Calculation of intragranular misorientation distributions in polycrystals

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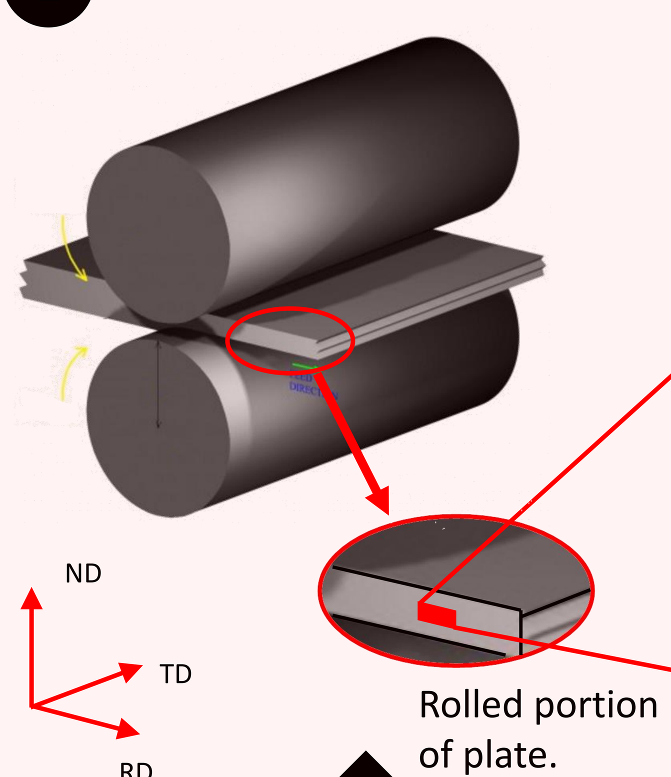
Introduction

We develop a methodology for calculation of intragranular misorientation distributions by integration of intragranular rotation rate distributions within the visco-plastic self-consistent model. We apply the model to tension and plane-strain compression of fcc polycrystal and compare the predictions to experiments and full-field simulation results. The developed procedure provides basis for fragmentation and recrystallization modeling and improves the texture predictions in computationally efficient manner.

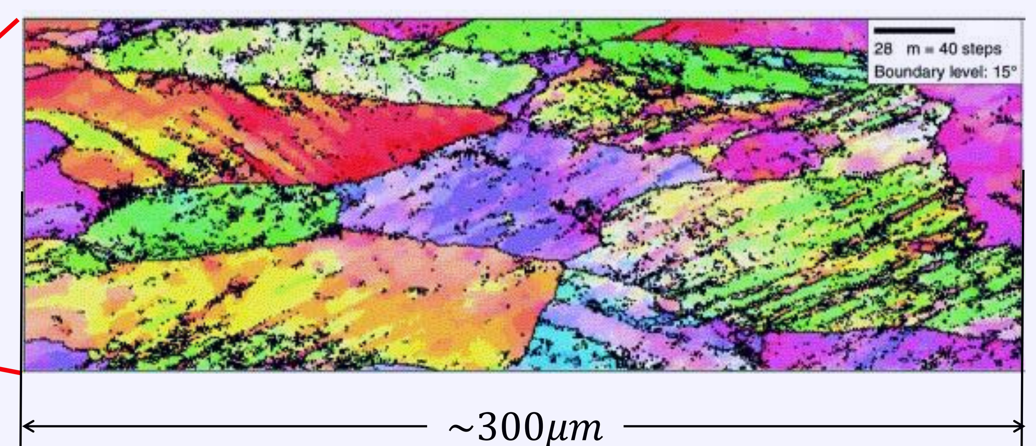
Intragranular misorientation development

1 Rolling process.

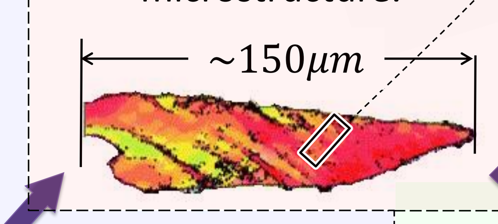


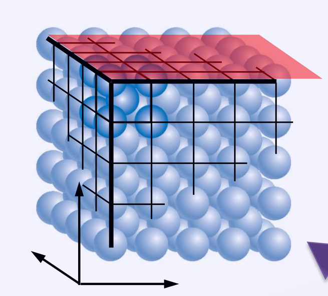
Rolled portion of plate.

