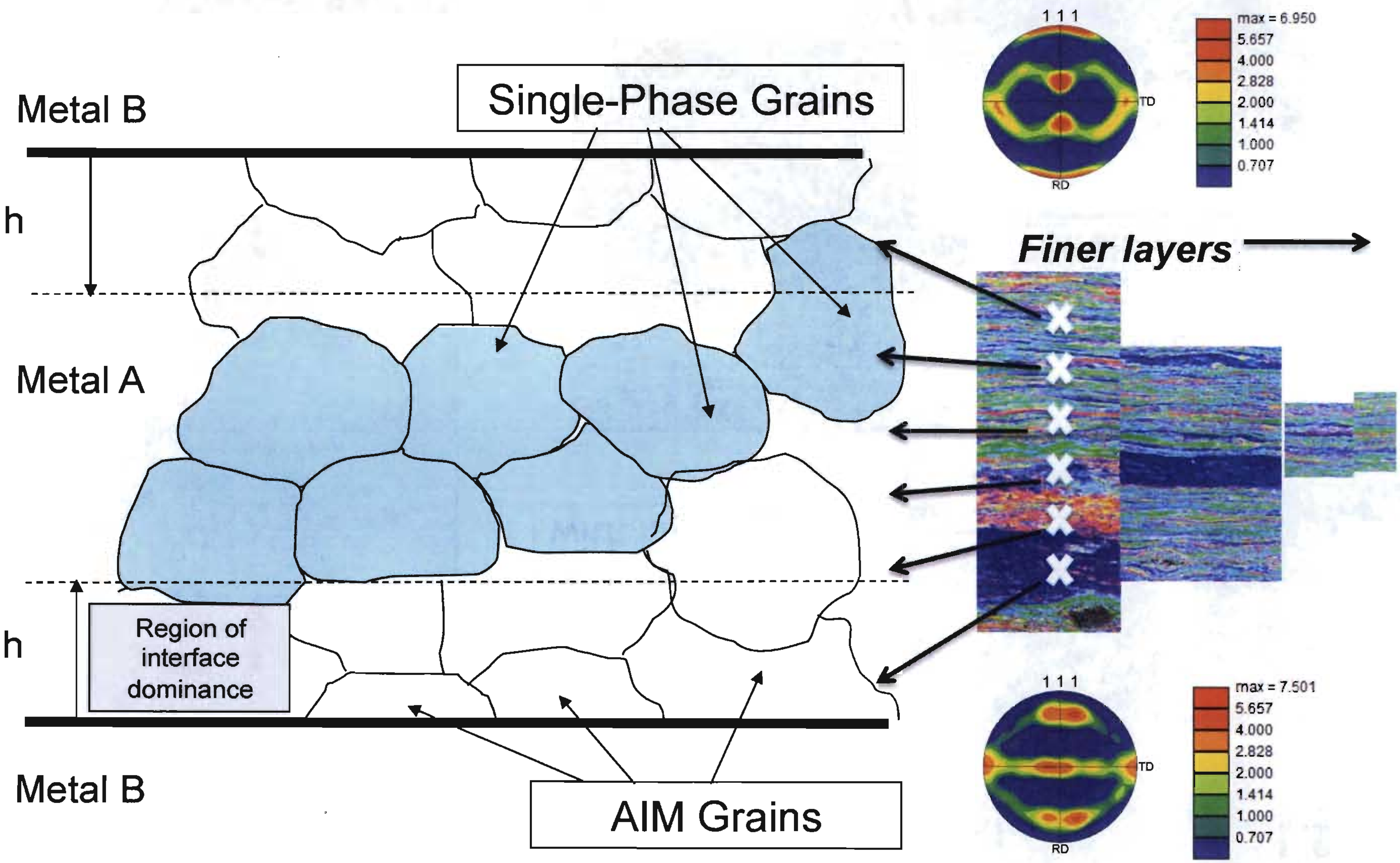
Single Interface Model



Predictions:

