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Title:	Multiscale Modeling of Interface-Defect Interaction in Multilayered Metallic Composites
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ABSTRACT

Multiscale modeling of interface-defect interaction in multilayered metallic composites

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We consider a multiscale modeling strategy for the behavior of composite materials consisting of alternating thin layers of two immiscible metals. Dislocations and other defects can be nucleated, annihilated, stored in or transmitted across the bi-metal interfaces in such composites. The effect of such interface-defect interactions on the macro-scale properties of the composite material is more pronounced when the thickness of individual layers is small, resulting in a high density of heterophase interfaces in the composite. In this interface-dominated regime, depending on their structure and properties, the bi-metal interfaces can endow their parent composite material with very desirable properties, e.g. outstanding damage resistance and significantly enhanced lifetimes, via their ability to mitigate damage accumulation induced under severe loading conditions. Metallic laminates with layer thicknesses in the sub-micron range can now be fabricated in bulk quantities ($\sim \mathrm{cm}^3$) using severe plastic deformation processes, such as accumulative roll bonding [1]. The proposed multiscale modeling strategy takes into consideration the structure of heterophase interfaces, and its evolution during the deformation process. This is crucial in elucidating the effect of interfaces on microstructural evolution under severe plastic deformation, with the goal of manipulating the fabrication process to produce composites with the desired properties.

REFERENCES:

[1] S.C.V. Lim and A.D. Rollett, "Length scale effects on recrystallization and texture evolution in Cu layers of a roll-bonded Cu-Nb composite," *Mater. Sci. Engng. A*, vol. 520, pp. 189–196, 2009.

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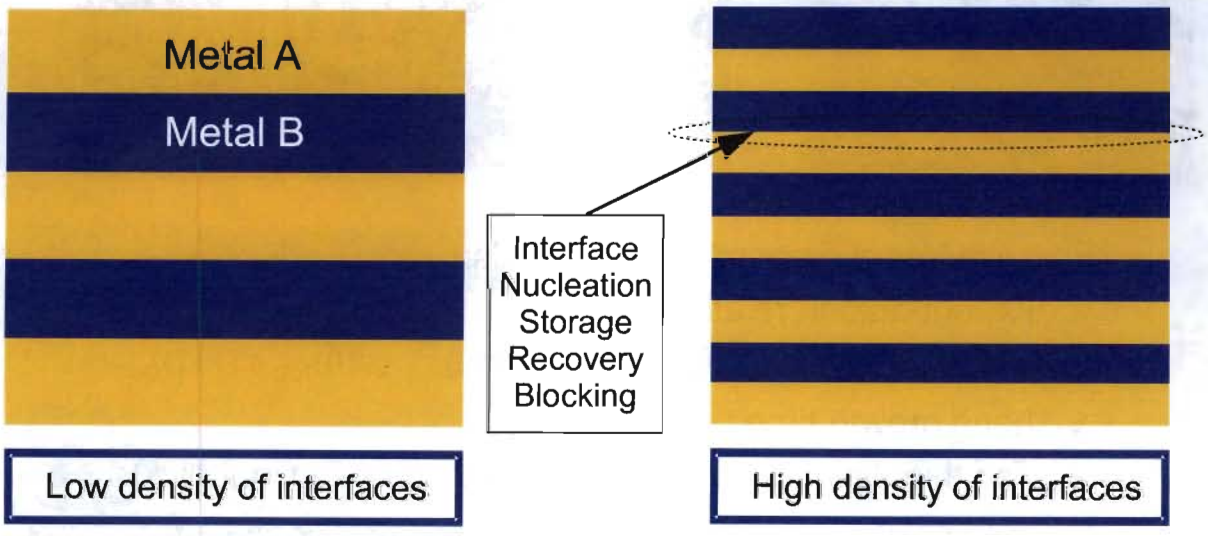
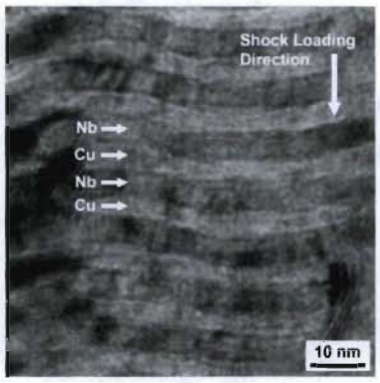
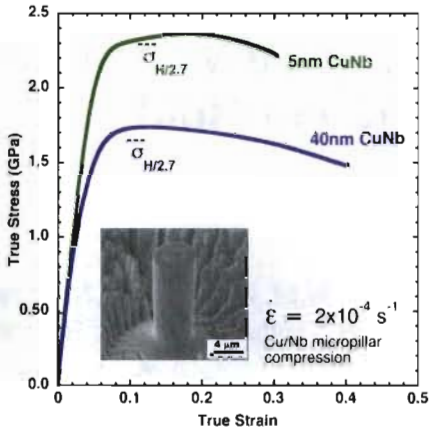
Interface Dominance

