Modeling of Texture Evolution in Ti Forgings

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Project requires either a rare graduate student or a postdoctoral fellow.

Explore the evolution of texture in Ti forgings.

We seek to simulate meaningful conditions:

- Ti-6Al-4V
- Reasonable strains (>20%)

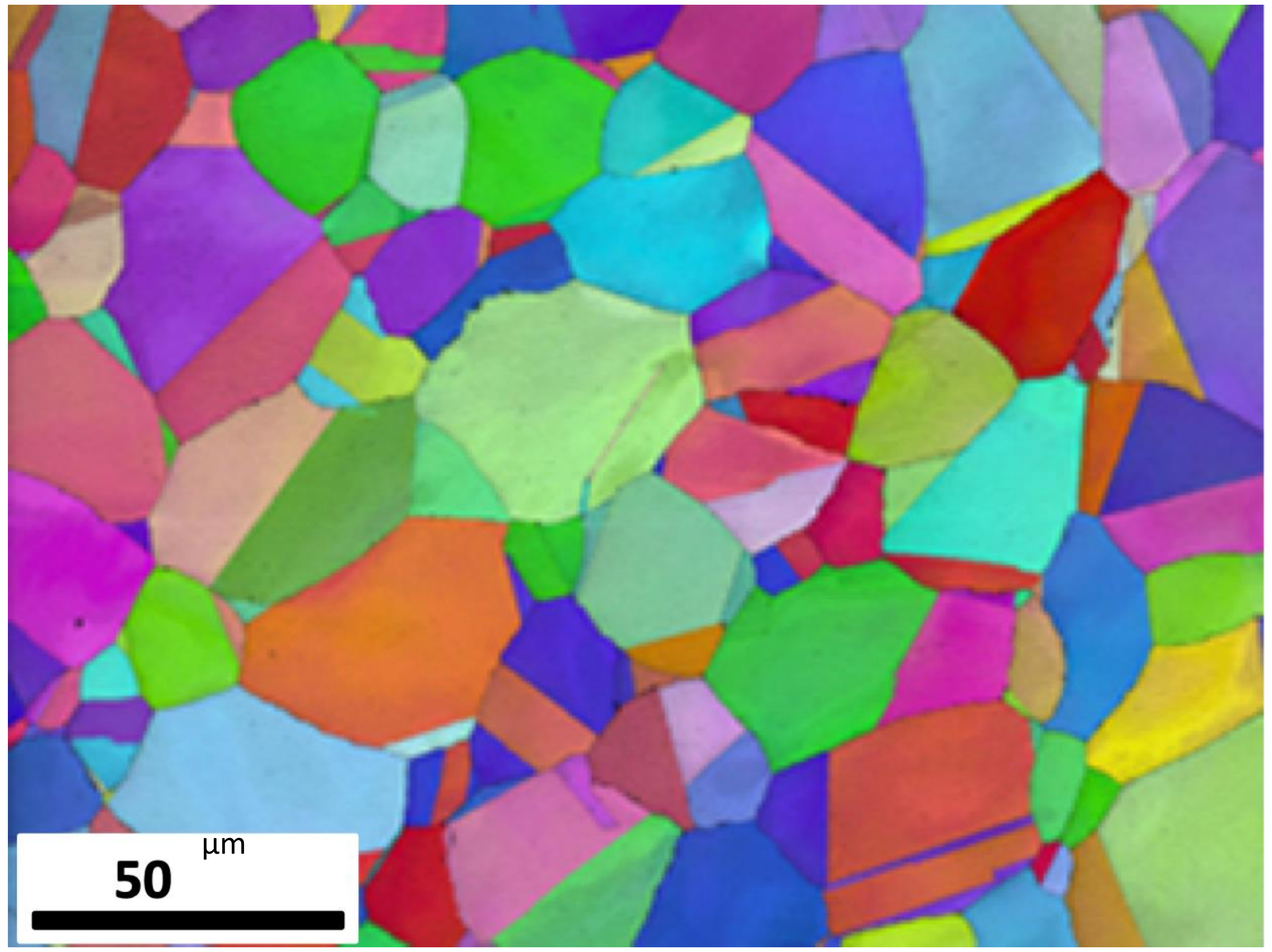
We are aware that the orientation, coupled with temperature, may be useful for studying other microstructural evolution

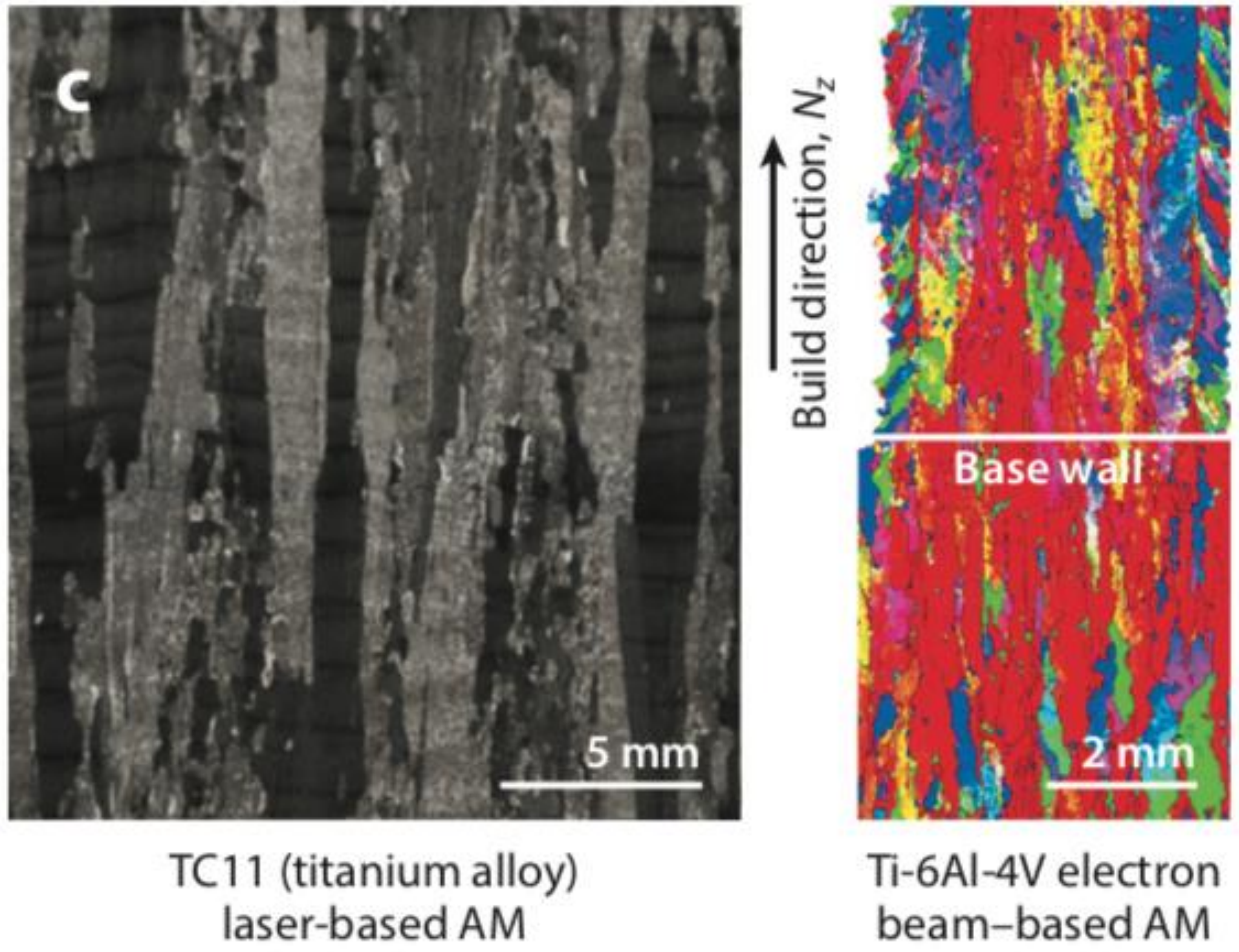
How does a polycrystalline metallic material deform under an external load?

