Modelling of Metal Microstructures by the Grain Size Orientation Distribution Function

Jesús Galán López
Monireh Azimi
Leo Kestens

j.galanlopez@tudelft.nl

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MuSTMeF

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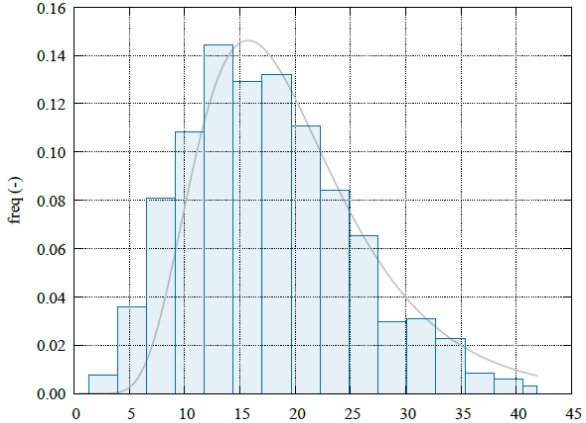
Introduction



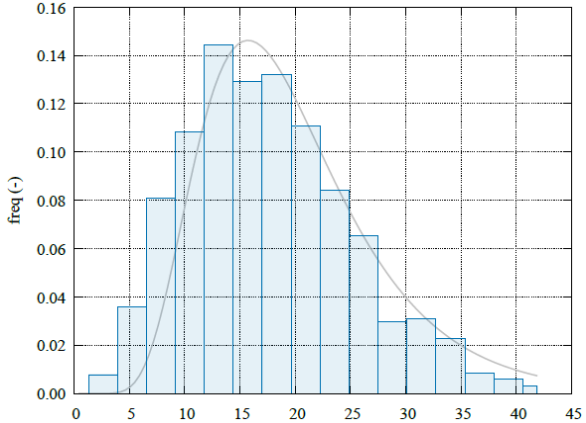
Grain size: lognormal or other distribution

$$p(d) = \mathcal{N}_{\mu,\sigma}\left(\log(d)\right)$$

Crystallographic texture: ODF (harmonic series)

$$f(g) = \sum_i c_i T_i(g)\,, \qquad g \equiv \varphi_1, \Phi, \varphi_2$$

Introduction



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$$p(d) = \mathcal{N}_{\mu,\sigma}\left(\log(d)\right)$$

Crystallographic texture: ODF (harmonic series)

$$f(g) = \sum_i c_i T_i(g)\,, \qquad g \equiv \varphi_1, \Phi, \varphi_2$$

GSODF

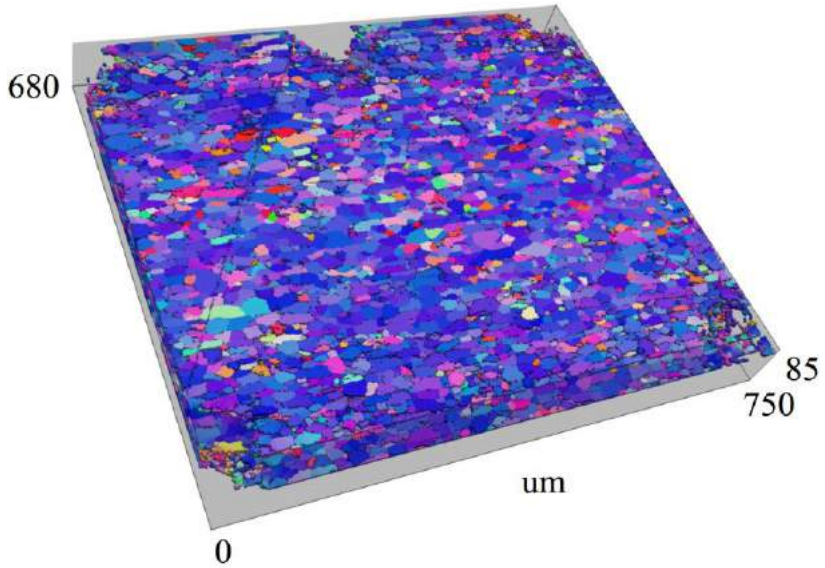
Grain size and orientation distribution function

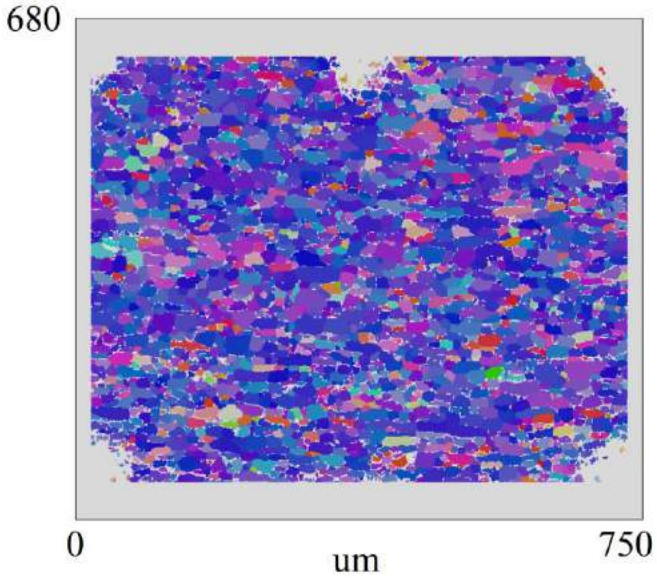
$$F(d, g\,) = ?$$

Outline

- Introduction
- GSODF calculation example (ELC steel, 2D/3D)
- Applications
  - DP steel (3D), IF steel (2D)
  - RVE generation (Dream3D)
  - Crystal plasticity simulations (VPSC)
- Conclusions

GSODF calculation

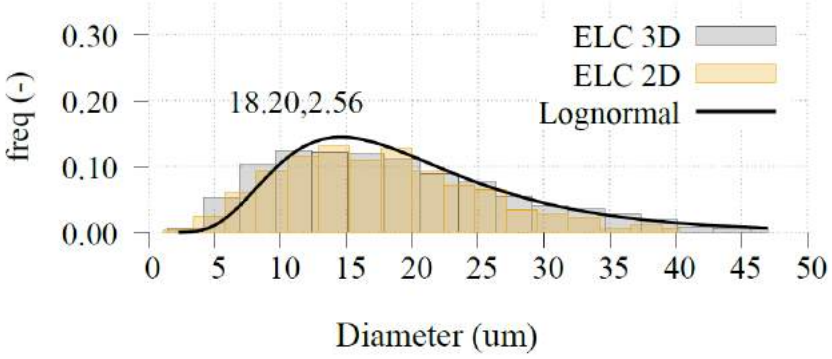


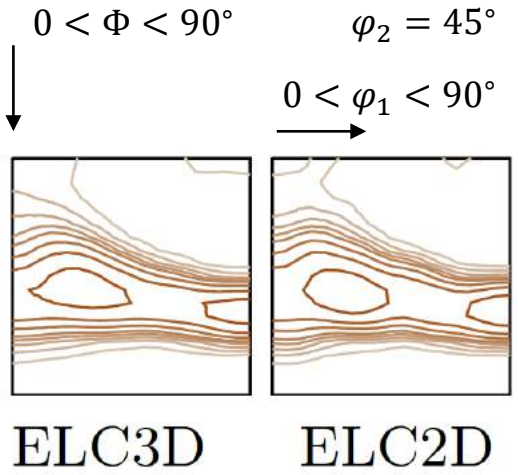


Extra Low Carbon (ELC) steel

3D-EBSD (40 layers)
9047108 points, 28605 valid grains

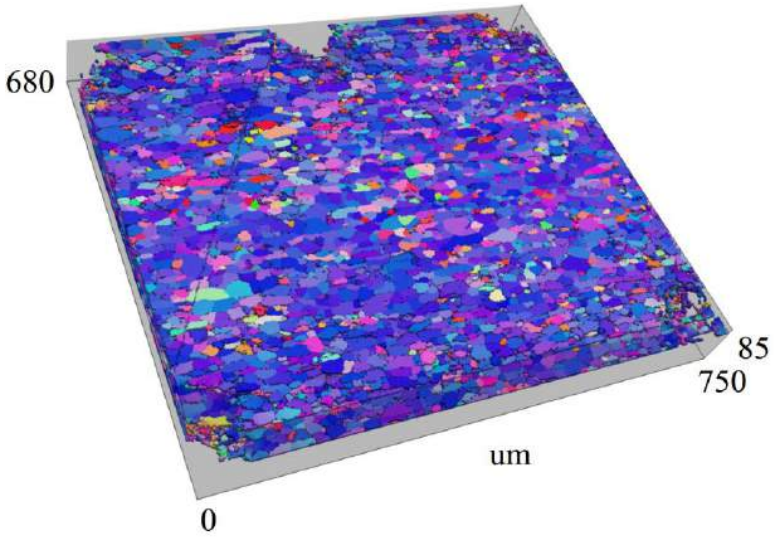
2D-EBSD (middle layer)
438755 points, 2679 valid grains





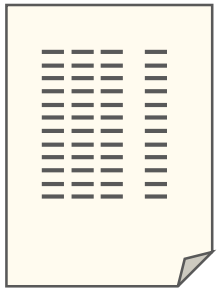
Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

GSODF calculation



DREAM 3D

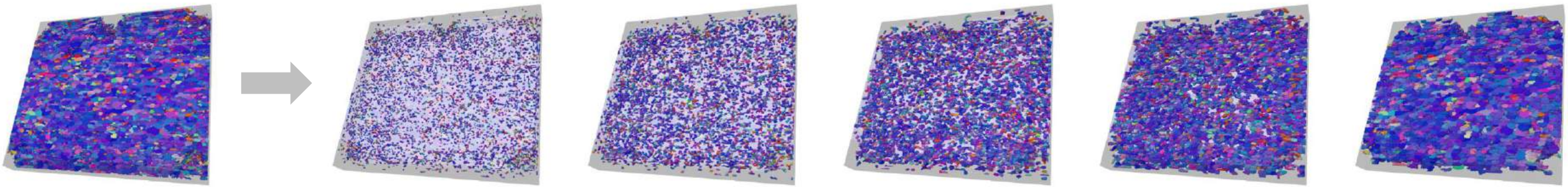
List of grains:



Euler angles
and volume

Step 0 (pre-processing)
Align all 2D-EBSD layers, clean-up data, divide into grains according to boundary misorientation and average over grains

GSODF calculation

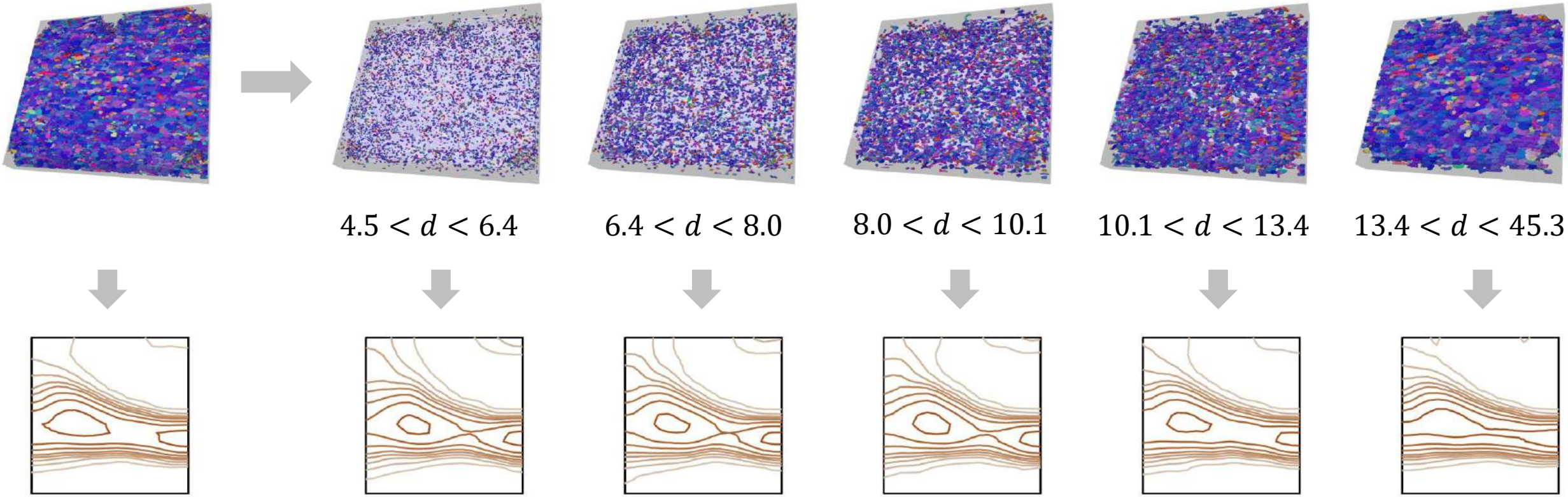


$4.5 < d < 6.4$ $6.4 < d < 8.0$ $8.0 < d < 10.1$ $10.1 < d < 13.4$ $13.4 < d < 45.3$

Step 1

Divide total number of grains in bins (with the same number of grains) depending on grain size

GSODF calculation

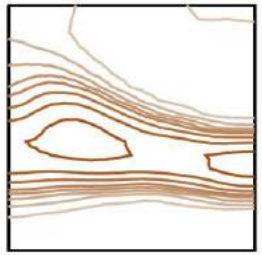
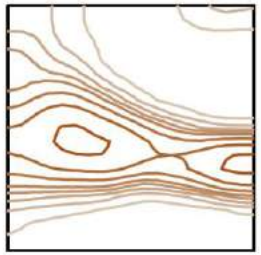
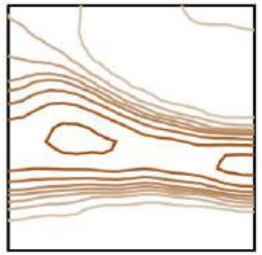


Step 2

Calculate ODF (harmonic series expansion) of each bin using MTM-FHM software

Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

GSODF calculation

ODF	$4.5 < d < 6.4$	$6.4 < d < 8.0$	$8.0 < d < 10.1$	$10.1 < d < 13.4$	$13.4 < d < 45.3$
					
$f(g) = \sum_i c_i T_i(g)$	$\sum_i c_i^{I} T_i(g)$	$\sum_i c_i^{II} T_i(g)$	$\sum_i c_i^{III} T_i(g)$	$\sum_i c_i^{IV} T_i(g)$	$\sum_i c_i^{V} T_i(g)$

