Electron Backscatter Diffraction Pattern Simulation for Interaction Volume Containing Lattice Defects

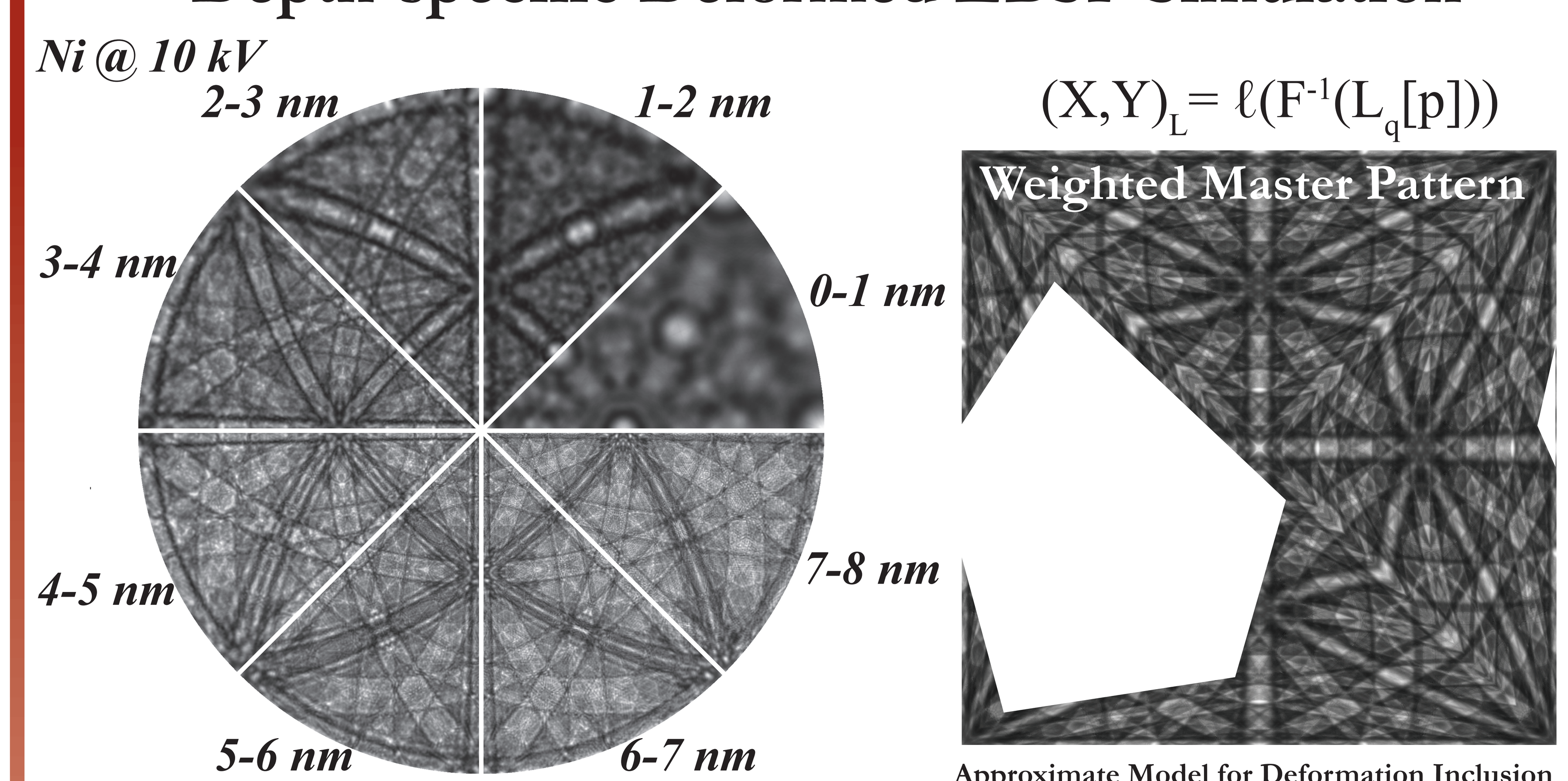
Chaoyi Zhu, Marc De Graef
Department of Materials Science and Engineering, Carnegie Mellon University
5000 Forbes Avenue, Pittsburgh PA 15213-3890, USA
Funding Source: DoD Vannevar-Bush Faculty Fellowship (# N00014-16-1-2821)

