Internal Elastic Fields and The Dislocation Density Tensor in Deformed FCC Crystals: Computational Modeling and Experimental Measurements

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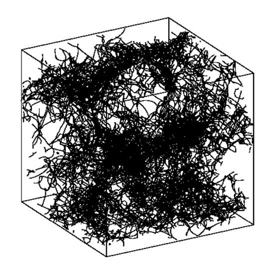
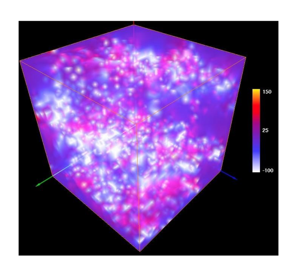
Motivation

- Mesoscale plastic deformation of crystals is governed by motion and interaction of large dislocation systems.
- The evolution of dislocation systems is connected to their internal elastic fields, which exhibit a statistical nature due to dislocation density fluctuations.
- 3D X-ray microscopy techniques now have the capability to measure internal elastic fields and dislocation density tensors with sub-micrometer resolution, making possible direct comparison with dislocation dynamics deformation simulations.
- Understanding the statistics of internal elastic fields and the dislocation density tensor helps complete the mesoscale crystal plasticity theory.
- Here we present initial investigation of these statistics using both computer simulations and experimental measurements.

A volume of deformed crystal showing mesoscale deformation features



Resolved region showing complex dislocation structure



Internal stress of dislocation system exhibits statistical features

Boundary Value Problem of Dislocations

- Dislocation stress in a bounded crystal volume consists of two contributions:

$$\sigma(r) = \sigma^{\infty}(r) + \sigma^{img}(r)$$

- Infinite-domain solution is obtained from non-singular analytic formula:

$$\sigma^{\infty,ns}_{\alpha\beta}(r) = -\frac{\mu}{8\pi}\oint_C b_m e_{im\alpha}\partial'_i\partial'_p\partial'_p R_a dr'_\beta - \frac{\mu}{8\pi}\oint_C b_m e_{im\beta}\partial'_i\partial'_p\partial'_p R_a dr'_\alpha - \frac{\mu}{4\pi(1-\nu)}\oint_C b_m e_{imk}\left(\partial'_i\partial'_\alpha\partial'_\beta R_a - \delta_{\alpha\beta}\partial'_i\partial'_p\partial'_p R_a\right)dr'_k$$

- Image stress is the solution of a boundary value problem of dislocations:

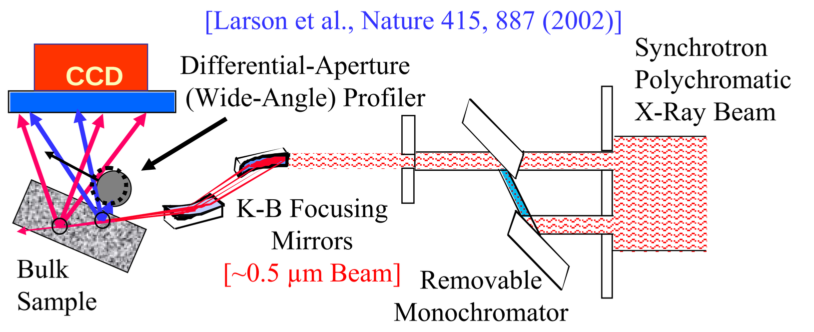
$$\nabla\cdot\sigma^{img}(r) + \nabla\cdot\sigma^{\infty}(r) = 0 \quad \text{with boundary conditions} \quad \sigma^{img}(r)n(r) = -\sigma^{\infty}(r)n(r)$$

- Internal elastic strain and lattice rotations by dislocations are part of the elastic solution.
- The dislocation density tensor is determined by lattice curvature and elastic strain gradients in the infinitesimal distortion regime:

$$\alpha_{ij} = \kappa_{ji} - \delta_{ij}\kappa_{kk} - e_{ikl}\partial_k\varepsilon_{lj}$$