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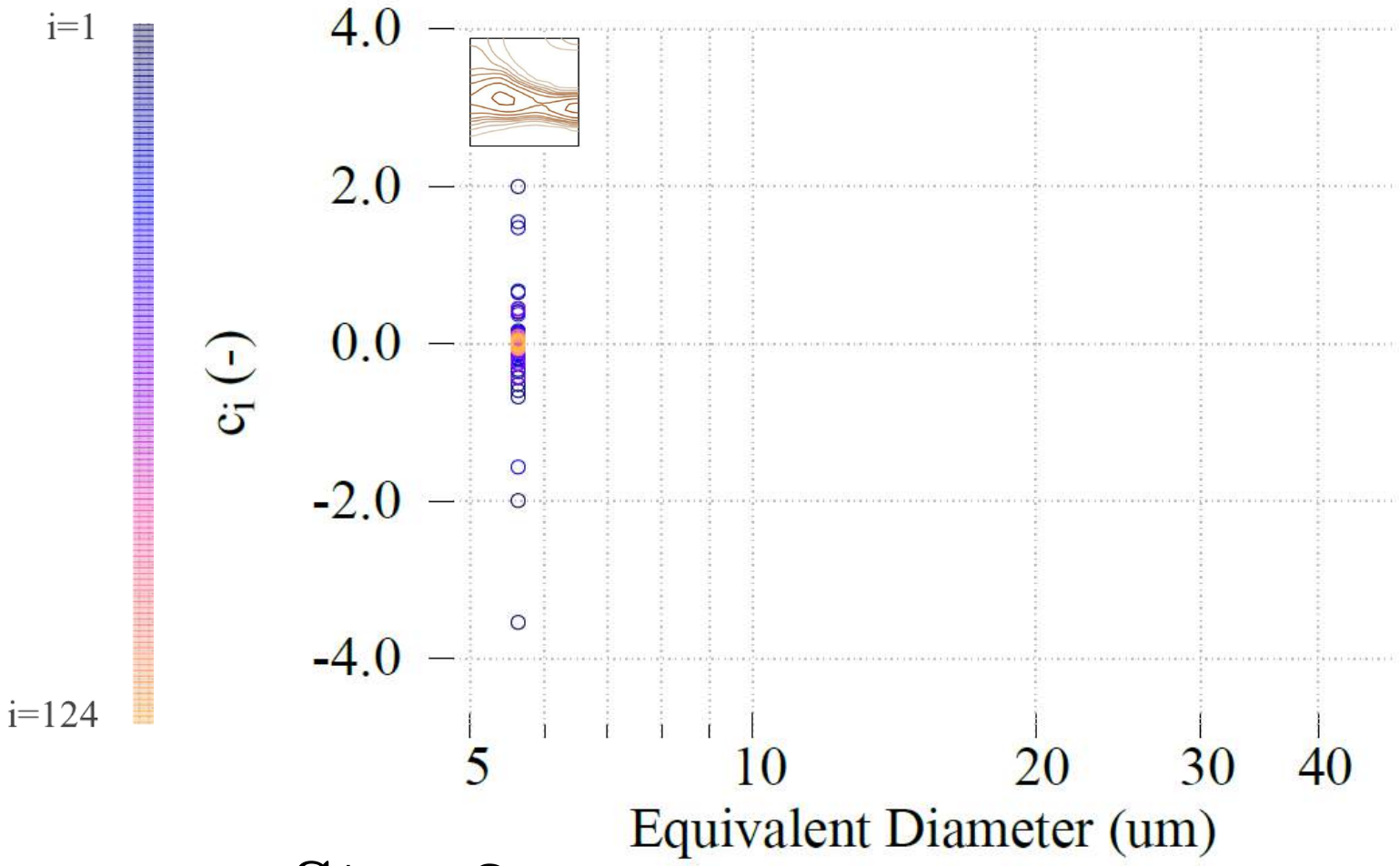
GSODF calculation

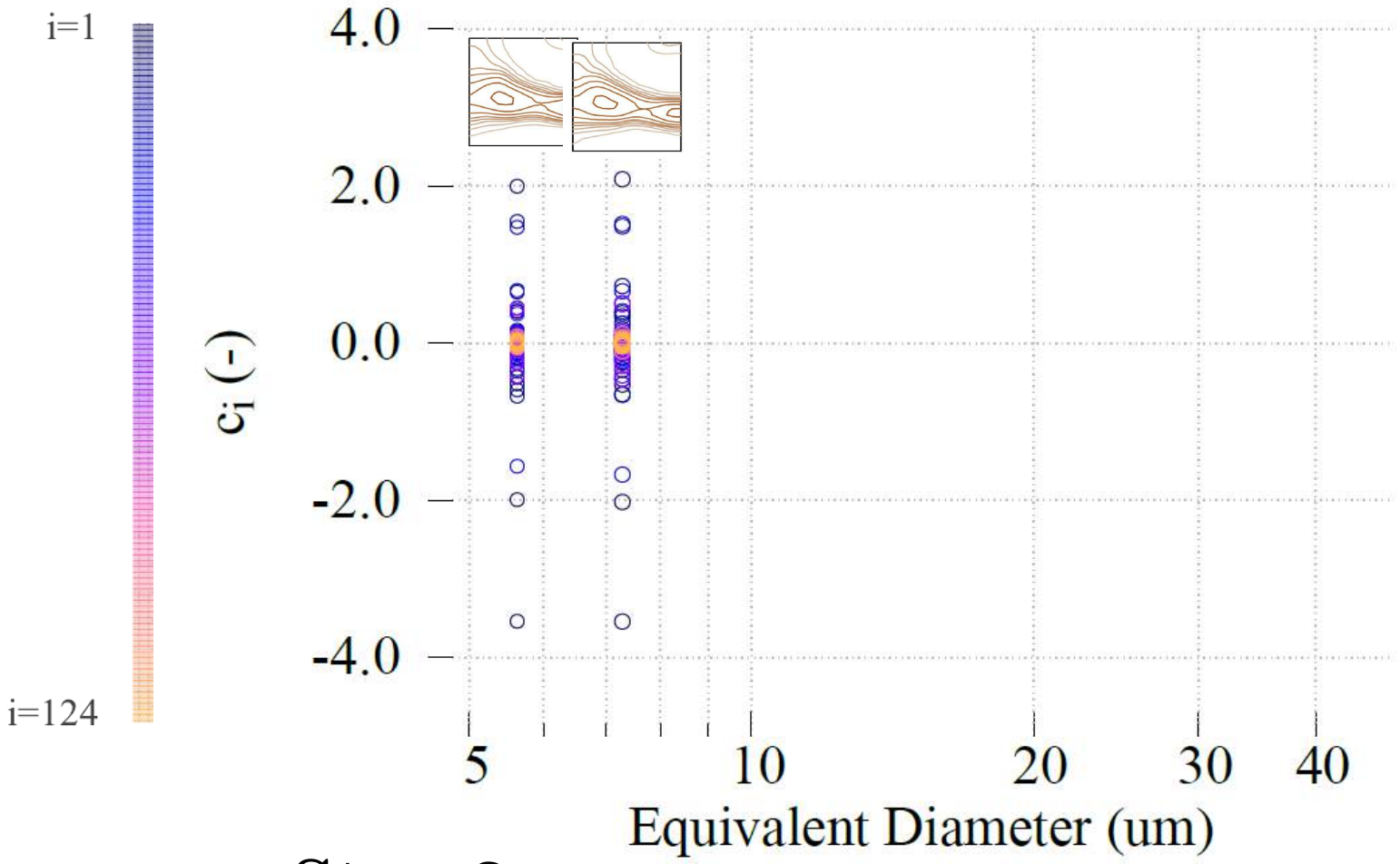


Step 3

Represent C-coefficients of the calculated ODFs with respect to grain size

Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

GSODF calculation



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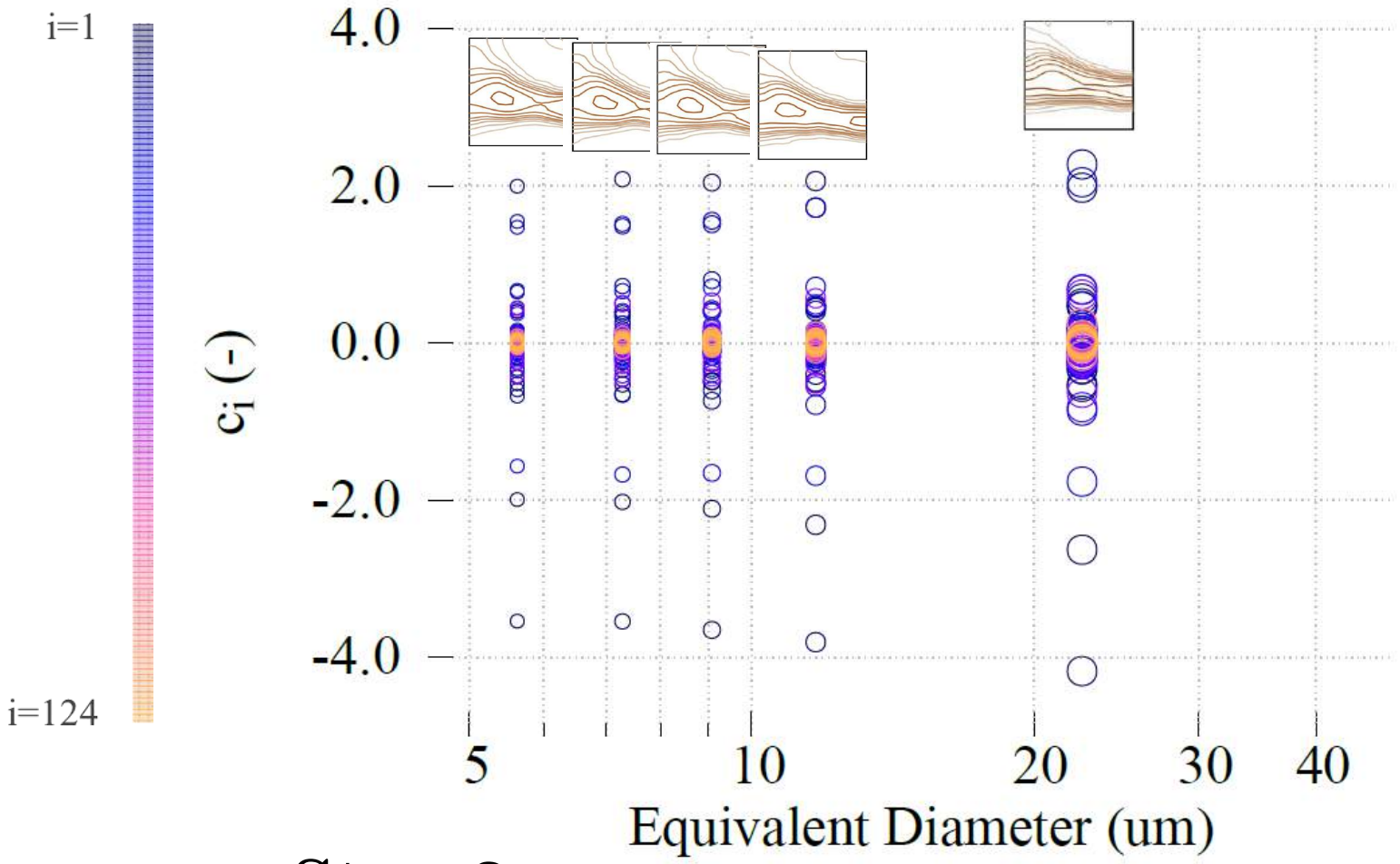

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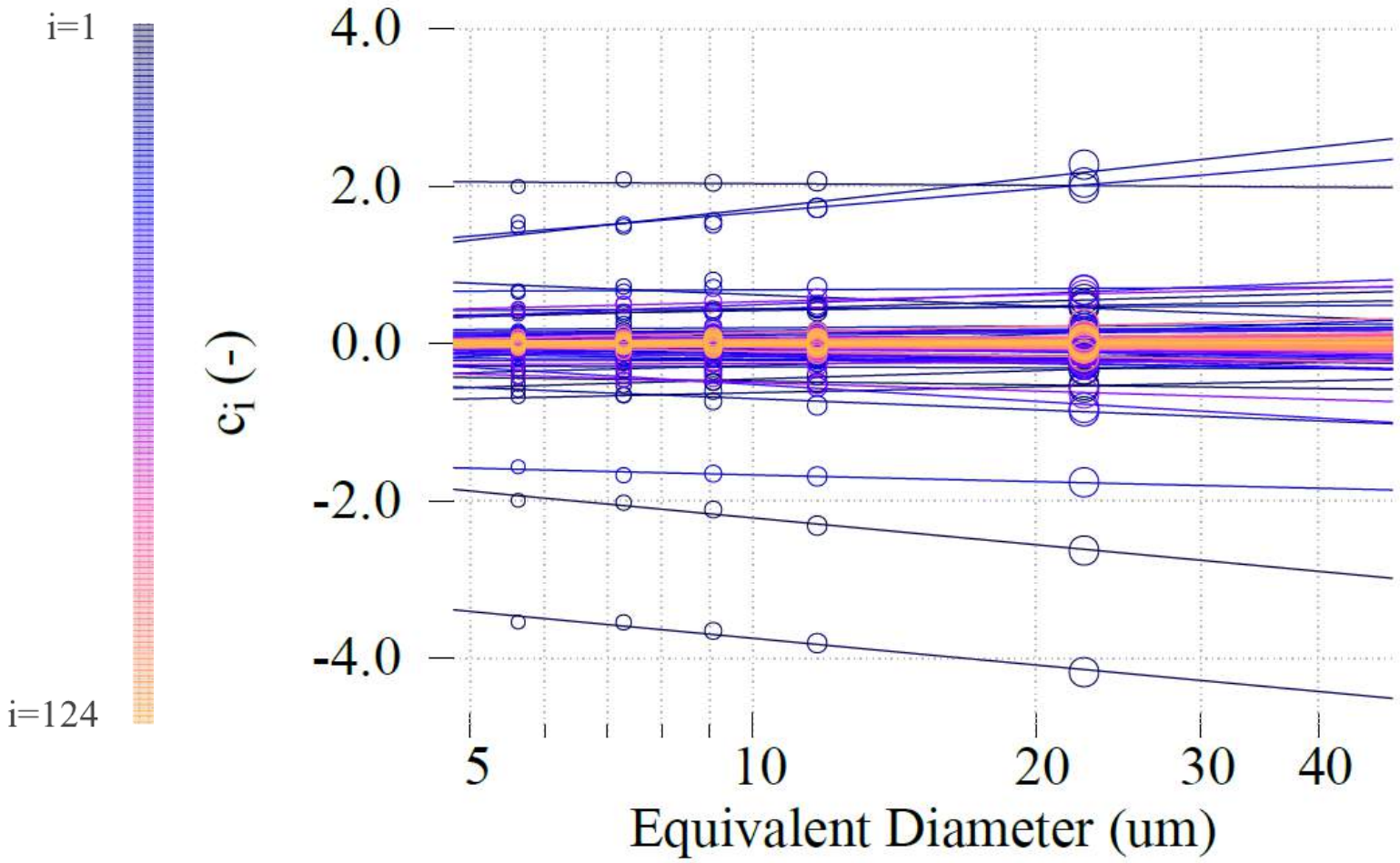


