Microstructure design

For multi scale simulation of advanced steel grades

Piet Kok, Carola Celada Casero, Wil Spanjer, Frank Korver

Together we make the difference

Agenda

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1	**Microstructure modelling**
2	Using 2D EBSD data
3	Crystal plasticity model
4	Spatial distribution of martensite: closed network
5	Spatial distribution of martensite: bands

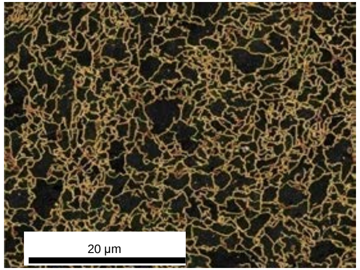
Typical microstructures of steel grade families

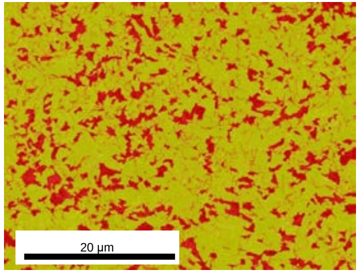
Microstructure is the ‘DNA’ of the material
Extensive range in microstructure parameters:

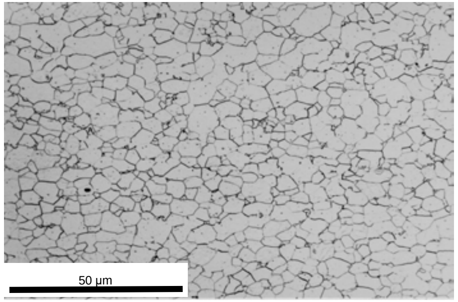
- Grain size and shape
- Volume fractions and spatial distribution of phases
- Texture and misorientation distribution

→ Development of a microstructure design tool based on multilevel Voronoi

HSLA







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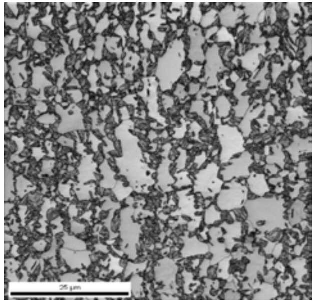


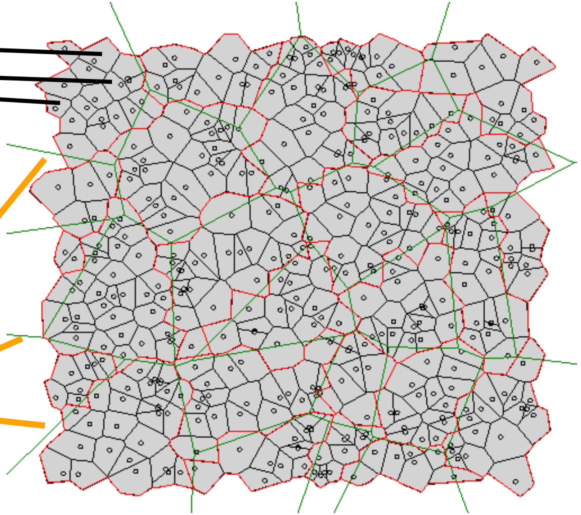
DP

CP

Construction of microstructure with advanced voronoi based algorithm

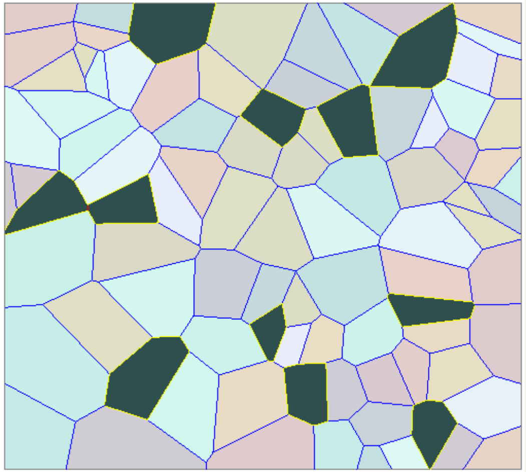
1st level: finer cell tessellation

2nd level: coarser grain tessellation



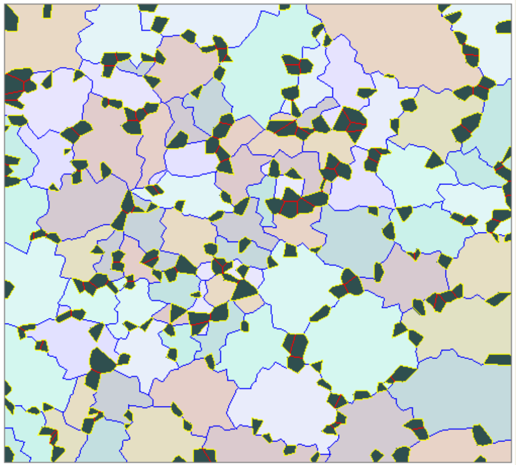
Voronoi principle: Every point that is closer to its generating site S_i will be part of cell *i.*
Multilevel voronoi: Every cell which generating site is closer to the generating site S_{gi} of the 2nd level will be part a grain *gi*.

