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Dislocation-induced Elastic Fields for FCC Crystals

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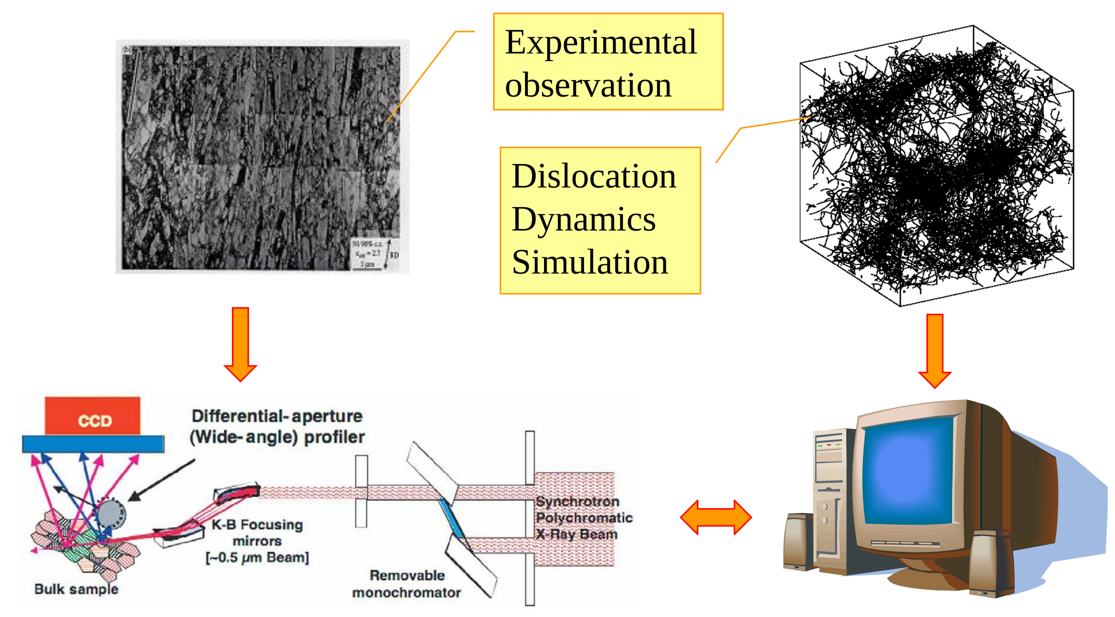
Introduction

- Plastic deformation leaves crystals highly dislocated.
- The **internal fields** of these dislocations represent the main signature of the dislocation structures that can be probed experimentally.
- Namely the **lattice rotation** and **elastic strain** can be used to compute the **dislocation density tensor**, a key geometric measure for the dislocation system in distorted crystals.



- X-ray microscopy currently provides spatially resolved measurements of local lattice orientation and dislocation density tensor in 3D and with sub-micron scale resolution.
- This provides a previously missing bridge between mesoscale deformation **experiments** and computer **simulations** results.
- We investigate the statistical behavior of those fields, as a step towards comparison between mesoscale simulations and experiments.

Theory and Results

Elastic Fields Calculation

- The elastic strain and lattice rotation fields of dislocations inside a finite crystal volume have two contributions:
  - Infinite contribution: from the classic line-integral form of the elastic solution of dislocations inside an infinite elastic medium.
  - Image contribution: is calculated by solving a traction boundary value problem .
- The dislocation density tensor can then be evaluated as:

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

where is δ_{ij} the Kronecker delta, e_{ikl} is the permutation symbol, and κ_{ij} is the lattice curvature tensor defined as the gradient of the lattice orientation $\kappa_{ij} = \partial_i \theta_j$, and θ_i is the lattice rotation, defined in terms of the lattice rotation field as $\omega_{ij} = e_{ijk}\theta_k$.