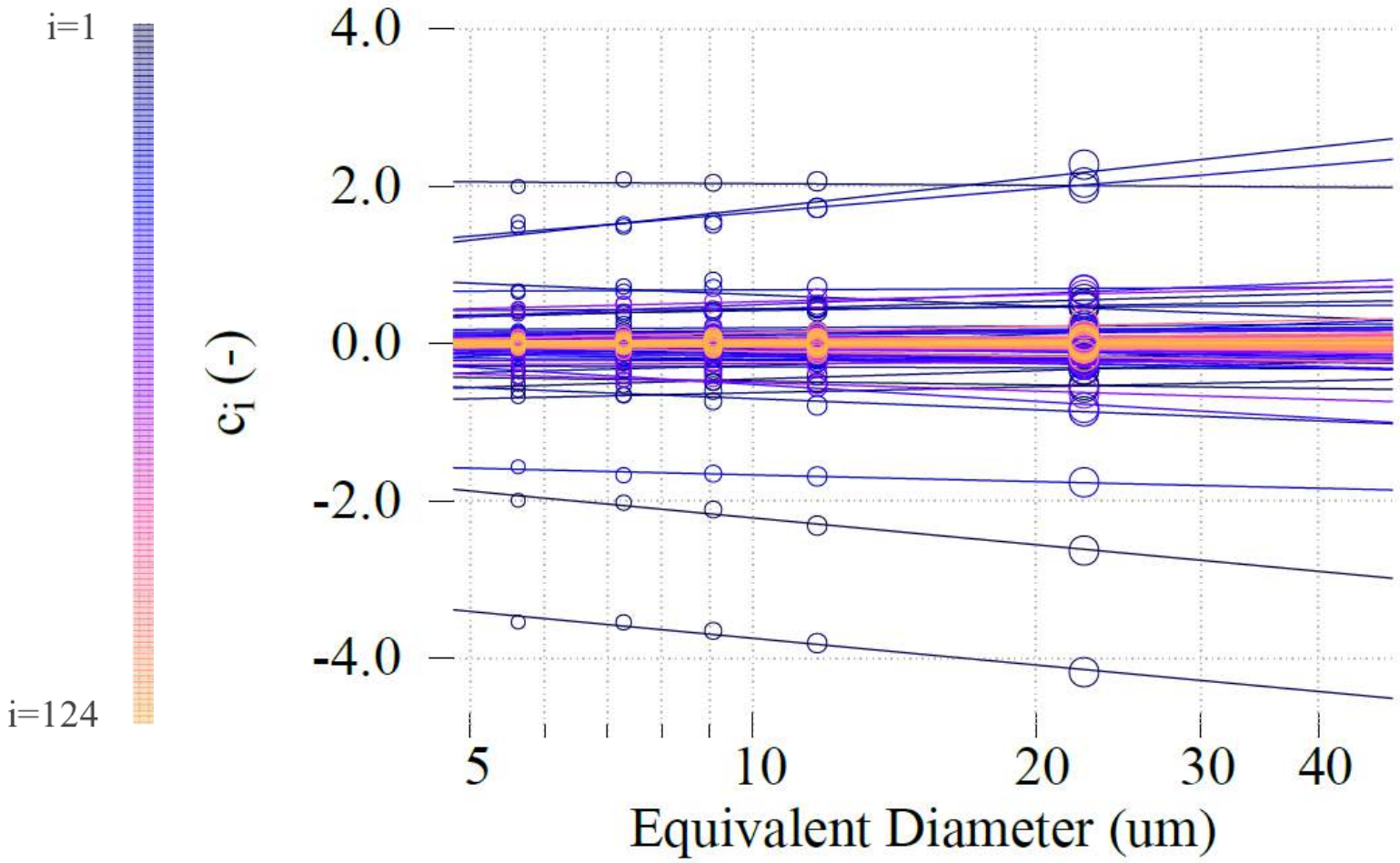
Linear relationship

$$c_i(d) = a_i + b_i \log(d)$$

Step 4

Linear fitting with respect to $\log(d)$

GSODF calculation



$$c_i(d) = a_i + b_i \log(d)$$

$$\Downarrow$$

Grain size dependent ODF:

$$f_d(g) = \sum_i (a_i + b_i \log(d)) T_i(g)$$

Step 4

Linear fitting with respect to $\log(d)$

GSODF

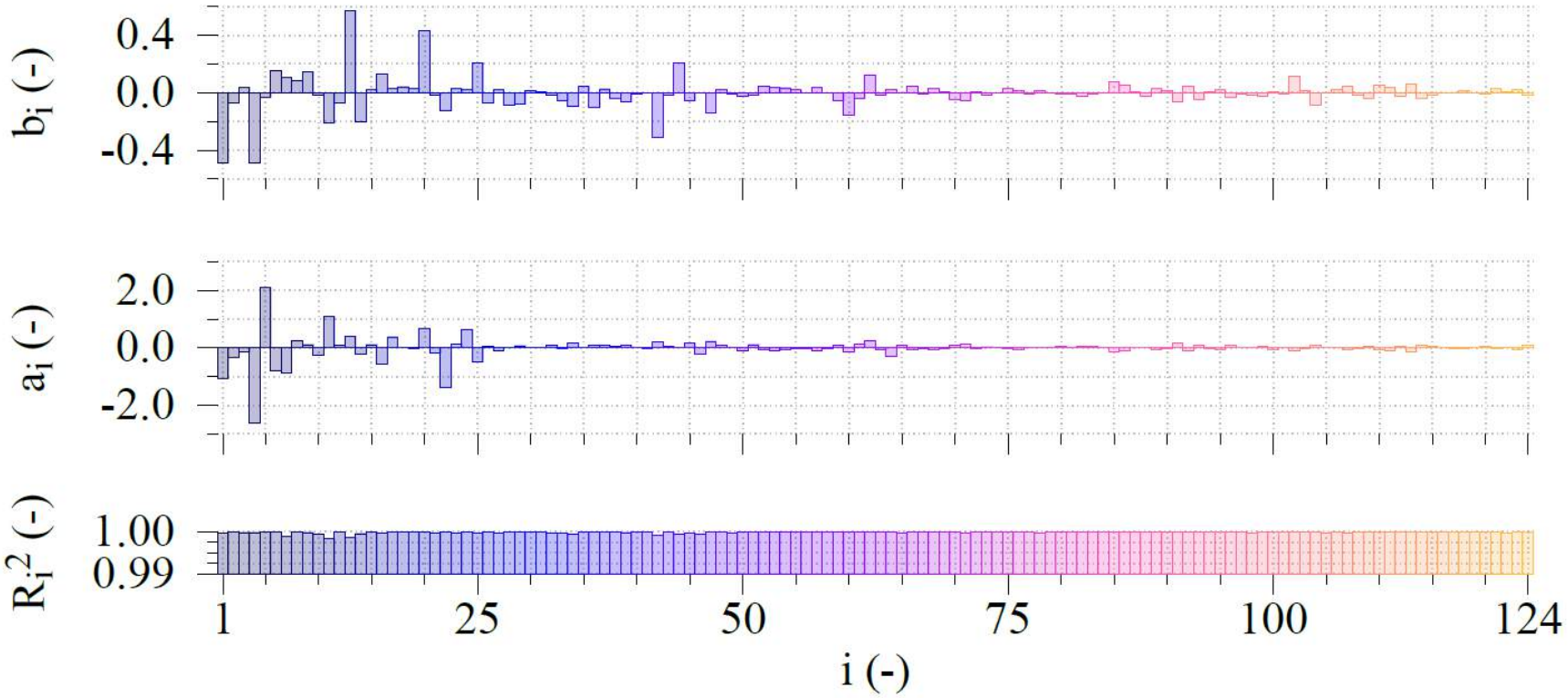
$$p(d) = \mathcal{N}_{\mu,\sigma}\left(\log(d)\right)$$

$$f_d(g) = \sum_i (a_i + b_i \log(d)) T_i(g)\,, \qquad g \equiv \varphi_1, \Phi, \varphi_2$$

$$F(d, g) = \mathcal{N}_{\mu,\sigma}\left(\log(d)\right) \sum_i (a_i + b_i \log(d)) T_i(g)$$

GSODF calculation

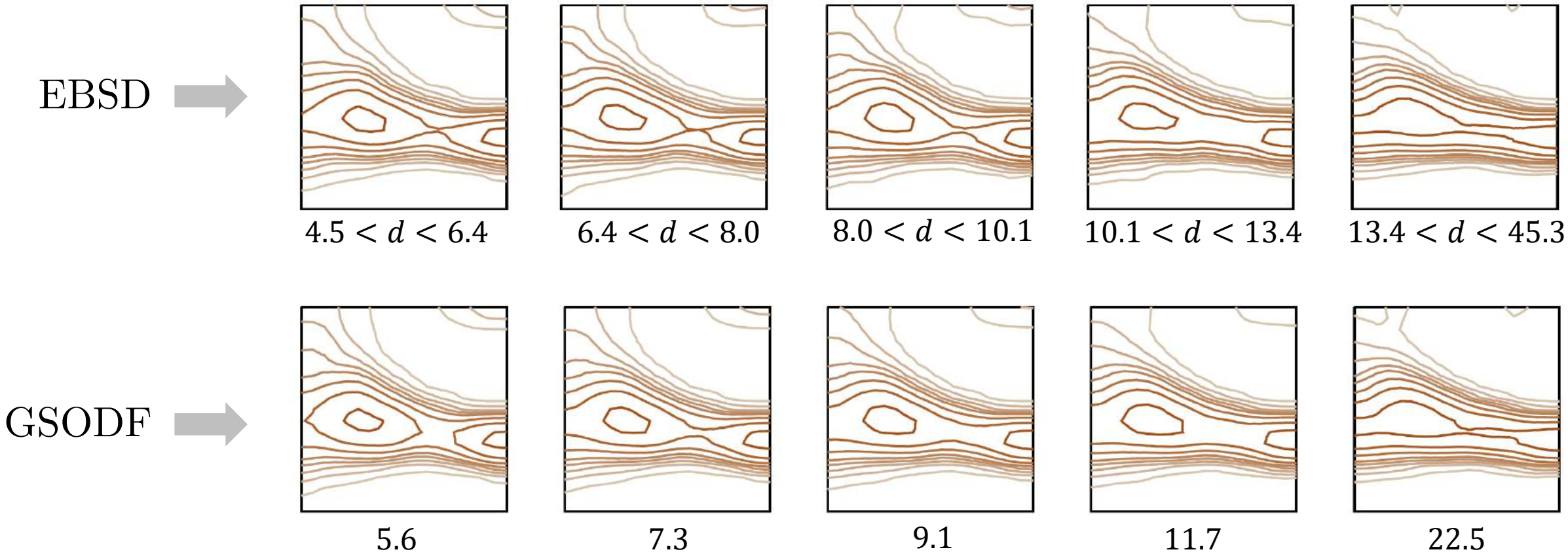
$$f_d(g) = \sum_i c_i(d) T_i(g) = \sum_i (a_i + b_i \log(d)) T_i(g)$$



