FLORIDA STATE UNIVERSITY

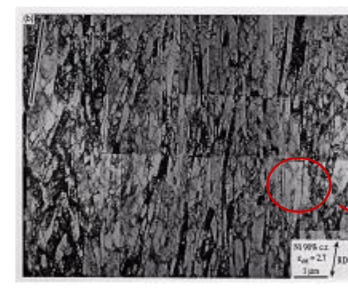
Department of Scientific Computing

Dislocation Statistics for FCC Crystals

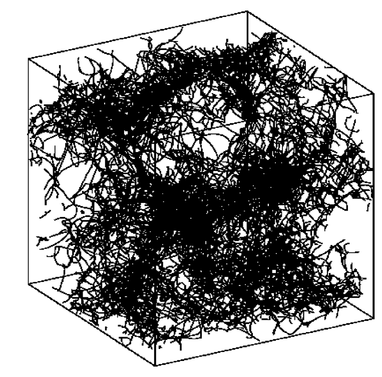
Mamdouh Mohamed, Jie Deng, and Anter El-Azab

Introduction

- Mesoscale plastic deformation of crystals is governed by motion and interaction of large dislocation systems.
- Density-based models are used to simulate the collective behavior of dislocations during plastic deformation.
- **Statistical analysis** is required to fix the average velocity term, and source terms appearing in the kinetic equations.



A volume of deformed crystal showing mesoscale deformation features



Resolved region showing complex dislocation structure

$$\frac{\partial \rho^{\alpha}(\mathbf{x},\theta,t)}{\partial t} + \nabla.\left(\bar{\mathbf{v}}\ \rho^{\alpha}(\mathbf{x},\theta,t)\right) = S_M^{\alpha} + S_{CS}^{\alpha}\left(\rho^{\alpha},\rho^{\beta}\right) + S_{SR}^{\alpha}\left(\overline{\rho^{\alpha}\rho^{\beta}}\right)$$

Dislocation Density (**for slip system α**) in volume $d\mathbf{x}$ around point $\mathbf{x}$

Source terms account for dislocations multiplication+ cross-slip + short range interactions.

Statistical Analysis

Temporal Statistics

- The Source terms are supposed to continuously represent the discrete processes (cross-slip, junctions formation,..) that take place at the level of individual dislocations, which requires temporal coarse-graining.

1. **Cross-slip source term:**

$$\bar{S}_{CS}^{\alpha}(\theta) = -\frac{\partial \bar{\rho}_{CS}^{\alpha}(\theta)}{\partial t} = -R_{CS}^{\alpha} 1_{\Theta_{CS}^{\alpha}}(\theta)\bar{\rho}^{\alpha}(\theta) \quad \text{and} \quad \bar{S}_{CS}^{\beta}(\theta) = \frac{\partial \bar{\rho}_{CS}^{\beta}(\theta)}{\partial t} = R_{CS}^{\beta} 1_{\Theta_{CS}^{\beta}}(\theta)\bar{\rho}^{\alpha}(\theta)$$

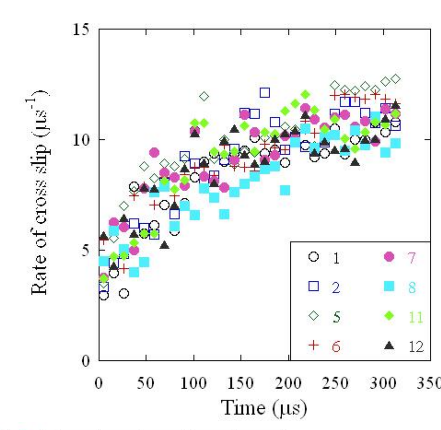
2. **Junctions formation source terms:**