Statistical measures

- The statistical behavior of those fields is demonstrated via probability density function (PDF) and pair correlation function (PCF).
- For any field β_{ij} , the **PDF** can be defined as:

$$p_{ij}(\beta_o) = \int_V p_{ij}(\beta_o, x)/V \quad \text{where}$$

$$p_{ij}(\beta_o, x) = \sum_{s_1,\dots,s_n}\int_\Omega f^{(s_1,\dots,s_n)}(x_1,\theta_1,\dots,x_n,\theta_n)\,\delta\left[\beta_o - \beta_{ij}(x)\right]dx_1 d\theta_1 .. dx_n d\theta_n$$

n : no. of segments
s_i : slip system index

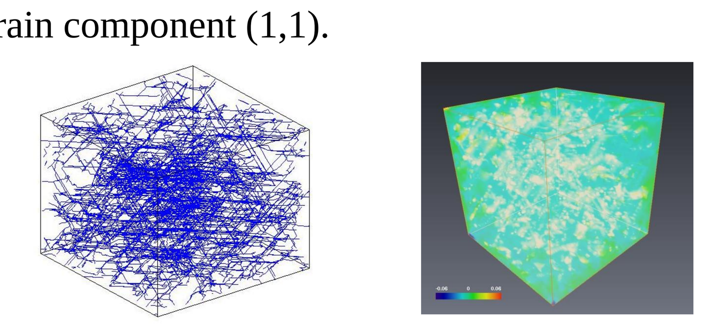
where $f^{(s_1,\dots,s_n)}(x_1,\theta_1,\dots,x_n,\theta_n)$ is the n-th order PDF for the dislocation density.

•The **PCF** can be defined as:

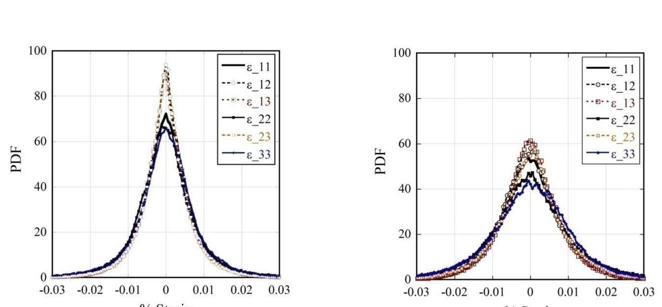
$$C_{ijkl}(\Delta\mathbf{x}) = \frac{Cov\left(\beta_{ij}(\mathbf{x}),\beta_{kl}(\mathbf{x}+\Delta\mathbf{x})\right)}{\sqrt{Var\left(\beta_{ij}(\mathbf{x})\right)Var\left(\beta_{kl}(\mathbf{x}+\Delta\mathbf{x})\right)}} = \frac{\langle\beta_{ij}(\mathbf{x})\,\beta_{kl}(\mathbf{x}+\Delta\mathbf{x})\rangle - \langle\beta_{ij}(\mathbf{x})\rangle\langle\beta_{kl}(\mathbf{x}+\Delta\mathbf{x})\rangle}{\sqrt{\left(\langle\beta_{ij}^2(\mathbf{x})\rangle - \langle\beta_{ij}(\mathbf{x})\rangle^2\right)\left(\langle\beta_{kl}^2(\mathbf{x}+\Delta\mathbf{x})\rangle - \langle\beta_{kl}(\mathbf{x}+\Delta\mathbf{x})\rangle^2\right)}}$$

Elastic Strain Field

- The below figures show the discrete dislocation structure at strain level ~ 0.65%, and the elastic strain component (1,1).

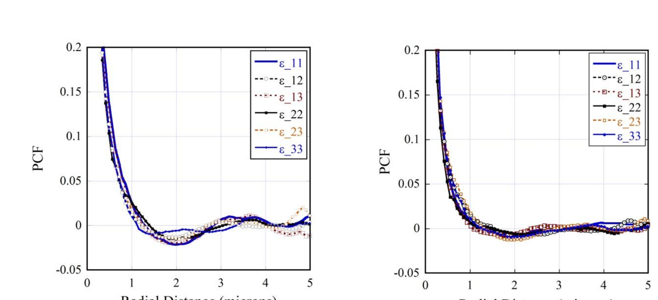


•The PDF for strain components is shown:



- The PDF is symmetric around zero mean, and its peak decays with strain level (similar to internal stress PDF).

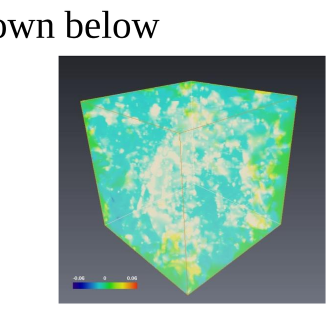
•The PCF for the elastic strain is shown below