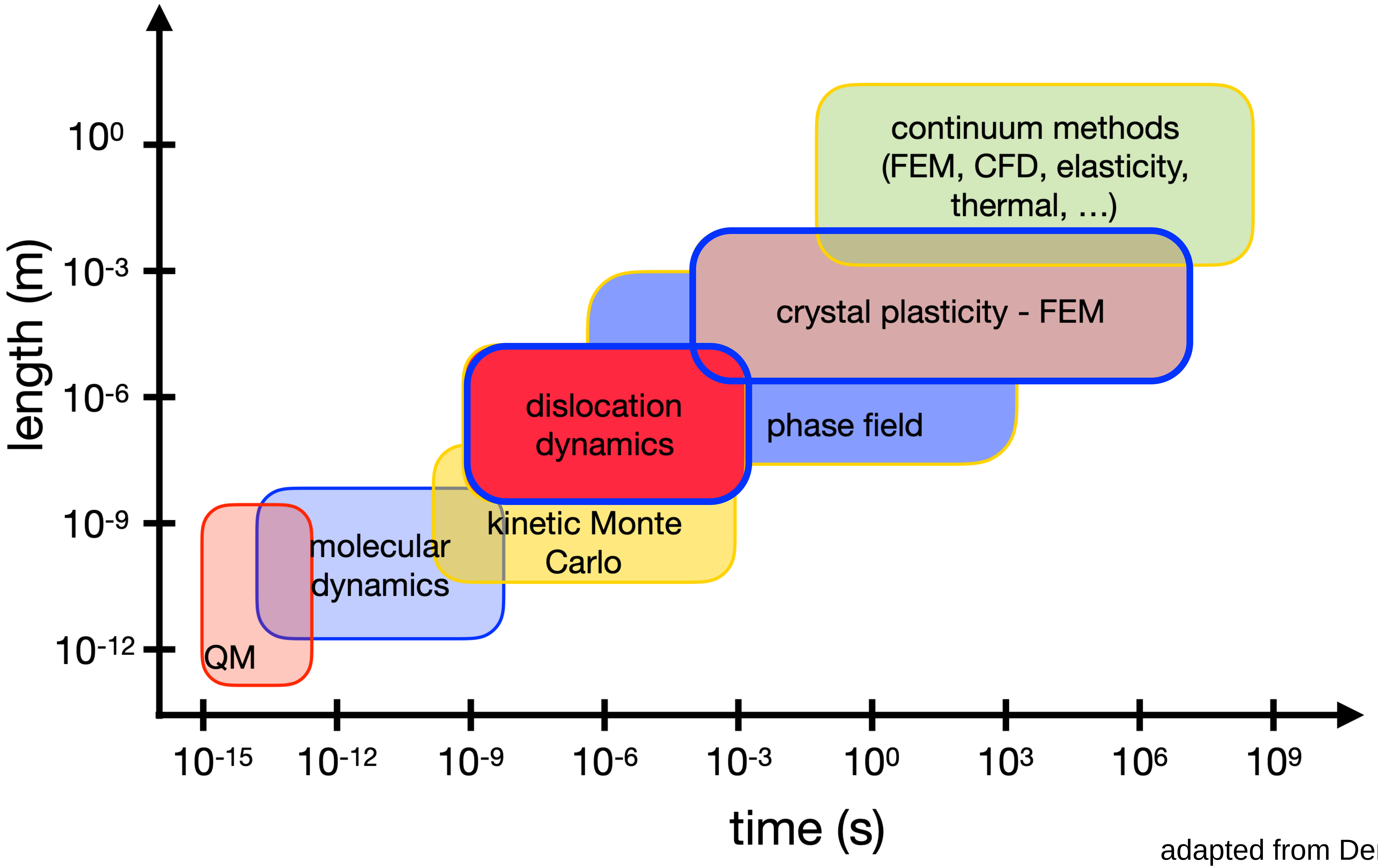
- role of grain size, shape, and orientations
- role of grain boundaries
- role of dislocations
- …