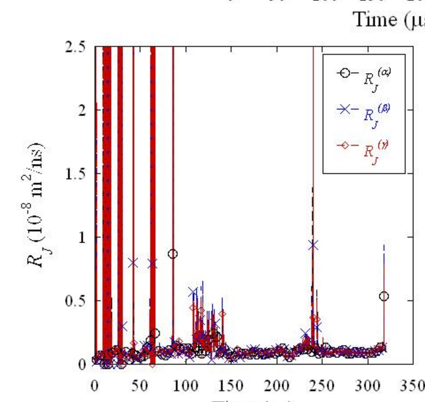
$$\bar{S}_J^{\alpha}(\theta) = -\partial\bar{\rho}_J^{\alpha}(\theta)/\partial t = -R_J^{\alpha}\int_{\Theta_J^{\beta}} \overline{\rho^{\alpha}(\theta)\rho^{\beta}(\theta')}d\theta' \ \bigstar$$

$$\bar{S}_J^{\beta}(\theta) = -\partial\bar{\rho}_J^{\beta}(\theta)/\partial t = -R_J^{\beta}\int_{\Theta_J^{\alpha}} \overline{\rho^{\beta}(\theta)\rho^{\alpha}(\theta')}d\theta'$$

$$\bar{S}_J^{\gamma}(\theta) = \partial\bar{\rho}_J^{\gamma}(\theta)/\partial t = R_J^{\gamma}\int_{\Theta_J^{\alpha}}\int_{\Theta_J^{\beta}} \overline{\rho^{\alpha}(\theta')\rho^{\beta}(\theta'')}d\theta' d\theta''.$$

★ Integrand gives rise to **spatial & orientation correlation** terms





Spatial Statistics

- The integrand in the junctions source term can be generally expressed as:

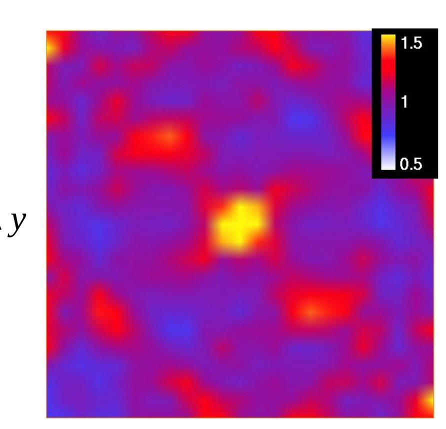
$$\overline{\rho^{\alpha}\ \rho^{\beta}} = \overline{\rho^{\alpha}}\ \overline{\rho^{\beta}}\ cor^{(\alpha,\beta)}(\mathbf{x}',\theta',\mathbf{x}'',\theta'',t)$$

- The general expression for the pair correlation function takes the form:

$$cor^{(\alpha,\beta)}(\mathbf{x}',\theta',\mathbf{x}'',\theta'') = \frac{\left\langle \Psi^{\alpha}(d\mathbf{x}'\times d\theta')\ \Psi^{\beta}(d\mathbf{x}''\times d\theta'')\right\rangle}{\left\langle \Psi^{\alpha}(d\mathbf{x}'\times d\theta')\right\rangle\left\langle \Psi^{\beta}(d\mathbf{x}''\times d\theta'')\right\rangle}$$

$\langle ... \rangle$: The ensemble average

- Assuming Statistical homogeneity, others expressions can be derived for correlations as function of coordinate difference in position and orientation spaces.
- Deriving a correlation for only one space (ex: spatial) requires the integration of the correlation expression over the other space (ex: orientation).
- This figure shows an example of the spatial correlation as function of coordinate difference $(\Delta x, \Delta y)$.