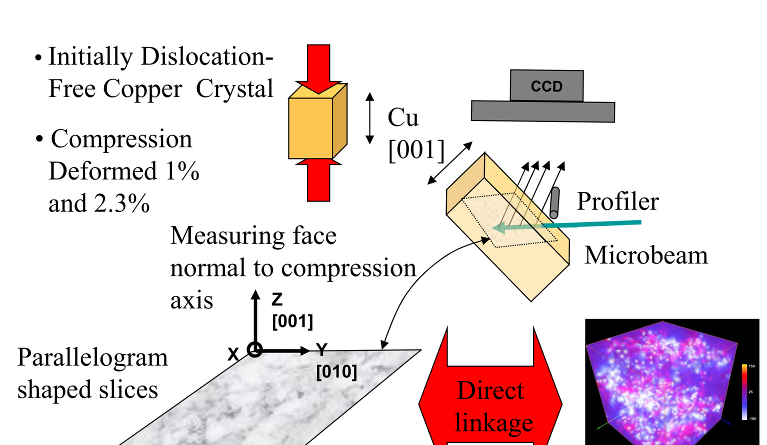
Experimental Measurement

Differential-Aperture 3D X-Ray Microscopy*



- White Beams Generate Full Laue Diffraction Pattern for Each Submicron Segment
- Local Structure, Orientation, Full Strain Tensor, Deformation Microstructure

Measurements on Compressed Cu



Schematic of 3D X-ray Microscopy Deformation Microstructure Measurement

Dislocation Dynamics Simulation of Deformation in [001] strained Cu

*Measurements performed on Sector 34 ID-E, Advanced Photon Source, ANL

Statistical Modeling

- The statistics of internal elastic fields and dislocation density tensor has been modeled by generalized n-th order probability density function of dislocation density $f^{(s_1,\cdots,s_n)}(r_1,\theta_1,\cdots,r_n,\theta_n)$
- First order probability density function of internal elastic fields:

$$p_{ij}(\beta_\circ,r) = \sum_{s_1,\cdots,s_n}\int_\Omega f^{(s_1,\cdots,s_n)}(r_1,\theta_1,\cdots,r_n,\theta_n)\delta\left[\beta_\circ - \beta_{ij}(r)\right]dr_1 d\theta_1\cdots dr_n d\theta_n \longrightarrow p_{ij}(\beta_\circ) = \int_V p_{ij}(\beta_\circ,r)/V$$

- Pair correlation function of internal elastic fields:

$$C_{ijkl}(r,r') = \langle\beta_{ij}(r)\beta_{kl}(r')\rangle / \left(\langle\beta_{ij}(r)\rangle\langle\beta_{kl}(r')\rangle\right) \longrightarrow C_{ijkl}(\Delta r) = \langle\beta_{ij}(r)\beta_{kl}(r+\Delta r)\rangle / \sqrt{\langle\beta^2_{ij}(r)\rangle\langle\beta^2_{kl}(r+\Delta r)\rangle}$$

- First order probability density function of dislocation density tensor:

$$p_{ij}(\alpha_\circ,r) = \sum_{s_1,\cdots,s_n}\int_\Omega f^{(s_1,\cdots,s_n)}(r_1,\theta_1,\cdots,r_n,\theta_n)\delta\left[\alpha_\circ - \alpha_{ij}(r)\right]dr_1 d\theta_1\cdots dr_n d\theta_n \longrightarrow p_{ij}(\alpha_\circ) = \int_V p_{ij}(\alpha_\circ,r)/V$$

- Higher order probability density functions and correlation functions can be formulated by following the same strategy.

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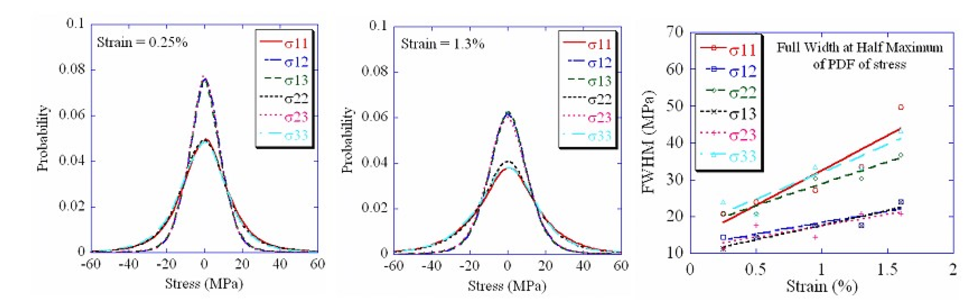
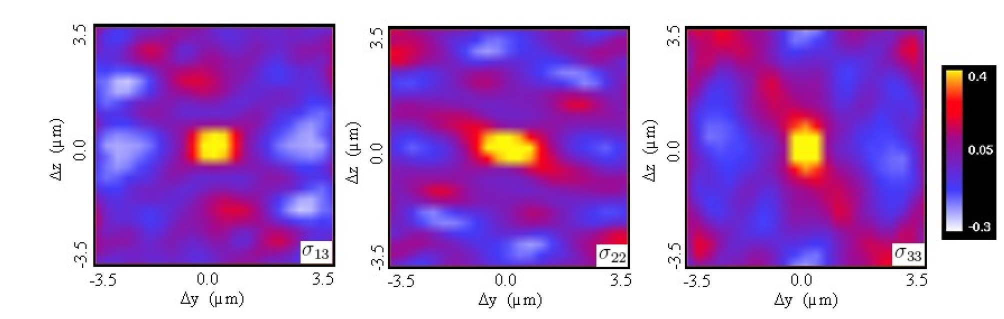
Preliminary Results