Result

The GSODF is given by the GS distribution and the coefficients a_i and b_i

GSODF calculation



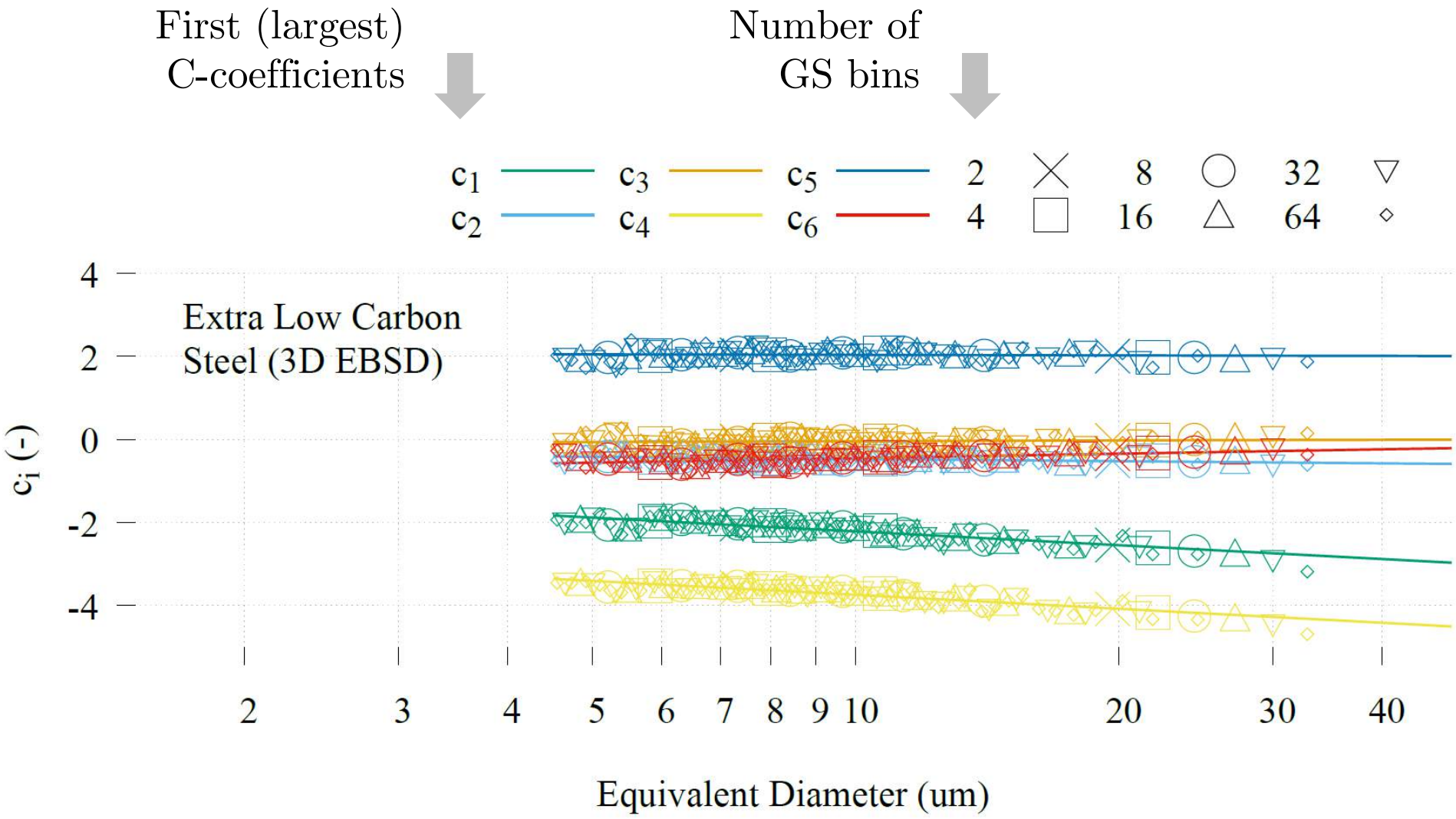
Validation

Predictions of GS dependent ODFs for the equivalent diameter of each bin

Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

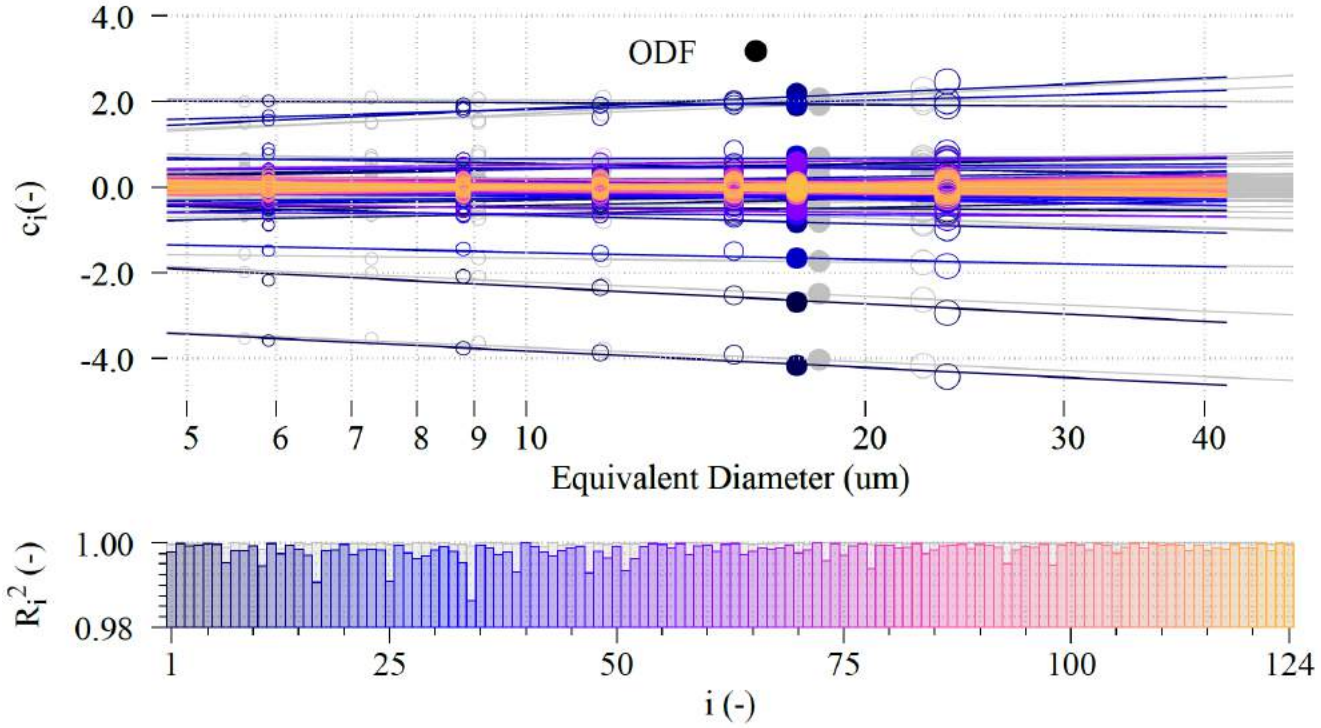
GSODF calculation

Dependence on number of grain size bins

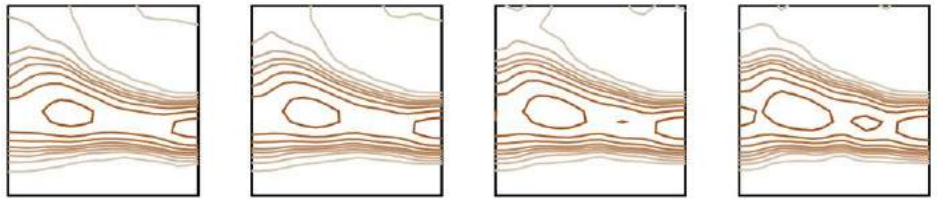


GSODF calculation (2D)

EBSD

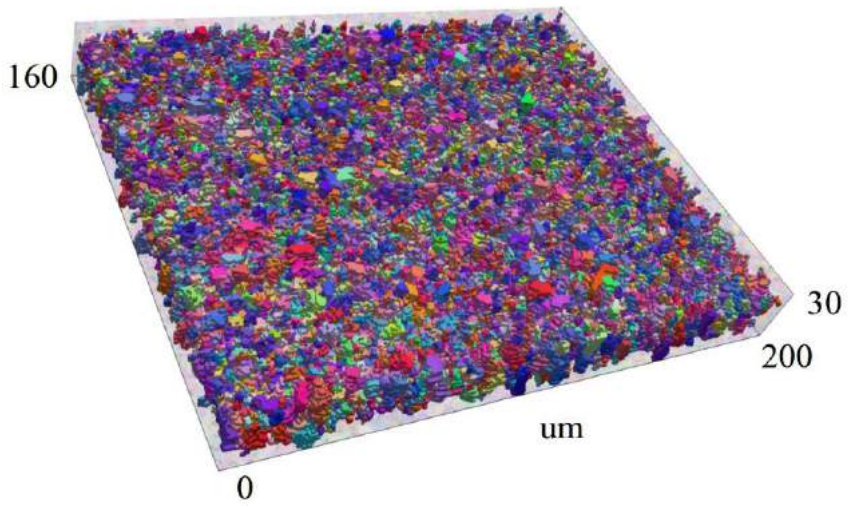


GSODF



Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

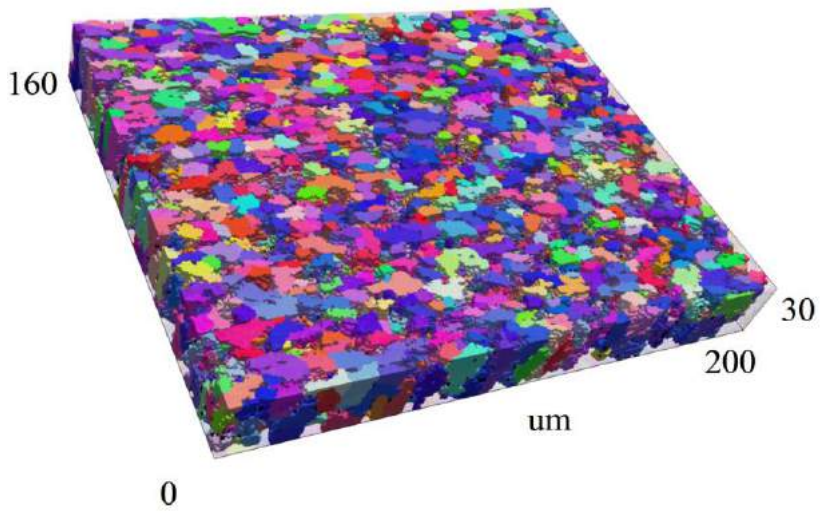
Dual Phase Steel

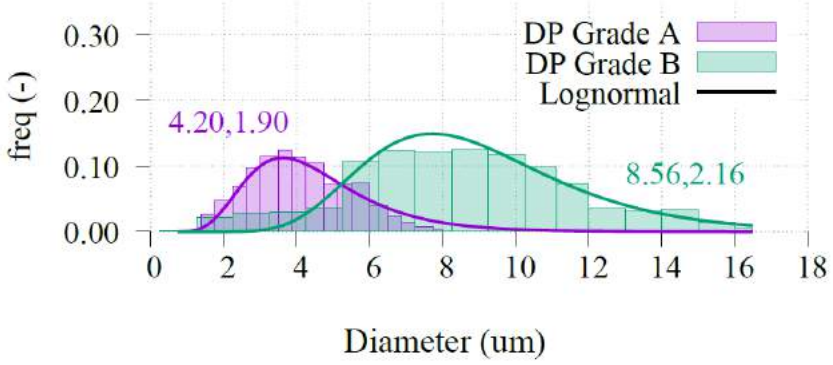


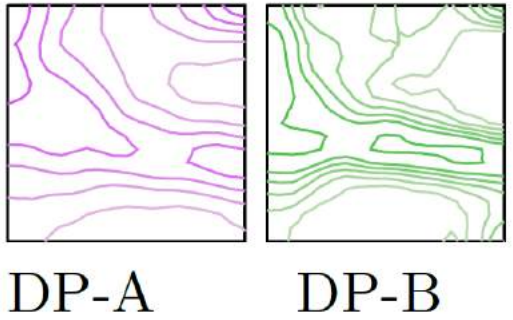
Dual Phase (DP) steel (ferrite)

