Lecture at the Workshop Labex DAMAS **What can we learn from diffraction on polycrystal behavior?**
Labex DAMAS, 18 November, 2015, LEM3-Metz

EBSD based GND densities in severe plastic deformed metals - The role of geometrically necessary dislocations in the plastic behavior of pure copper at extreme large strains

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Outline

The role of dislocations in polycrystal deformation

Geometrically necessary dislocation measurements

Modeling of polycrystal deformation

Relation between disorientation distributions and GNDs

Conclusions

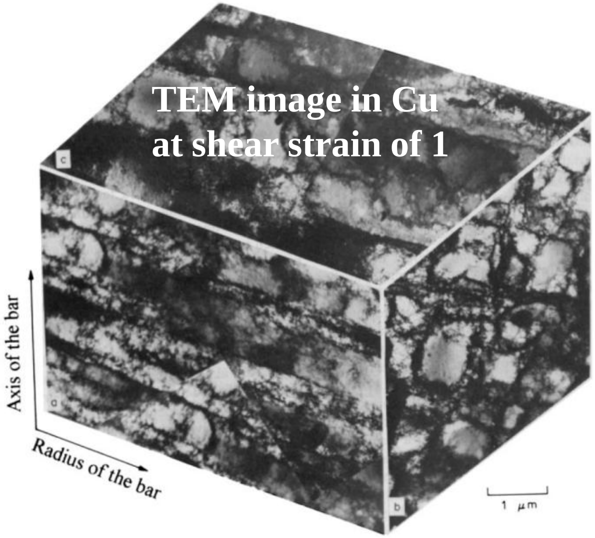
The role of dislocations in polycrystal deformation

Two types of dislocations

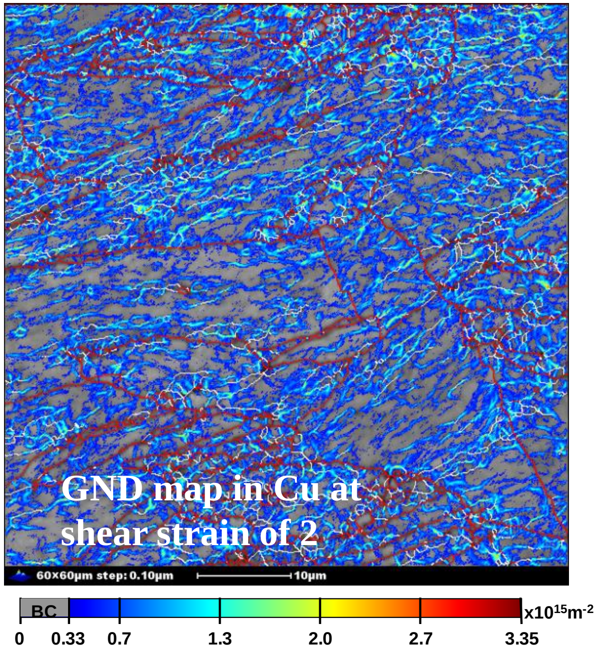
Statistical dislocations $\rho_{total} = \rho_{stat.} + \rho_{GND}$ Geometrically necessary dislocations

→ To achieve imposed deformation
→ For strain hardening
→ No orientation gradient
→ Patterning

→For deformation gradients
→ Orientation differences are produced
→Patterning

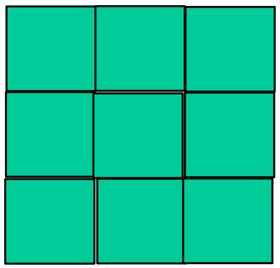


GNDs are needed in crystals of a polycrystal to account for deformation heterogeneities at mesoscopic level.



C.F. Gu, L.S. Tóth, B. Beausir, *Scripta Materialia*, 2012.

GND from lattice curvature



$$\rho_{GND} = \frac{\theta}{bd}$$

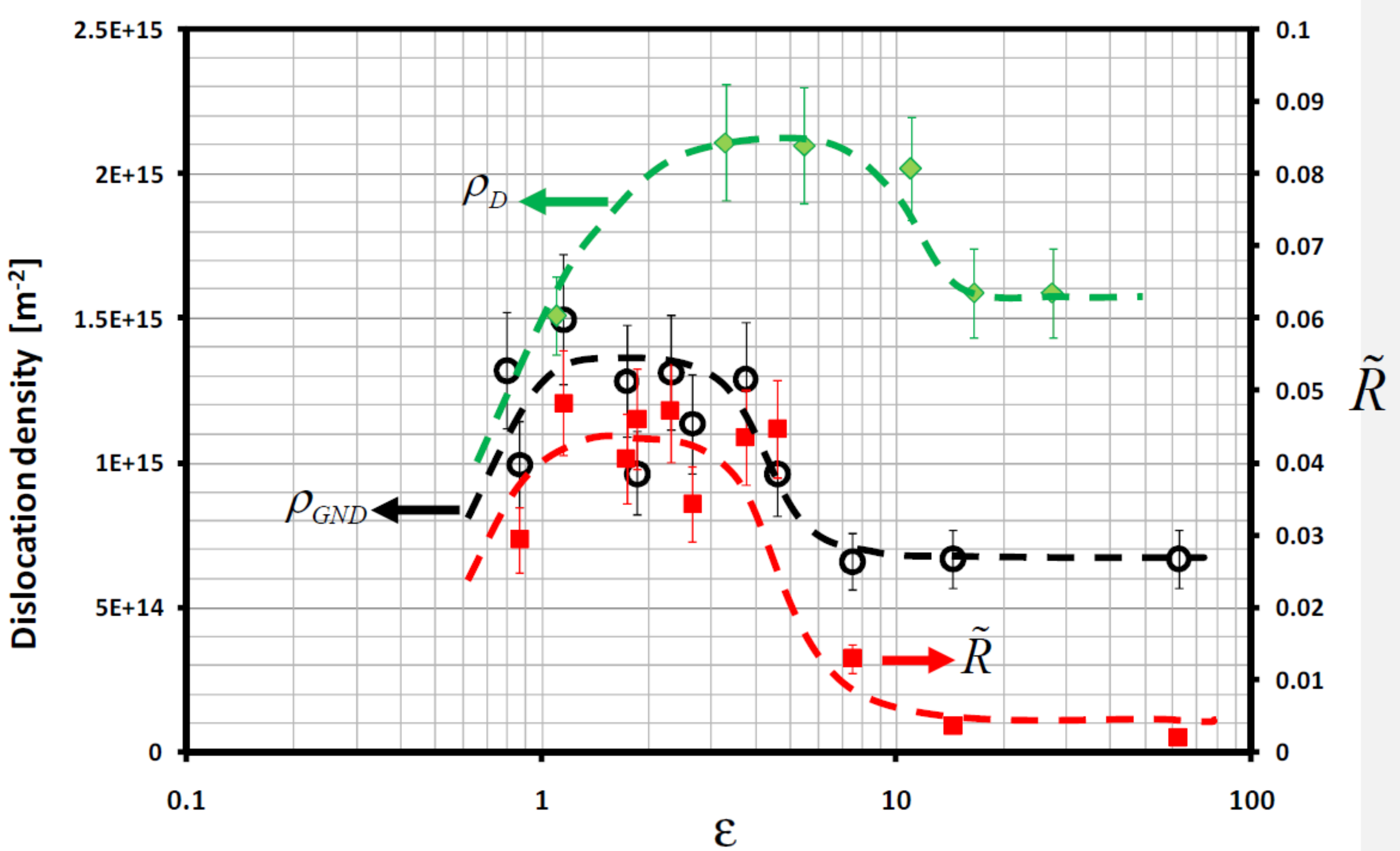
$$\alpha_{12},\ \alpha_{13},\ \alpha_{21},\ \alpha_{23},\ \alpha_{33}$$