Usual modeling approach is a method referred to as *polycrystal plasticity*

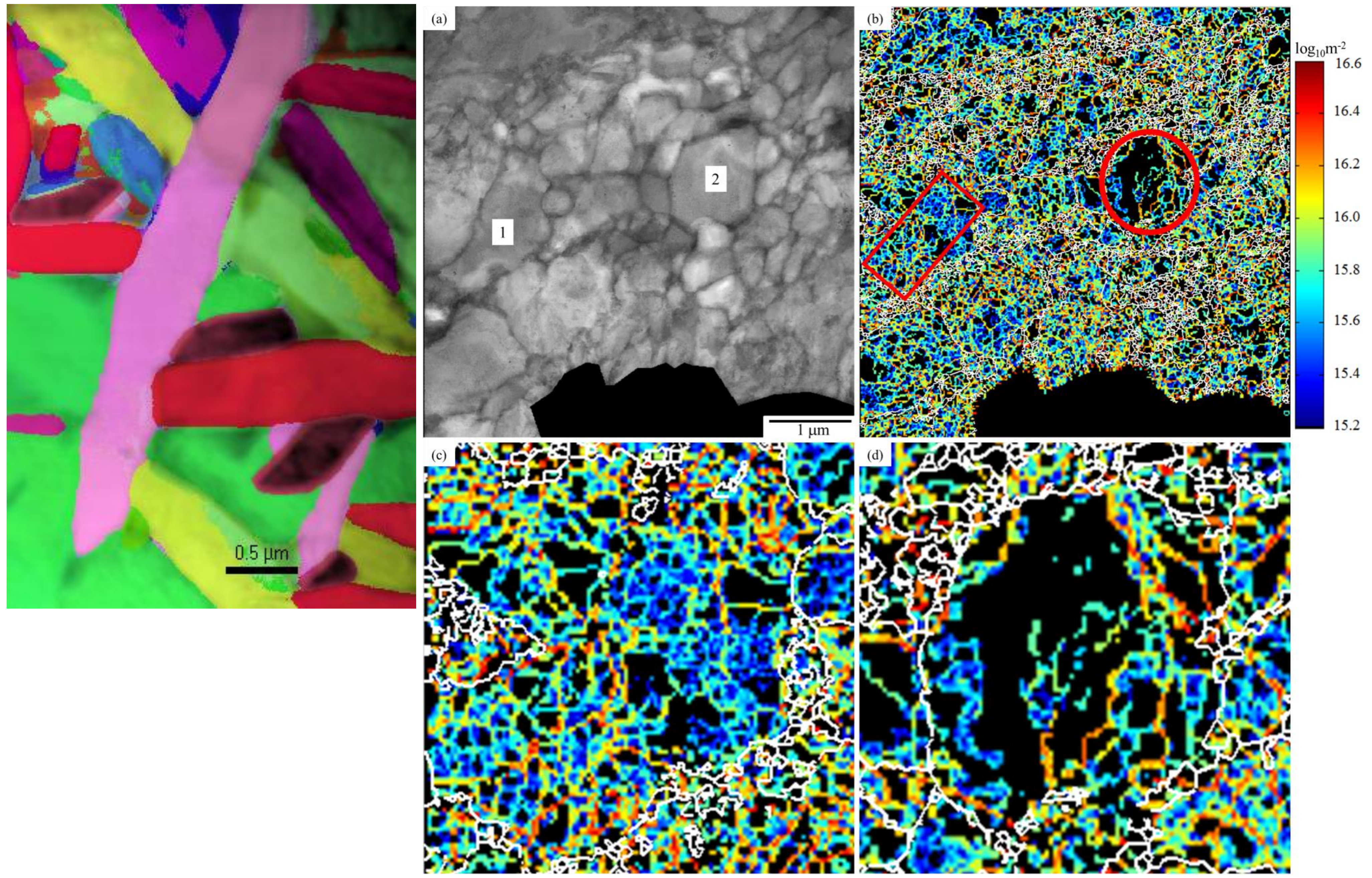
- predicts deformation of individual grains
- does not describe details of dislocation behavior