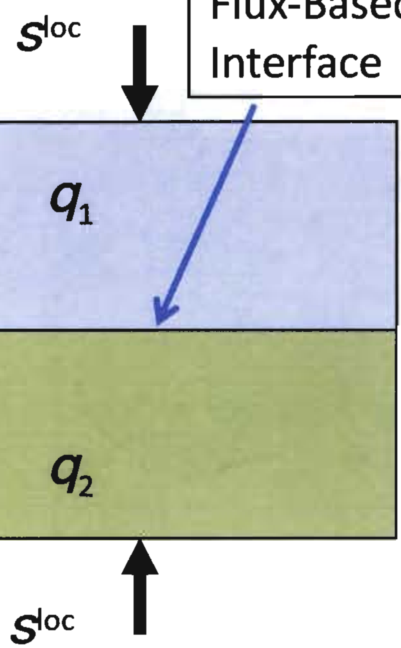
- How flux-controlling interfaces affect slip activity and reorientation
- Interface affected region (internal stress, dislocation density)
- Interfacial density

Interface-affected grains in the multiple interface model

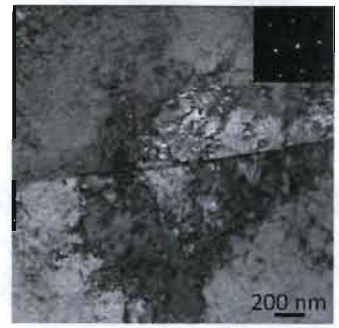


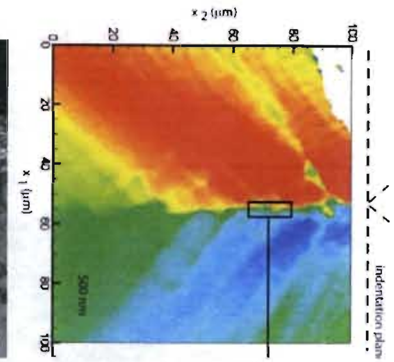
Single Interface Model

Flux-Based Interface

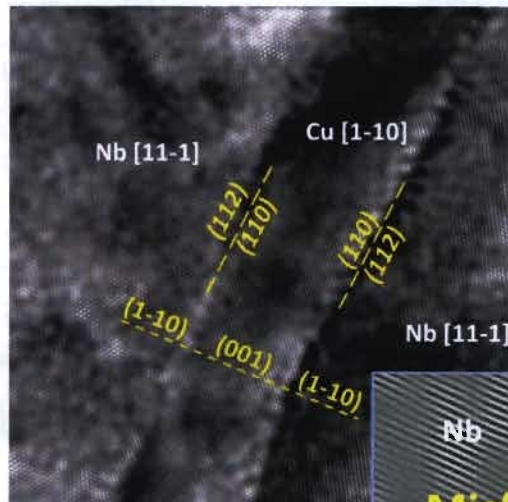


Bulk dislocation density, rotations, & strain gradients with layer h

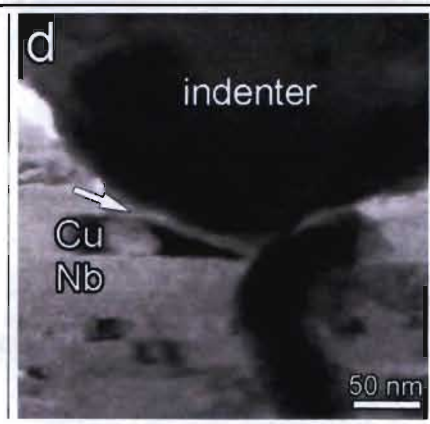




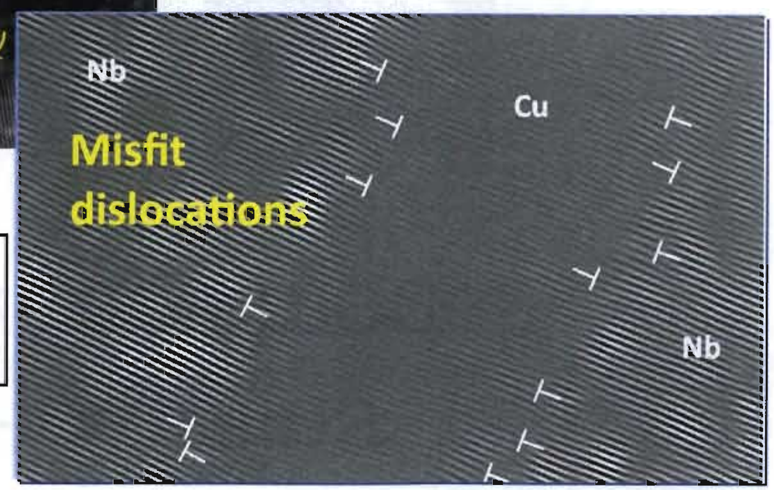
Interface crystallography as a function of strain and layer h