2 Electron backscatter diffraction scan of the microstructure, color-coded according to crystal orientation. Grain boundaries are plotted as black lines.



3 One grain within the microstructure.

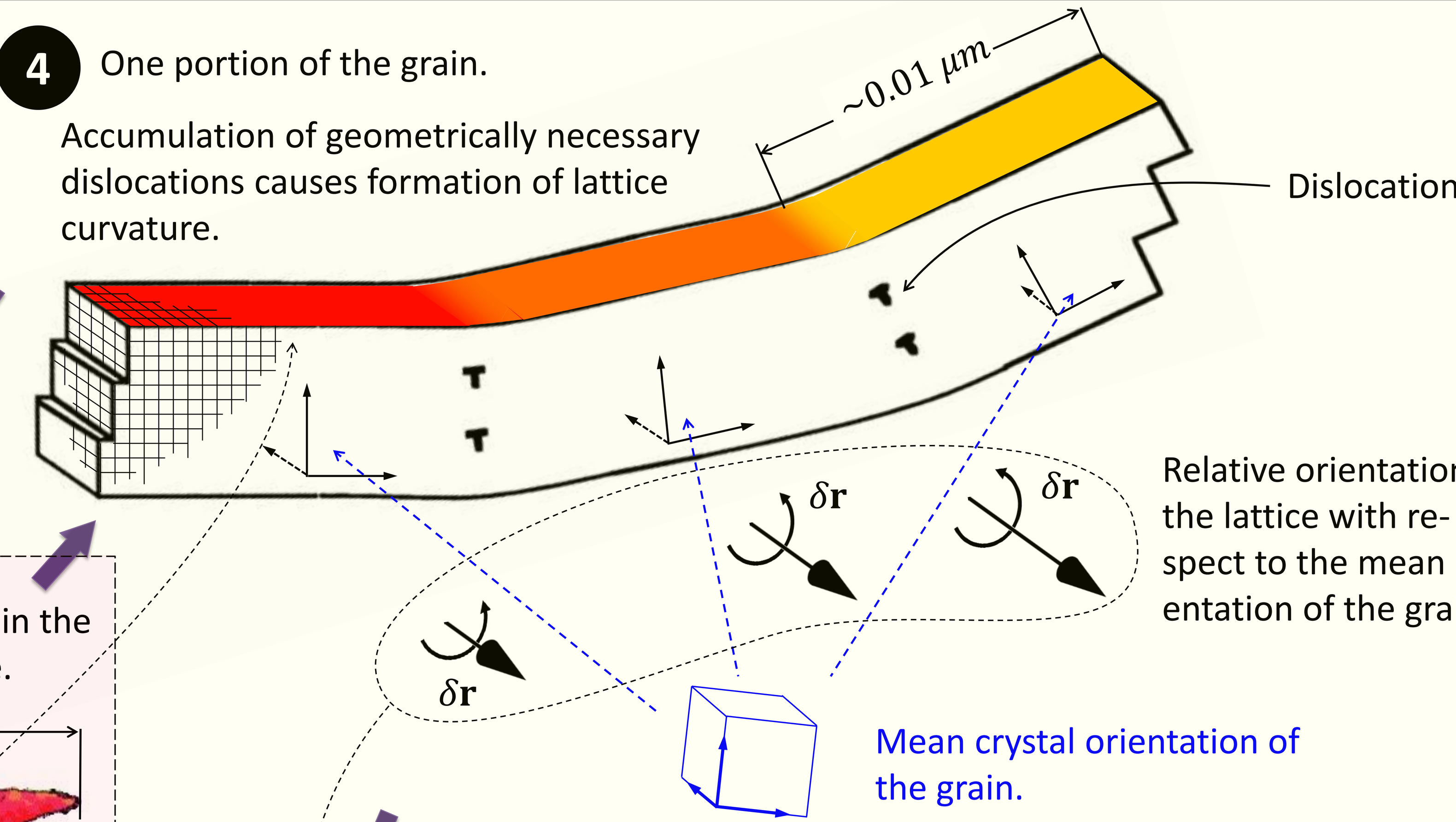




Atoms ordered into lattice