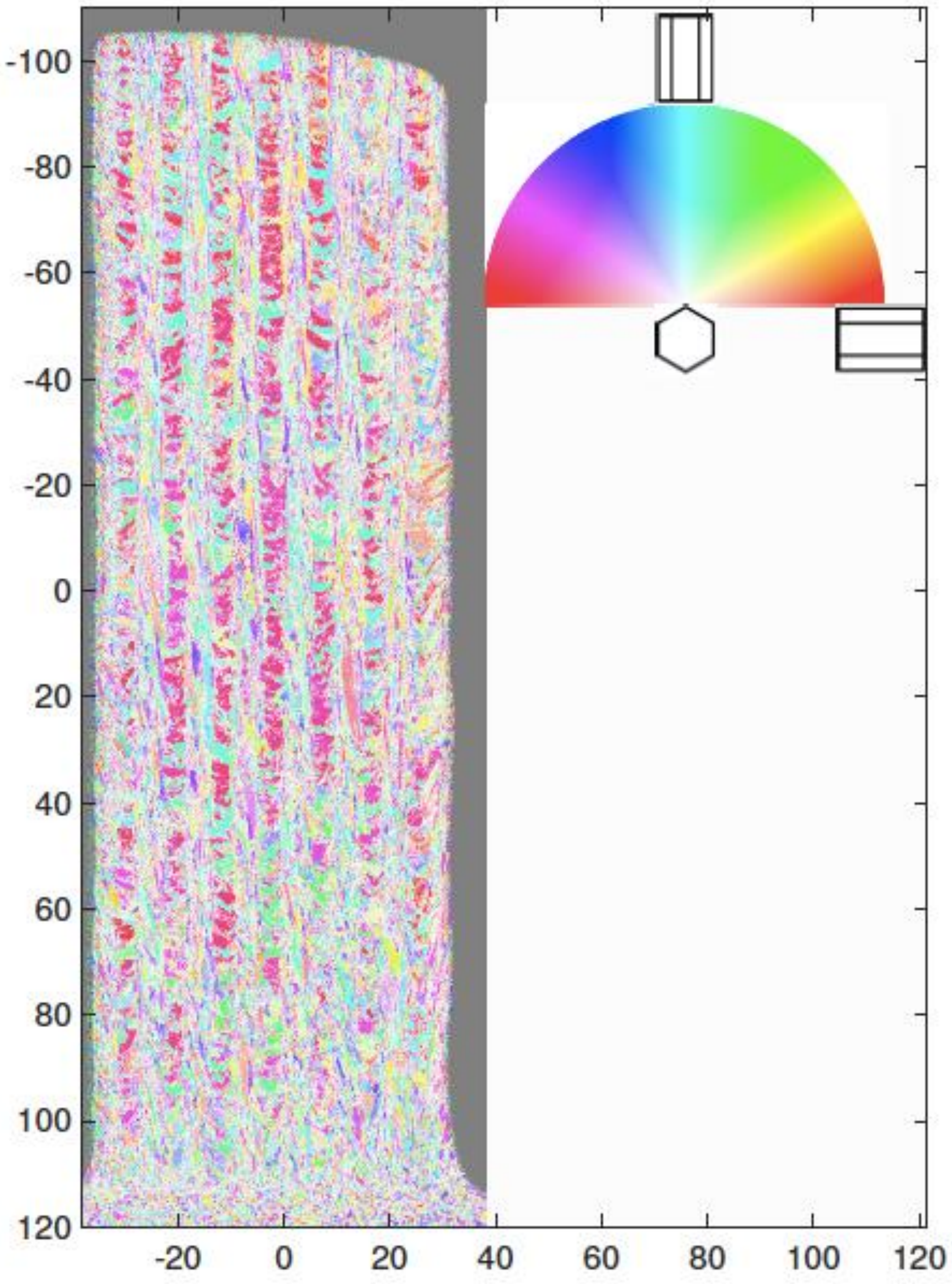


adapted from Dennis Dimiduk

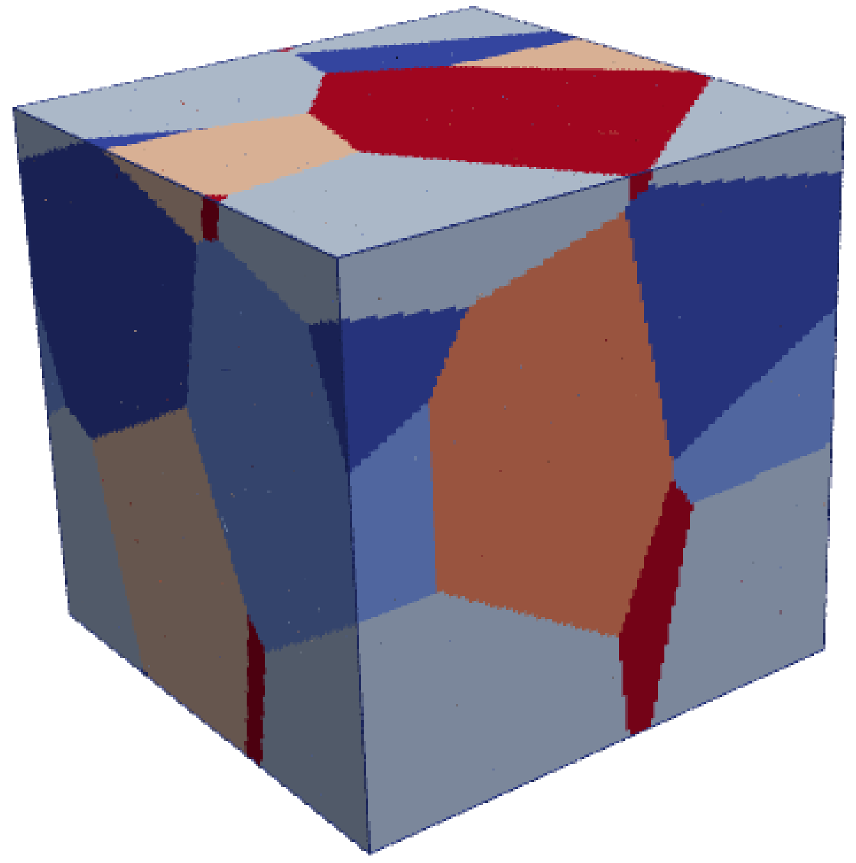


We will analyze both the dislocation content to understand strength and deformation behavior along with 2D large-scale texture (and EBSD / beam line studies if needed).

We will measure texture across cross-sections of forgings to support and validate the modeling efforts.