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



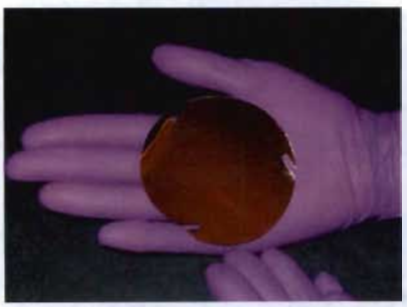
Motivation and Background

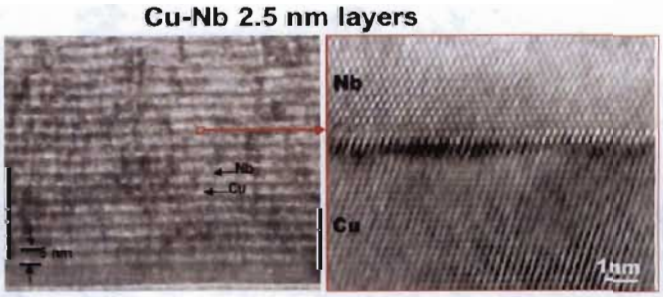




- Interfaces can absorb and eliminate defects
- provide the layered composite with an efficient mechanism for mitigating damage accumulation, and
- give this class of materials very desirable properties

Motivation and Background: PVD

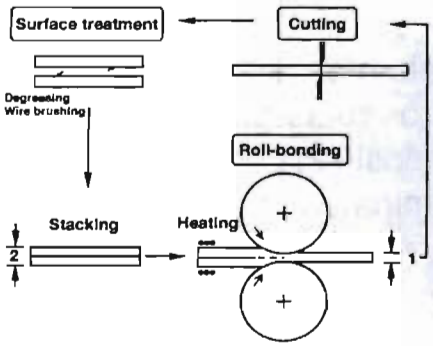




- Physical Vapor Deposition (PVD) foils:
  - KS orientation relationship:
    $\{111\}_{fcc} \parallel \{110\}_{bcc}$ (interface plane), $\langle 110\rangle_{fcc} \parallel \langle 111\rangle_{bcc}$
  - Long growth time (~ 24 hours).
  - Too thin even for some testing methods ($\sim 20\ \mu m$ thick)
- Need bulk fabrication technique for ID layered composites

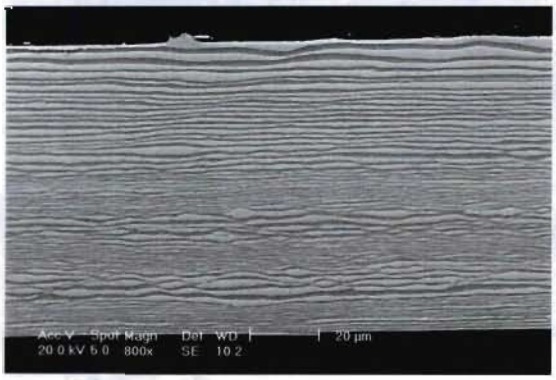
Motivation and Background: ARB

- SPD bulk fabrication technique
- High-purity polycrystalline Cu, Nb
- Rolling: 60% thickness reduction
- Anneal: 615°C for 3 hours
- Layer thickness: 1 mm → 10 nm



Bordeaux F and Yavari R. Z Metall 1990; 81: 130.

Motivation and Background: ARB



- Two-dimensional layered microstructure
- Controllable layer thicknesses
- Monotonic deformation imposed in a familiar manner
- Requirement: The ability to predict microstructural evolution under extreme strains