Grade A: 3D-EBSD (40 layers)
4200420 points, 15446 valid grains

Grade B: 3D-EBSD (40 layers)
2691220 points, 5635 valid grains

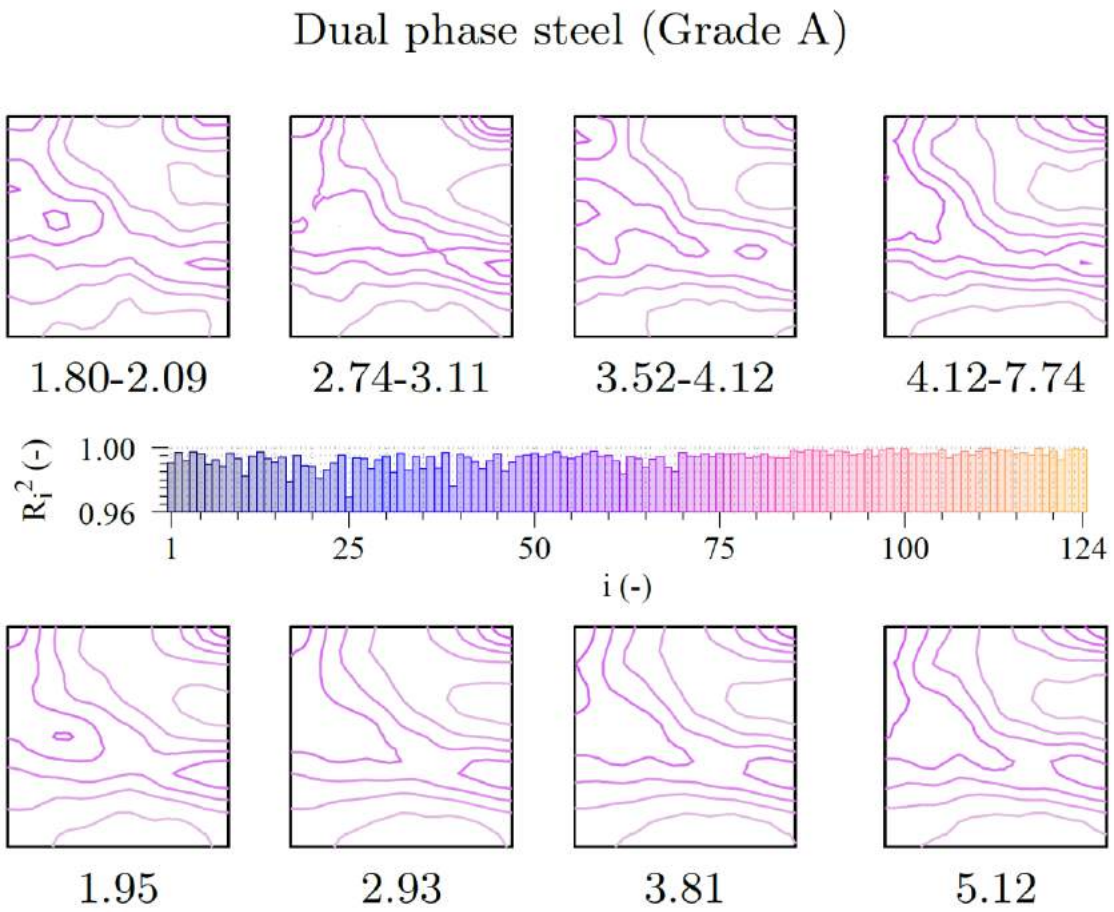


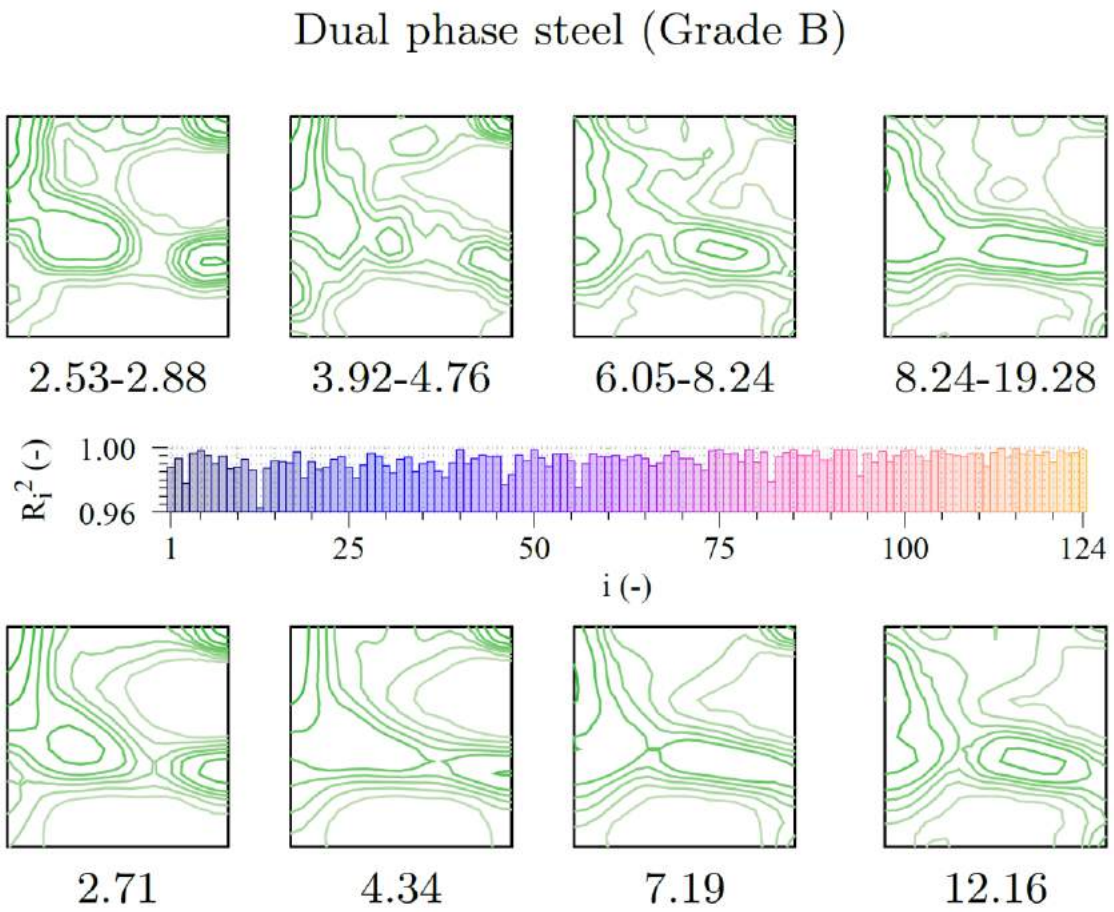




Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

Dual Phase Steel

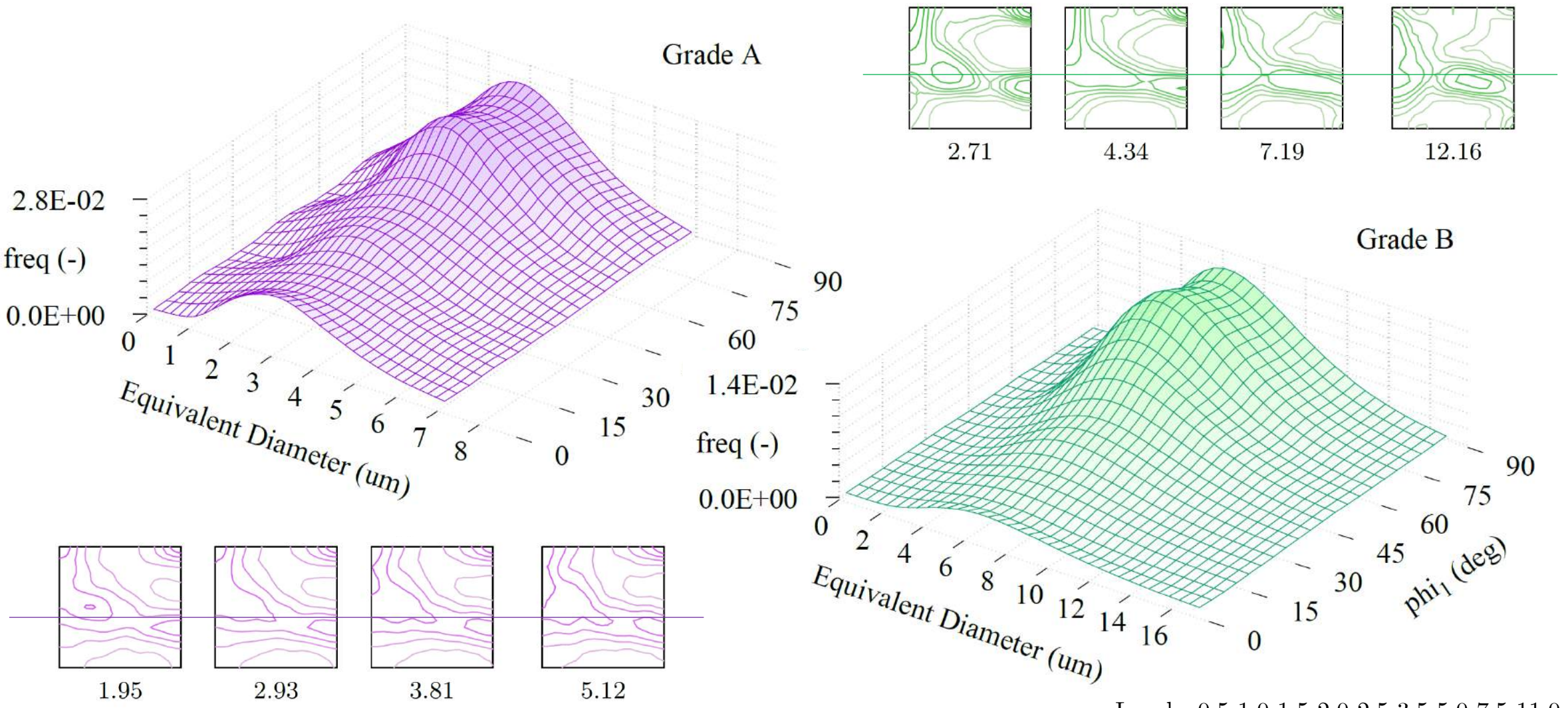




Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

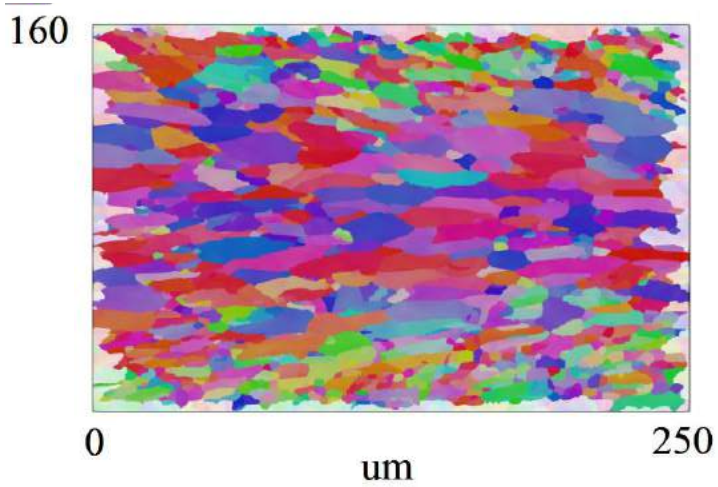
Dual Phase Steel

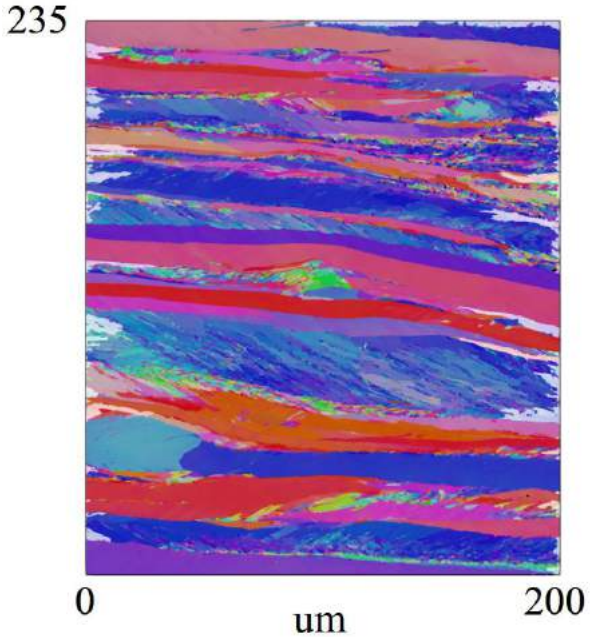
Grain size distribution along gamma fibre



Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

Interstitial Free Steel

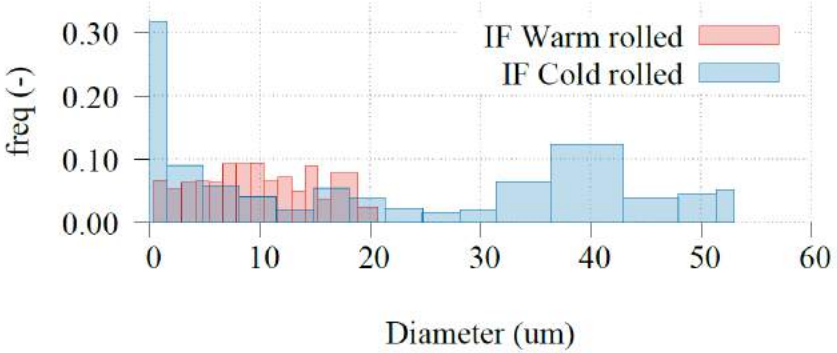


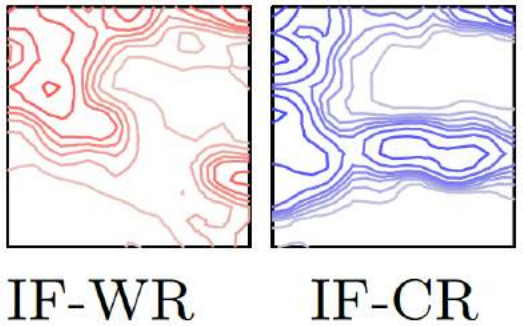


Interstitial free steel (GB=2deg)

Warm-rolled (2D-EBSD):
4200420 points, 15446 valid grains

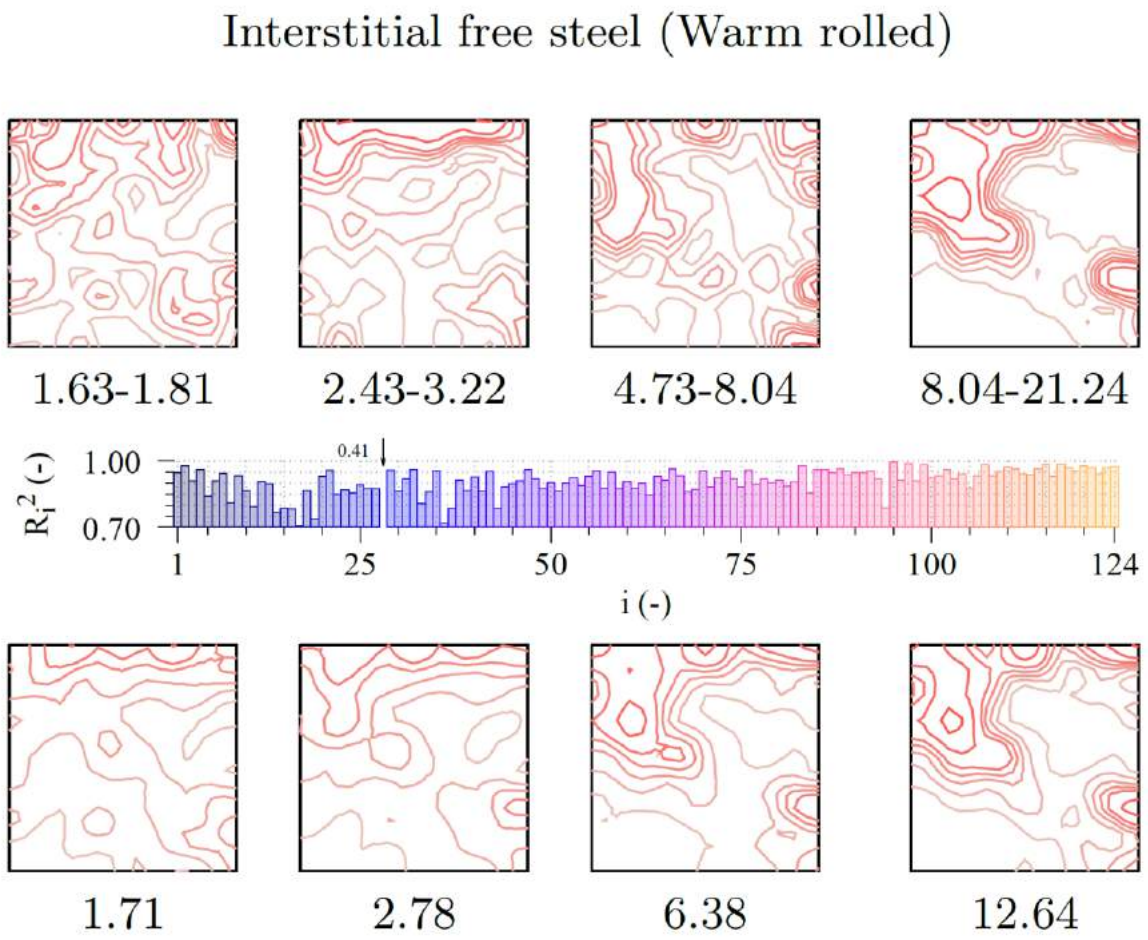
Cold-rolled (2D-EBSD):
2691220 points, 5635 valid grains