$$\rho_{GND}^{(2D)} = \frac{1}{b}\sqrt{\alpha_{12}^2 + \alpha_{13}^2 + \alpha_{21}^2 + \alpha_{23}^2 + \alpha_{33}^2}$$

$$\rho_{GND} = 3\rho_{GND}^{(2D)} \Big/ \sqrt{5}$$

GND density variations vs strain in SPD of copper

GND from EBSD - lattice curvature → 2D Ney GND tensor → isotropic assumption → 3D Ney GND tensor → scalar norme

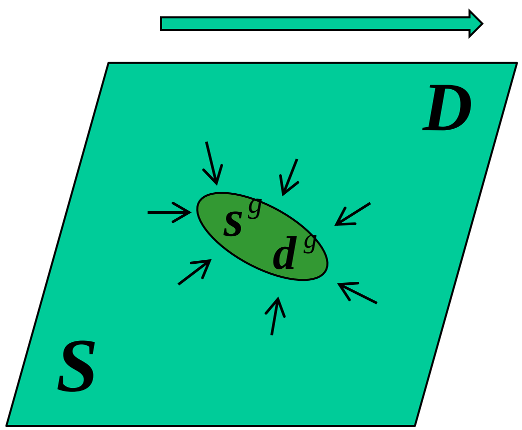


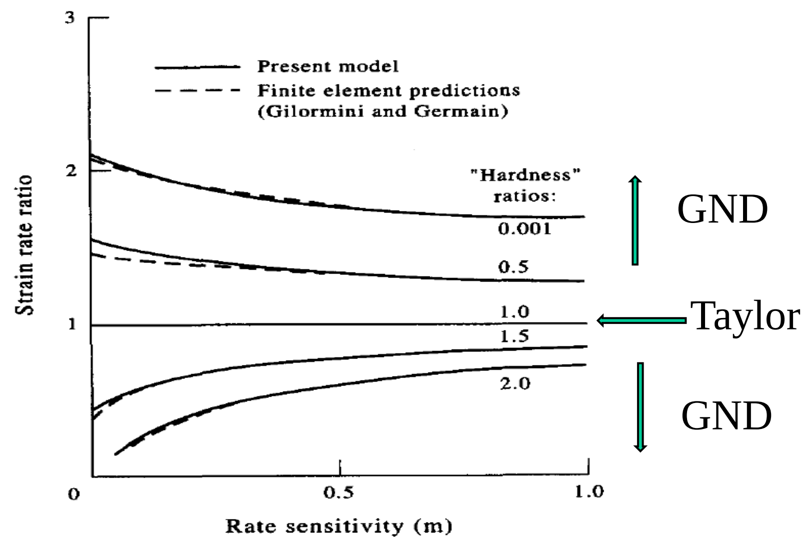
Modeling of polycrystal deformation

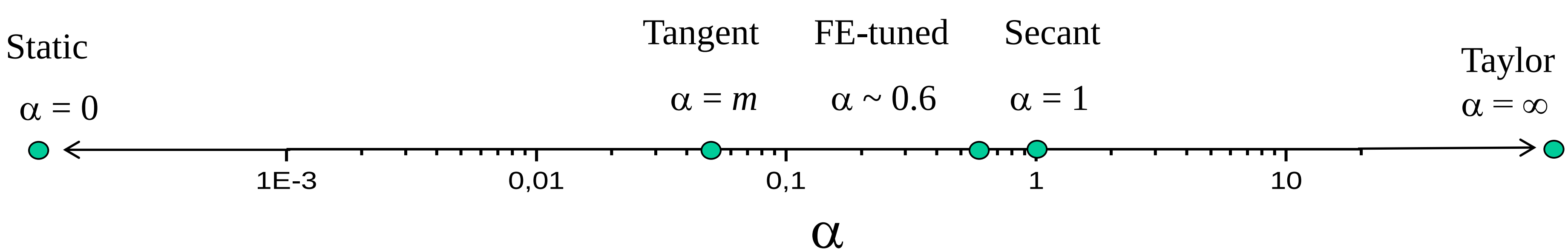
Viscoplastic Self Consistent Model (VPSC)

A. Molinari, L.S. Toth, Tuning a self consistent viscoplastic model by finite element results, Part I: Modelling, *Acta Metallurgica et Materialia*, 42, 2453-2458, 1994.

Localization equation: $$s^g - S = \alpha\left(\Gamma^{sgg^{-1}} + A^s\right)\left(d^g - D\right)$$