Introduction and Background

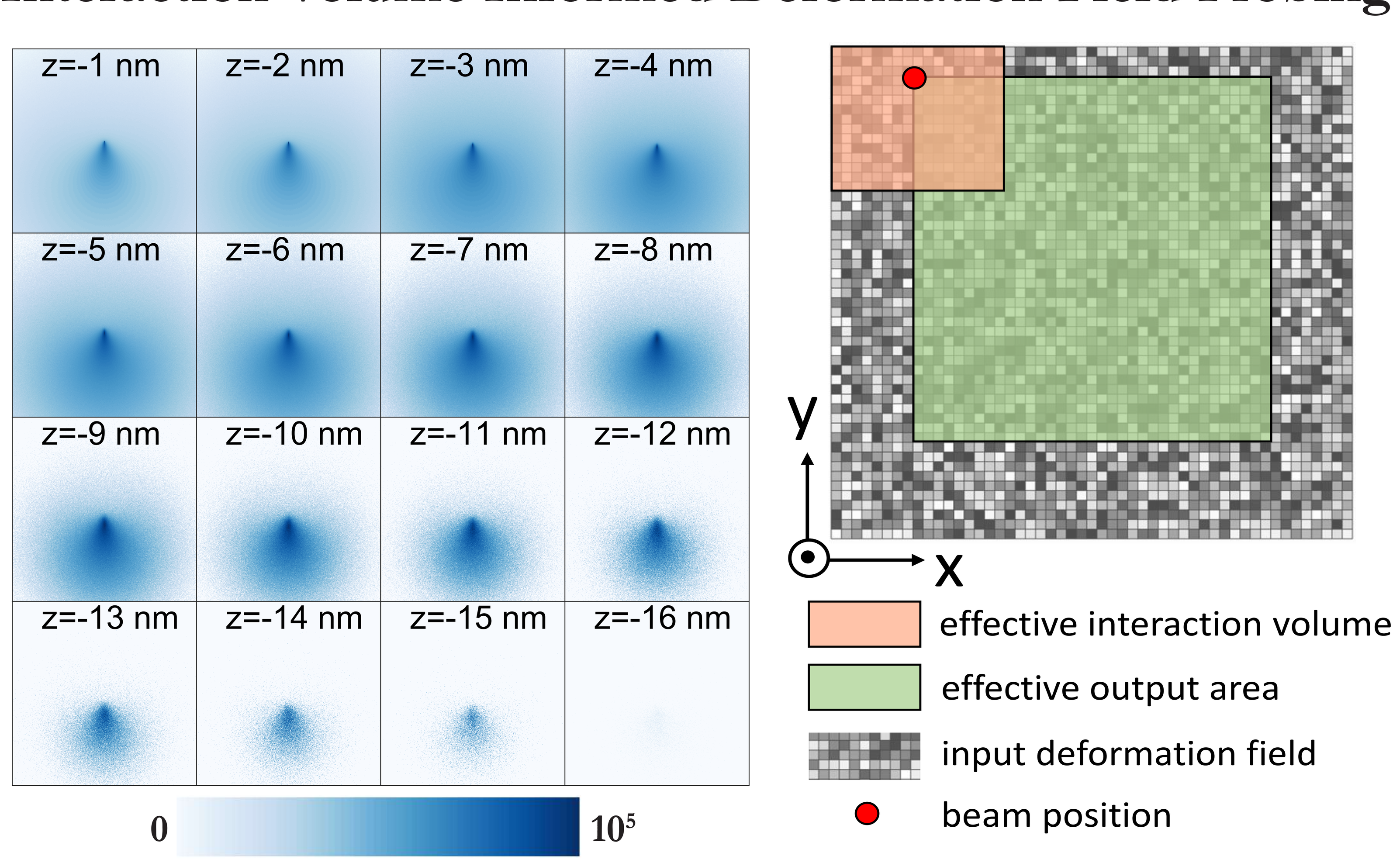
Electron backscatter diffraction (EBSD) is a SEM based characterization technique which allows researchers to speedily probe surface information of a crystalline sample e.g. local texture, defect density, etc over a large area of interest. Despite the existence of numerous experimental studies on lattice defects with EBSD, no study has been done so far to systematically investigate these effect from the perspective of pattern simulation. In this study, we have implemented dynamical depth-specific deformed pattern simulation over the entire interaction volume, which allows us to map deformation field of single dislocation and a low angle grain boundary under low accelerating voltage (10kV).