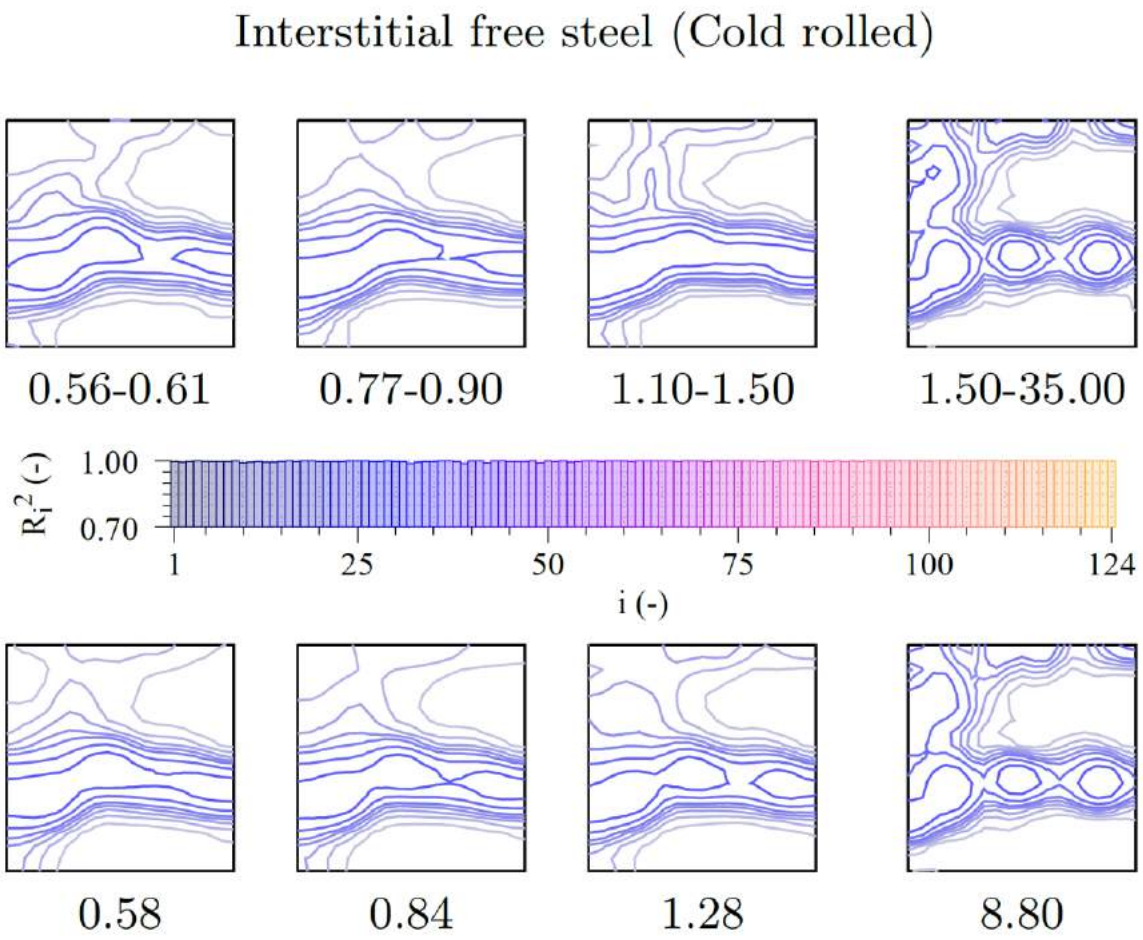




Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

Interstitial Free Steel

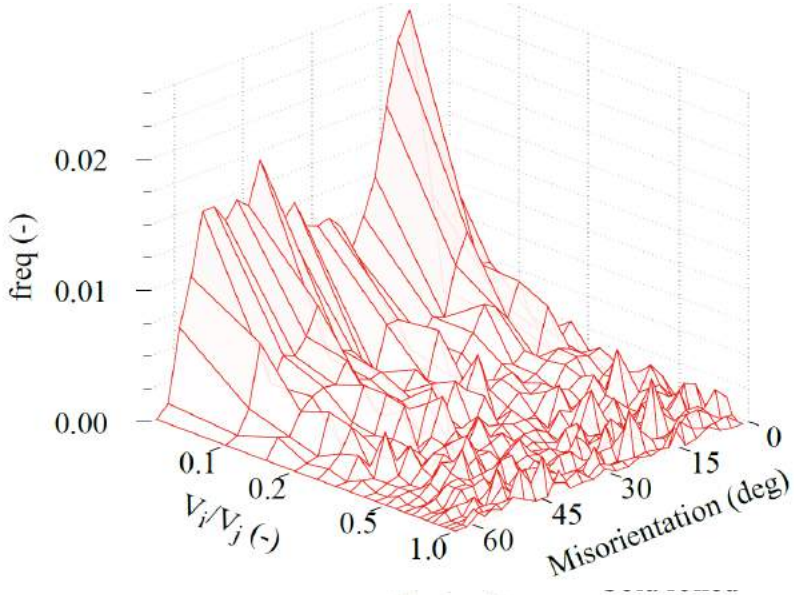


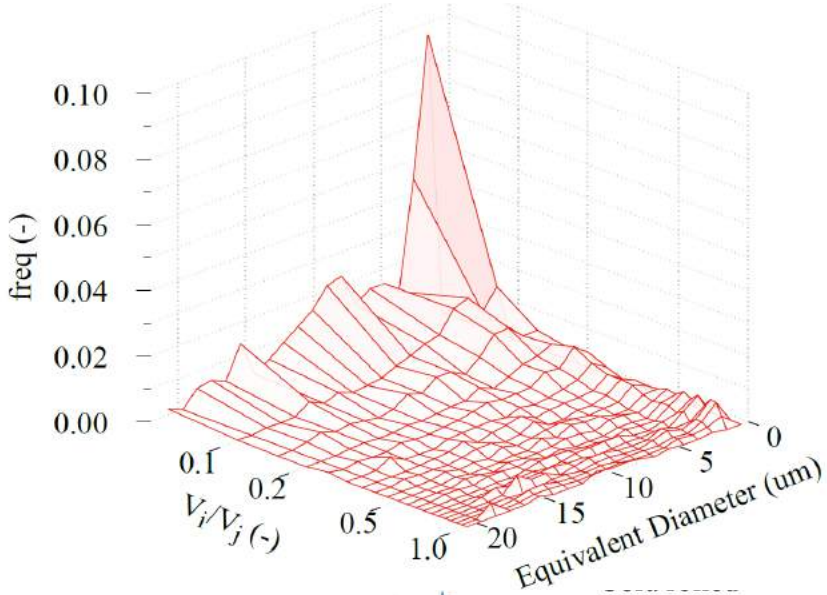


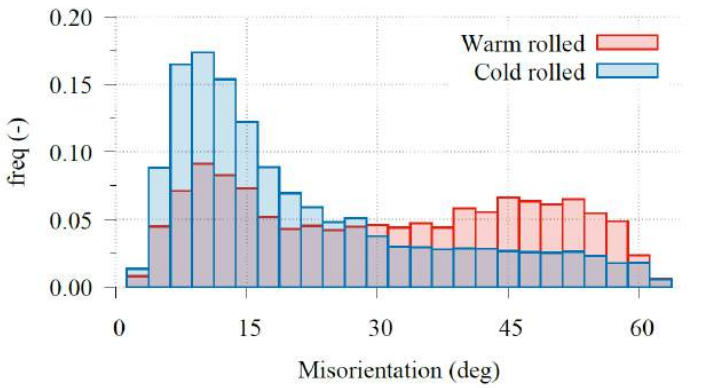
Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

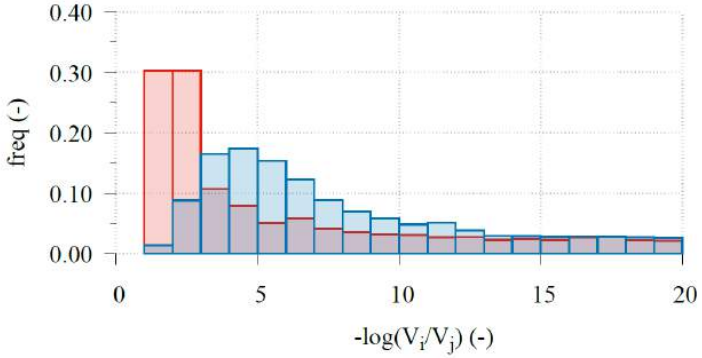
Interstitial Free Steel

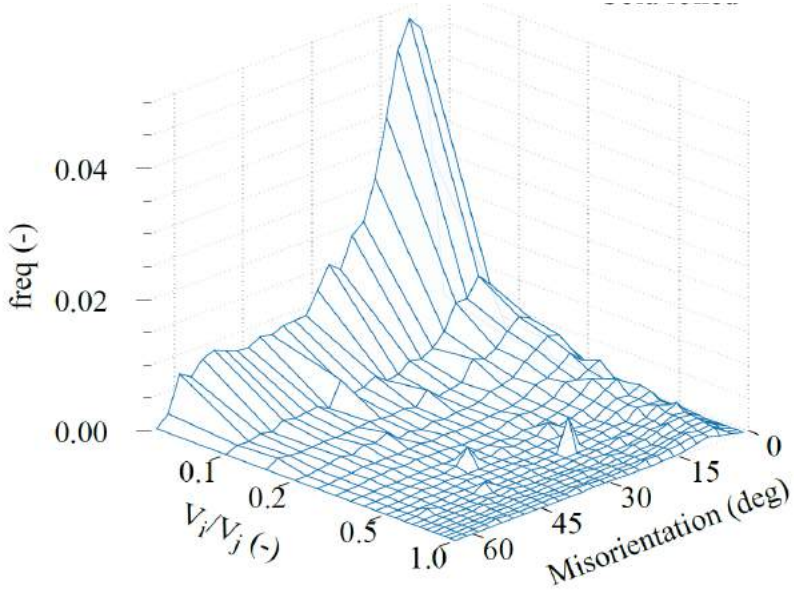
Misorientations and grain size ratio distributions

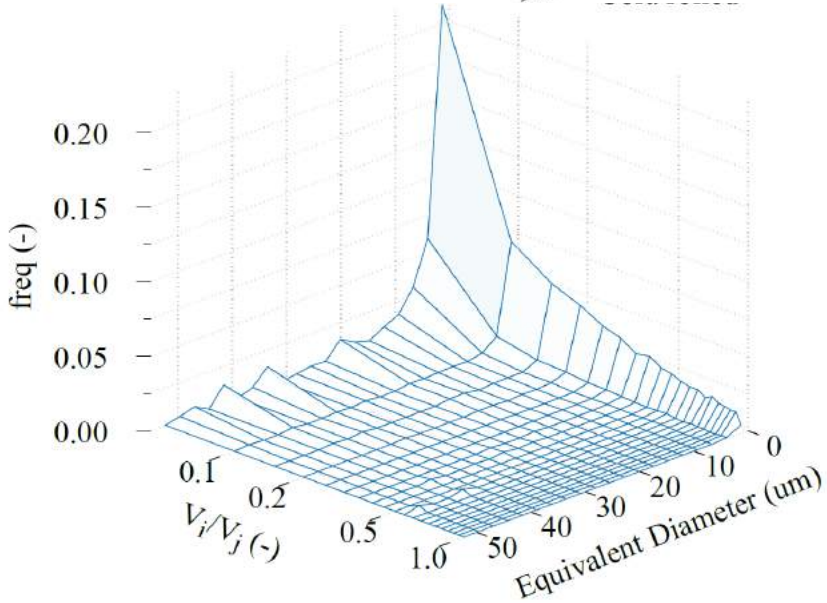


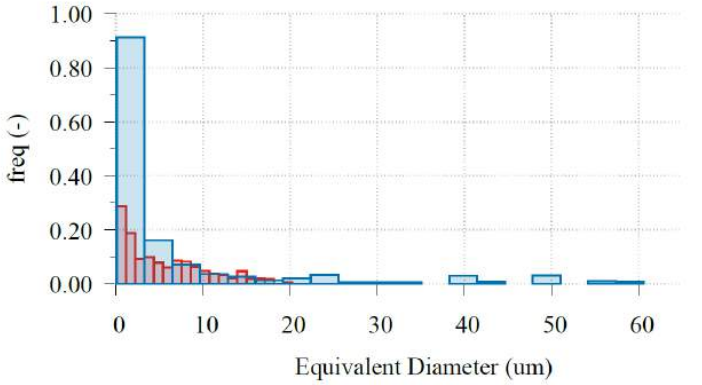








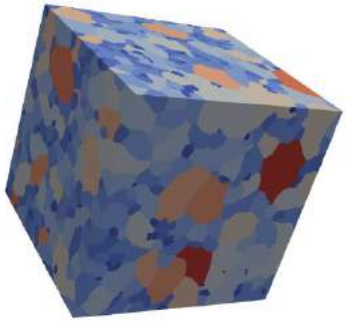




RVEs

DREAM 3D

64x64x64 points (resolution: 1.00um)
246 grains



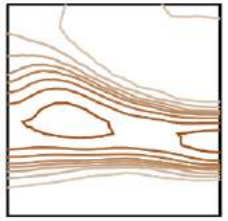
196x196x196 points (resolution: 0.75um)
2984 grains