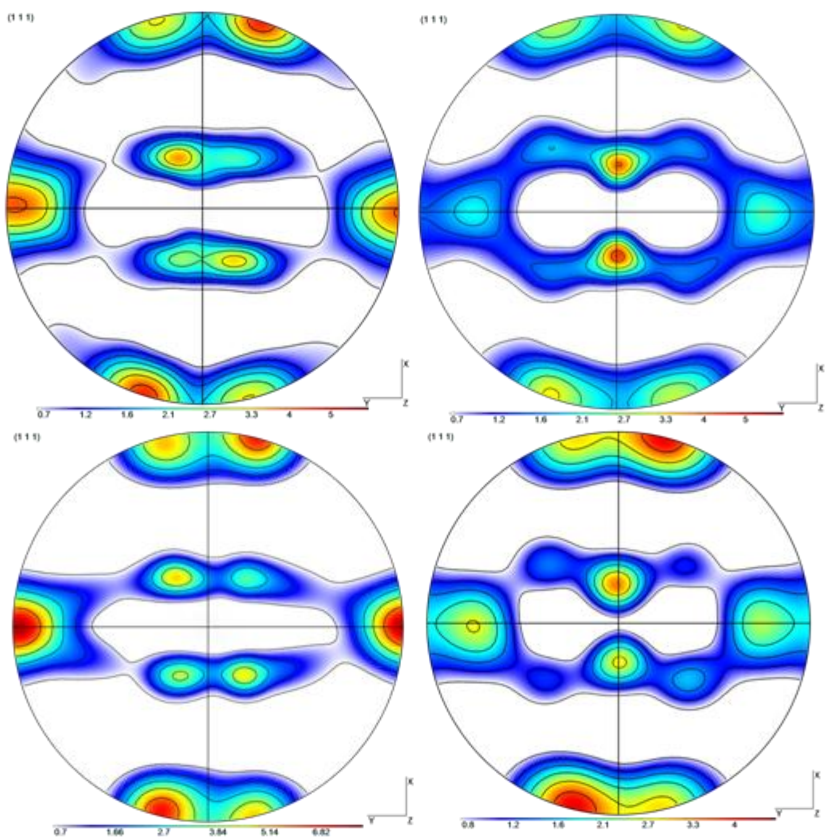
Rolling texture simulations

UFG rolling
11.2% Cu, 39% S and 34% Bs

CG rolling
17% Cu, 41% S and 17% Bs

Experiment

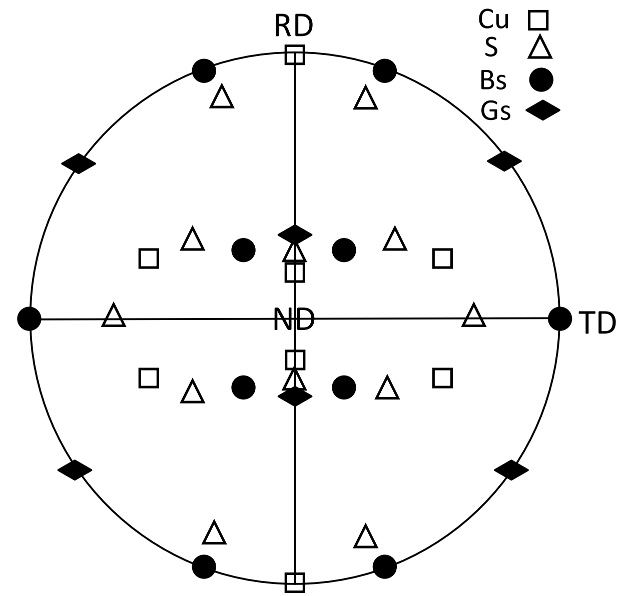
Simulation (VPSC)



<110> + <112> slip
Near-Taylor model (α = 20)

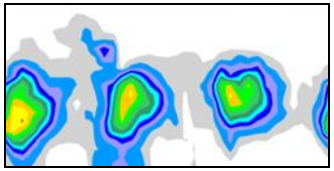
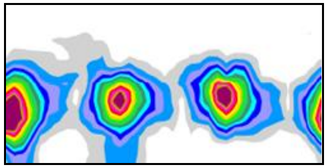
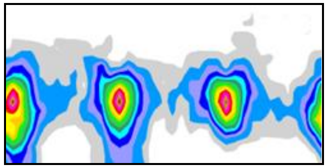
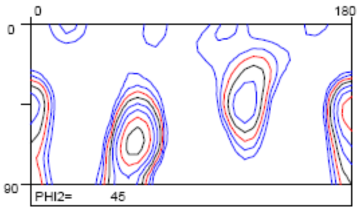
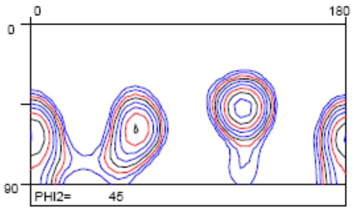
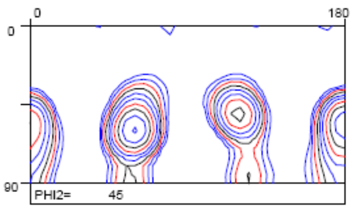
<110> slip
Tangent model

Key {111} pole figure in rolling



C. F. Gu, M. Hoffman, L.S. Toth, Y.D. Zhang, Materials Characterization, 101 (2015) 180–188.

High Pressure Torsion (HPT) of nano-polycrystalline Pd-10%Au

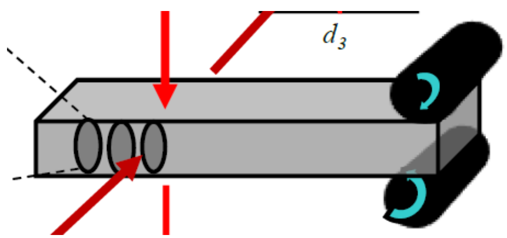
		γ = 2.83	γ = 8.38	γ = 16.76
(a)	Experiment			
(b)	Taylor with <110>+<112> CRSS 1.5 : 1			

Electro-deposited, initial grain size: 14 nm, coarsening to 24 nm, refinement to 20 nm, 2-3 dislocations per grain.

Werner Skrotzki, Andy Eschke, Bertolan Jonas, Tamas Ungar, Laszlo S. Toth; Yulia Ivanisenko; Lydia Kurmanaeva, *Acta* Materialia, 61 (2013) 7271–7284.

Rolling of nano-polycrystalline Ni-18%Fe

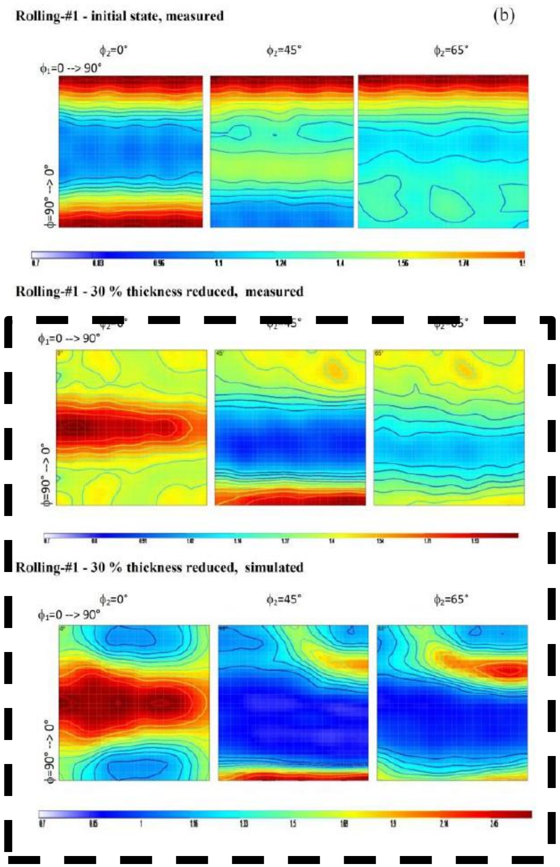
Electro-deposited, initial grain size: 20-40 nm, elongated parallel to <100> axis