Theory

Depth-specific Deformed EBSP Simulation



Interaction Volume Informed Deformation Field Probing



Callahan, P.G. *and De Graef, M.,* 2013. Microscopy and Microanalysis.
Winkelmann, A., *et al*, *2007.* Ultramicroscopy.
Joy, D.C., *1995;* De Graef, M., *2003;* Schwartz, A.J., *et al eds.,* 2009.

Validation

Yoffe's Screw Dislocation Model

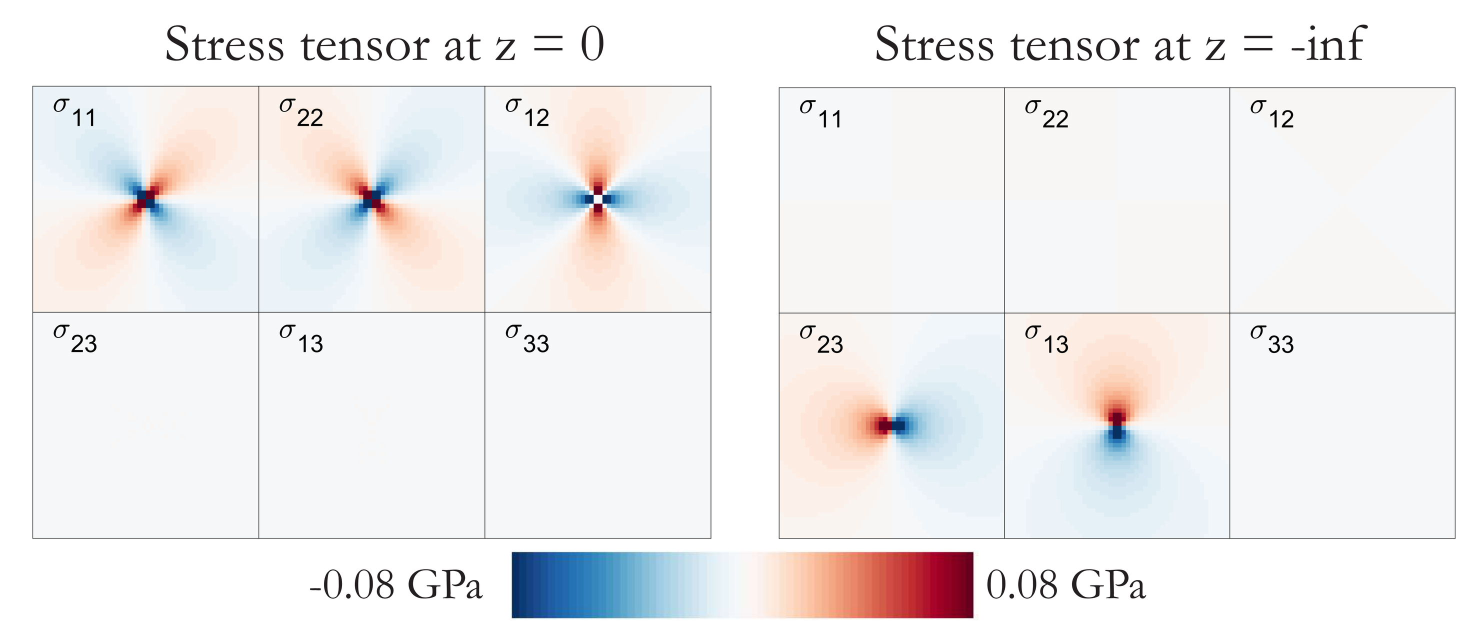