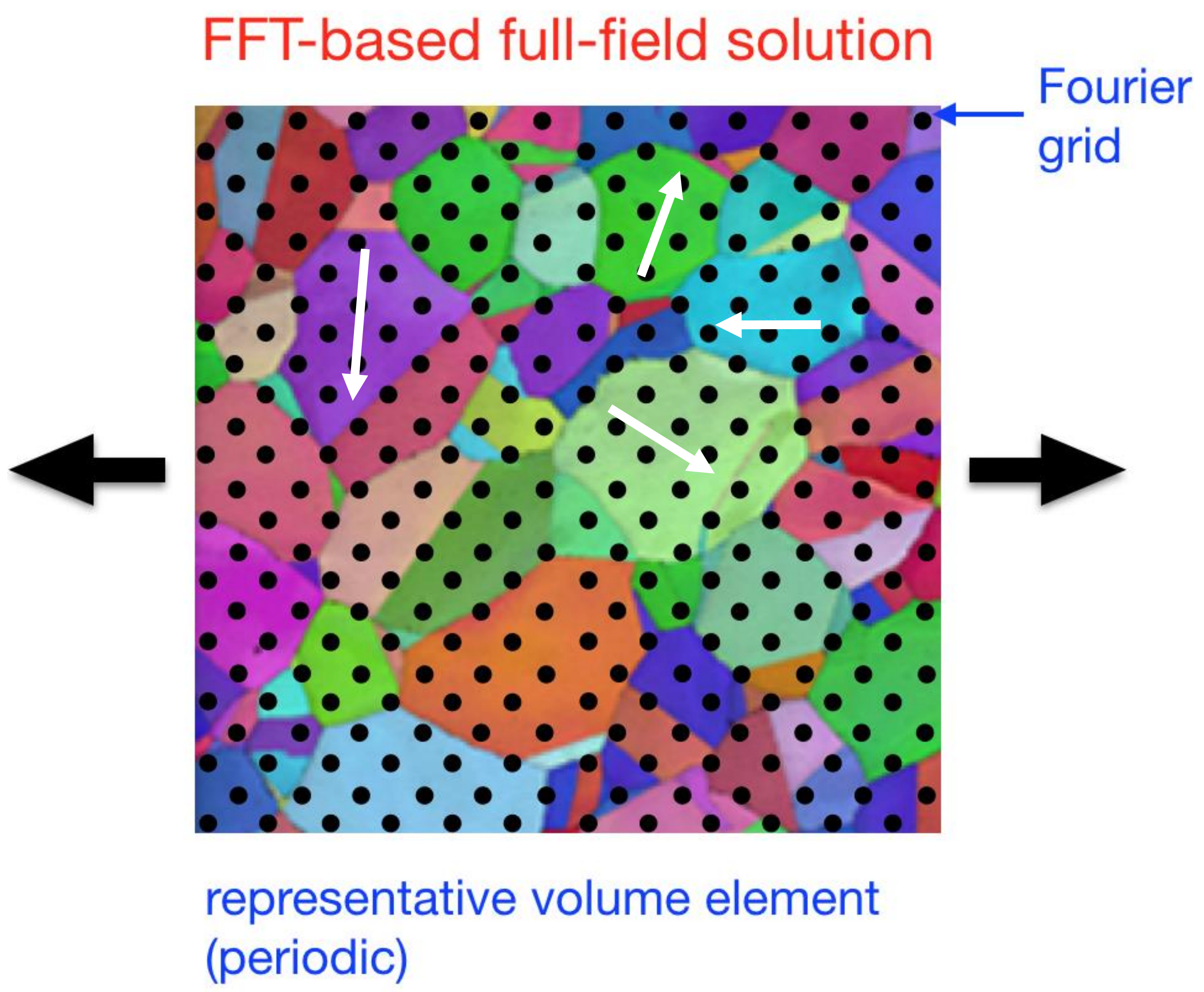


A full-field elasto-viscoplastic fast Fourier transform (EVP-FFT) crystal plasticity formulation will be used to simulate uniaxial tensile deformation in the generated microstructures (Lebensohn, IJP 32,59 (2012)).



Microstructure can be read in from external files using Dream3D (experimental or generated).

Microstructure images are discretized on a regular Fourier grid and material properties (e.g., elastic stiffness tensor and slip systems for plastic loading) are defined for each grain.



The output is the stress, strain-rate and orientation fields at each grid point.

Elasto-viscoplastic model (EVP) is used:

$$\dot{\varepsilon}_{ij}^{p}(\mathbf{x}) = \sum_{s=1}^{N_s} m_{ij}^{s}(\mathbf{x})\dot{\gamma}_s = \dot{\gamma}_o \sum_{s=1}^{N_s} m_{ij}^{s}(\mathbf{x})\left(\frac{|\mathbf{m}^{s}(\mathbf{x}):\boldsymbol{\sigma}(\mathbf{x})|}{\tau^{s}(\mathbf{x})}\right)^{n} sgn(\mathbf{m}^{s}(\mathbf{x}):\boldsymbol{\sigma}(\mathbf{x}))$$

- **m** is the Schmid tensor, $\dot{\gamma}_o$ is the strain rate, and $\tau^{s}(\mathbf{x})$ is the critical resolved shear stress (CRSS) for slip system s
- the change of the plastic strain at each time step is $\Delta\boldsymbol{\epsilon}^{p}(\mathbf{x}) = \dot{\boldsymbol{\epsilon}}^{p}(\mathbf{x})\Delta t$

The rotation-rate of the crystallographic lattice associated with a material point **x** is

$$-\dot{\omega}_{ij}^{p}(\mathbf{x}) = -\sum_{s=1}^{N_s} \alpha_{ij}^{s}(\mathbf{x})\dot{\gamma}_s$$

- $\boldsymbol{\alpha}$ is the anti-symmetric Schmid tensor

We will examine various hardening laws:

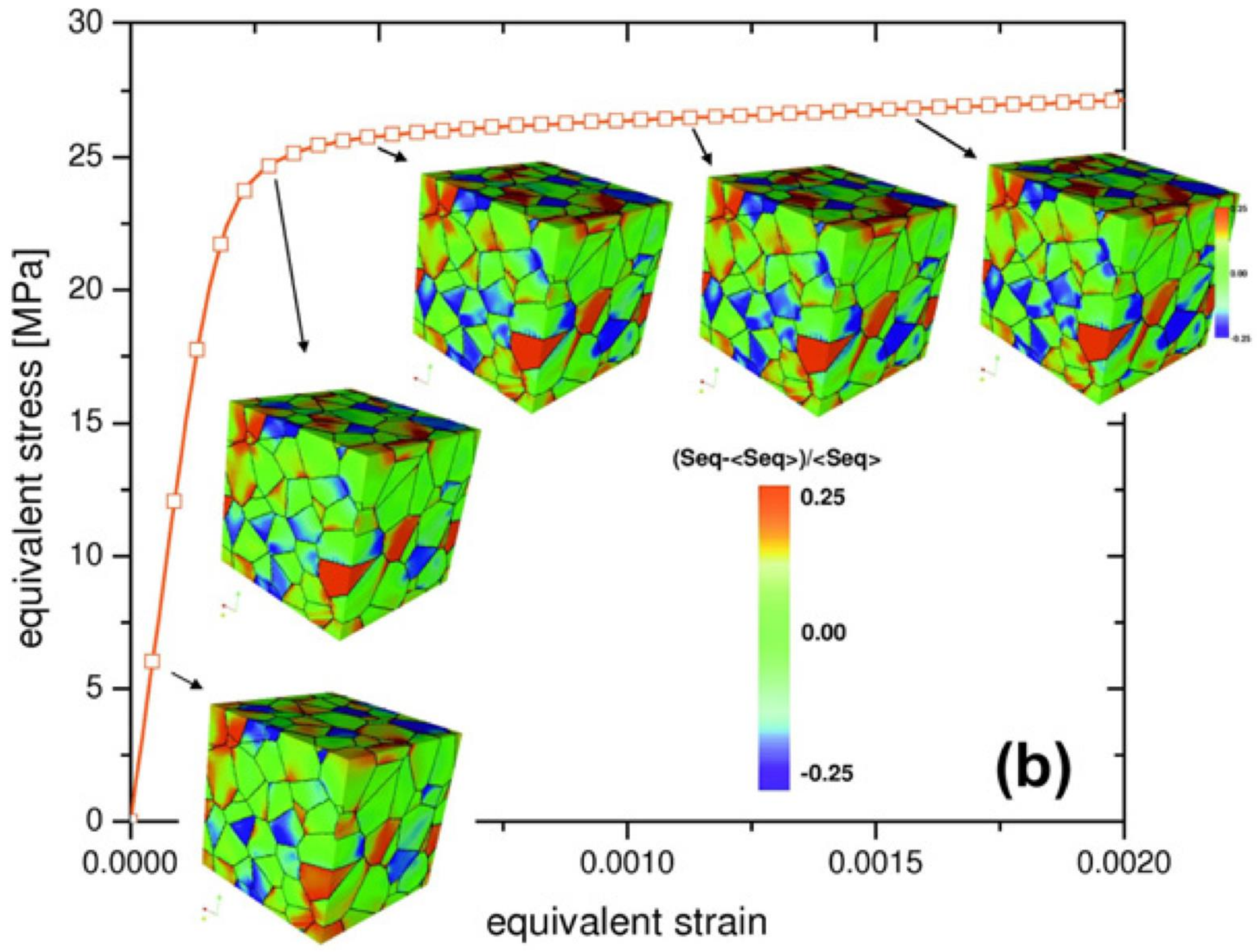
- As one example, the Voce hardening law can be used to model evolution of CRSS of each slip plane (Γ is the accumulated strain in the grains).