512x512x512 points (resolution: 0.50um)
15459 grains

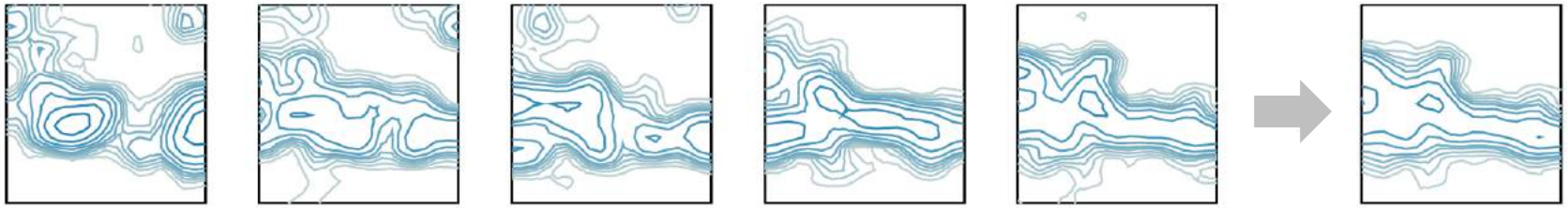
Blue: smaller size
Red: larger size

RVEs

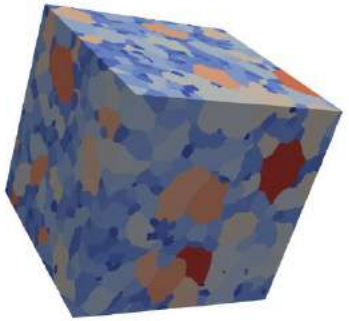
ELC steel

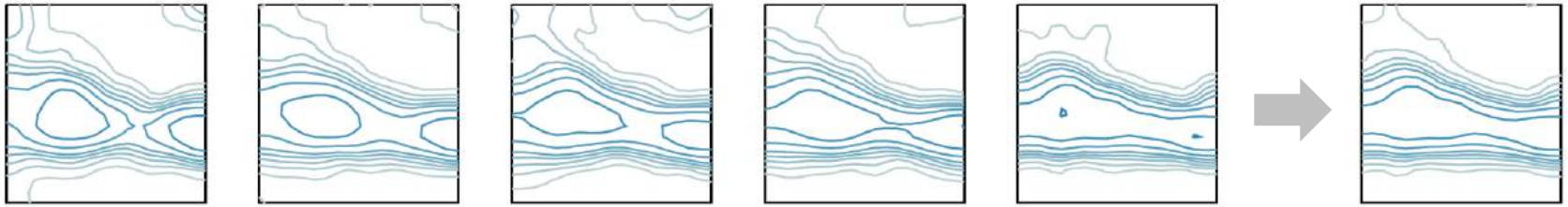


64x64x64

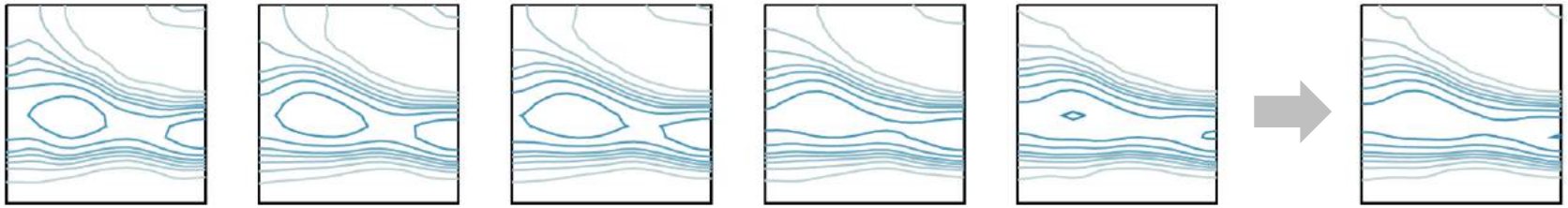


196x196x196





512x512x512



0.00-7.26 | 7.26-9.10 | 9.10-10.54 | 10.54-12.05 | 12.05-13.80 | Total

Blue: smaller size

Red: larger size

Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

VPSC

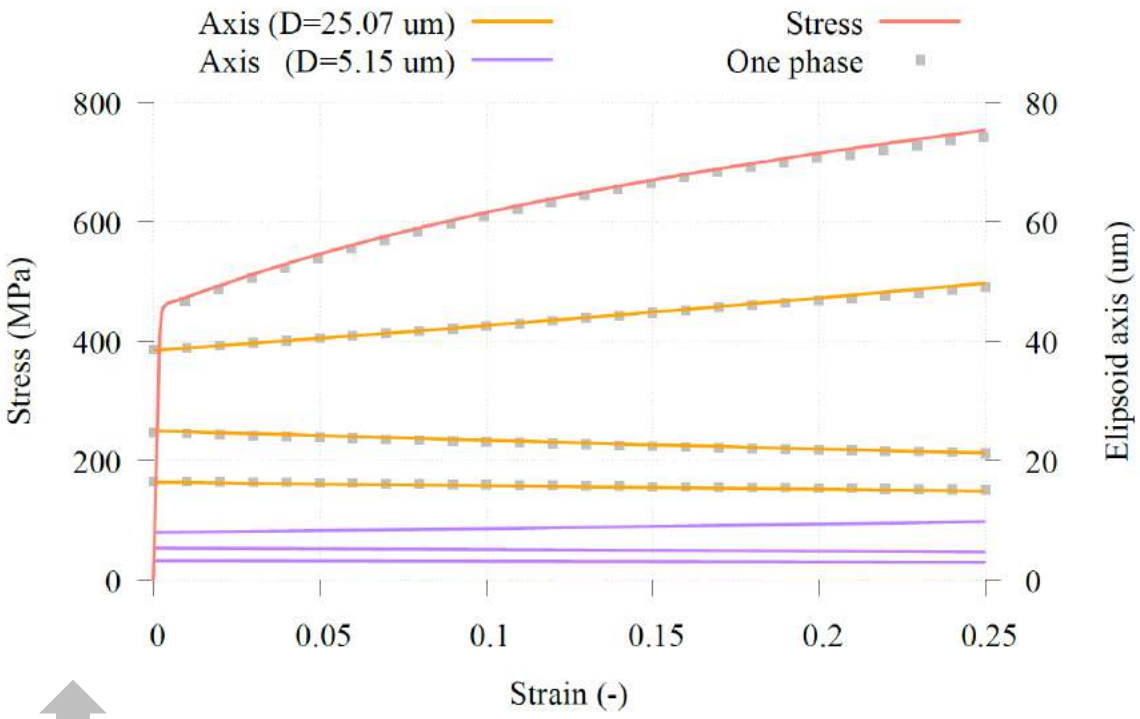
Crystal plasticity simulation using viscoplastic self-consistent model (25% uniaxial tension in 250s)

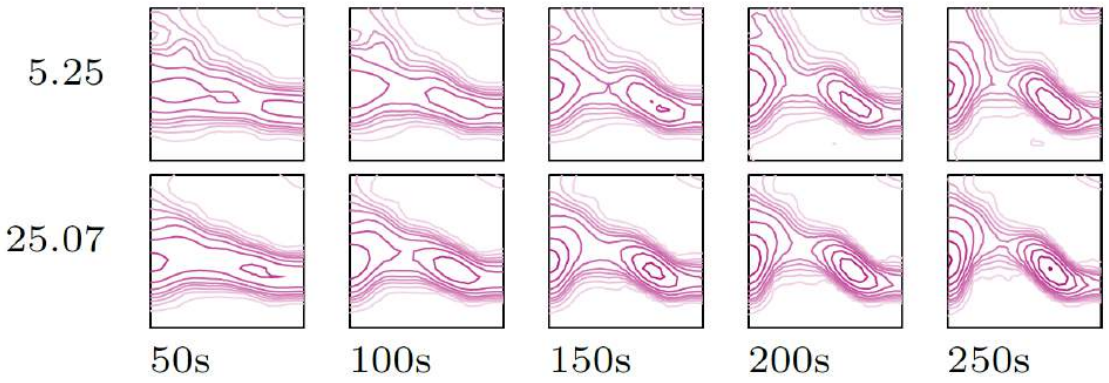
8 ferrite phases, 1 for each grain size bin:

- Phase fraction depending on GS distribution
- Discrete texture (500 grains) extracted from GSODF
- Hardening (Voce) parameters depending on grain size according to Hall-Petch relationship
- Shape (ellipsoid ratios) averaged by size

VPSC

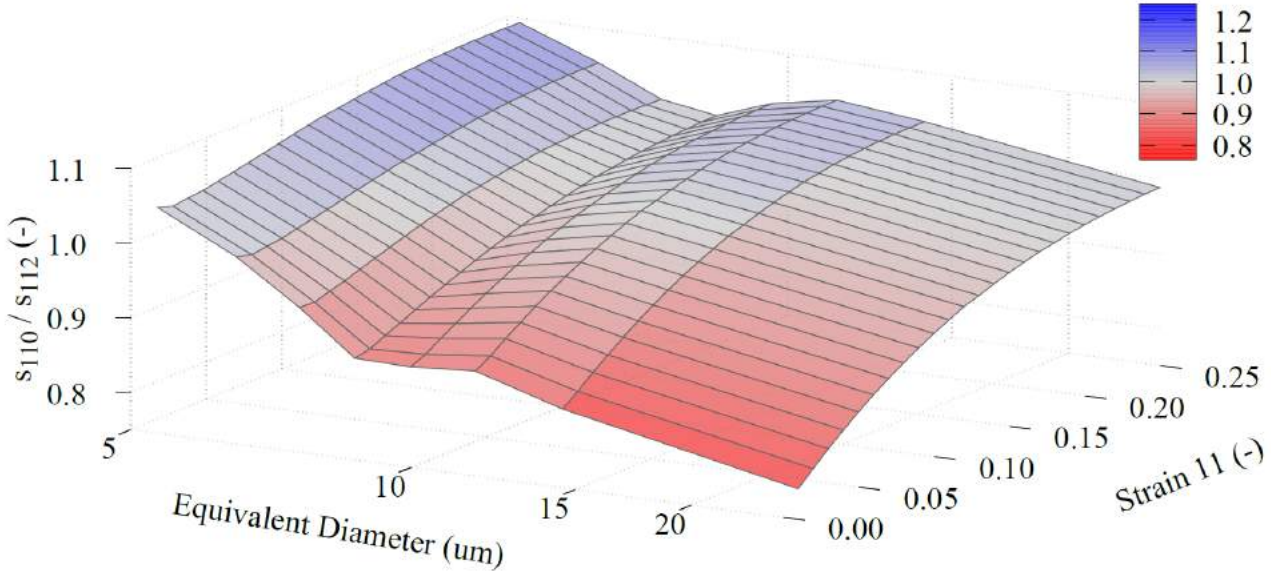
Texture evolution of largest and smallest grains





Tensile curve and shape evolution of largest and smallest grains

Relative slip system activity by grain size

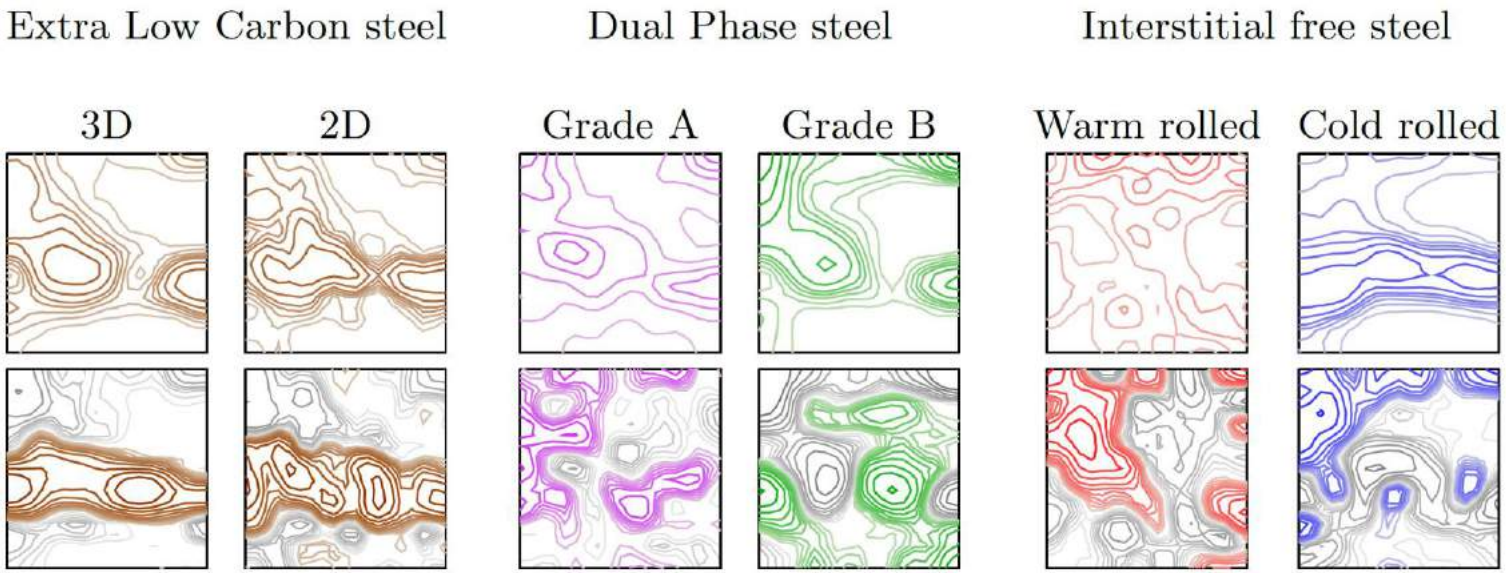


Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

Representation

$$f_0 = \sum_i a_i T_i(g)$$

$$\frac{f_d}{\log(d)} = \sum_i b_i T_i(g)$$



Negative values in grey

$\sum_i a_i T_i(g) \equiv$ Orientation distribution for grain size 0

$\log(d) \sum_i b_i T_i(g) \equiv$ Intensity increment for grain size d

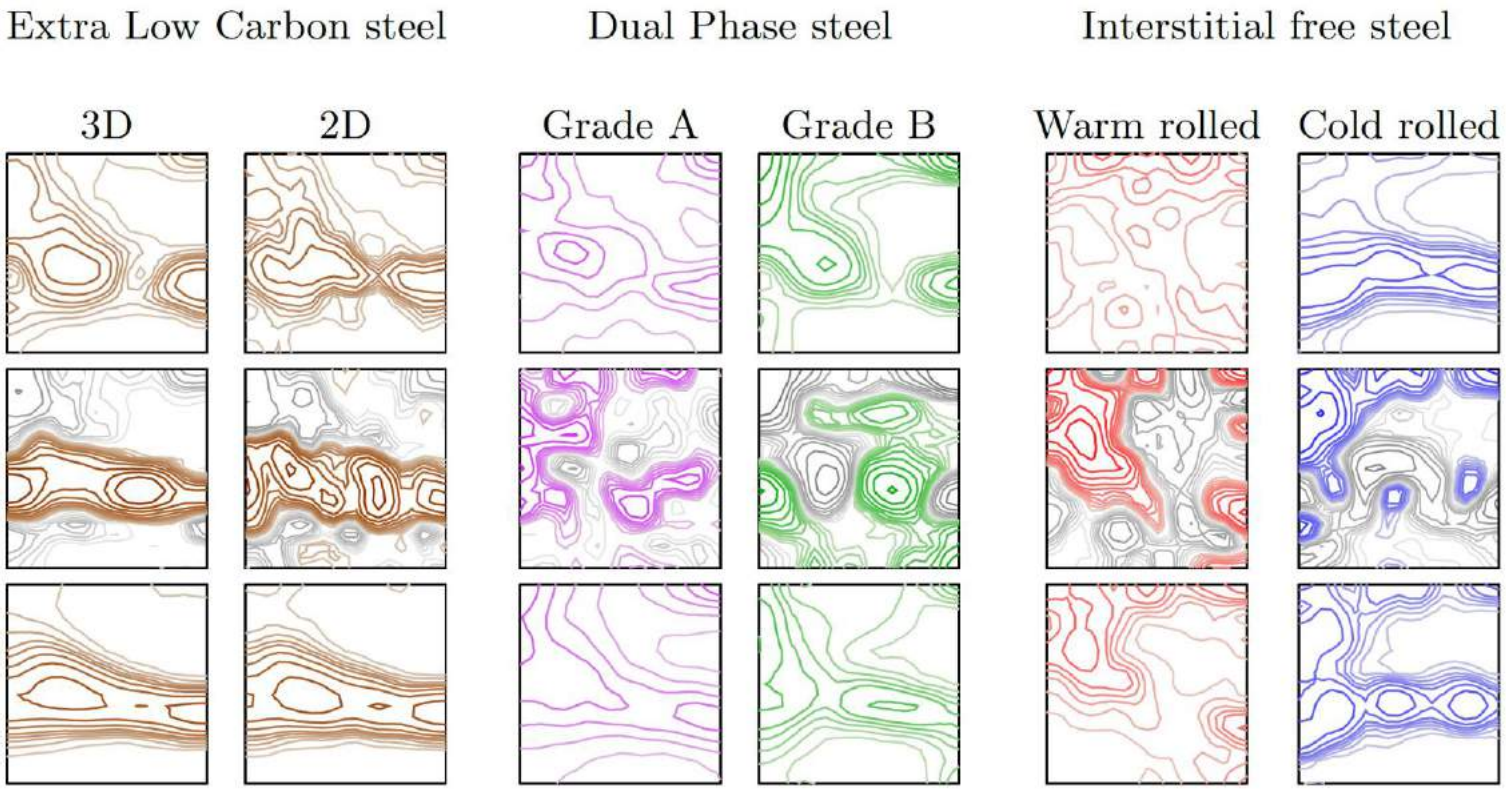
Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

