

Currently in Texture analysis:

- We have great tools for describing orientation likelihoods
- But new techniques can measure intragranular strain
- Past research has extracted strain Expectation from HEDM
- But now we want the orientation dependent strain likelihood
- This is much harder, but also much more directly useful!

Pythonic ODFs and SODFs for EBSD and far field HEDM

Austin Gerlt, The Ohio State University

Scan here to read more!



Orientations (w/ Bunge angles): $g = g(\phi_1, \Phi, \phi_2)$

Strain tensor: $\epsilon = \epsilon(\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}, \epsilon_{xy}, \epsilon_{yz}, \epsilon_{xz})$

Note: Orientations exist in the Lie Space SO3, and thus use non-Euclidean probability functions

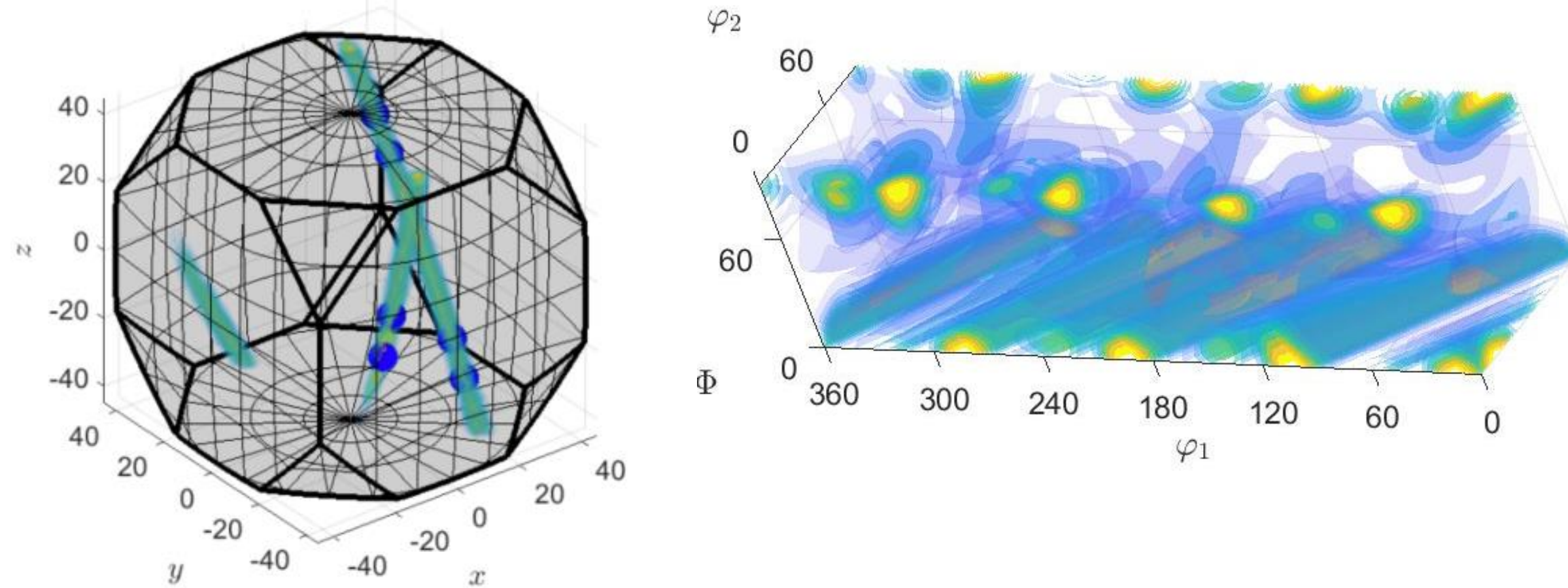
Orientation Distribution Function (ODF):

Gives scalar **Likelihood** of a given orientation.