$$\tau_s(\Gamma) = \tau_0^s + (\tau_1^s + \theta_1^s \Gamma)\left(1 - \exp\left(-\Gamma \left|\frac{\theta_0^s}{\tau_1^s}\right|\right)\right)$$

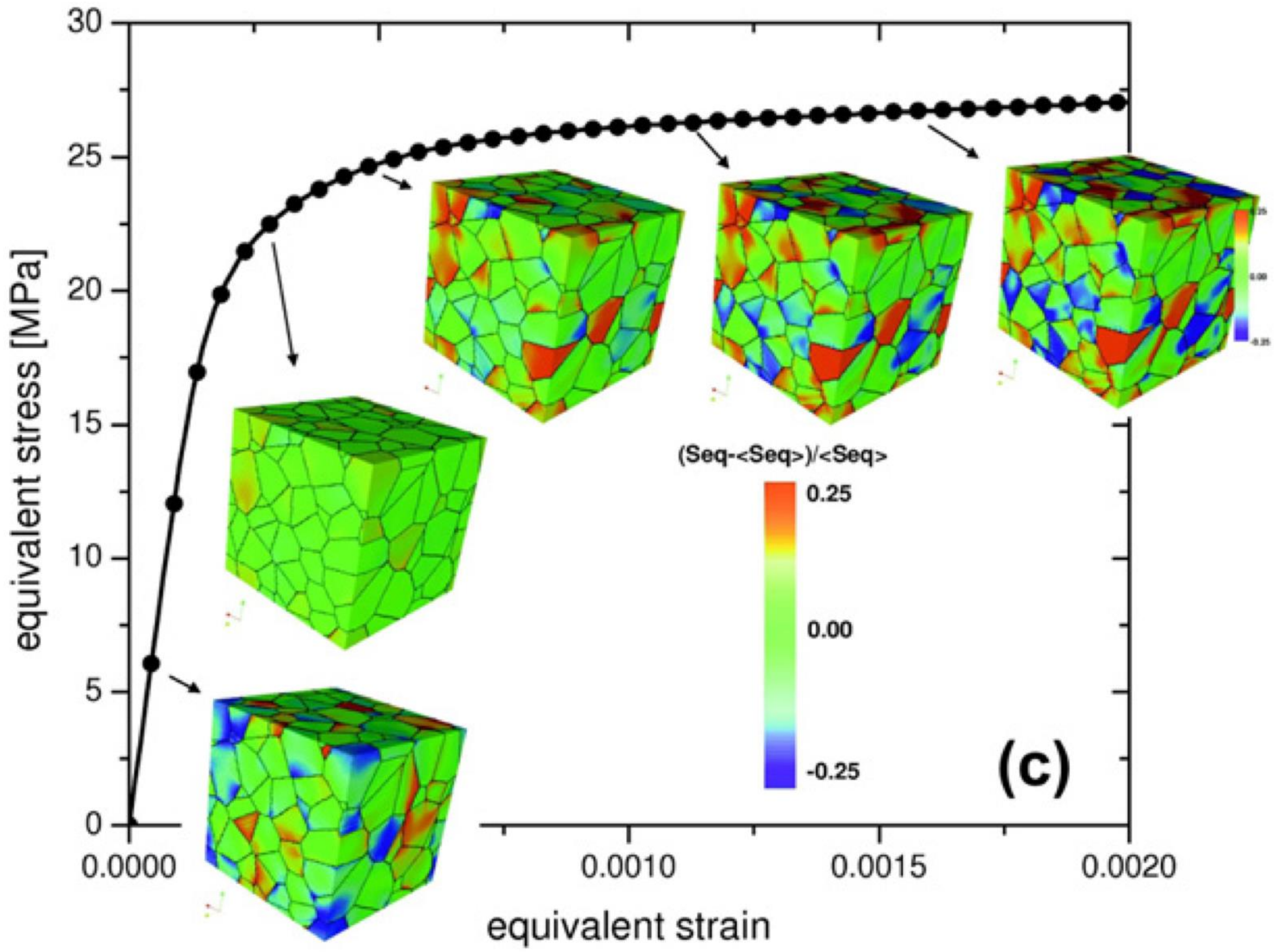
Lebensohn, IJP 32, 59 (2012)

Random fcc polycrystals (EVP-FFT calculations)

“Cu” (A = 2.2)



“Cu” (isotropic)