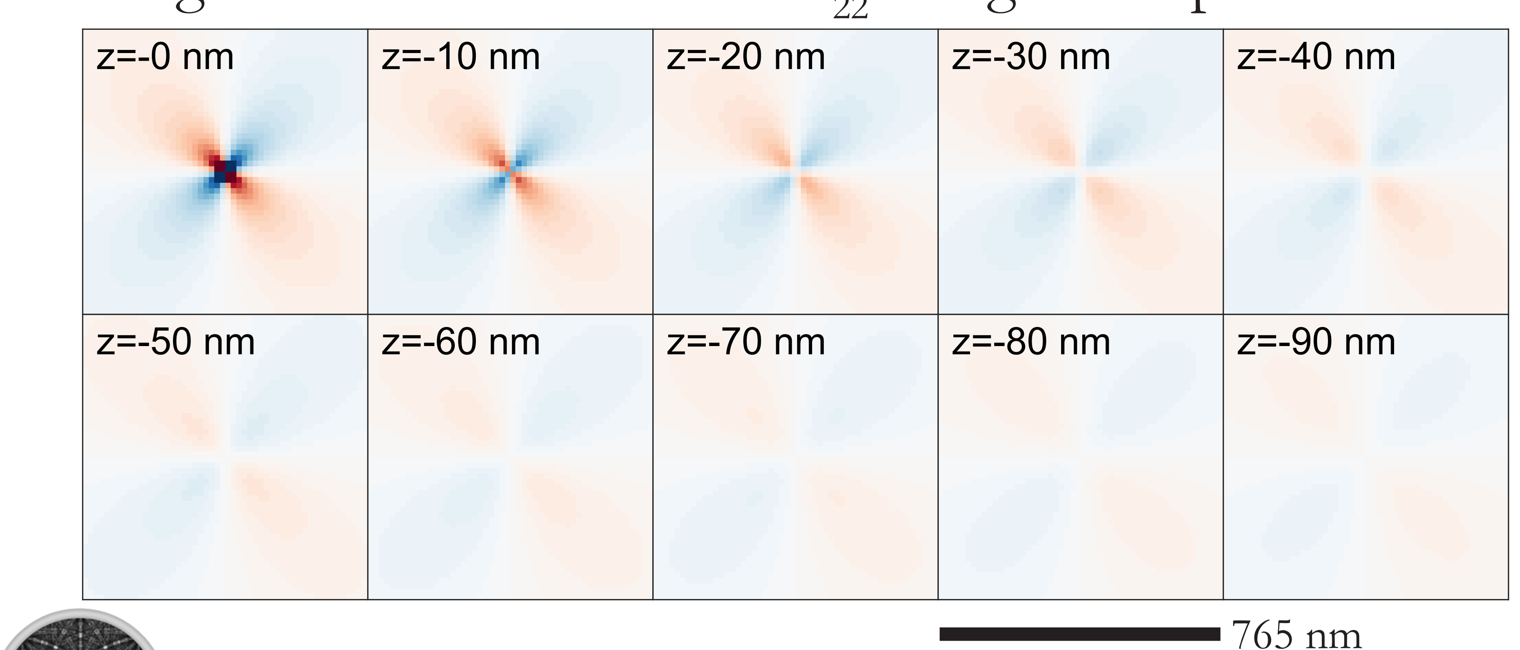
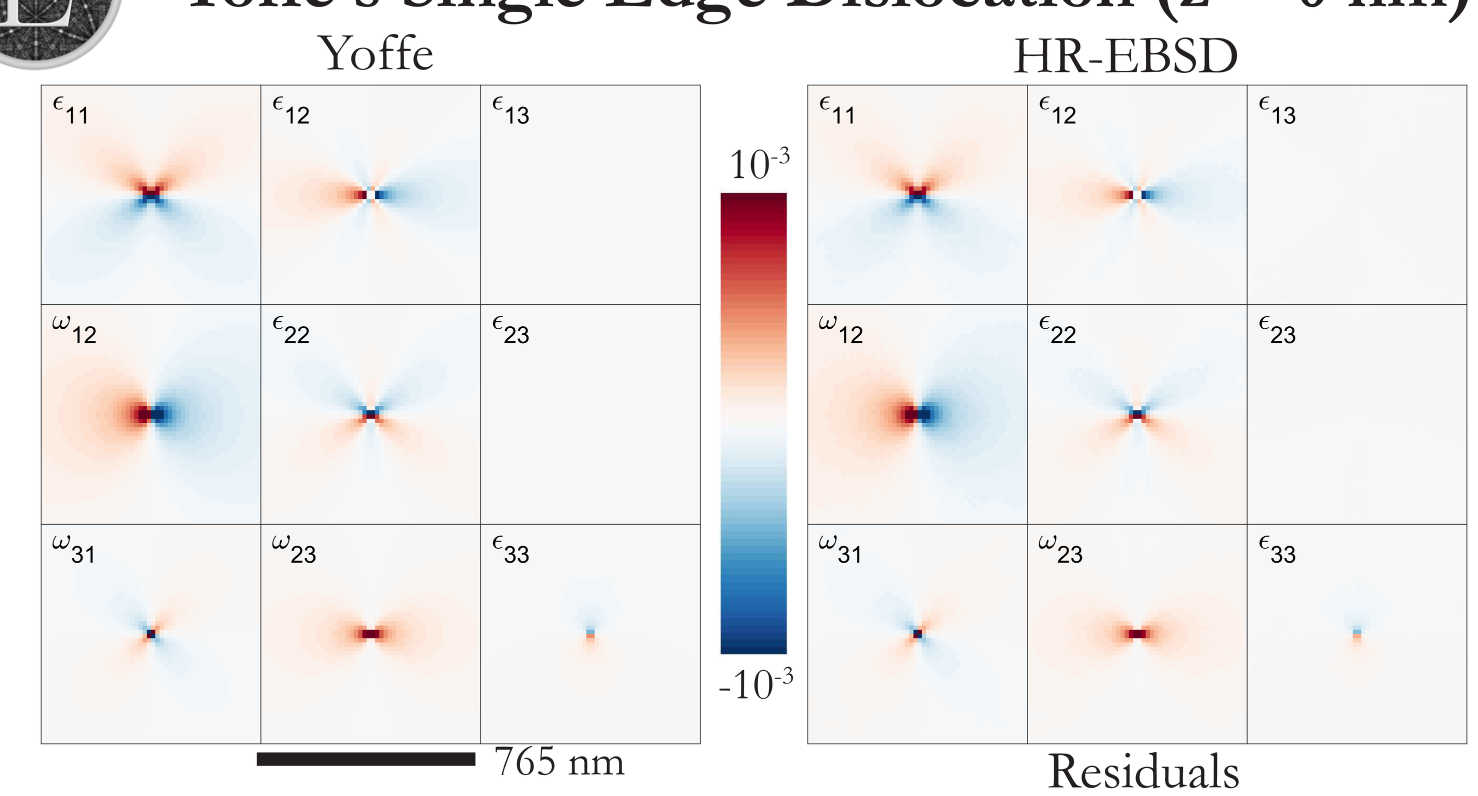
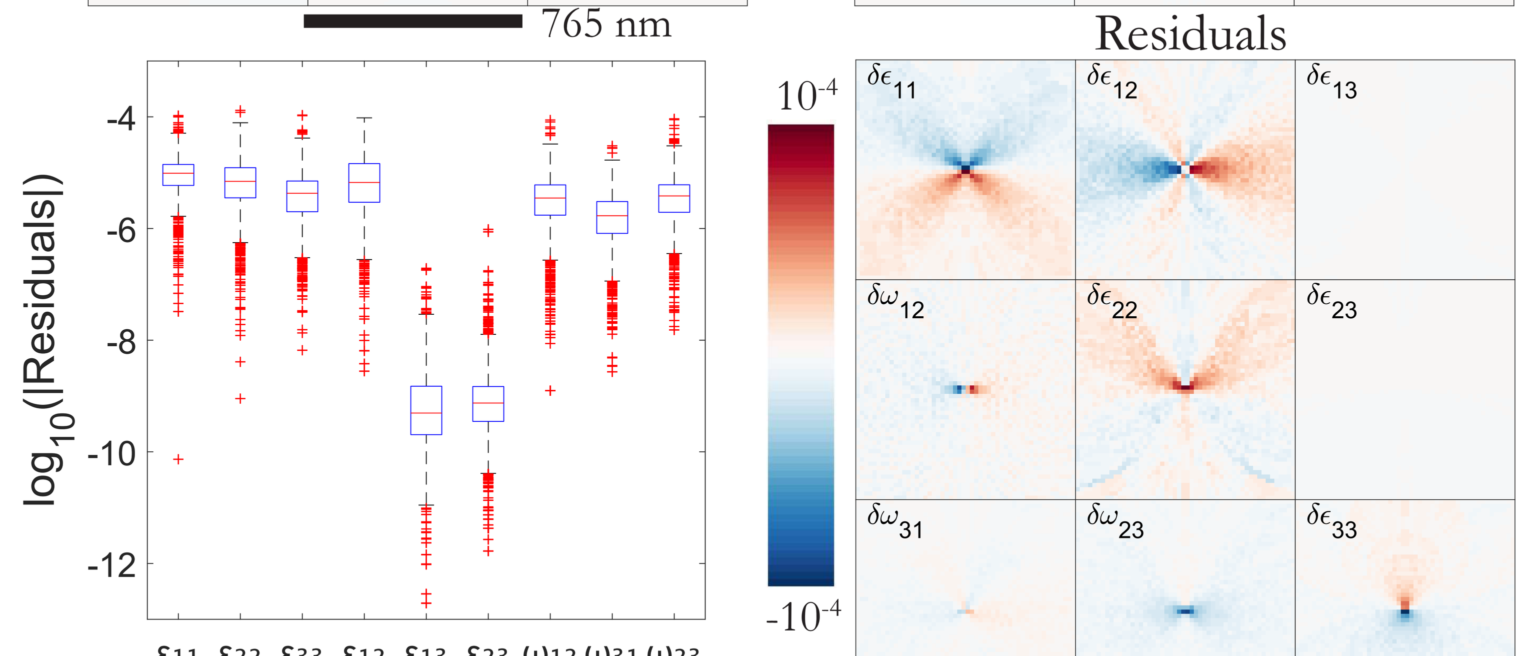