- Probability distribution for internal stress fields of dislocations in deformed Cu



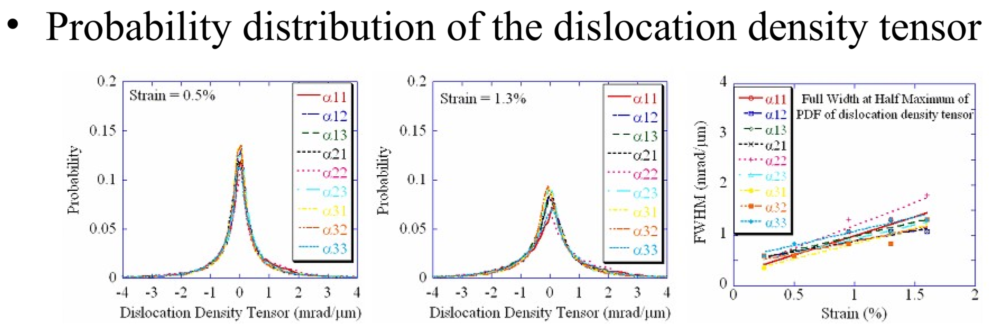
- All stress components are distributed similarly.
- Stress fluctuations increase as the strain level and dislocation density increase.

- Pair correlation of internal stress fields of dislocations in deformed Cu



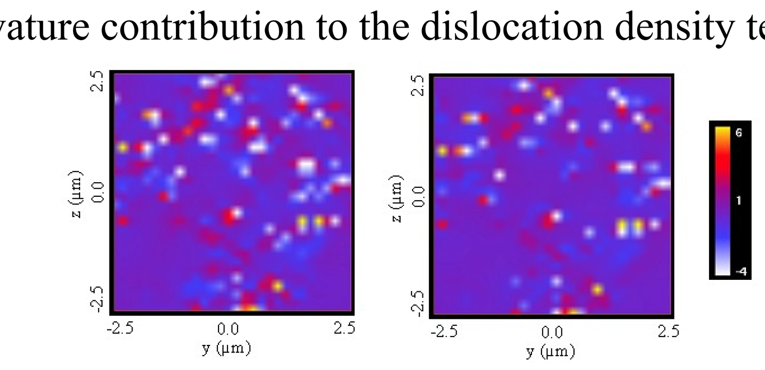
- Distributions are dependent on the dislocation density and related to its correlation.
- Anisotropic distribution indicates stress patterning.

- Probability distribution of the dislocation density tensor in deformed Cu



- The probability distributions for dislocation density tensor components in deformed Cu are symmetric with widths that increase linearly with strain.