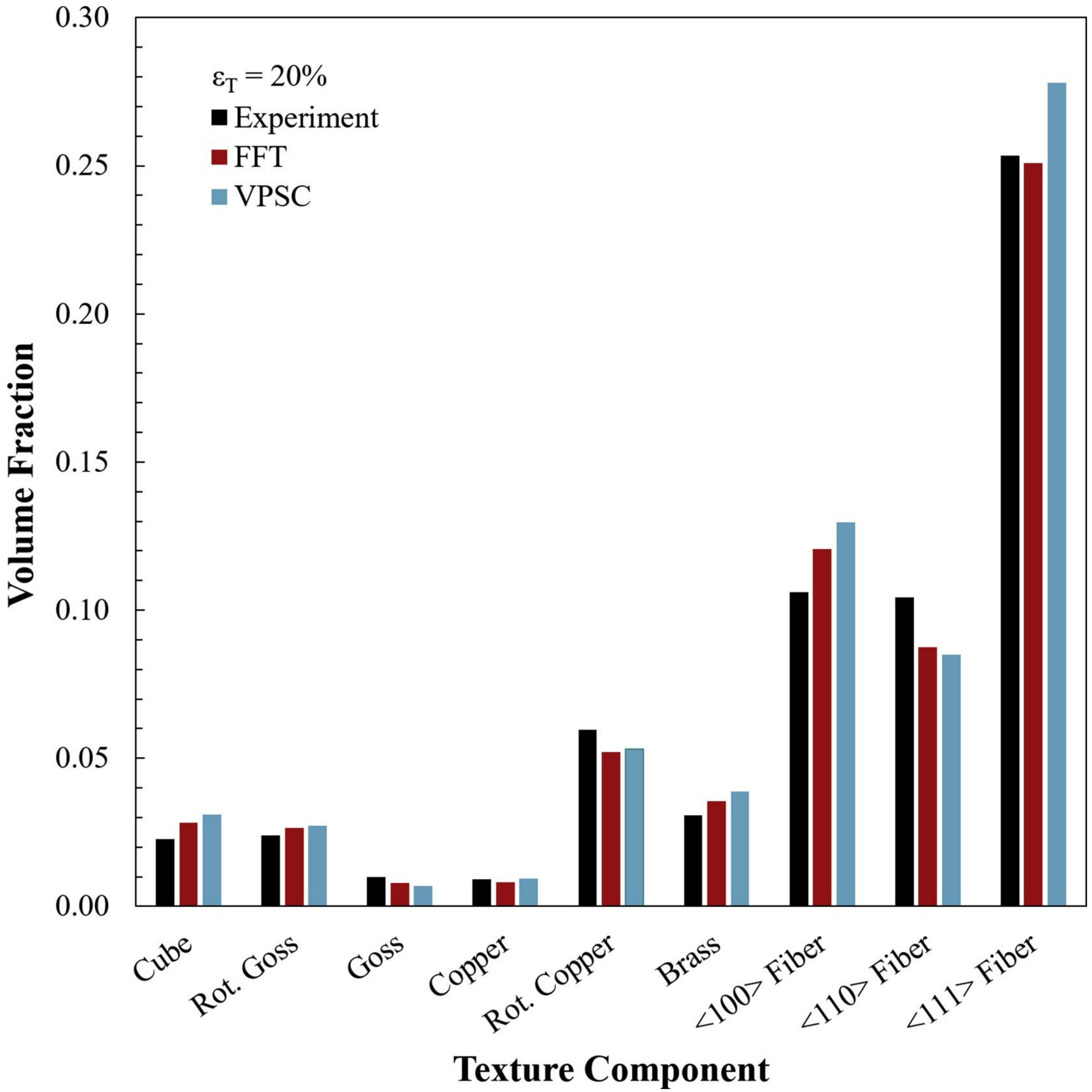
Lebensohn, IJP 32, 59 (2012)

Loaded under tensile stress to 20% true strain.

Comparison of texture predictions:

- FFT: elastoviscoplastic-FFT
- VPSC: viscoplastic self constant (mean field)

We will use the EVP-FFT model to examine texture development under forging conditions in Ti alloys. Will determine which constitutive relation yields best predictions.



Slone et al, Acta Mater. 158, 38 (2018)

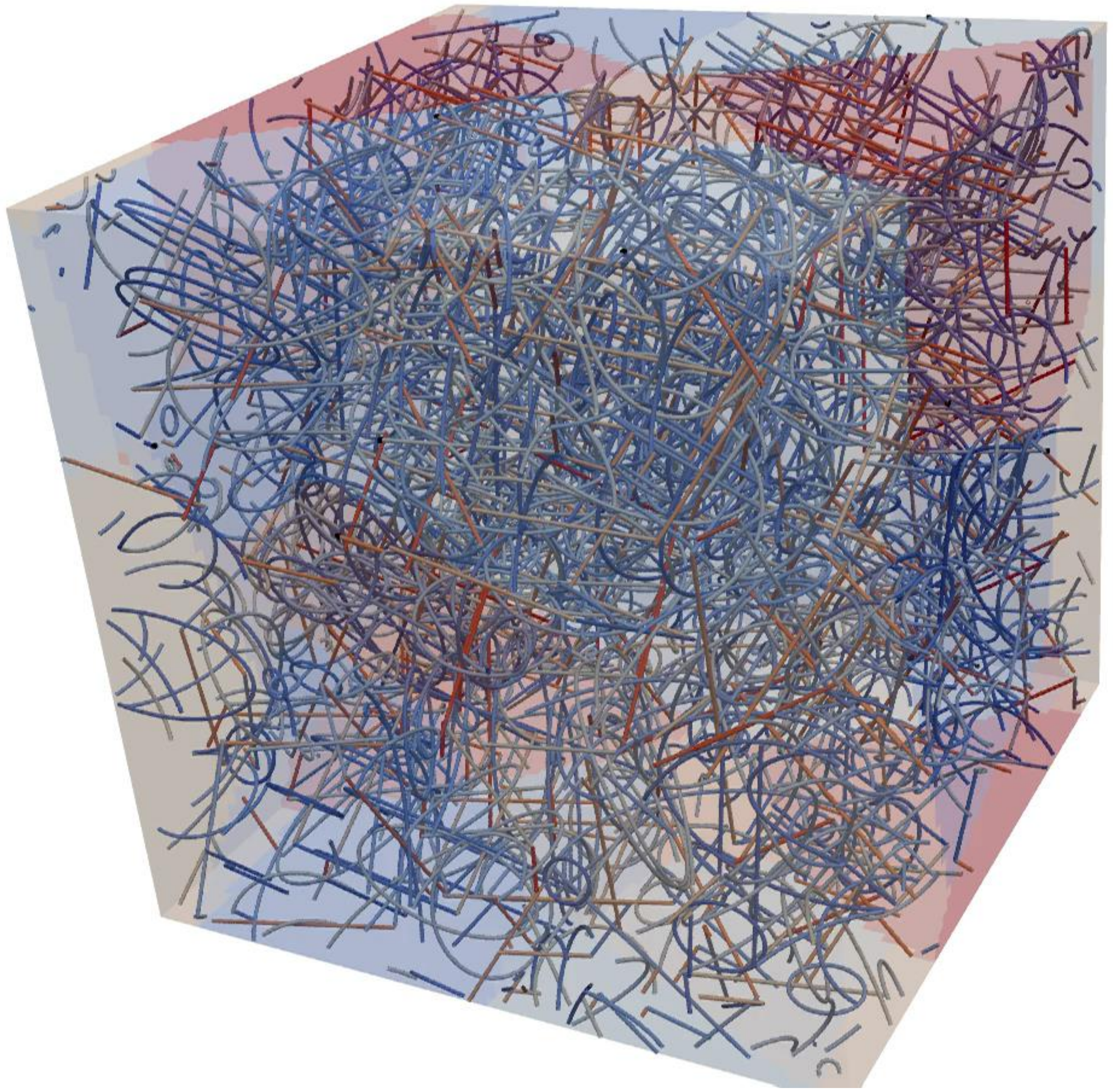
Texture development in CrCoNi under tensile load

Holm and students used the mean-field EVP-FFT crystal plasticity model to study fcc and hcp polycrystals (2 studies, each with 10,000 simulations) with different generated grain structures to identify hotspots (stresses greater than 90th percentile of the stress distribution).