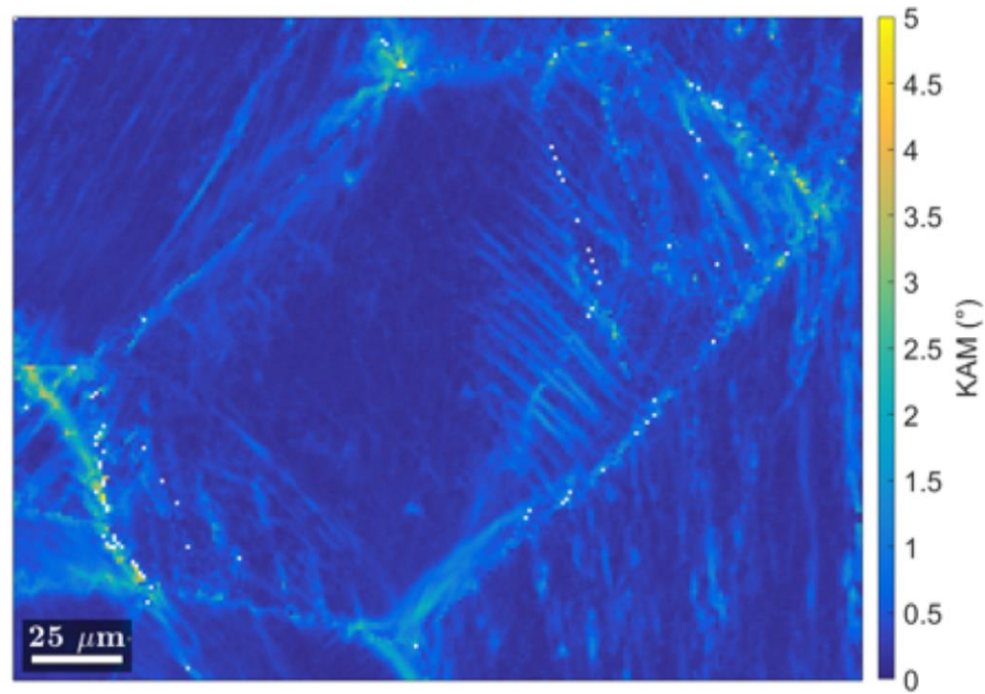
Usually a truncated series of Wigner D matrices (eg: TSL/MTEX)

$$ODF(g) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} c_{mn}^{\ell} D_{mn}^{\ell}(g) = \mathcal{P}(g)$$

For the original Bunge version, the corrected C.S. Mann representation, and details on ODFs, [Scan this QR →](#)