Orientation Statistics

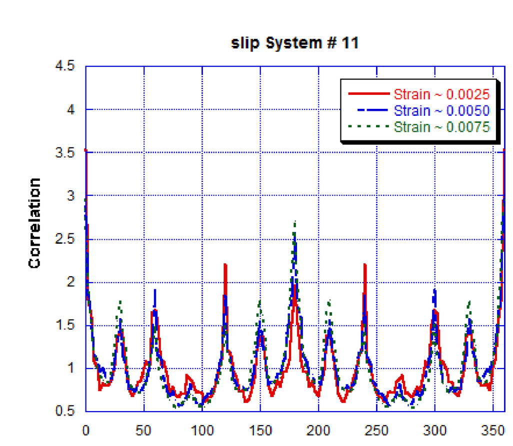
- Since junction formation depends on the orientation of both reacting segments, junction source terms will include terms representing the orientation pair correlation.
- Assuming statistical homogeneity, pair correlations depend only on the angle difference

$$C^{(\alpha_1,\alpha_2)}(\Delta\theta) = \frac{\left\langle \rho^{\alpha_1}(\theta_1)\,\rho^{\alpha_2}(\theta_2)\,1_{C_{\Delta\theta}}(\theta_1,\theta_2)\right\rangle}{\left\langle \rho^{\alpha_1}(\theta_1)\,1_{C_{\Delta\theta}}(\theta_1,\theta_2)\right\rangle\left\langle \rho^{\alpha_2}(\theta_2)\,1_{C_{\Delta\theta}}(\theta_1,\theta_2)\right\rangle}$$

$$\left\langle \rho^{\alpha_1}(\theta_1)\,\rho^{\alpha_2}(\theta_2)\,1_{C_{\Delta\theta}}(\theta_1,\theta_2)\right\rangle = \frac{\sum_{i,j}^{n}\rho^{\alpha_1}(\theta_i)\,\rho^{\alpha_2}(\theta_j)\,1_{C_{\Delta\theta}}(\theta_i,\theta_j)}{\sum_{i,j}^{n} 1_{C_{\Delta\theta}}(\theta_i,\theta_j)}$$

$$\left\langle \rho^{\alpha_1}(\theta_1)\ 1_{C_{\Delta\theta}}(\theta_1,\theta_2)\right\rangle = \frac{\sum_{i,j}^{n}\rho^{\alpha_1}(\theta_i)\ 1_{C_{\Delta\theta}}(\theta_i,\theta_j)}{\sum_{i,j}^{n} 1_{C_{\Delta\theta}}(\theta_i,\theta_j)}$$

$$\left\langle \rho^{\alpha_2}(\theta_2)\,1_{C_{\Delta\theta}}(\theta_1,\theta_2)\right\rangle = \frac{\sum_{i,j}^{n}\rho^{\alpha_2}(\theta_j)\,1_{C_{\Delta\theta}}(\theta_i,\theta_j)}{\sum_{i,j}^{n} 1_{C_{\Delta\theta}}(\theta_i,\theta_j)}$$



Internal Stress Statistics

- The ultimate goal here is to find the ensemble average of the internal stress field acting on segments.
- Defining generalized probability density function (PDF) of the dislocation system:

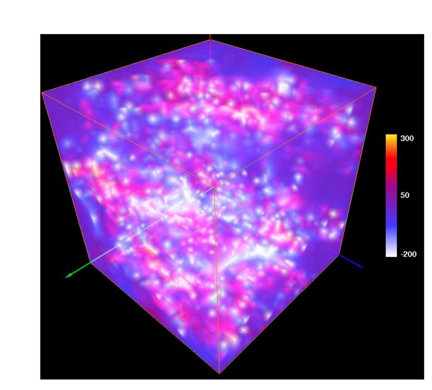
$$\int_{\Gamma} f^{(\alpha_1,\dots,\alpha_n)}(\mathbf{x}_1,\theta_1,\dots,\mathbf{x}_n,\theta_n)\ d\mathbf{x}_1 d\theta_1 \dots d\mathbf{x}_n d\theta_n = 1 \qquad \Gamma \equiv \Omega\times O$$

- The first order PDF of internal stress, generated by the entire dislocation system, can be written as:

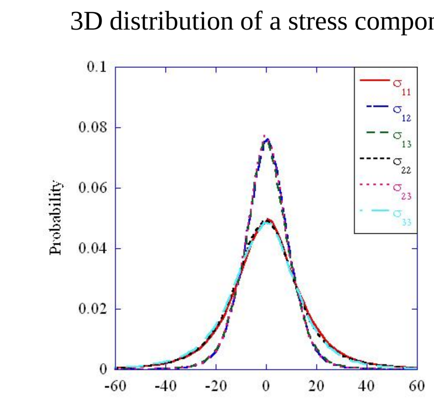
$$p_{ij}(\sigma_{\circ};\mathbf{x}) = \int_{\Gamma} f^{(\alpha_1,\dots,\alpha_n)}(\mathbf{x}_1,\theta_1,\dots,\mathbf{x}_n,\theta_n)\ \delta[\sigma_{\circ}-\sigma_{ij}(\mathbf{x})]\ d\mathbf{x}_1 d\theta_1 \dots d\mathbf{x}_n d\theta_n$$

- For statistically homogeneous stress field : $p_{ij}(\sigma_{\circ}) = \frac{1}{\Omega}\int_{\Omega} p_{ij}(\sigma_{\circ};\mathbf{x})\,d\mathbf{x}$
- The pair correlation function can be written as:

$$C_{ijkl}(\mathbf{r}) = \frac{Cov(\sigma_{ij}(\mathbf{x}),\sigma_{kl}(\mathbf{x}+\mathbf{r}))}{\sqrt{Var(\sigma_{ij}(\mathbf{x}))\ Var(\sigma_{kl}(\mathbf{x}+\mathbf{r}))}}$$

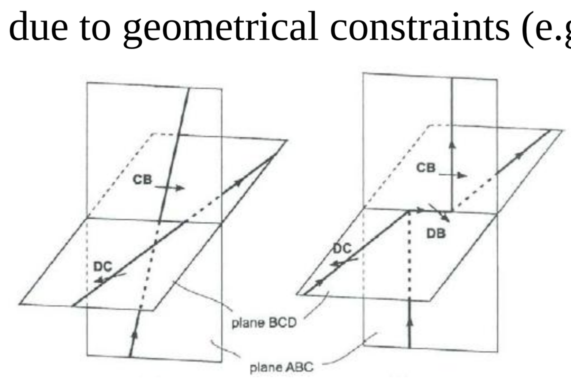


3D distribution of a stress component



Velocity Statistics

- After evaluating the ensemble average of the internal stress field on segments, and summing it to contributions from external fields and self forces, we need establish a formula calculating the ensemble average of segments' velocity as a function of average stress field.
- Ideally, the dislocation motion is governed by a linear relation between force and velocity. However, some dislocation segments violate this relation due to geometrical constraints (e.g.; non-coplaner junctions).
- Considering this effect, an average mobility law can be established to calculate the average dislocations' velocity.
- Research is proceeding in this direction in order to establish this formula.



Formation of non-coplaner junction. Hull and Bacon. P (141).

Temporal Statistics → Rate constants
+
Orientation Statistics → Orientation Correlations
+
Spatial Statistics → Spatial Correlations
=
Source Terms

$$\frac{\partial \rho^{\alpha}}{\partial t} + \nabla.\left(\bar{\mathbf{v}}\ \rho^{\alpha}\right) = S^{\alpha}$$

Average Velocity Term
=
Velocity Statistics → Average Mobility Law
↑
Stress Statistics → Average internal Stress + Other Contributions

Summary

- An approach, based on the statistical mechanics concepts, was introduced to solve the plasticity problem, and it resulted in a set of kinetic equation for the evolution of the dislocation density. It was shown that the closure of these equations requires statistical analysis in terms of fixing the average velocity and source terms.
- Source terms like cross slip term will be fixed via the temporal statistics, however other terms like the junction formation term will additionally require spatial and orientation statistics in order to find the corresponding pair correlation functions in the source term equations.
- The average internal stress field obtained from the internal stress statistics, should be added to the other stress contributions to get the average total stress field acting on segments. This stress field will be substituted in the average mobility law, establish via the velocity statistics, to evaluate the average velocity term.
- Sample results were demonstrated as examples for the statistical measures.