Machine learning was used to develop correlations between the hotspots and the local grain neighborhoods.

We will examine the development of hotspots in the EVP-FFT calculations and see if the local neighborhoods are similar to those in fcc/hcp materials.

Replace the constitutive relations of Lebensohn with a direct calculation of dislocation stresses and motion calculated with FFT-Discrete Dislocation Dynamics (DDD) method:



We will:

- examine dislocation substructures in hotspots in representative grain neighborhoods
- compare with experimental results

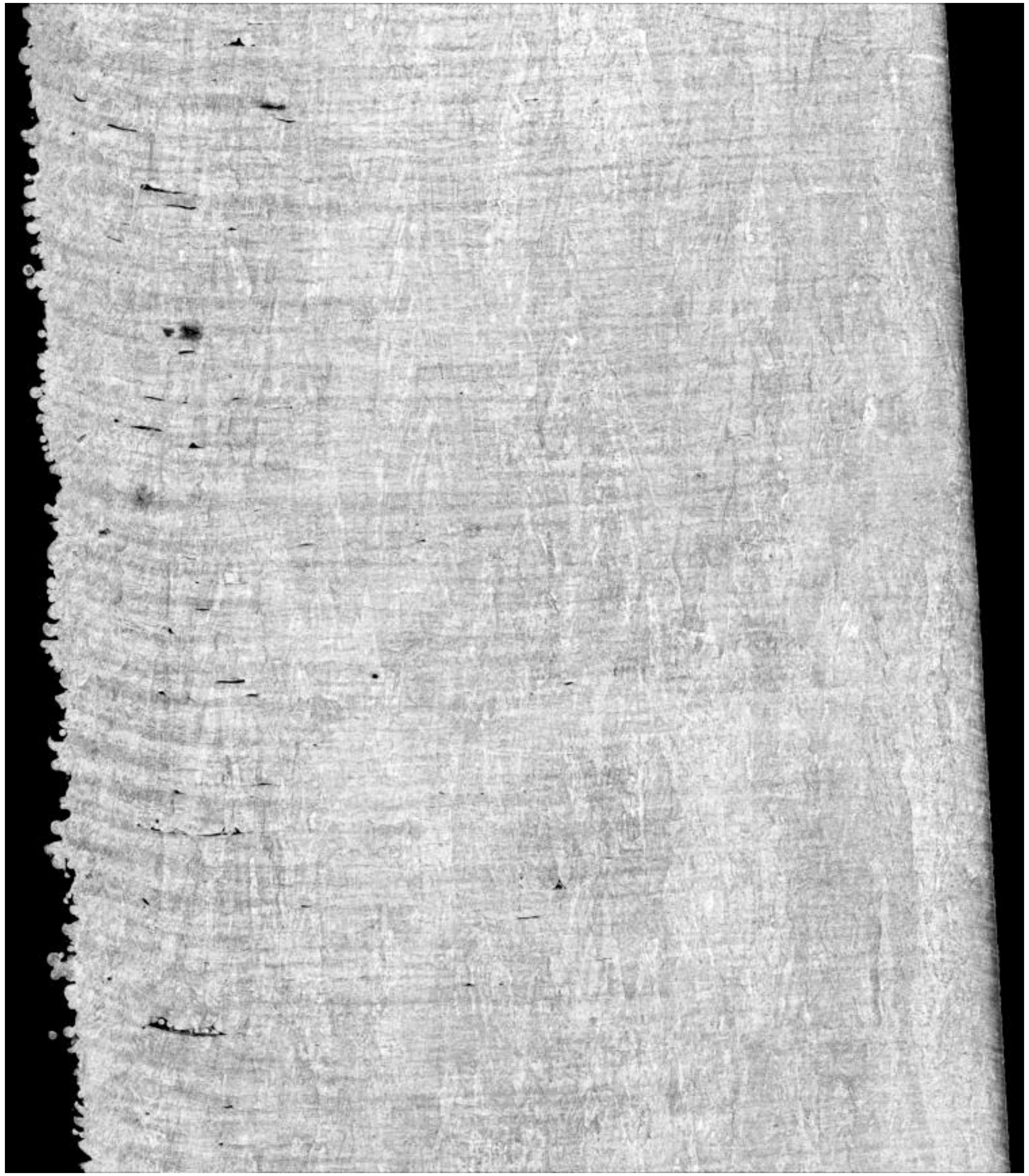
Rapid Defect Assessment of Non-Ferrous Materials Processed via Additive Manufacturing

Peter Collins
Martin Thuo

Initial work being conducted by an undergraduate team

Challenge: Low defect density (porosity) additively manufactured material (1-2%), CT does not give sufficiently accurate metrics.

Archimedes method is promising, but has some intrinsic challenges, including speed and the prospect of rough surfaces capturing small bubbles.



Initial plan: Develop methods for accurate measurements of density using the Archimedes method (i.e., establish a SOP).

Extend: We plan on exploring

(i) higher density liquids to more easily/accurately measure low porosity levels
(ii) Surfactants to promote hydrophilicity
(iii) The effect of phases/microstructure on density

We will look toward chemistry to promote hydrophilicity (i.e., compounds like “AcuWet”) and increase the density of liquids (including density separating liquids like fickle gradients)

The primary objective is to develop the following.

(i) The chemistries of surface coatings to make them hydrophilic and temporary (perhaps multifunctional to enhance imaging strategies for surface roughness).
(ii) The chemistries of the liquid to replace water for a new Archimedes approach for additively manufactured materials.
(iii) A standard operating procedure that is reproducible and fast.
(iv) Potentially explore an automated system for analysis.

We will wrestle with how to handle latent porosity with internal unmelted powder.

We will validate our measurements by:

(i) Assessing human factors (reproducibility from different users)

(ii) CT scanning (on a new 225 kV tomography system at ISU) and possible beam line studies

(iii) Robo-Met serial sectioning

We will wrestle with how to handle latent porosity with internal unmelted powder. This will involve other methods beyond the Archimedes method. Possibilities include: multimeasurement data fusion and modeling, emerging NDE methods, surface sensitive NDE techniques, …