Taylor

relaxed

0	1	0
1	0	0
0	0	0



Initial

Rolled

Simulated

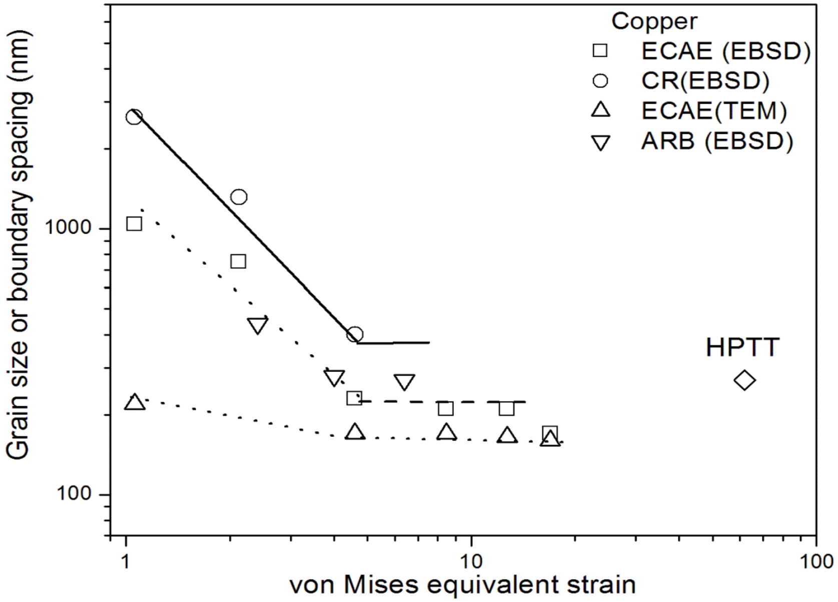
Grain Growth in a Nanocrystalline Ni-Fe Alloy during Cold Rolling, L. Li, T. Ungár, L. S. Toth, Z. Fogarassy, W. Skrotzki, Y. D. Wang, Y. Ren, H. Choo, X. T. Zhou, and P. K. Liaw, to submit, 2015.

Conclusion on polycrystal modelling:

Deformation mode is grain size dependent.

Large grain size:	**Tangent model – strain heterogeneities**
Ultra fine grain size:	**Near Taylor model, <111> and partial slip**
Nano-polycrystal:	**Taylor model, <111> and partial slip**

During severe plastic deformation: deformation mode is changing due to decrease in grain size:



Laszlo S. Toth, Chengfan Gu, Ultrafine-grain metals by severe plastic deformation,
A tutorial review, Materials Characterization, http://dx.doi.org/10.1016/j.matchar.2014.02.003

Example of grain fragmentation in severe plastic deformation

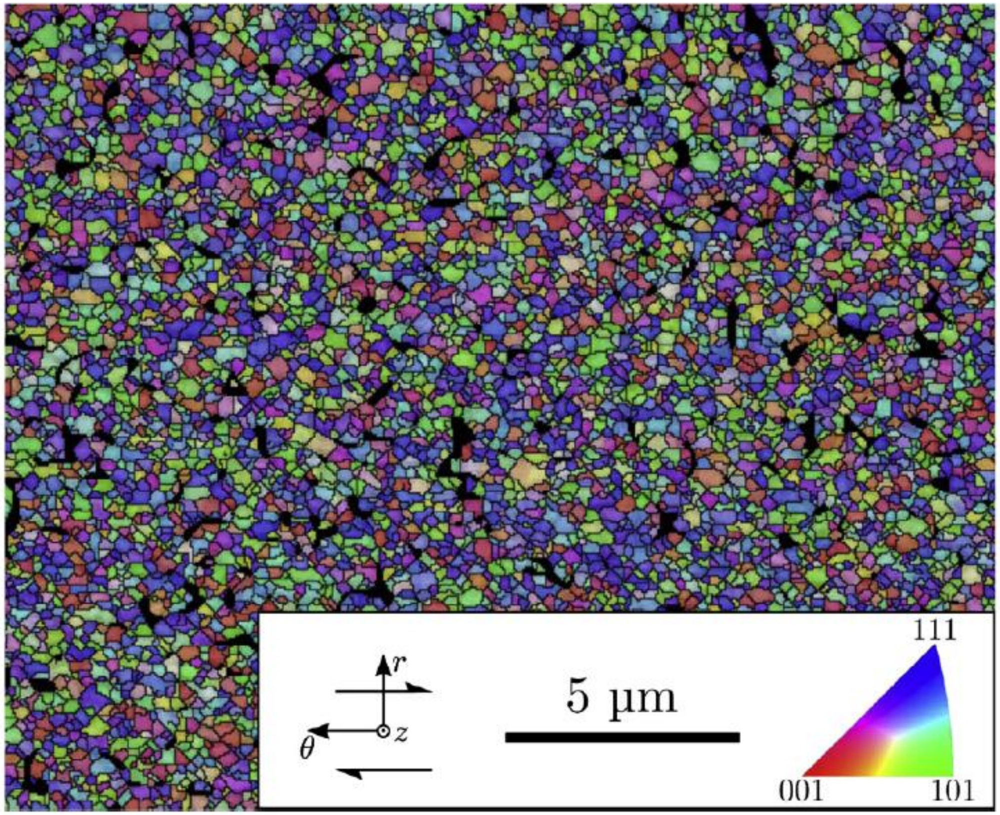


Figure 2. Inverse pole figure map obtained by EBSD after room temperature HPTT of Cu in the steady state after $\gamma = 108$ shear strain.

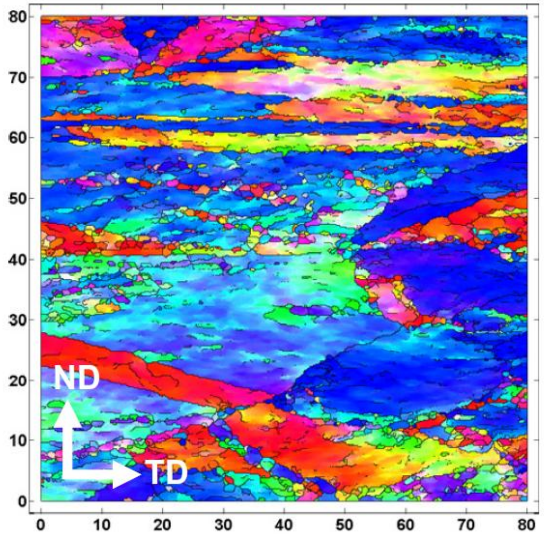
A. Pougis, L.S. Toth, J.J. Fundenberger, A. Borbely, Scripta Mater., 72-73 (2014) 59-62.
Extension of the Derby-relation to metals severely deformed to their steady state ultra-fine grain size,

How can we connect polycrystal deformation mode to GNDs?