Image stress attenuation for σ_{22} along the depth direction



Yoffe's Single Edge Dislocation (z = 0 nm)

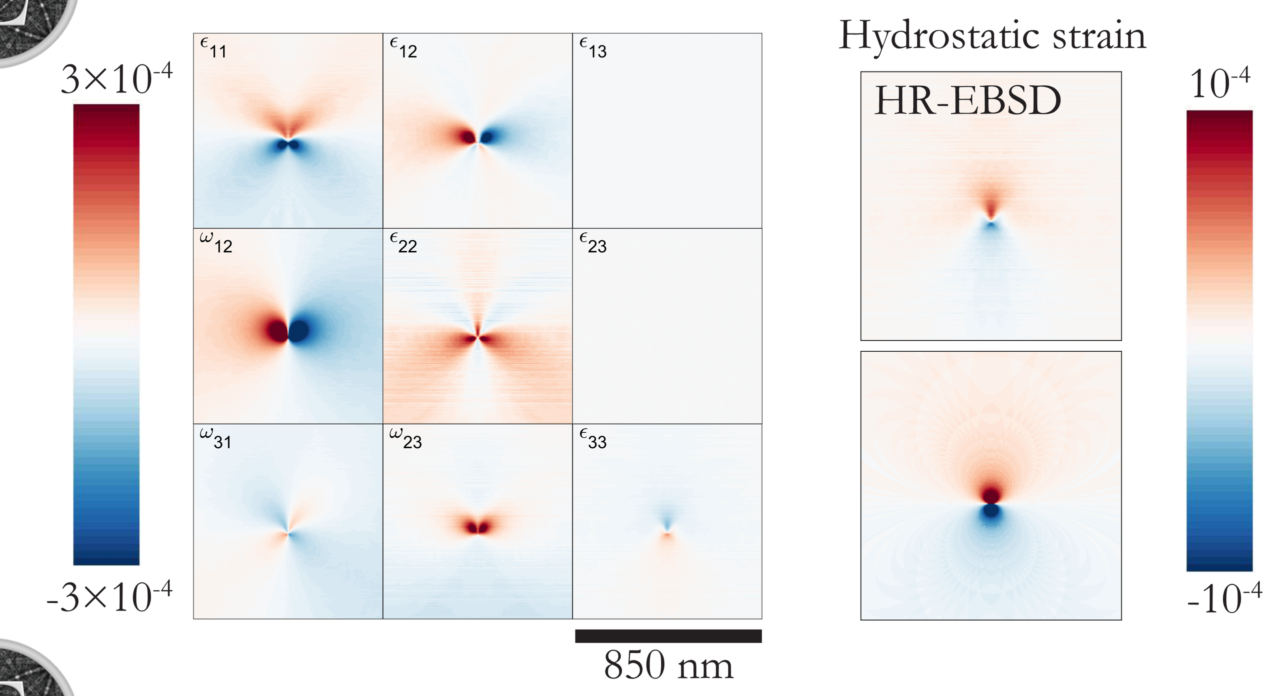




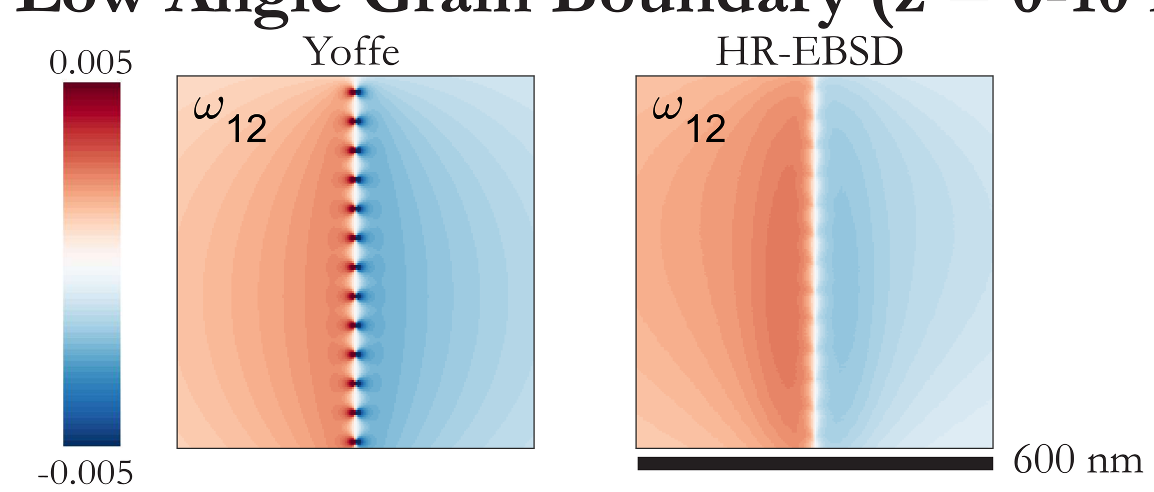
Yoffe, E.H., *1961.* Philosophical Magazine.
Shaibani, S.J. and Hazzledine, P.M., *1981.* Philosophical Magazine A