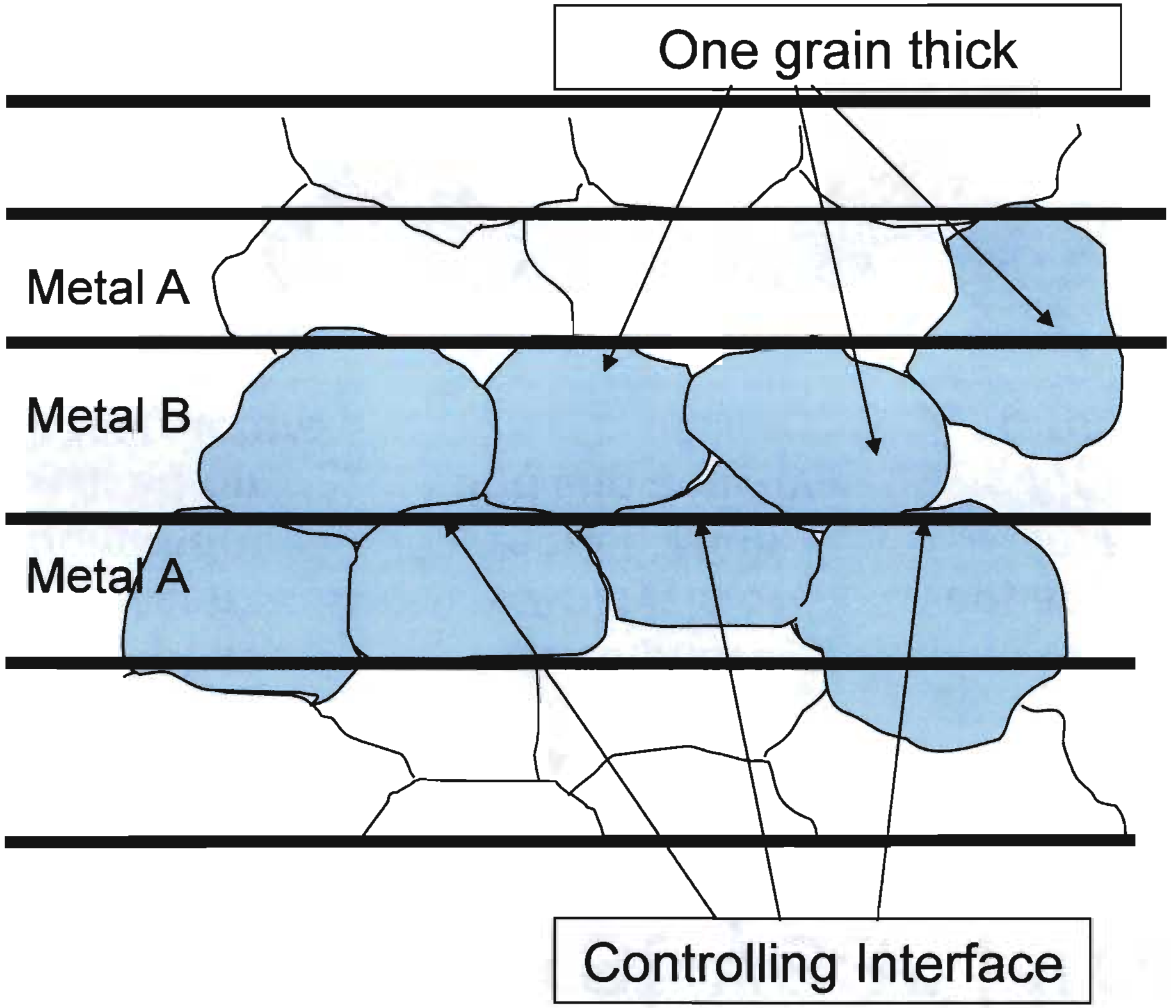
Kinetics: In-situ TEM

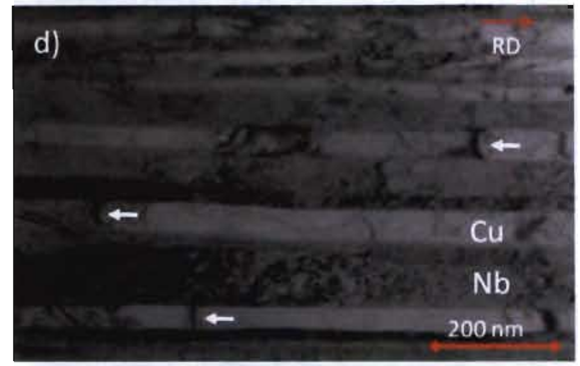


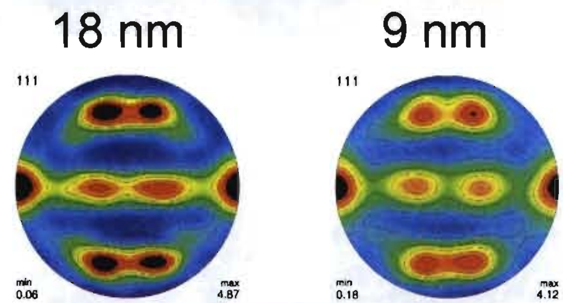
Defect density in the interface

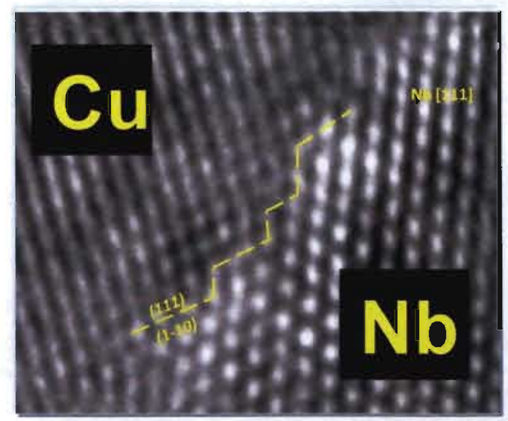


Multiple interface model: Evolution to finer layers