GNDs appear inside grains because of the potential incompatibilities between neighbouring grains.

Examine then the neighbour characteristics in deformed polycrystals!

→ Disorientations measured by EBSD



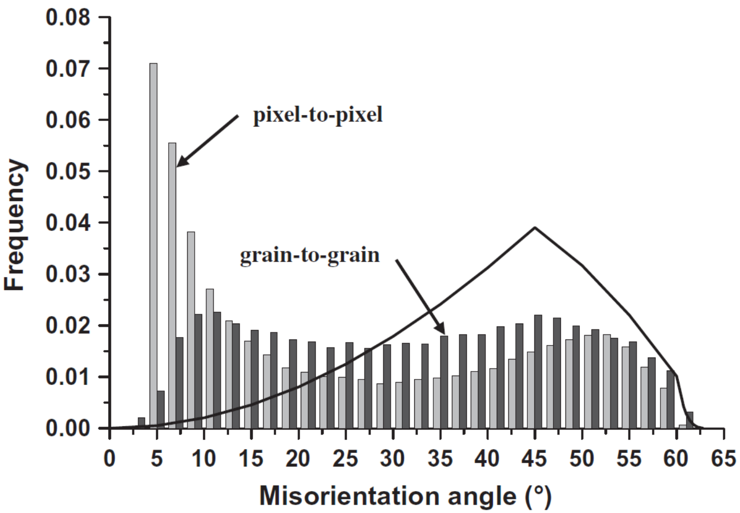
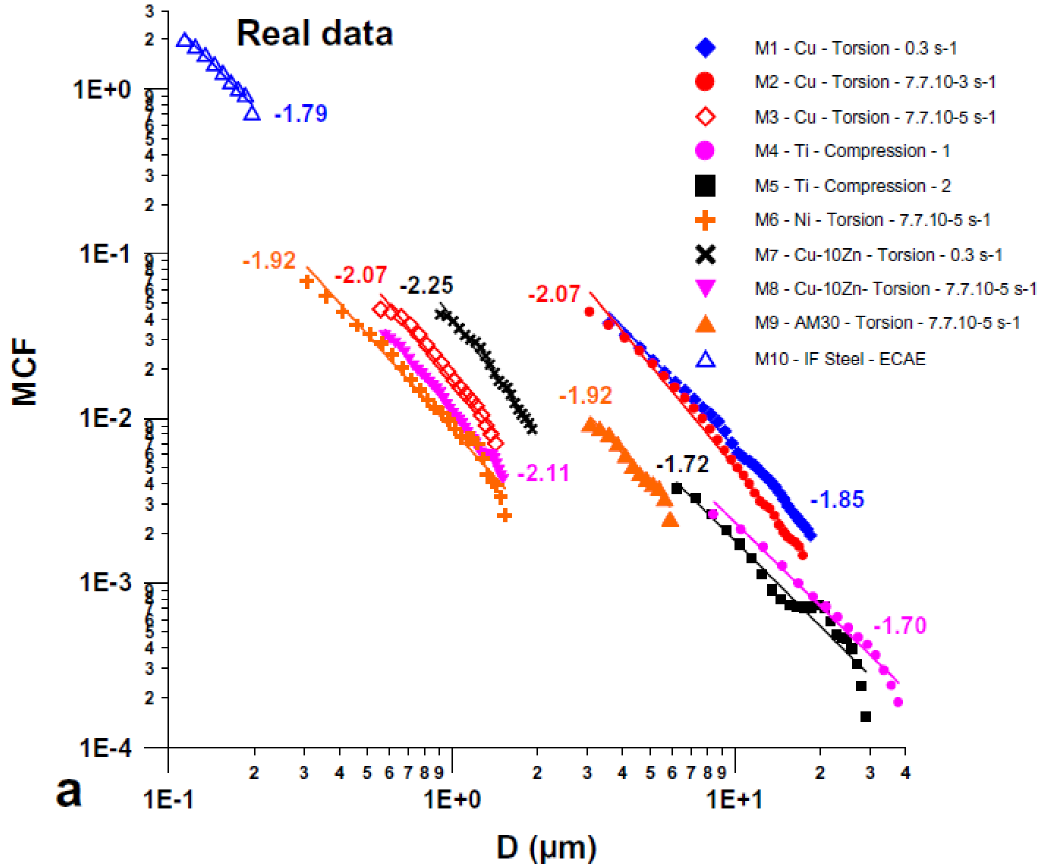


Fig. 1. Comparison between pixel-to-pixel (light gray) and grain-to-grain (dark gray) misorientation distributions (correlated) after three passes of Cu in ECAP on the TD plane. The theoretical Mackenzie distribution (uncorrelated) is plotted by the solid black line.

L.S. Toth, B. Beausir, C.F. Gu, Y. Estrin, N. Scheerbaum, C.H.J. Davies, Effect of grain refinement by severe plastic deformation on the next-neighbour misorientation distribution, *Acta Materialia*, 58 (**2010**) 6706-6716