4 One portion of the grain.

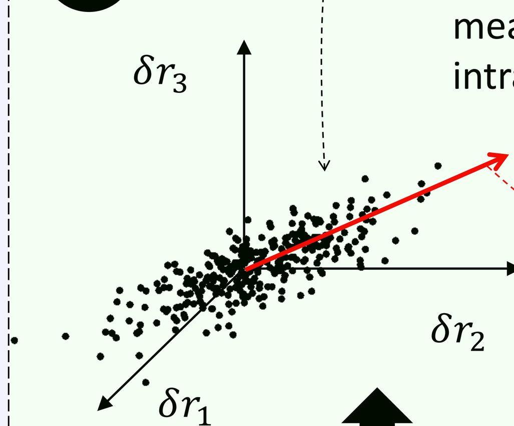
Accumulation of geometrically necessary dislocations causes formation of lattice curvature.



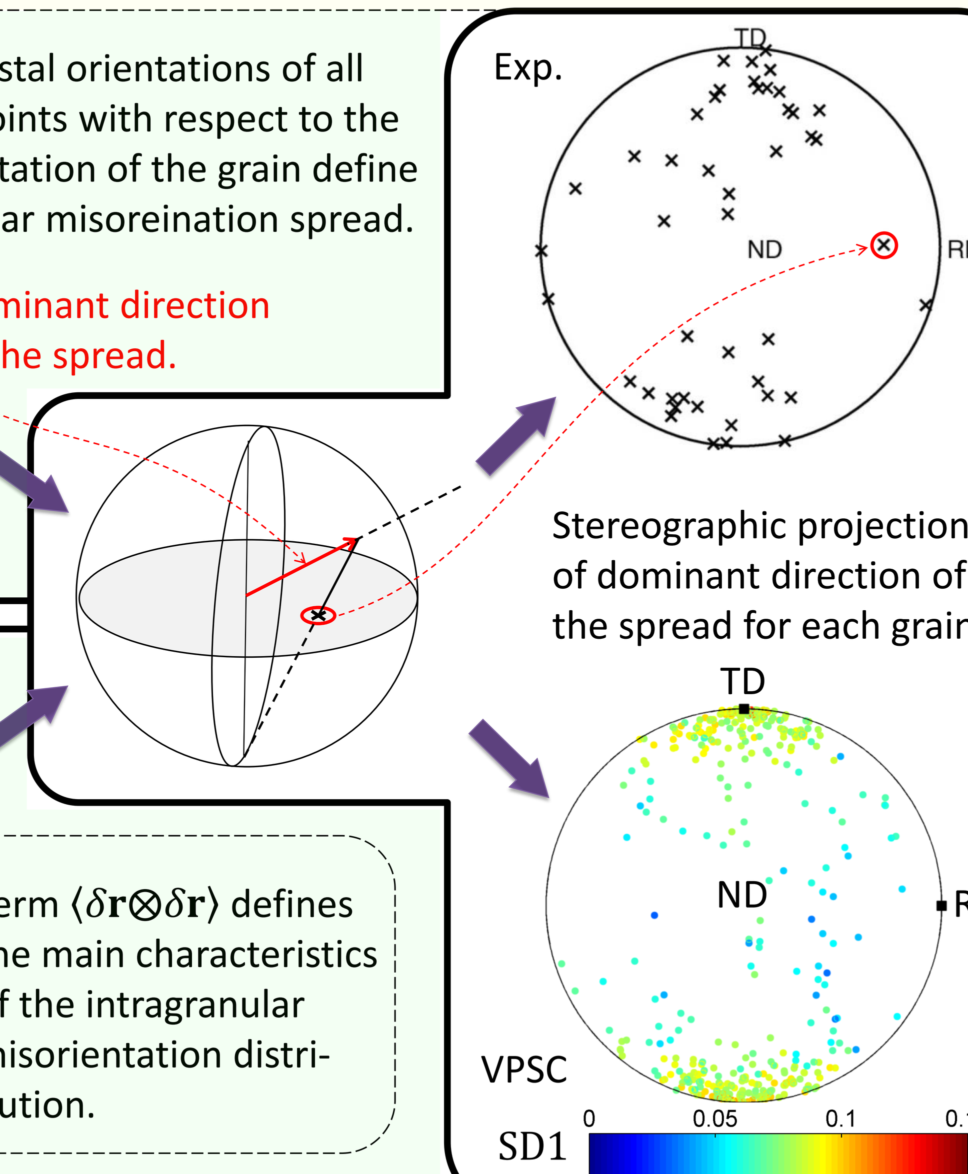
Relative orientation of the lattice with respect to the mean orientation of the grain.