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First-year Progress

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Multi-interface Models

- Two phase
- Mesh generation based on microstructure

Single-interface Models

- Two phase
- Analysis of reorientation and slip activity

Interface Flux Models

- Rate equations for an interface
- Flux based formulation

Dislocation Models

- Interface formulation
- Interface physics

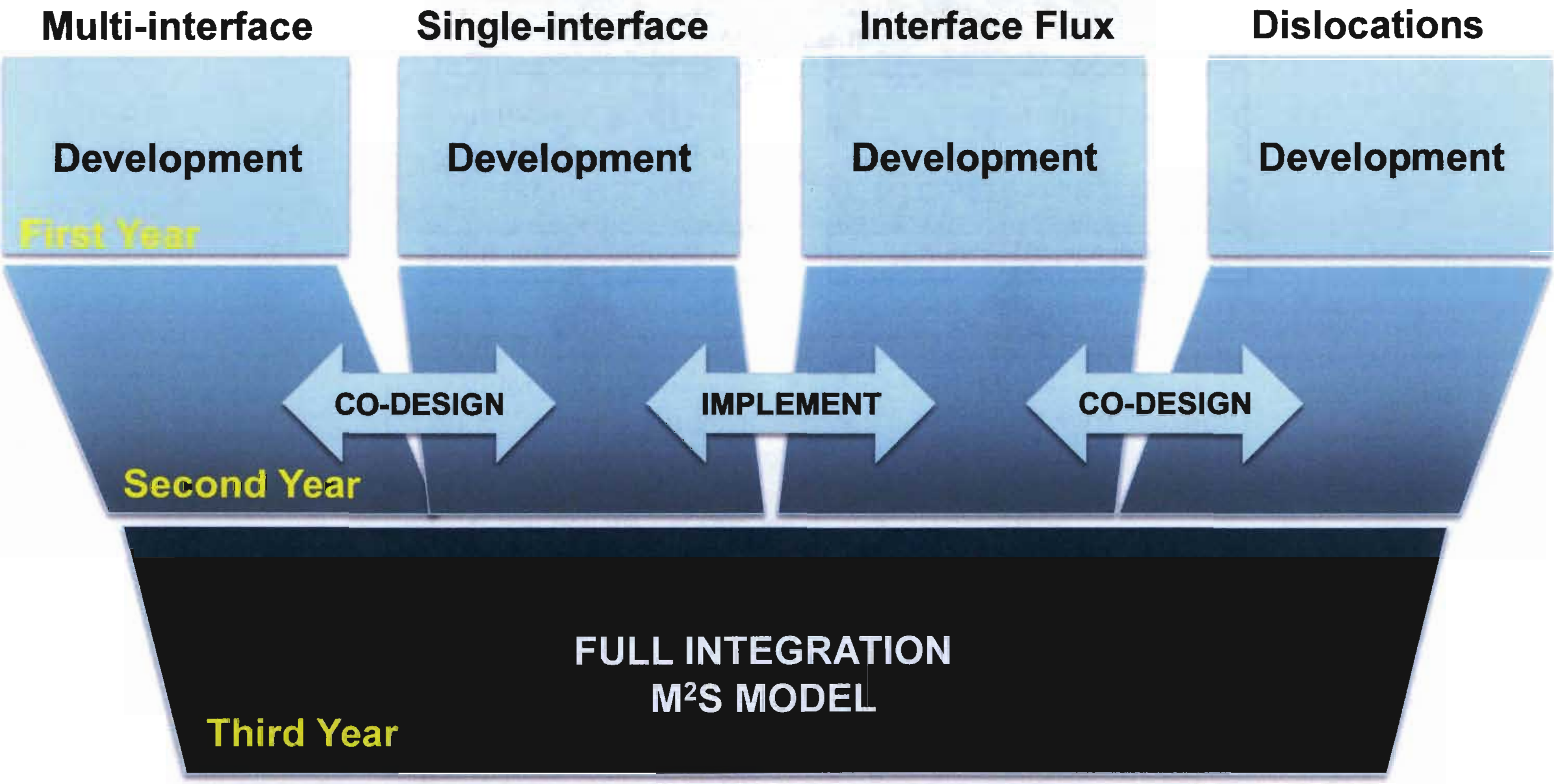
- CPFE framework
- Boundary conditions
- Single crystal model for bulk