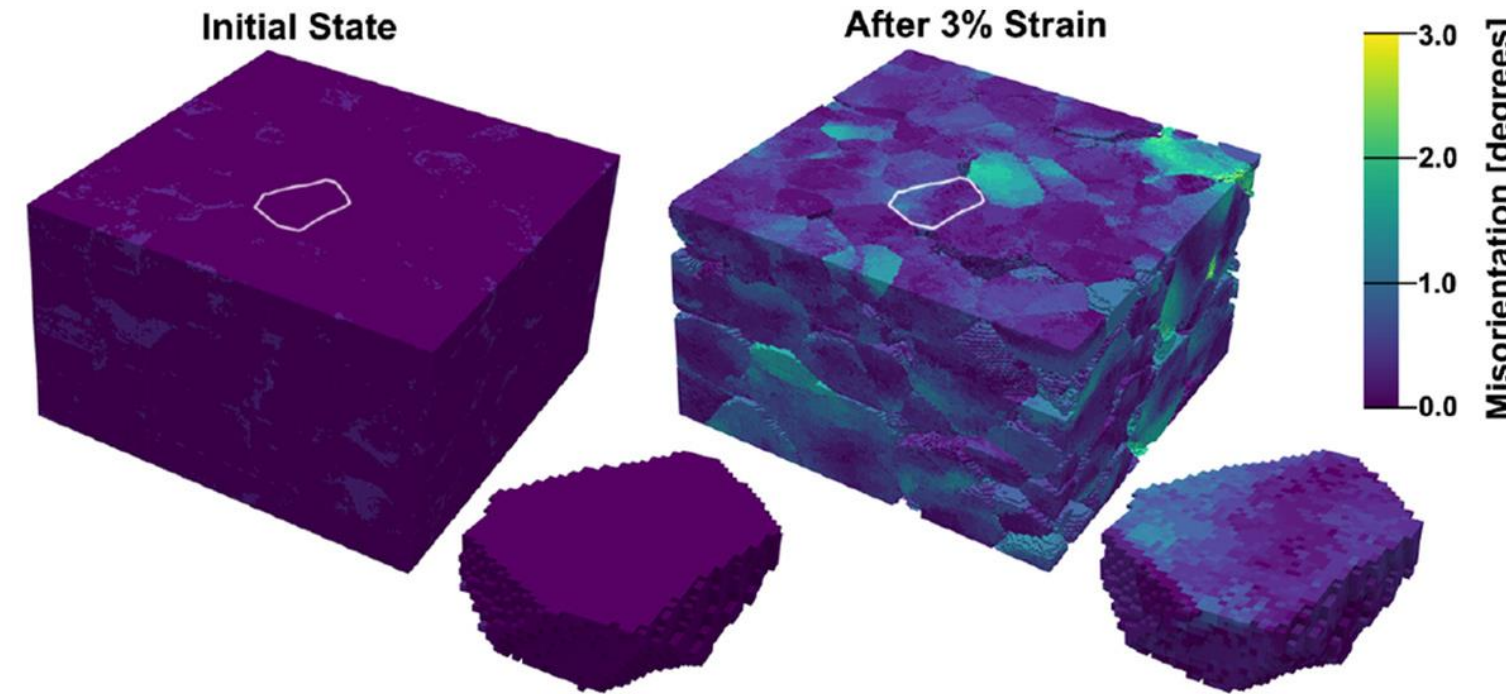
High Resolution EBSD



Gregory Sparks, G. et al, 2021 *Ultramicroscopy*, 2021

← HR-EBSD with 0.02° angular resolution showing slip in Ti-7Al

High Energy Diffraction Microscopy



Kelly Nygren et al, *Materials Characterization*, 2020

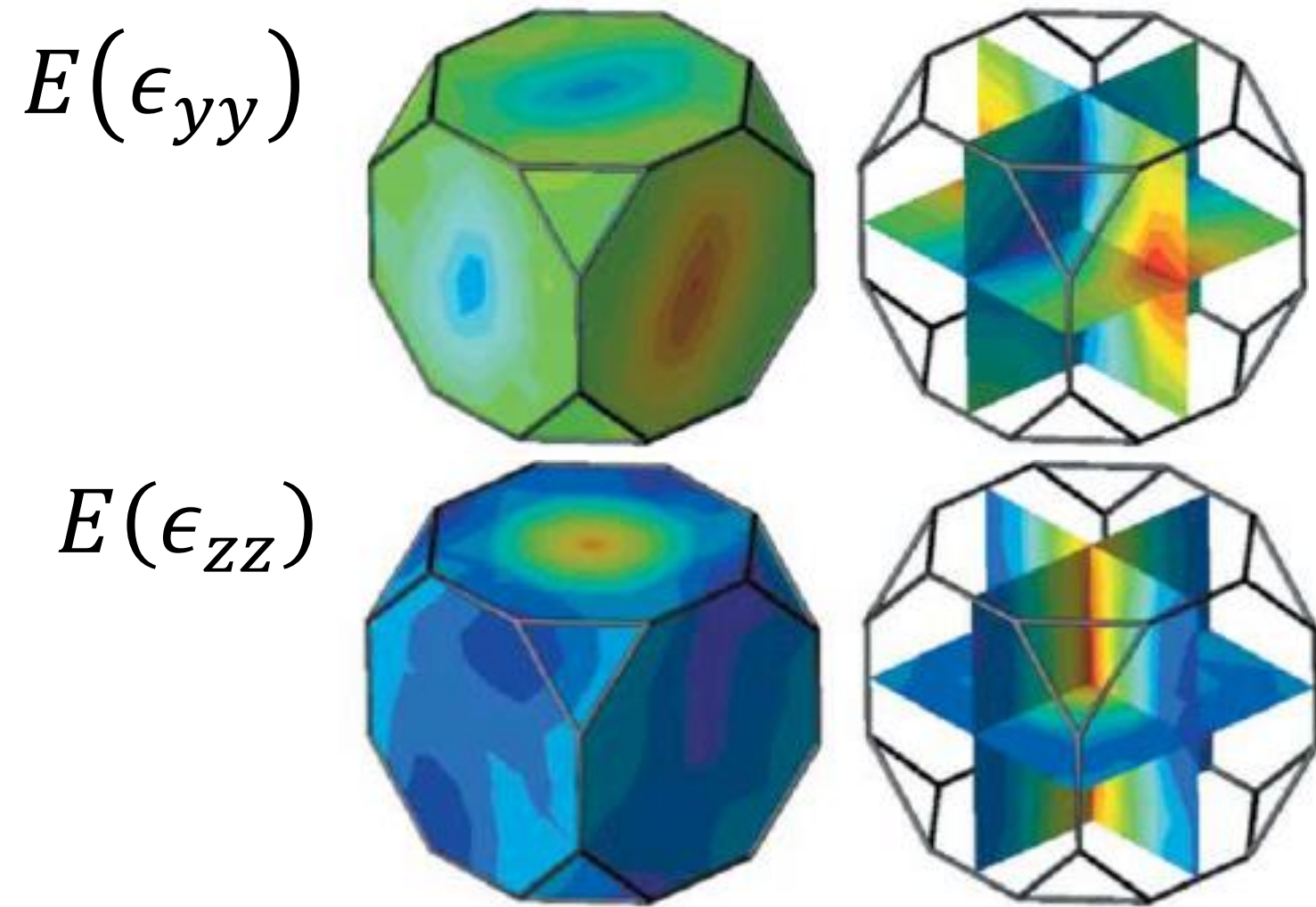
Combined near and far field HEDM showing intragranular strain →