Mean crystal orientation of the grain.

5 Relative crystal orientations of all the grain points with respect to the mean orientation of the grain define intra-granular misoreination spread.



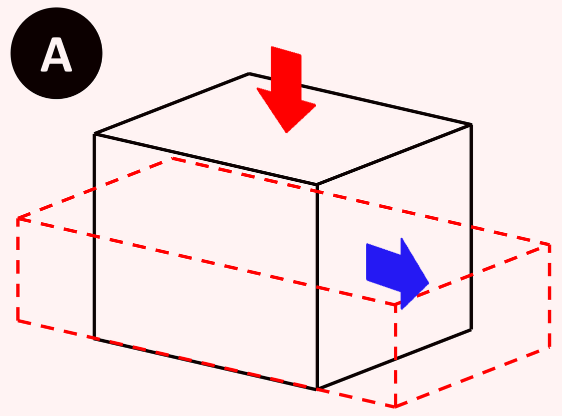
Dominant direction of the spread.



Stereographic projection of dominant direction of the spread for each grain.

Model

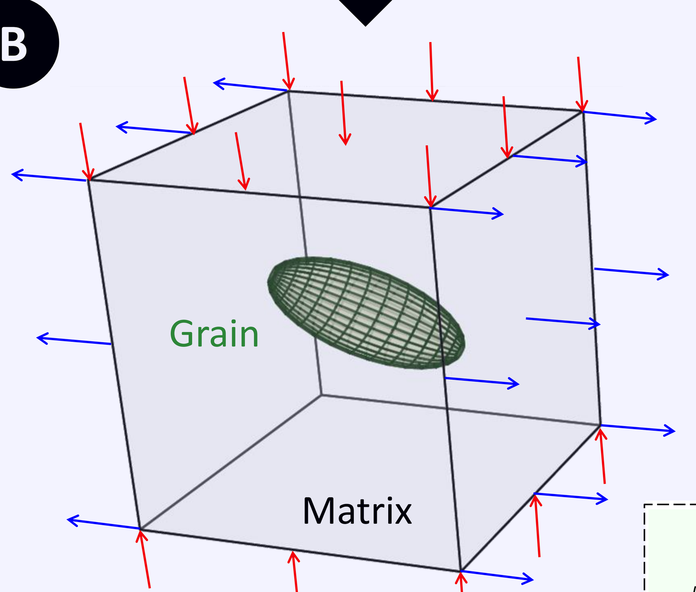
A



Rolling process is simulated as plane strain compression:

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} s^{-1}$$

B



Representation of a grain within the model.

In visco-plastic self-consistent (VPSC) model the boundary conditions are applied to the matrix with embedded ellipsoidal grain. Response of the grain depends on the crystal orientation while the properties of the matrix correspond to the average over all grains.

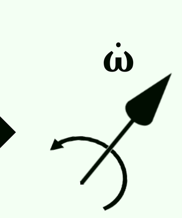
C $\langle \delta\boldsymbol{\sigma} \otimes \delta\boldsymbol{\sigma} \rangle$

Evolution of stress distribution within the grain during the process.

Assumption #1
Linearity of rotation rate with respect to stress:
$\dot{\boldsymbol{\omega}} \approx \mathbf{W}:\boldsymbol{\sigma} + \mathbf{w}^0$

D $\langle \delta\dot{\boldsymbol{\omega}} \otimes \delta\dot{\boldsymbol{\omega}} \rangle$

Evolution of rotation rate distributions [1].

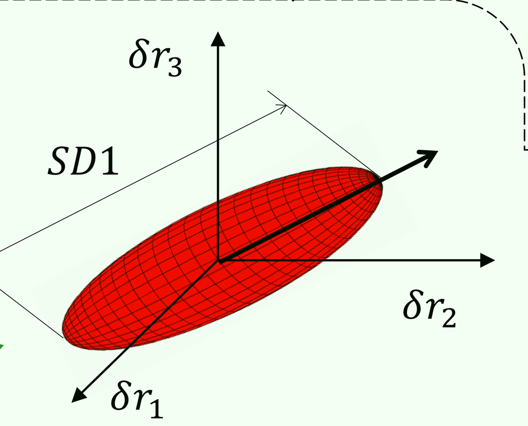


Rate of lattice rotation.