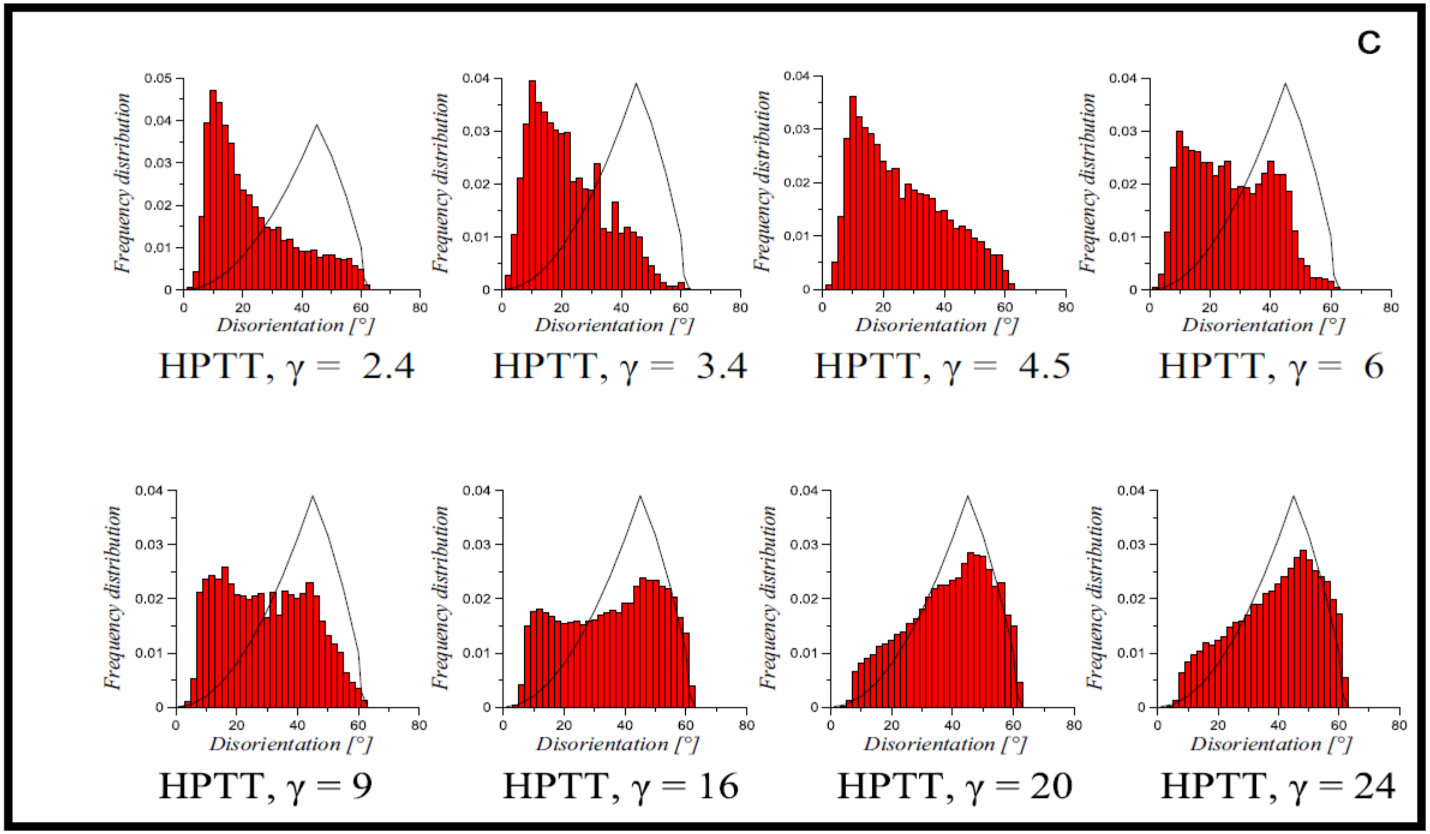
Disorientation correlation

Probality density at maximum disorientation – vs distance between neighbor grains for plastically deformed materials



B. Beausir, C. Fressengeas, N. Gurao, Laszlo S. Toth, Satyam Suwas,
Spatial correlation in grain misorientation distribution, *Acta Materialia*, 57 (2009) 5382-5395

Evolution of correlated disorientation angle distribution between first neighbours (Al – simple shear)



Cai Chen, Yan Beygelzimer, Laszlo S.Toth, Jean-Jacques Fundenberger, Microstructure and strain in protrusions formed during severe plastic deformation of aluminum, Materials Letters159 (2015) 253–256

Evolution of correlated and non-correlated disorientation angle distribution between first neighbours (SPD of Cu)

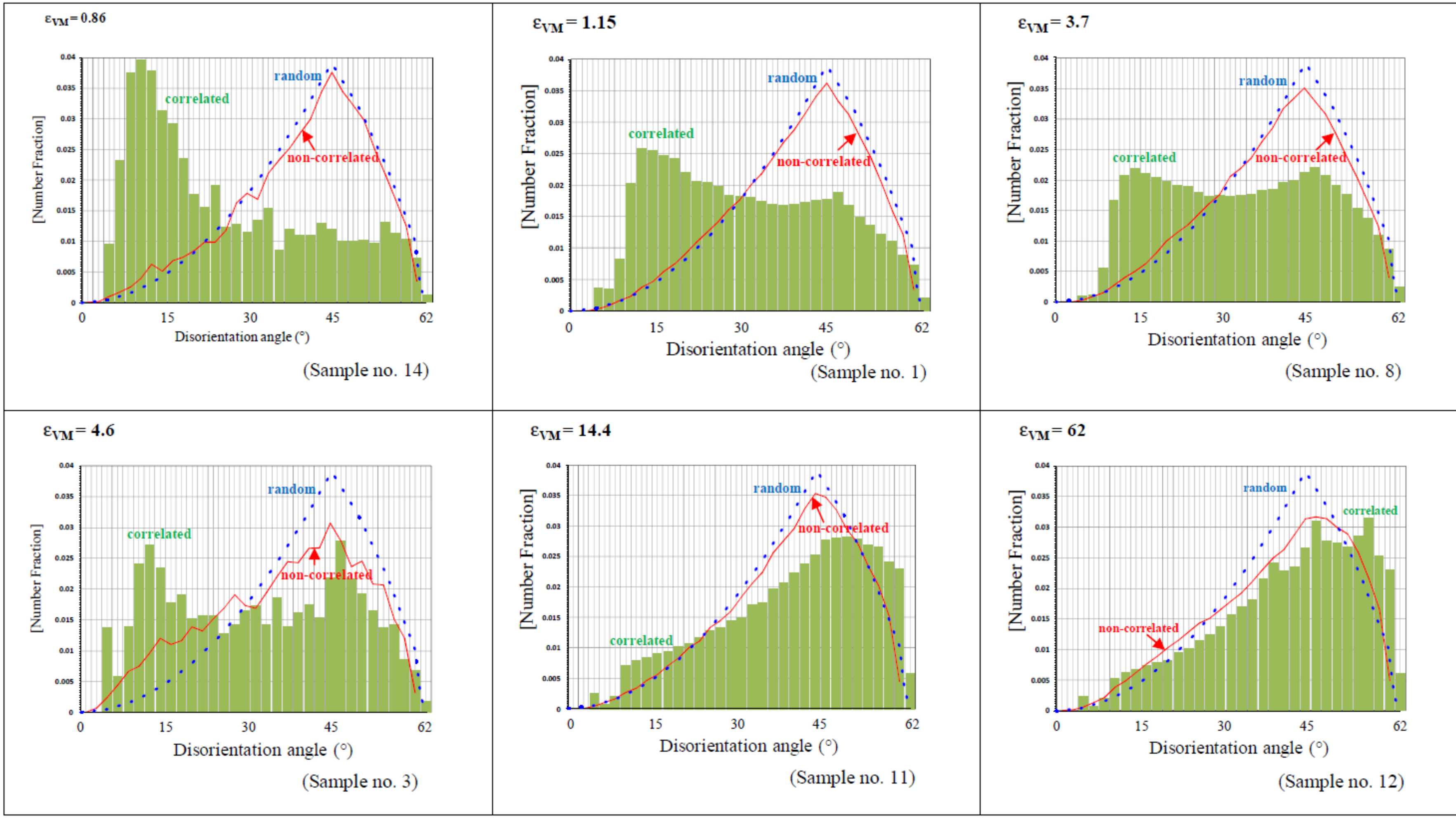


Fig. 2. Disorientation distributions between neighbor grains as a function of large strains for commercially pure copper