Results

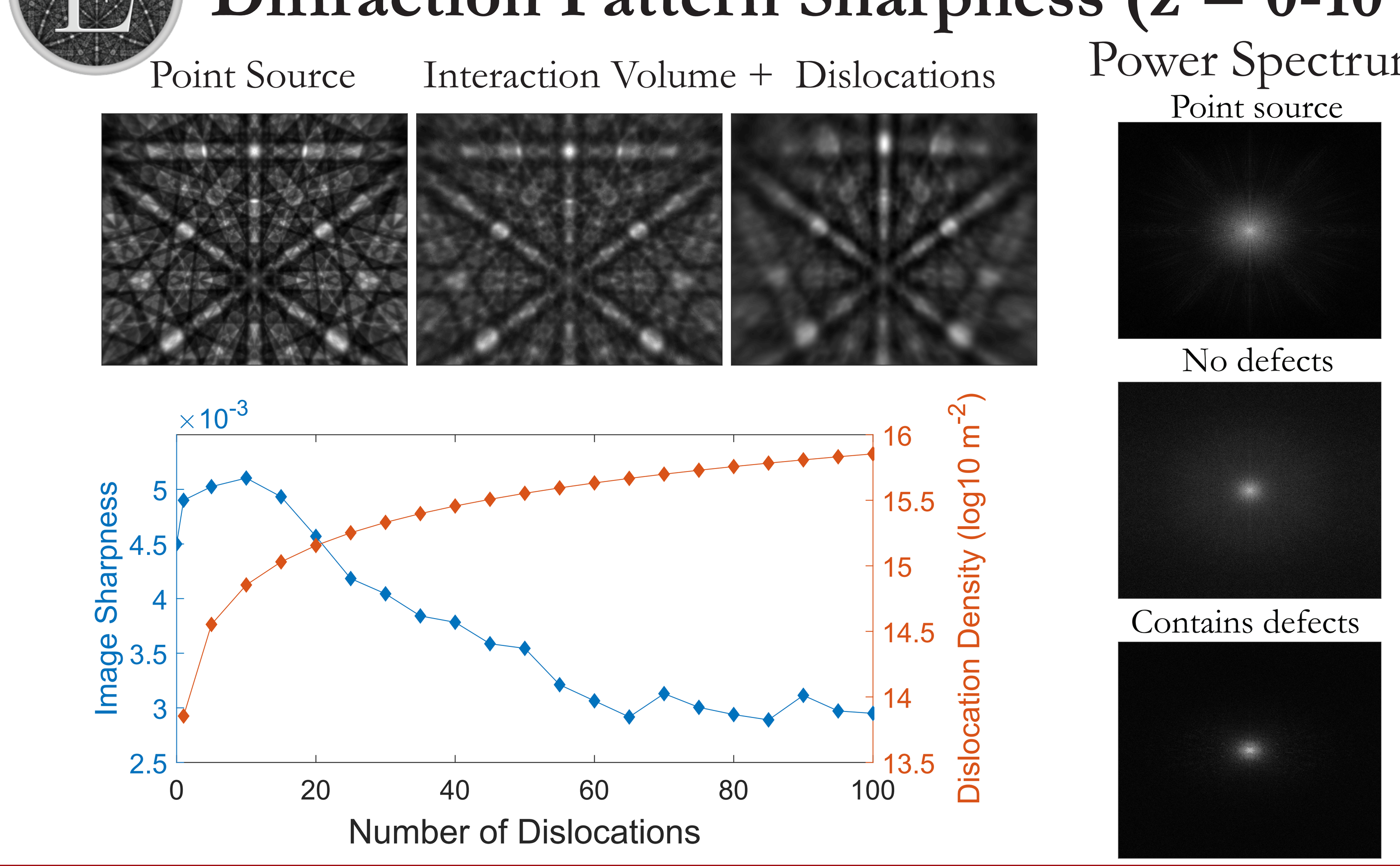
Yoffe's Single Edge Dislocation (z = 0-10 nm)



Low Angle Grain Boundary (z = 0-10 nm)



Diffraction Pattern Sharpness (z = 0-10 nm)



Conclusion

- interaction volume for Ni at 10 kV occupies ~16 nm surface material.
- image stress attenuates rapidly in the first 20 nm surface material.
- approximate model for deformation inclusion in pattern simulation is an accurate for surface deformation with a sensitivity $\leq 10^{-4}$.
- interaction volume containting defects reduces the pattern sharpness.
- interaction volume approach for pattern simulation reduces the magnitude/sharpness of deformation field around dislocations and distort the shape of deformation field.

Github: https://github.com/EMsoft-org/EMsoft