Objectives and Approach

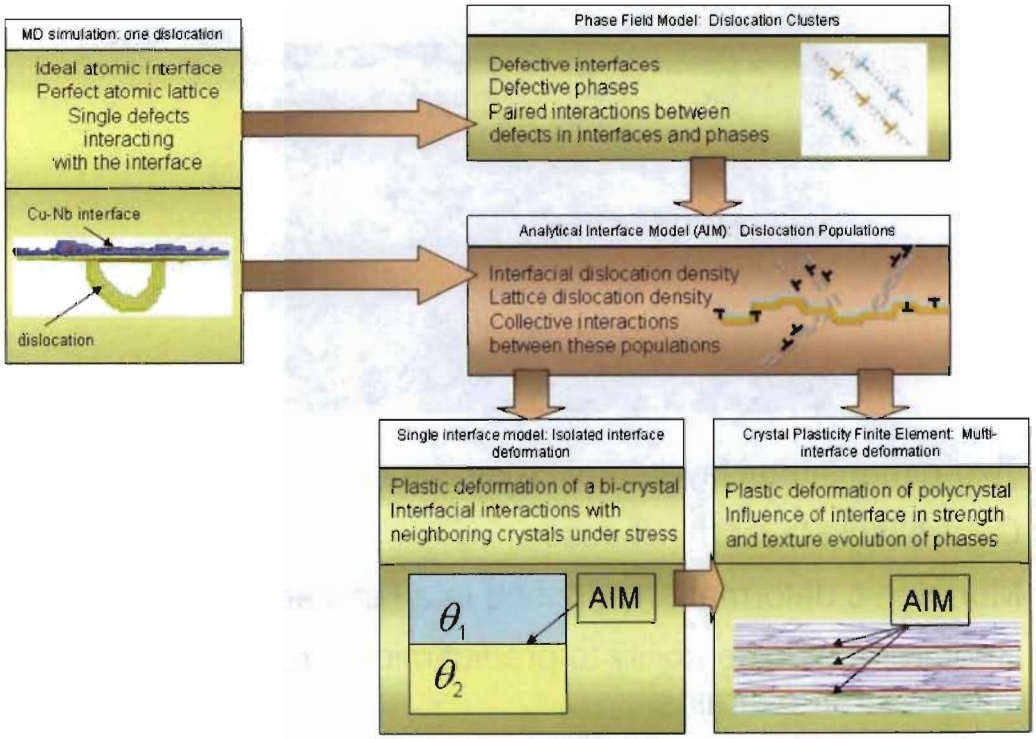
- **Objectives:**

  Manipulate the ARB process (short term) and/or other bulk fabrication processes (long term) to produce layered composite materials with optimal properties.

- **Approach:**

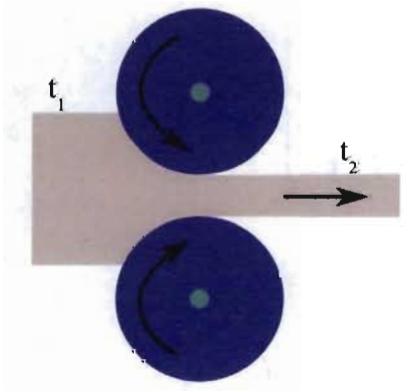
  Develop a meso (nm to μm) multi-scale modeling framework, capable of predicting microstructural evolution in multilayered metallic composites, during the transition from the constituent-dominated to the interface-dominated regime.

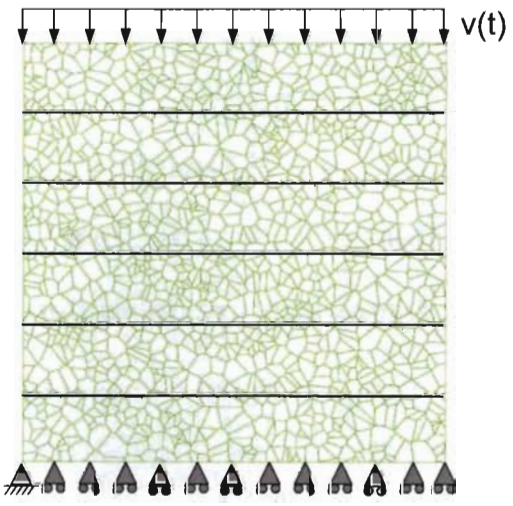
Modeling At Multiple Scales: Overview



Crystal Plasticity FEM

Modeling the Rolling Process





$$\dot{\bar{\epsilon}} = \frac{\dot{\theta}\log(t_2/t_1)}{\cos^{-1}\left(1-\frac{t_1-t_2}{r}\right)}$$

- Plane strain compression is an idealization of the rolling process, approached as $r \to \infty$

Mechanics BVP

- **Governing PDE and boundary conditions:**

$$\nabla \cdot \boldsymbol{\sigma} + \boldsymbol{b} = \mathbf{0} \qquad \text{in } \Omega$$

$$\boldsymbol{u} = \bar{\boldsymbol{u}} \qquad \text{on } \Gamma^u$$

$$\boldsymbol{n} \cdot \boldsymbol{\sigma} = \bar{\boldsymbol{t}} \qquad \text{on } \Gamma^\sigma$$

- **Kinematics:**

$$\boldsymbol{F} = \boldsymbol{F}^* \boldsymbol{F}^p \qquad \dot{\boldsymbol{F}}^p = \boldsymbol{L}^p \boldsymbol{F}^p$$

$$\boldsymbol{L}^p = \sum_\alpha \dot{\gamma}^{(\alpha)} \boldsymbol{m}^{(\alpha)} \otimes \boldsymbol{n}^{(\alpha)} \qquad \boldsymbol{E}^e = \frac{1}{2}\left(\boldsymbol{F}^{*\,T} \boldsymbol{F}^* - \boldsymbol{I} \right) - \boldsymbol{A}(T - T_0)$$

- **Stress-strain relations:**

$$\boldsymbol{S} = \mathbb{C} : \boldsymbol{E}^e \qquad \boldsymbol{\sigma} = \frac{1}{\det \boldsymbol{F}^*} \boldsymbol{F}^* \boldsymbol{S}\, \boldsymbol{F}^{*\,T}$$

Local Single Crystal Plasticity Model

- **Slip rate:**

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \exp\left\{ -\frac{F_0}{kT} \left[1 - \left(\frac{\left|\tau^{(\alpha)}\right| - s^{(\alpha)} \dfrac{\mu}{\mu_0}}{s_l^{(\alpha)} \dfrac{\mu}{\mu_0}} \right)^p \right]^q \right\} \operatorname{sgn}\left(\tau^{(\alpha)}\right)$$

where $\tau^{(\alpha)} = \boldsymbol{\sigma} : \left(\boldsymbol{m}^{(\alpha)} \otimes \boldsymbol{n}^{(\alpha)} \right)$