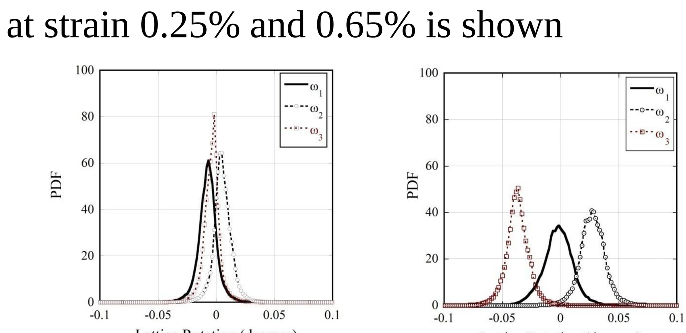
•The correlation decays fast to the uncorrelation value, followed by fluctuations

Lattice Rotation

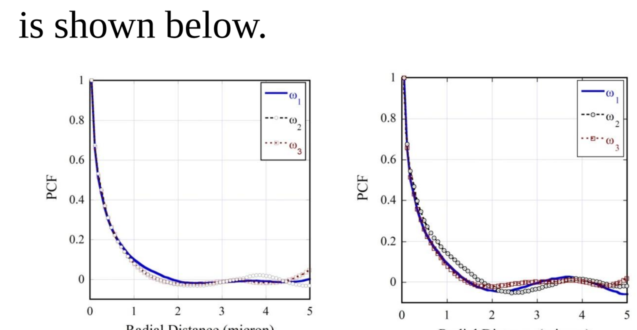
- 3D map for the lattice rotation components (1) is shown below



- The PDF for the lattice rotation components at strain 0.25% and 0.65% is shown



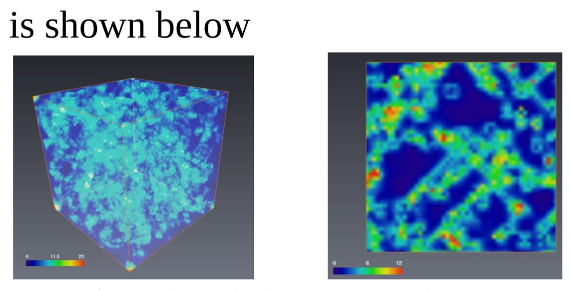
- The PDF is almost symmetric around non-zero mean, and also its peak decays with strain level.
- The PCF for the lattice rotation components is shown below.



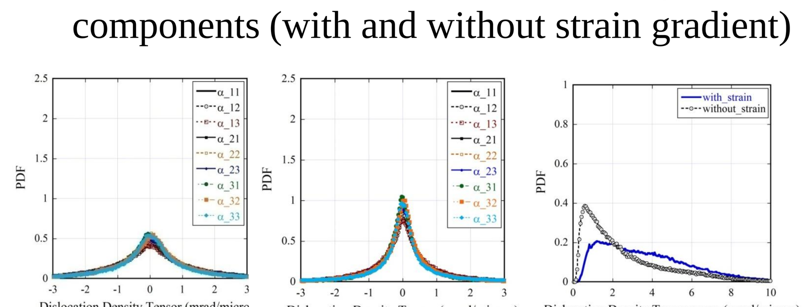
- The PCF decays fast to the uncorrelation value, followed by fluctuations that seems to get enhanced with the strain level

Dislocation Density Tensor

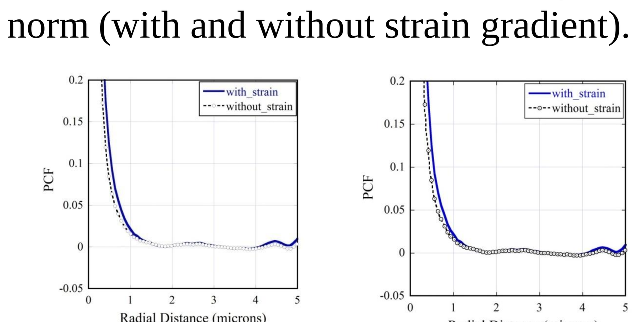
- 3D map for the dislocation density tensor norm is shown below



- The PDF for the dislocation density tensor components (with and without strain gradient)