E

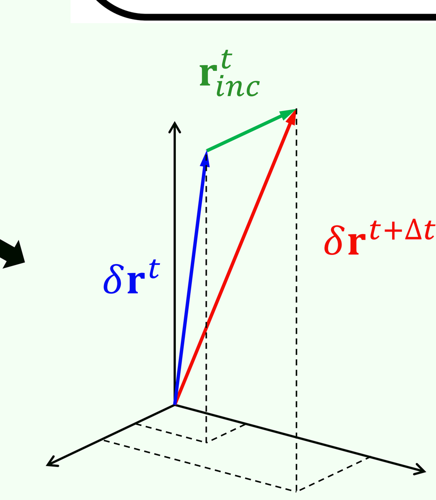
Evolution of intragranular misorientation distribution with strain [2].

$\langle \delta\mathbf{r} \otimes \delta\mathbf{r} \rangle$



Term $\langle \delta\mathbf{r} \otimes \delta\mathbf{r} \rangle$ defines the main characteristics of the intragranular misorientation distribution.

Assumption #2
Additive accumulation of misorientations:
$\delta\mathbf{r}^{t+\Delta t} \approx \delta\mathbf{r}^{t} + \delta\mathbf{r}^{t}_{inc}$

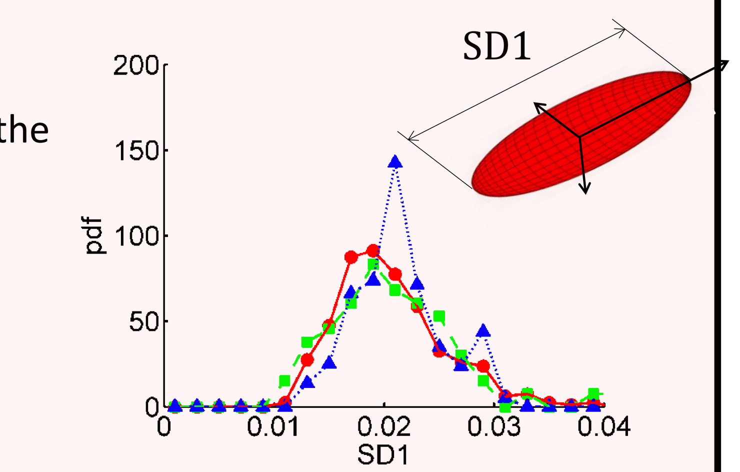


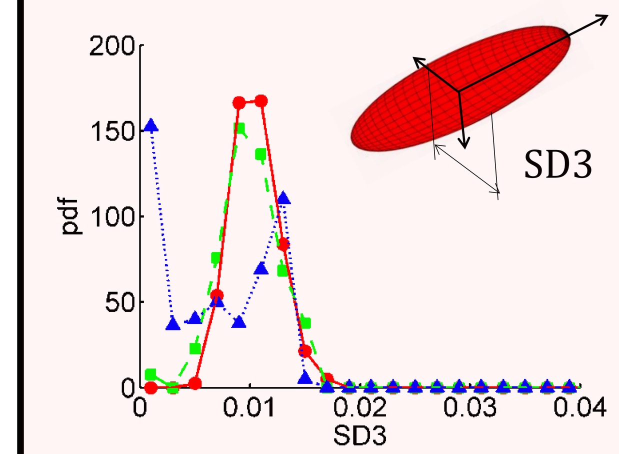
Results for tension to 11% strain

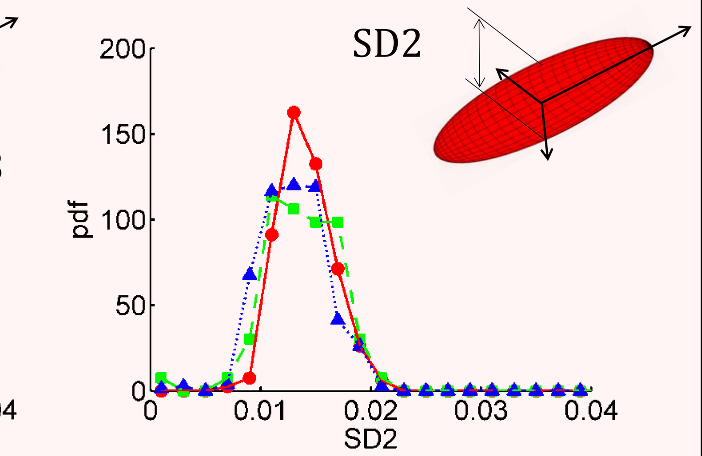
VPSC model predictions after tension to 11% strain are compared to experiment and full-field simulations.