- Curvature contribution to the dislocation density tensor in deformed Cu

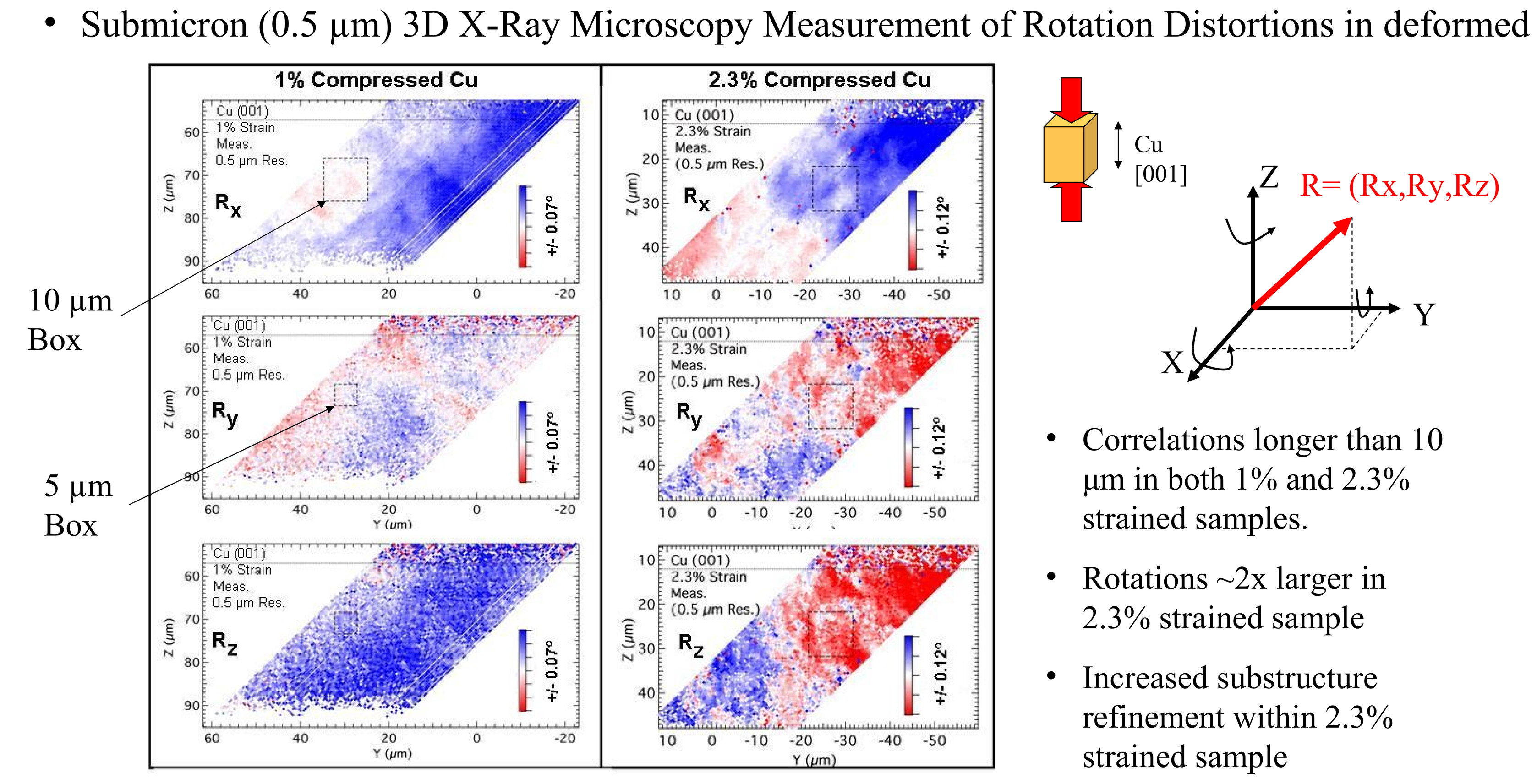


Left: Dislocation density tensor component α_{12} (mrad/µm)

Right: Curvature contribution

- The dislocation density tensor is determined mainly by the curvature part in deformed metals.

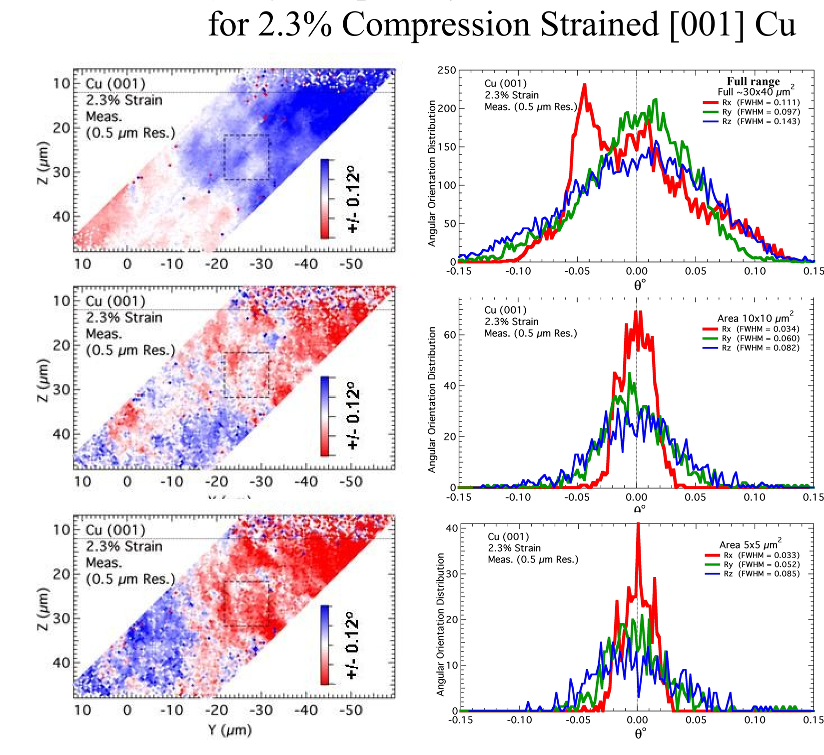
- Submicron (0.5 µm) 3D X-Ray Microscopy Measurement of Rotation Distortions in deformed Cu