Representation

$$f_0 = \sum_i a_i T_i(g)$$

$$\frac{f_d - f_{d_\mu}}{\log(d/d_\mu)} = \sum_i b_i T_i(g)$$

$$f_{d_\mu} = \sum_i (a_i + b_i \log(d_\mu)) T_i(g)$$



Negative values in grey

$\sum_i a_i T_i(g) \equiv$ Orientation distribution for grain size 0

$\log\left(\frac{d}{d_\mu}\right) \sum_i b_i T_i(g) \equiv$ Intensity increment for grain size d with respect to d_μ

$\sum_i (a_i + b_i \log(d_\mu)) T_i(g) \equiv$ ODF for grain size $d_\mu \equiv$ ODF

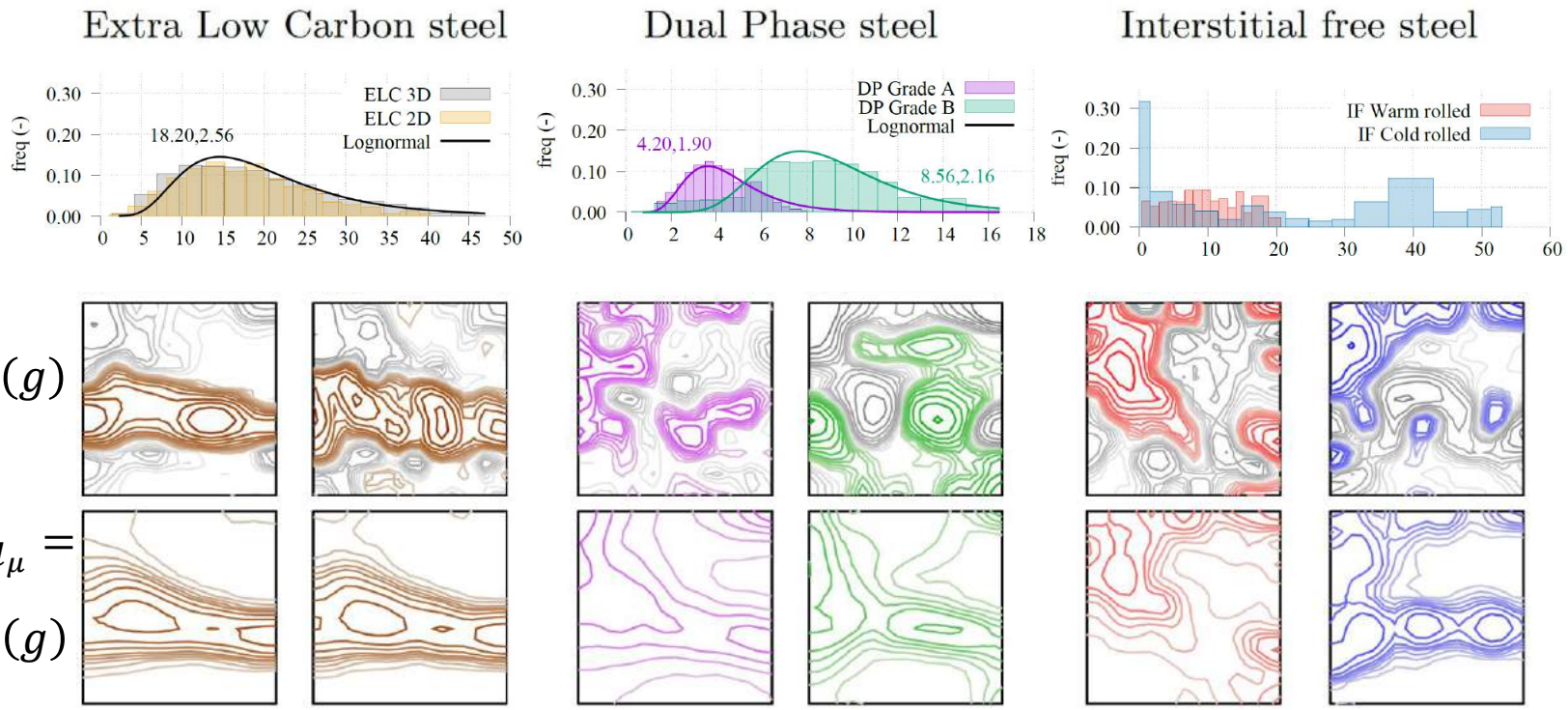
Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

Representation

$$p(d) = \mathcal{N}_{\mu,\sigma}\left(\log(d)\right)$$

$$\frac{f_d - f_{d_\mu}}{\log(d/d_\mu)} = \sum_i b_i T_i(g)$$

$$f_{d_\mu} = \sum_i (a_i + b_i \log(d_\mu)) T_i(g)$$

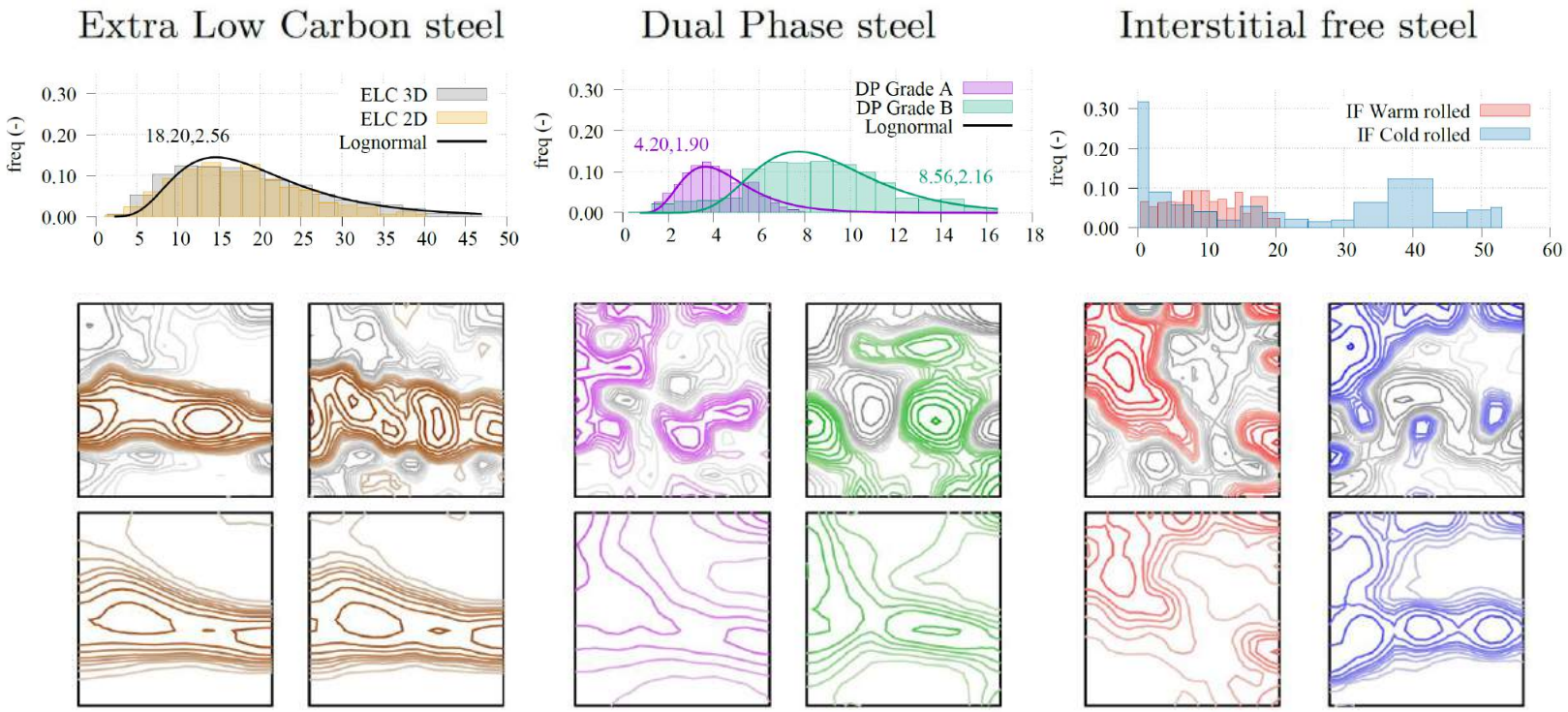


Negative values in grey

$$F(d,g) = \mathcal{N}_{\mu,\sigma}\left(\log(d)\right)\left(\sum_i (a_i + b_i \log(d_\mu)) T_i(g) + \sum_i b_i \log\left(\frac{d}{d_\mu}\right) T_i(g)\right)$$

Levels: 0.5 1.0 1.5 2.0 2.5 3.5 5.0 7.5 11.0 16.0

Conclusions



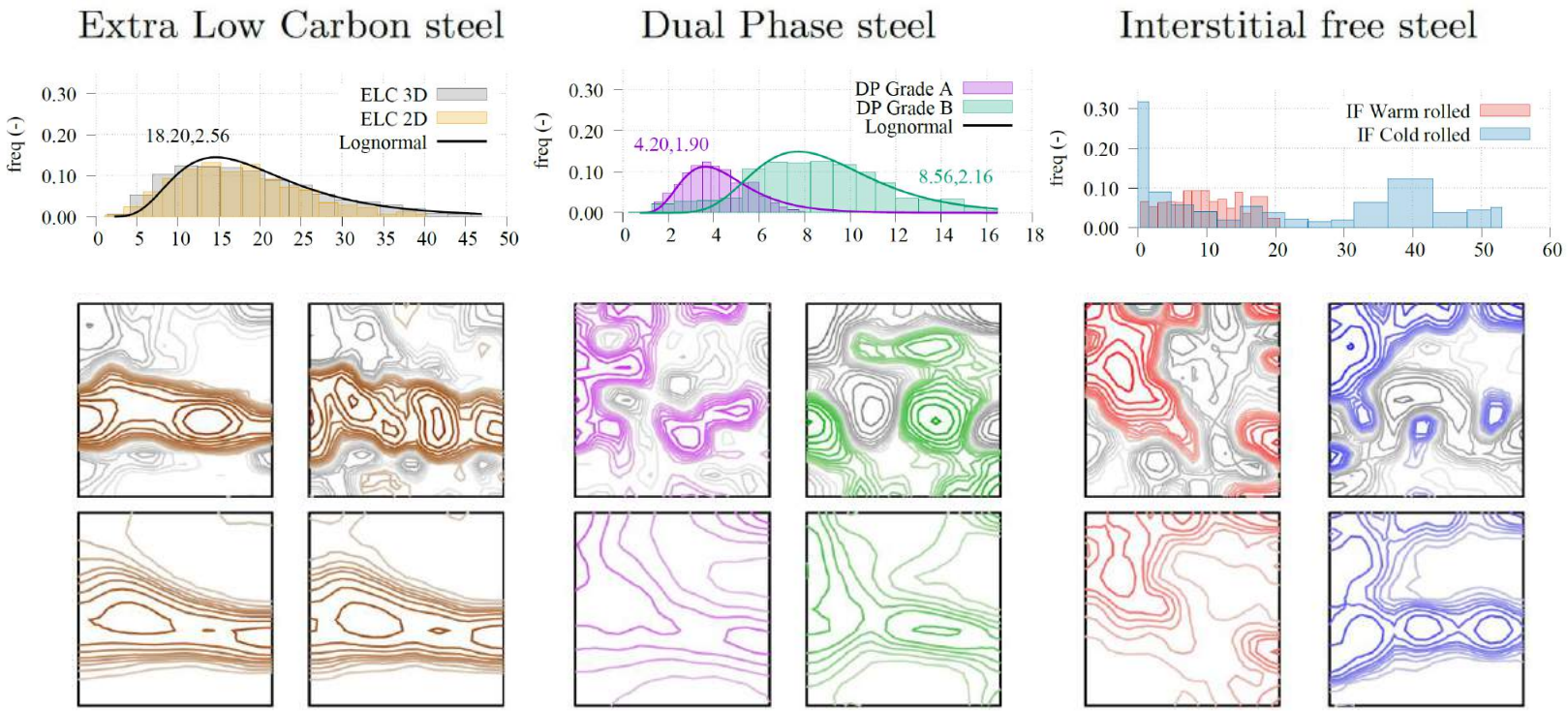
- Continuous GSODF that subsumes grain size and orientation distribution functions
- Application to material characterization, generation of RVEs, and CP simulations

Modelling of Metal Microstructures by the Grain Size Orientation Distribution Function

RFCS project 2015-709418
MuSTMeF

j.galanlopez@tudelft.nl

Jesús Galán López
Monireh Azimi
Leo Kestens



- Continuous GSODF that subsumes grain size and orientation distribution functions
- Application to material characterization, generation of RVEs, and CP simulations

Thank you for your attention