Strain Expectation Function (SEF):

Gives the **Expected** strain, but **NOT the probability**.

$$SEF(g) = E(\epsilon) \text{ or } E(\epsilon|g)$$

- Several papers (Wang, Bernier, and Barton), yet no public code.
- Incorrectly call it an SODF, also ignore conditional probabilities.
- Still, incredible works that laid the groundwork for this study.



Bernier et al, *J. Appl. Cryst.*, 2006

This is already powerful, but we can go further!

Strain Orientation Distribution Function (SODF):

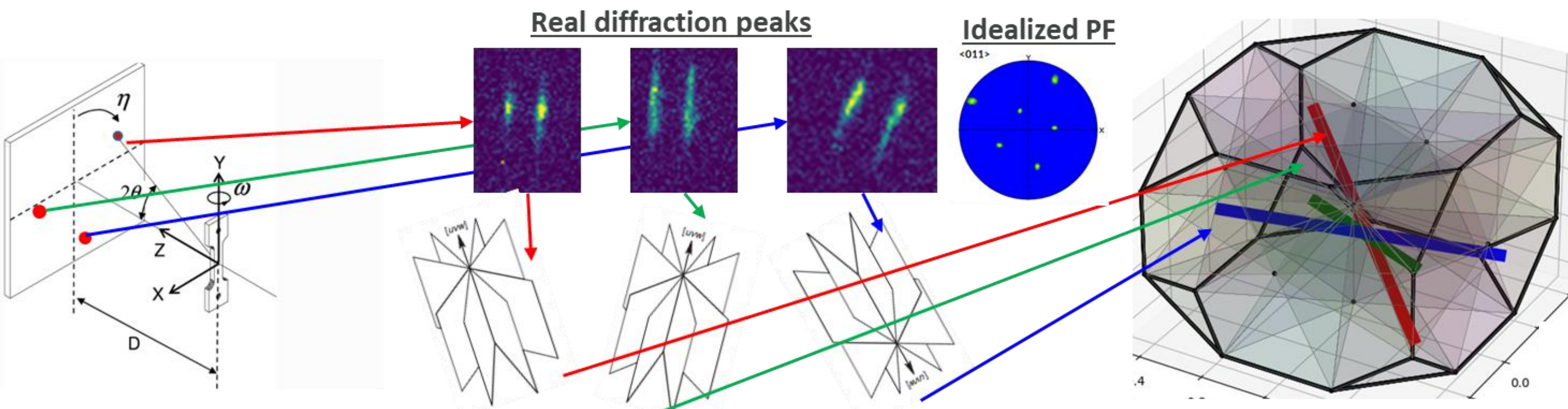
Gives the scalar **Likelihood** of finding any given combination of **Orientation AND Strain**.