The Idea

The quantity of GNDs is proportional to the difference between the correlated and non-correlated disorientation distributions:

$$\tilde{R} = \sqrt{\int \left[N(g) - R(g) \right]^2 dg}$$

correlated: $N(g)$ non-correlated: $R(g)$

$$\rho_{GND} \sim \tilde{R}$$

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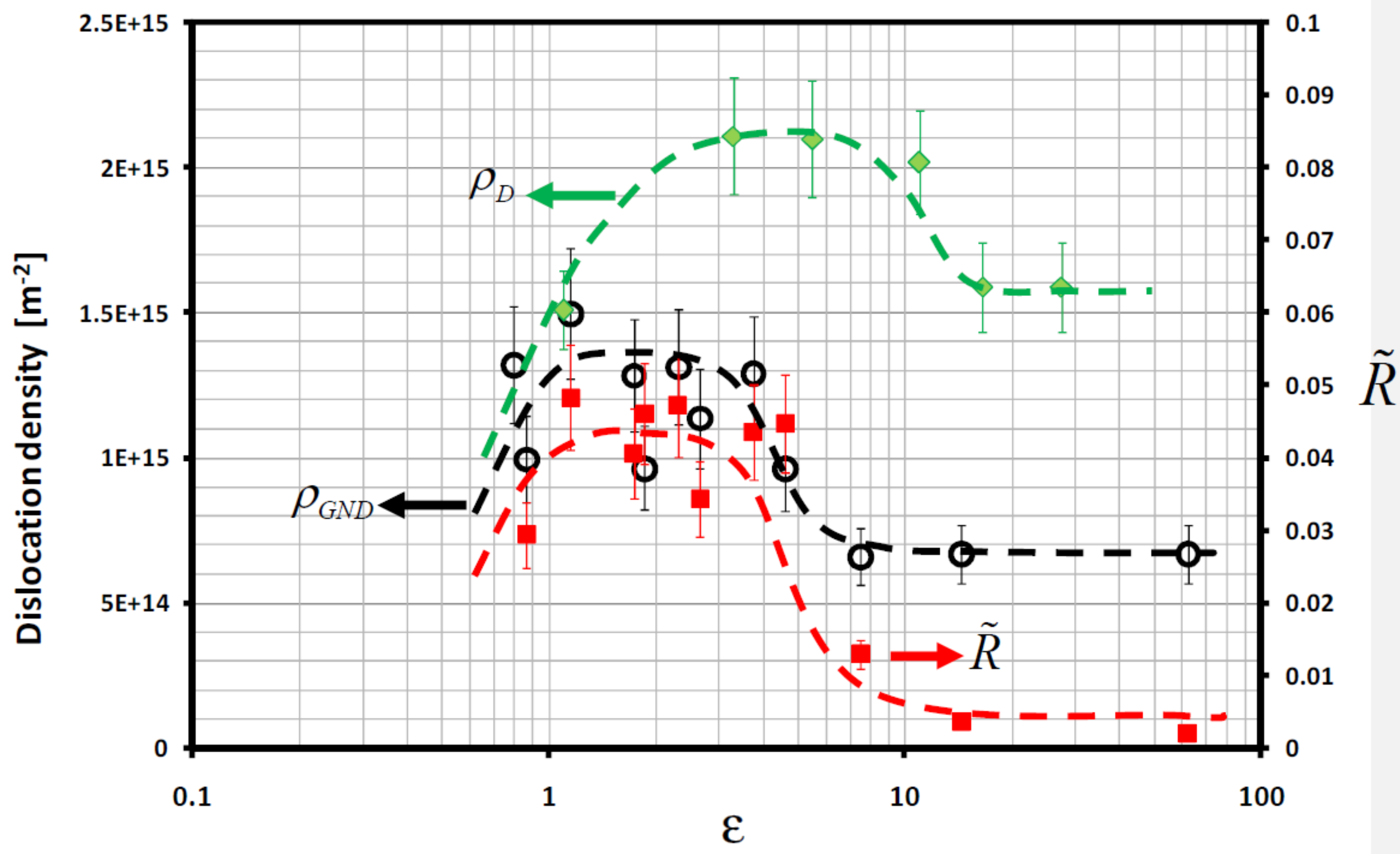
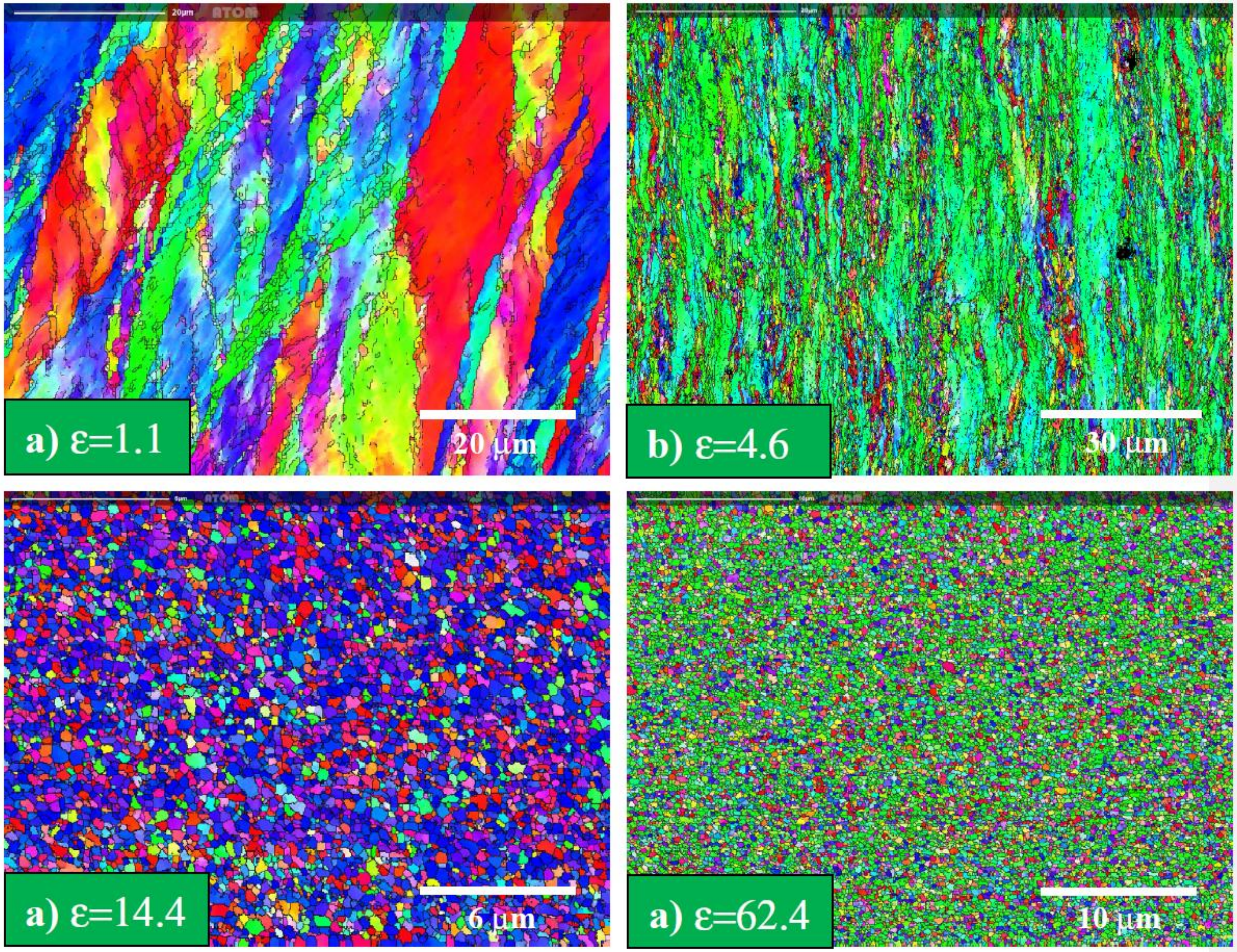