- **Rate & temperature dependent hardening law:**

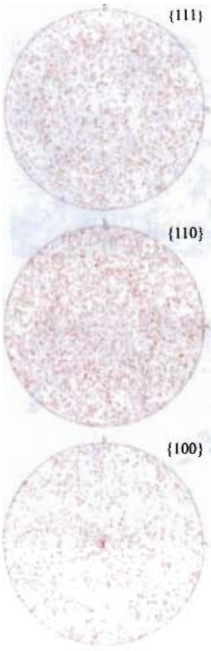
$$\dot{s}^{(\alpha)} = \sum_\beta h^{(\alpha\beta)} \left| \dot{\gamma}^{(\beta)} \right| \qquad h^{(\alpha\beta)} = h_0 \left[r + (1 - r)\delta_{\alpha\beta} \right] \left(\frac{s_s^{(\beta)} - s^{(\beta)}}{s_s^{(\beta)} - s_0^{(\beta)}} \right)$$

$$s_s^{(\beta)} = s_{s_0}^{(\beta)} \left(\frac{\dot{\gamma}^{(\beta)}}{\dot{\gamma}_0} \right)^{\frac{kT}{A}} \qquad \frac{\mu}{\mu_0} = 1 - \frac{m_{12}}{C_{12_0}} T$$

- **Adiabatic heating:** $\dot{T} = \dfrac{\eta}{\rho c_p} \sum_\alpha \tau^{(\alpha)} \dot{\gamma}^{(\alpha)}$

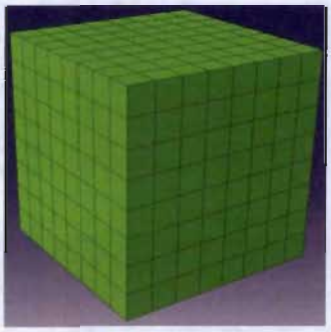
Single Crystal Plasticity Model Parameters

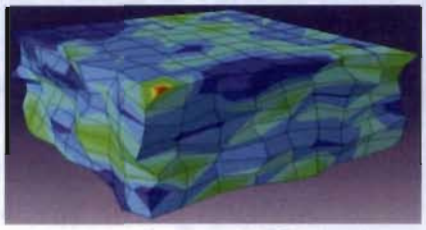
Initial texture



Cu	Nb
$\rho = 8960$ kg/m^3	$\rho = 8400$ kg/m^3
$c_p = 380$ J/kg-K	$c_p = 268$ J/kg - K
$\alpha = 17.7$ μm/m-K	$\alpha = 8.7$ μm/m - K
$\eta = 0.0, 0.95$	$\eta = 0.0, 0.95$
$m_{11} = -36.3$ MPa/K	$m_{11} = -17.7$ MPa/K
$C_{11_0} = 179.5$ GPa	$C_{11_0} = 242.0$ GPa
$m_{12} = -16.4$ MPa/K	$m_{12} = 1.92$ MPa/K
$C_{12_0} = 126.4$ GPa	$C_{12_0} = 121.2$ GPa
$m_{44} = -25.7$ MPa/K	$m_{44} = 2.18$ MPa/K
$C_{44_0} = 82.5$ GPa	$C_{44_0} = 28.0$ GPa
$r = 1.4$	$r = 1.4$
$\dot{\gamma}_0 = 10^7$ sec^{-1}	$\dot{\gamma}_0 = 10^7$ sec^{-1}
$s_0 = 1$ MPa	$s_0 = 40$ MPa
$s_i = 20$ MPa	$s_i = 700$ MPa
$F_0 = 1.0\times10^{-18}$ J	$F_0 = 2.1\times10^{-19}$
$p = 0.33$	$p = 0.34$
$q = 1.66$	$q = 1.66$
$s_{s_0} = 205$ MPa	$s_{s_0} = 140$ MPa
$h_{s_0} = 200$ MPa	$h_{s_0} = 300$ MPa
$A = 1.5\times10^{-19}$ J	$A = 1.0\times10^{-1}$

Cu: 12 systems – {111}⟨110⟩
Nb: 24 systems – {110}⟨111⟩, {112}⟨111⟩





512 Elements (Grains)

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Single Layer PSC Simulation

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Single Layer Cu / Nb PSC Simulation