- Programming for direct implementation

- Identifying key processes
- quantifying coefficients

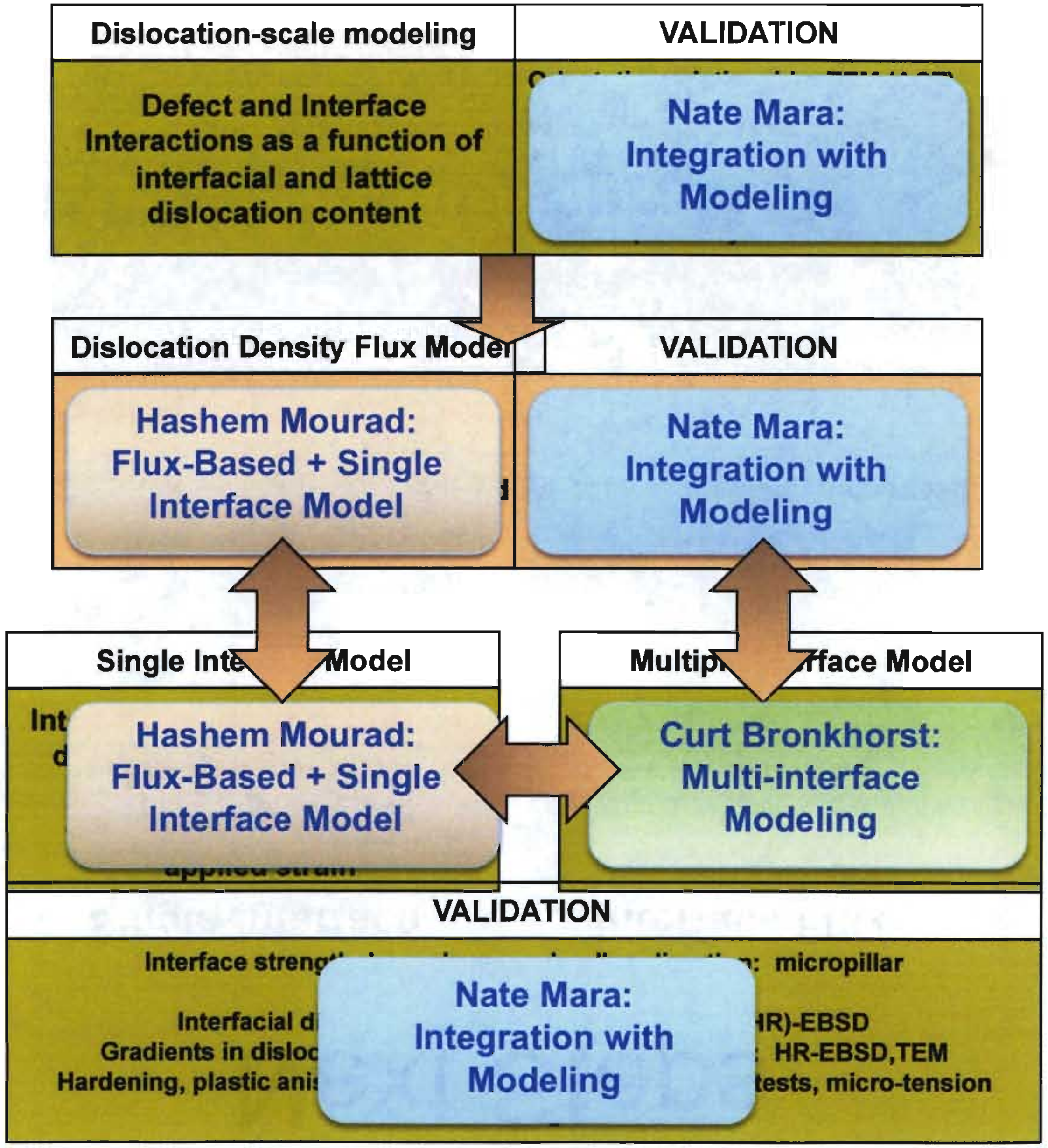
Integration with experiment

Next Steps



Multi-interface
Single-interface
Interface Flux
Dislocations
Development
Development
Development
Development
First Year
CO-DESIGN
IMPLEMENT
CO-DESIGN
Second Year
FULL INTEGRATION
M²S MODEL
Third Year

Upcoming Talks



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Upcoming Posters

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