Evolution of the microstructure (SPD of Cu)



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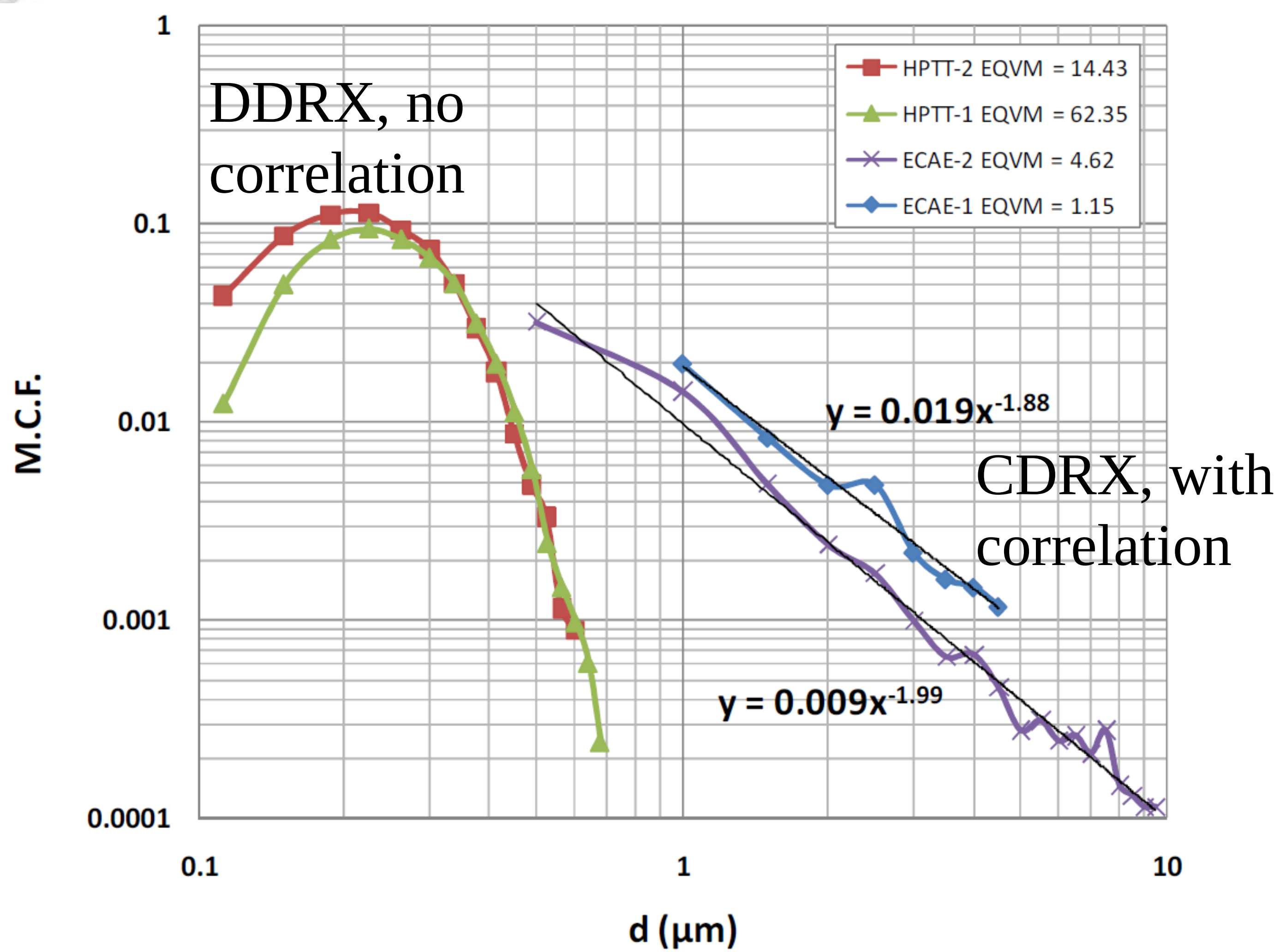
Probality density at maximum disorientation – vs distance between neighbor grains for plastically deformed materials



Conclusions

1. **GND density is initially rapidly increasing, reaches a maximum at strains of about 2-3 and then decreases. Radical decrease leads to approaching the Taylor type behavior of the polycrystal. Nano-polycrystalline materials deform by the Taylor mode.**

2. **The difference between the correlated and non-correlated disorientation distributions of the deformed polycrystal correlates with the GND density.**