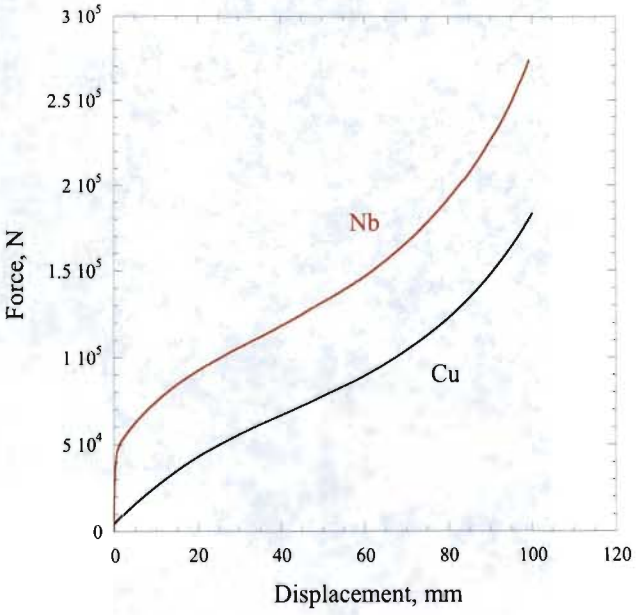
Cu: 12 systems – $\{111\}\langle 110\rangle$

Nb: 24 systems – $\{110\}\langle 111\rangle, \{112\}\langle 111\rangle$

- Same microstructure morphology, initial crystallographic texture, strain ($\bar{\epsilon} = -0.8$)

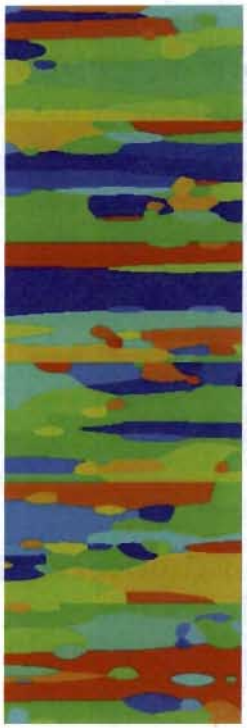
Single Layer PSC Simulation

- Substantial difference in rolling resistance between Cu and Nb
- Load–deflection curves are expected to be different in the multilayered case due to mutual kinematic constraints between layers
- How do these differences manifest themselves in the multilayered case?



Six-Layer Cu/Nb PSC Simulation

- Two-dimensional six-layer problem
- Aspect ratio 3:1
- 169 grains, 71,876 elements
- Currently in progress
- Local CPFEM can be used to simulate the rolling process until layer thicknesses reach $\sim 1\ \mu\mathrm{m}$
- In sub-micron (ID) regime, a non-local CPFEM model must be used to capture relevant size effects



Non-local Crystal Plasticity FEM

Flux-based Crystal Plasticity Model

- **Governing PDE and boundary conditions:** for each slip system α, and dislocation type $p \in \{e+, e-, s+, s-\}$

$$\dot{\varrho}^{(\alpha)}_{(p)} + \nabla \cdot \boldsymbol{f}^{(\alpha)}_{(p)} = \Phi^{(\alpha)}_{(p)} \qquad \text{in } \Omega$$

$$\varrho^{(\alpha)}_{(p)} = \varrho^{(\alpha)}_{0(p)} \qquad \text{in } \Omega \text{ at } t = 0$$

$$\varrho^{(\alpha)}_{(p)} = \bar{\varrho}^{(\alpha)}_{(p)} \qquad \text{on } \Gamma^{\varrho}$$

$$\boldsymbol{n} \cdot \boldsymbol{f}^{(\alpha)}_{(p)} = \bar{f}^{(\alpha)}_{(p)} \qquad \text{on } \Gamma^{f}$$

- **Constitutive relations:**

$$\boldsymbol{f}^{(\alpha)}_{(p)} = \varrho^{(\alpha)}_{(p)} \boldsymbol{v}^{(\alpha)}_{(p)}$$

Flux-based Crystal Plasticity Model

- **Coupling with Mechanics:**
  - **Slip rate:**

$$\dot{\gamma}^{(\alpha)} = \sum_{p} b^{(\alpha)} \| \boldsymbol{f}^{(\alpha)}_{(p)} \| \quad \text{(Orowan's equation)}$$

  - **Dislocation kinetics:**

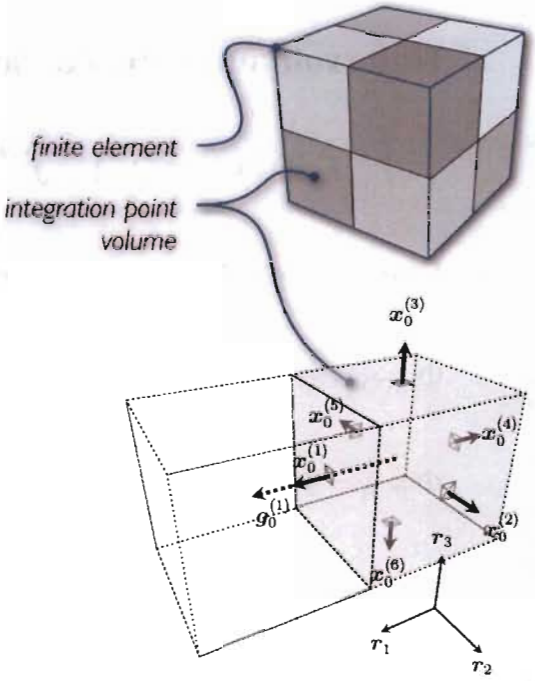
$$v^{(\alpha)}_{(p)} = v_0 \exp\left[-\frac{G_0}{kT} \left(1 - \frac{|\tau^{(\alpha)}|}{\hat{\tau}^{(\alpha)}} \right) \right] \operatorname{sgn}\left(\tau^{(\alpha)}\right) \qquad \text{(glide, } \forall p)$$