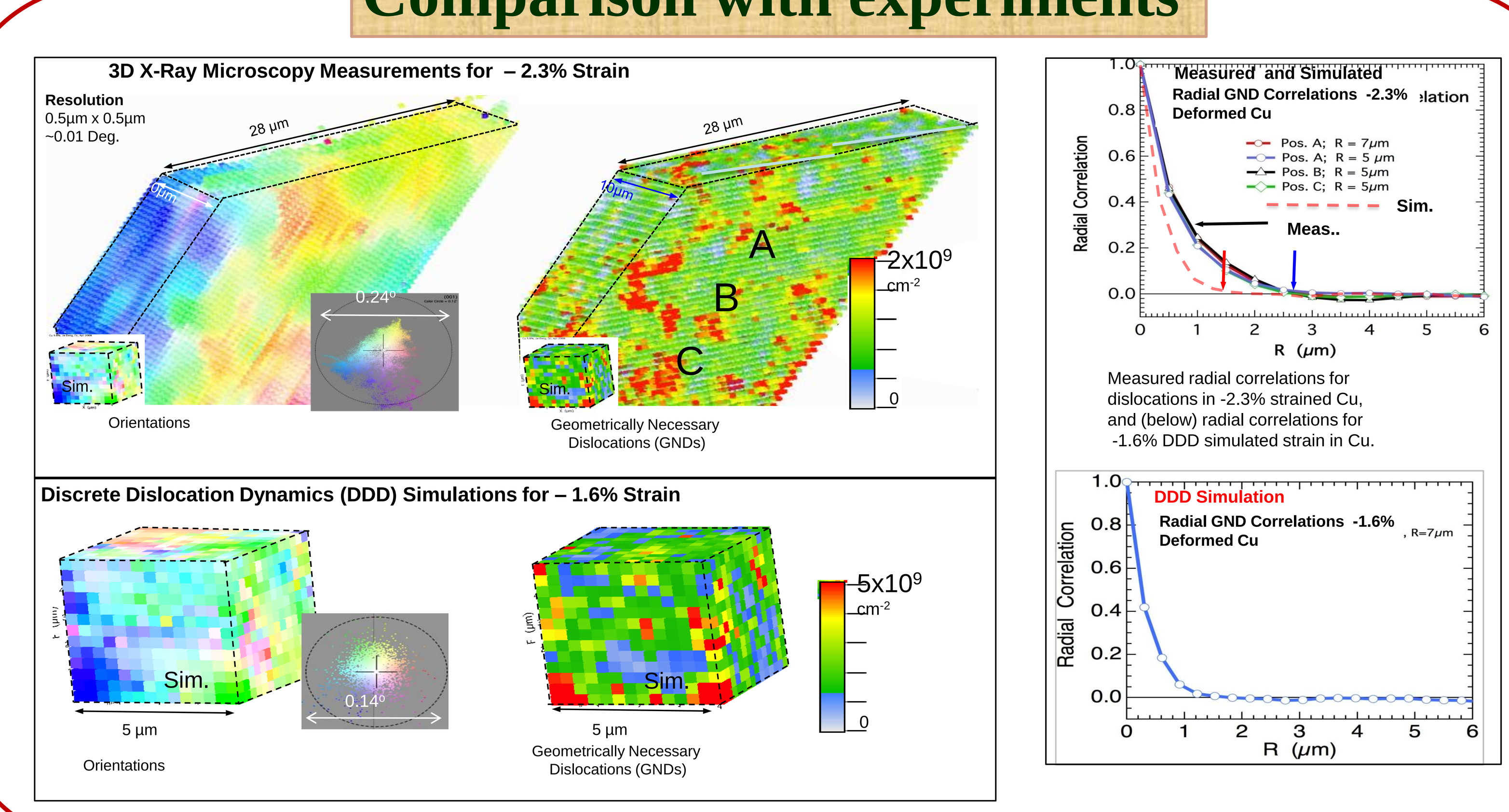


- Strain gradient contribution has significant contribution to the dislocation density tensor.
- The figures also reflect the increase in the dislocation density with strain level.
- The PCF for the dislocation density tensor norm (with and without strain gradient).



- The correlation also decays fast to the uncorrelation value, followed by fluctuations that seems much weaker that the constitutive elastic fields.

Comparison with experiments



Summary

- A preliminary investigation for the statistical analysis of internal elastic fields and dislocation density tensor has been conducted.
- The statistical characteristics of these fields were revealed via probability density, pair correlation function and 3D maps (not shown here).
- The elastic strain field shows PDF and PCF in agreement with those done before for the internal stress field.
- The results show a symmetric distribution of the lattice orientation, with nonzero mean value. The distribution of the dislocation density tensor was symmetric, in agreement with the simulated dislocation structure.
- The radial correlation functions for lattice rotation and dislocation density tensor exhibit slow initial decay followed by slight oscillations about no-correlation values.
- Preliminary comparison with experiments was conducted.