$$SODF(g, \epsilon) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} \begin{bmatrix} c_{mn}^{\ell} D_{mnxx}^{\ell}(g) & c_{mn}^{\ell} D_{mnxy}^{\ell}(g) & c_{mn}^{\ell} D_{mnxz}^{\ell}(g) \\ c_{mn}^{\ell} D_{mnyy}^{\ell}(g) & c_{mn}^{\ell} D_{mnyz}^{\ell}(g) & c_{mn}^{\ell} D_{mnzz}^{\ell}(g) \end{bmatrix} = \mathcal{P}(g, \epsilon)$$

- Could also be reframed as the conditional probability, $\mathcal{P}(g|\epsilon)$
- This hasn't been done before, and the best method for doing so is still unclear
 - Currently trying a 4D FEM, as well as a variant on Generalized Spherical Harmonics.

Challenge 1: create open source pythonic ODFs

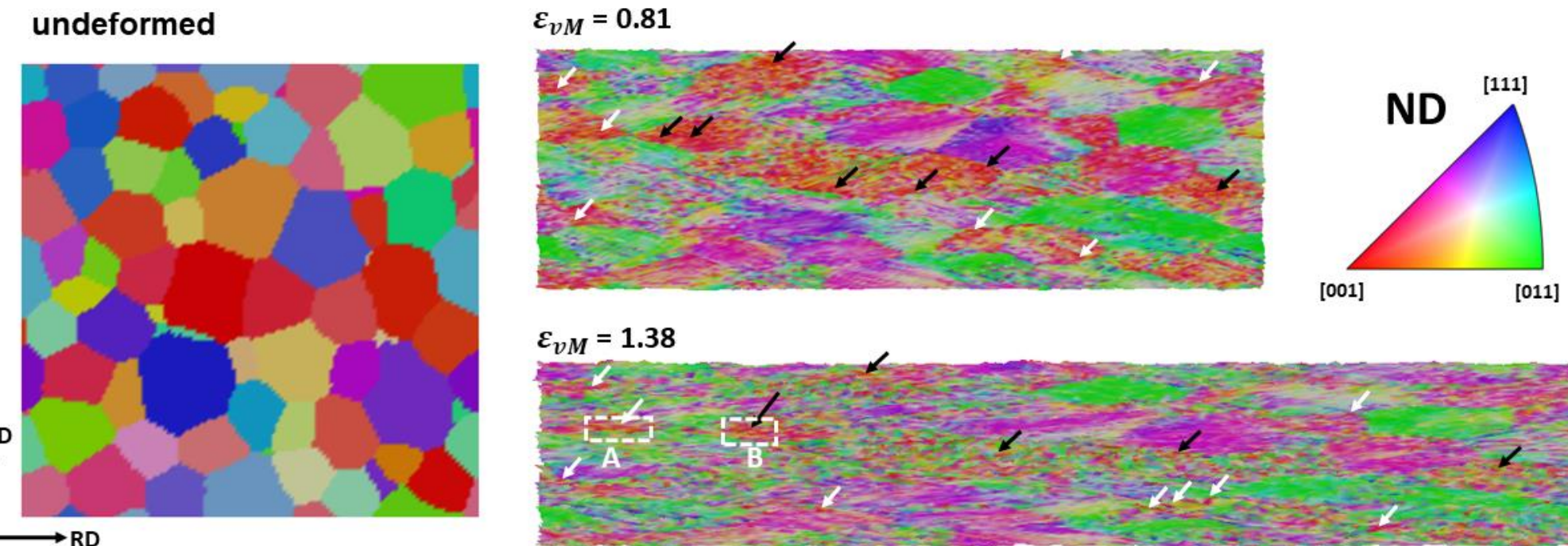
Need a user-friendly MTEX-like solution, but for HEDM (thus must also solve Pole figure inversion)



Challenge 2: Extrapolate to create the SODF

Crucial to building better Plasticity models. An **SEF** tell how far a solution **differs from the mean**, but an **SODF** states **how likely a solution is**.

Dislocation-Density Plastic Deformation Model



Chakraborty et al, *Met Trans A*, 2022

Background Information



Citations



Sparks 2021



Nygren 2020



Wang 2001



Barton 2012



Chakraborty 2022



Bernier 2006

Repos and Results