where $\tau^{(\alpha)} = \boldsymbol{S} : \left(\boldsymbol{m}^{(\alpha)} \otimes \boldsymbol{n}^{(\alpha)} \right)$, $\quad \hat{\tau}^{(\alpha)} = \mu b^{(\alpha)} \left[\sum_{\beta} \xi^{(\alpha\beta)} \left(\varrho^{(\beta)} + \varrho^{(\beta)}_{\text{dip}} \right) \right]^{0.5}$

- **Advantages:**
  - Accounts correctly for the underlying physics in plasticity
  - Resolves boundary layers and captures size effects
  - Facilitates linking AIM with CPFEM framework

Spatial Discretization

- Dislocations are carriers of plastic slip
- Dislocation transport is driven by stress
- Mechanics BVP is solved using FEM
- Dislocation transport IBVP is solved using FVM
- FV discretization is piggy-backed on Gauss quadrature point cloud associated with FE mesh



Divergence of the Dislocation Flux

- **Volume integration:**

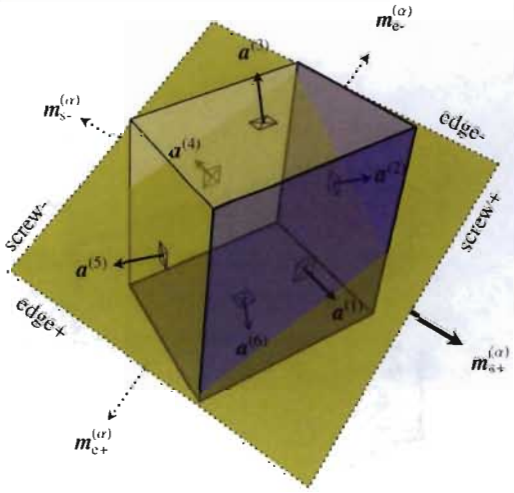
$$\int_V \dot{\rho}\,\mathrm{dV} + \int_V \nabla\cdot\boldsymbol{f}\,\mathrm{dV} = \int_V \Phi\,\mathrm{dV}$$

- **Volume averaging:**

$$\dot{\rho} + \frac{1}{V}\int_V \nabla\cdot\boldsymbol{f}\,\mathrm{dV} = \Phi$$

- **Divergence theorem:**

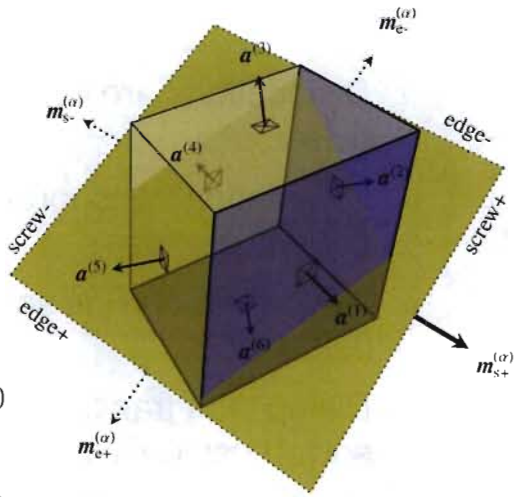
$$\dot{\rho} + \frac{1}{V}\int_{\partial V} \boldsymbol{f}\cdot\mathbf{a}\,\mathrm{dA} = \Phi$$



Divergence of the Dislocation Flux

- **Finite volume approximation:**

$$\frac{1}{V}\int_{\partial V} \boldsymbol{f}\cdot\mathbf{a}\,\mathrm{dA} \approx \frac{1}{V}\sum_{n}\chi^{(n)}\tilde{\boldsymbol{f}}^{(n)}\cdot\mathbf{a}^{(n)}\mathrm{A}^{(n)}$$



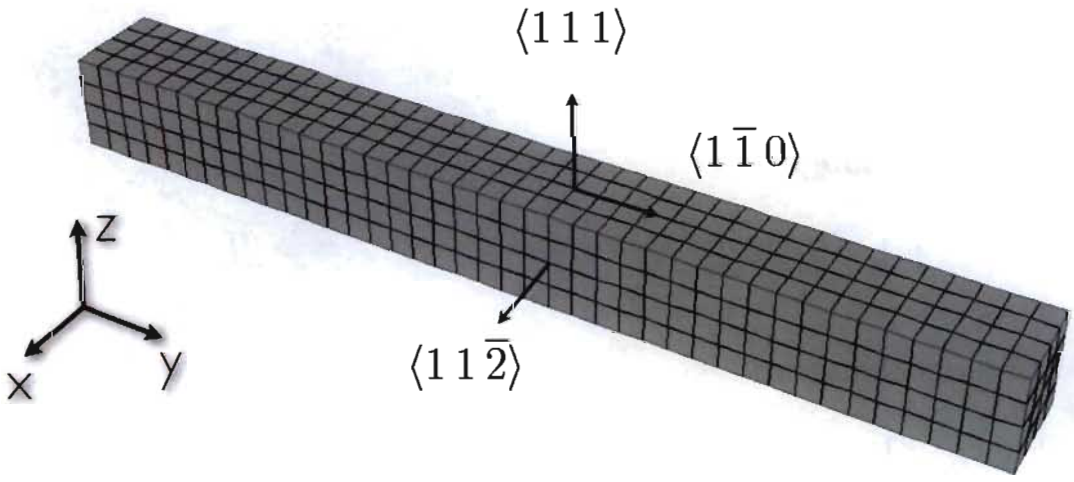
- **Dislocation blocking at interfaces:**