Comparison of magnitudes along principal directions of the misorientation spread.

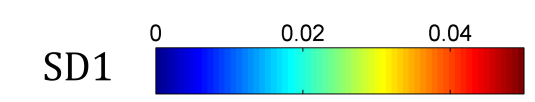
- Full-field
- Experiment
- VPSC

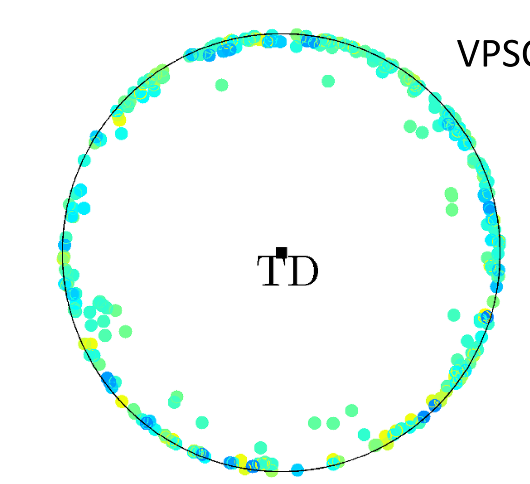


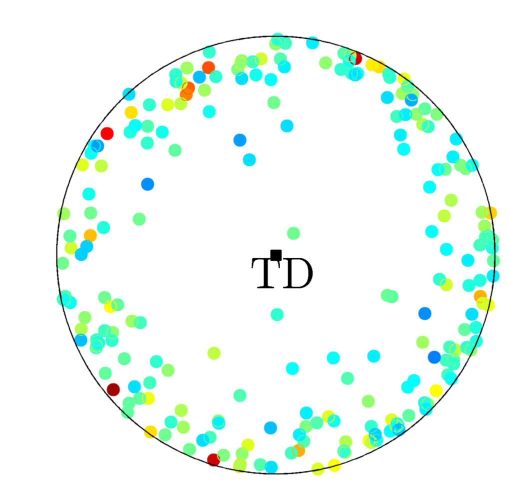




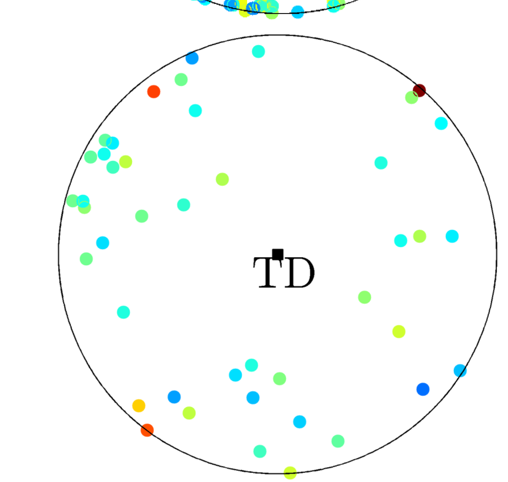
Comparison of dominant directions of the misorientation spread. Color-coding is according to magnitude of the spread along dominant direction.







Full-field



Exp.

Conclusions

Acceptable predictions of orientation spreads were achieved using VPSC, with tremendous computational advantages over full-field models. It was observed that at higher strains, some of the grains develop quite large misorientation spreads requiring fragmentation.

Literature cited

[1] R. A. Lebensohn, M. Zecevic, M. Knezevic and R. J. McCabe (2016), "Average intragranular misorientation trends in polycrystalline materials predicted by a viscoplastic self-consistent approach", Acta Materialia, 104, 228-236.

[2] M. Zecevic, R. A. Lebensohn, R. J. McCabe, W. Pantleon and M. Knezevic, "Predicting intragranular misorientation distributions in polycrystalline metals using the viscoplastic self-consistent formulation" – to be subbmitted

Acknowledgments

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