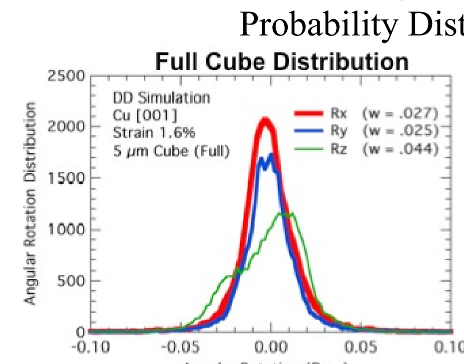
- Correlations longer than 10 µm in both 1% and 2.3% strained samples.
- Rotations ~2x larger in 2.3% strained sample
- Increased substructure refinement within 2.3% strained sample

- Initial Quantitative Comparison of Rotation Probability Distribution Measurements with Dislocation Dynamics Simulations for [001] Compression Strain in Copper

Submicron (0.5 µm) Spatially Resolved Rotation Measurements for 2.3% Compression Strained [001] Cu

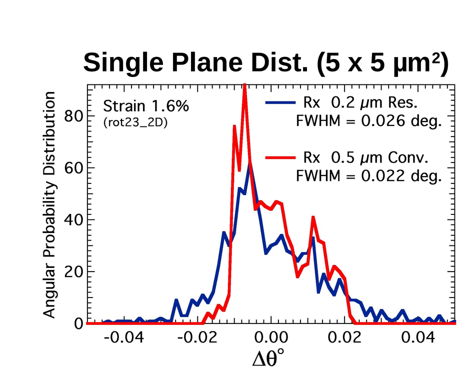


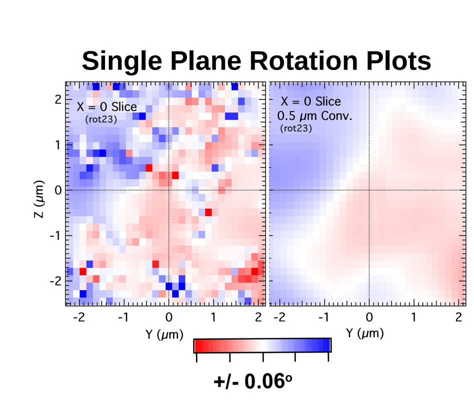
Dislocation Dynamics Simulations of the Rotation Probability Distribution in 1.6% Strained Cu



Comments

- Rotation probability distributions show non-symmetric distributions for measurements and simulations
- Single plane 5 x 5 µm² rotation probability distributions are more narrow than full sample measurements and simulations
- Impact of 0.5 µm measurement spatial resolution on the rotation probability distribution is moderate





Discussion

- Statistical analysis shows the internal elastic fields and dislocation density tensor are distributed anisotropically, with zero mean value and strain-dependent fluctuations.
- The internal elastic fields exhibit long-range correlations that are related to the distribution and correlations within the underlying dislocation structure.
- The analysis shows that the dislocation density tensor components exhibit symmetric distributions, which can be attributed to the zero mean lattice curvature and the statistical homogeneity of deformation process.
- The analysis has also shown that local curvature is the main contributor to the dislocation density tensor in deformed metals.
- Initial comparison between 3D x-ray microscopy measurements and dislocation dynamics simulations of deformation in Cu show semi-quantitative agreement, but also indicate the need for larger simulation volumes and measurements with improved spatial resolution.