$$\Phi_{\mathrm{mob}} = -\frac{1}{V}\sum_{n\in\mathscr{L}}\left(1-\chi^{(n)}\right)\tilde{\boldsymbol{f}}^{(n)}\cdot\mathbf{a}^{(n)}\mathrm{A}^{(n)}$$

$$\Phi_{\mathrm{imm}} = +\frac{1}{V}\sum_{n\in\mathscr{L}}\left(1-\chi^{(n)}\right)\tilde{\boldsymbol{f}}^{(n)}\cdot\mathbf{a}^{(n)}\mathrm{A}^{(n)}\mathrm{sgn}(v)$$

$$\text{where } \mathscr{L} = \left\{n \,\middle|\, \tilde{\boldsymbol{f}}^{(n)}\cdot\mathbf{a}^{(n)} > 0\right\}, \quad 0 \le \chi^{(n)} \le 1$$

Example: Al Bi-crystal in Single Slip



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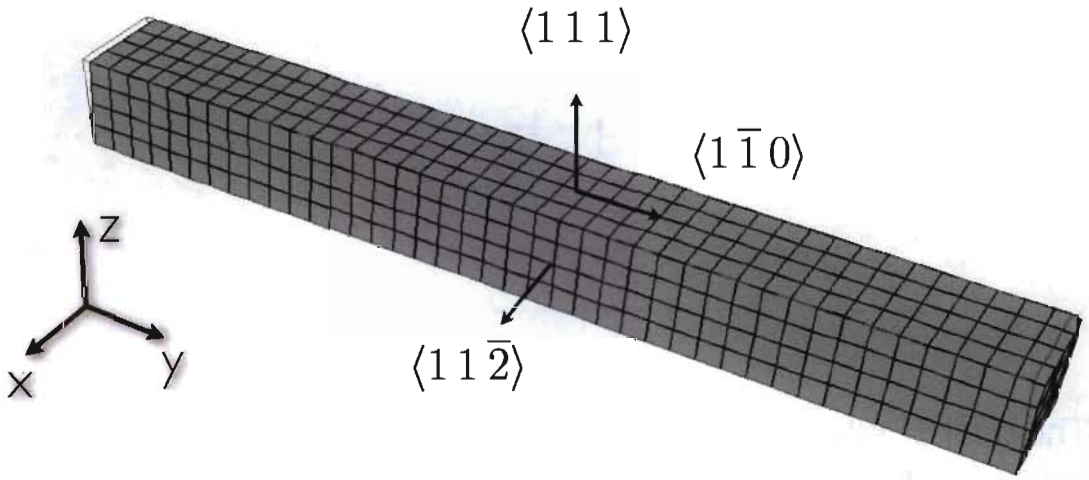
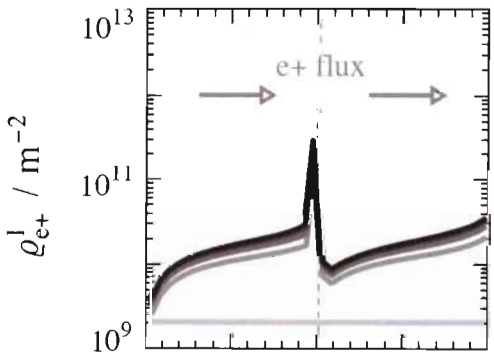
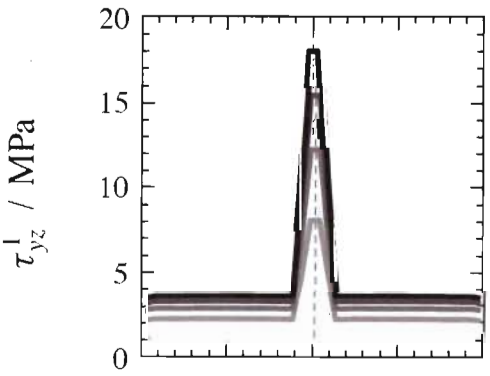
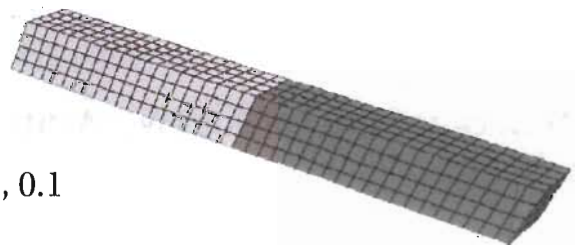


Example: Al Bi-crystal in Single Slip

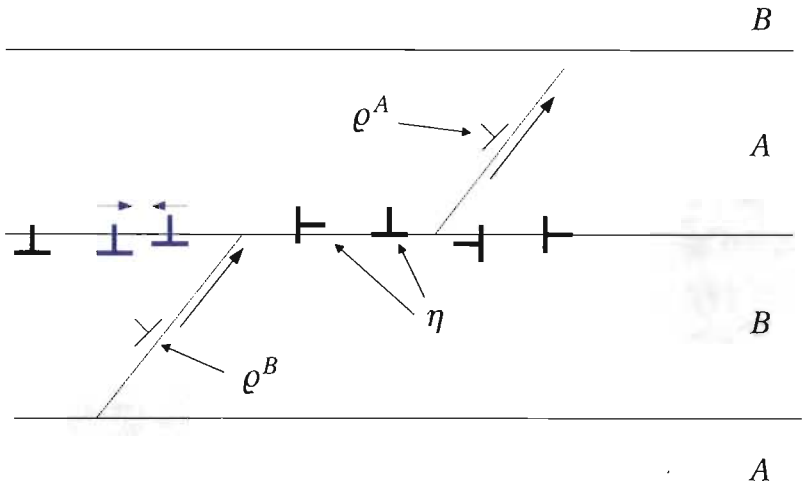






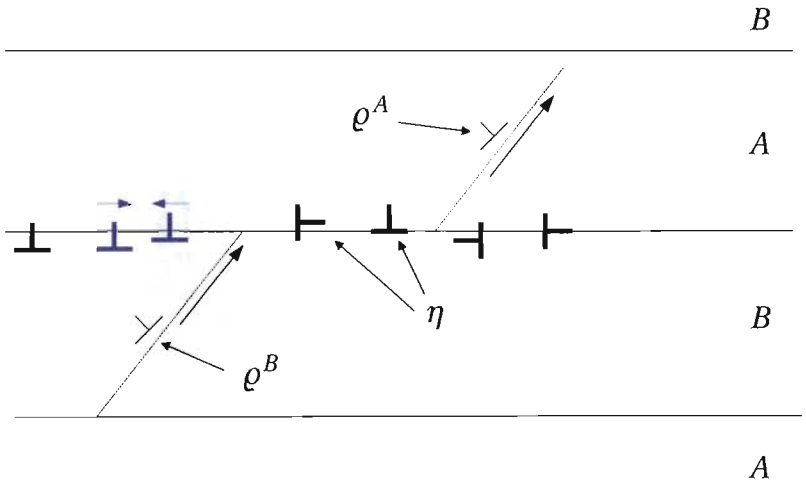
- GB has $\chi = 0.5$
- $\bar{\epsilon}_{yz} = 0, 0.025, 0.05, 0.075, 0.1$

Analytical Interface Model



- The goal of AIM is to predict the evolution of lattice and interface defect populations, based on the ability of the interface to absorb, store, annihilate, and emit lattice dislocations

Analytical Interface Model



- **Dislocation flux leaving layer A into the interface:**

$$\mathbf{a}\cdot\boldsymbol{f}\big|_{\Gamma^A_{int}} \equiv j^A = j^A_{\text{abs}} + j^A_{\text{bloc}} - j^A_{\text{emit}} - j^{BA}_{\text{tran}}$$

Evolution of Interfacial Dislocation Populations

- **Rate of absorption:**

$$j_{\text{abs}}^{A} = \sum_{\alpha \in \alpha^{A}} j_{\text{abs}}^{A(\alpha)} = \sum_{\alpha \in \alpha^{A}} \chi_{\text{abs}}^{(\alpha)} j^{A(\alpha)}$$

- **Rate of transmission:**

$$j_{\text{tran}}^{BA} = \sum_{\alpha \in \alpha^{A}} j_{\text{tran}}^{BA(\alpha)} = \sum_{\alpha \in \alpha^{A}} \sum_{\beta \in \beta^{B}} \chi_{\text{tran}}^{(\beta\alpha)} j_{\text{abs}}^{B(\beta)}$$

- **Extrinsic dislocations:**

$$\dot{\eta}^{E} = \underbrace{j_{\text{tran}}^{BA} + j_{\text{tran}}^{AB}}_{\text{Residuals}} - \phi_{\text{rxn}}^{EA} - \phi_{\text{rxn}}^{EB} - \phi_{\text{ann}}^{E}$$

- **Interfacial dislocations with A-lattice Burgers vector:**

$$\dot{\eta}^{A} = \underbrace{\sum_{\alpha \in \alpha^{A}} \sum_{\beta \in \beta^{B}} \left(1 - \chi_{\text{tran}}^{(\alpha\beta)}\right) j_{\text{abs}}^{A(\alpha)}}_{\text{Storage}} + \phi_{\text{rxn}}^{EA} - \phi_{\text{emit}}^{A}$$

Thank you