Standard Voronoi versus Multilevel Voronoi



Standard Voronoi

One size distribution of only convex shaped polygons

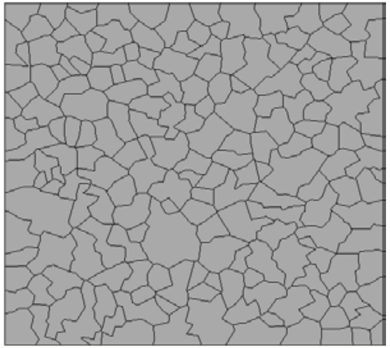


Multi Level Voronoi

User defined size distributions of complex shaped polygons

‘Black’ area fraction is 18% in both cases and the number of coloured polygons is 80

Artificial microstructures



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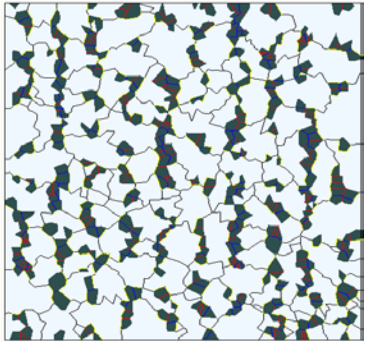

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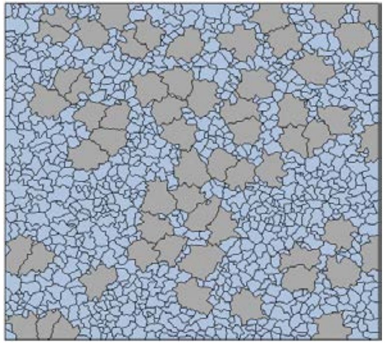

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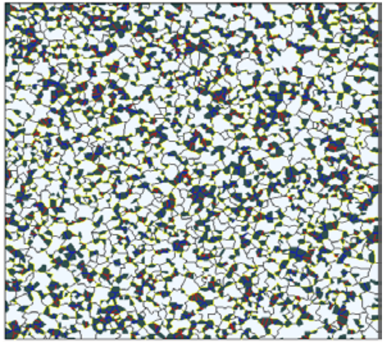
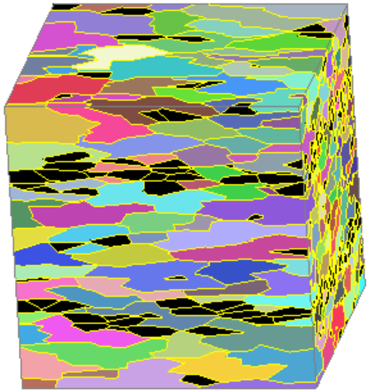


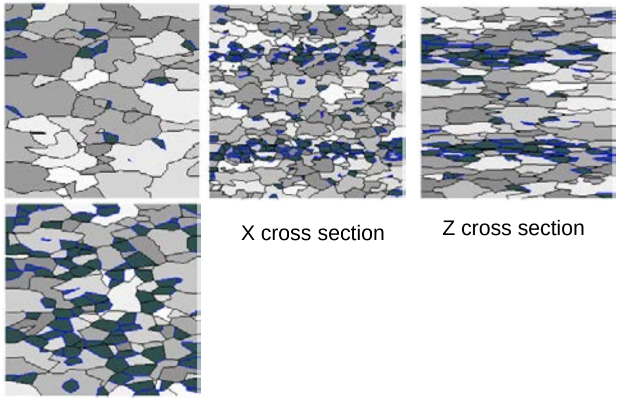
CP

We can already build Representative Volume Elements for several important steel grades (single, dual phase and multi-phase) within minutes!

Different microstructure aspects:
-volume fraction, morphology, size distributions, spatial distribution, anisotropy

Parametric study: elongated microstructure





X cross section

Z cross section

Y cross sections

- To build a 3D microstructure out of one sample takes at least a month experimenting, using skilled technicians and expensive facilities! (e.g. 3D EBSD)

- Virtual 3D microstructures → Standard computer: < 30 min.
  - Cross sections out of 3D are made in secs.
  - Many different 3D microstructures can be studied

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From 2D EBSD to 3D orientation distribution

ODF (Orientation Distribution function) or $f(g)$ is defined by

$$\frac{\mathrm{d}V}{V} = f(g)\mathrm{d}g$$

$$\mathrm{d}g = \frac{1}{8\pi^2} \sin \Phi \, \mathrm{d}\Phi \, \mathrm{d}\varphi_1 \, \mathrm{d}\varphi_2$$

dV = all volume elements with orientation g in orientation element dg
V = sample volume
φ_1, ϕ, φ_2 = Euler angles

$$\frac{\mathrm{d}V}{V} = \frac{\mathrm{d}O}{O}$$

dO = area elements on sample section with an orientation g
O = total section area

**) [H.J. Bunge: Texture analysis in materials science, resp. pg 42 , pg 49, pg 280 (1982)]*

From 2D EBSD to 3D orientation distribution

Monte Carlo Algorithm:
Iteration loop:
Weight of orientation g_i *:* $w_i = dO_i/O$
Assign EBSD orientation g_i*(j1, f, j2) randomly to 3D grains*
If weight is larger → more grains will get the same orientation
Calculate total volume dV of all grains with orientation g_i
Transform into volume fraction $x_i = dV(g_i) / V$
Calculate the sum $\sum (x_i - w_i)(x_i - w_i)$ *over all n orientations (=~TI *))*
End iteration loop

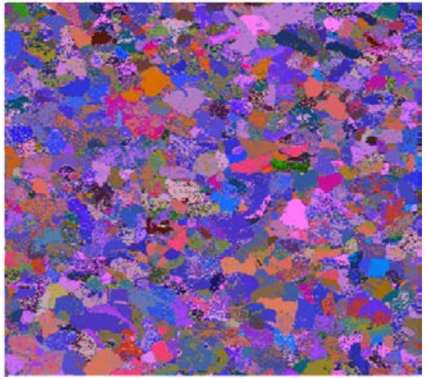
→ The minimum sum of ∑ over all n orientations will give the best fit

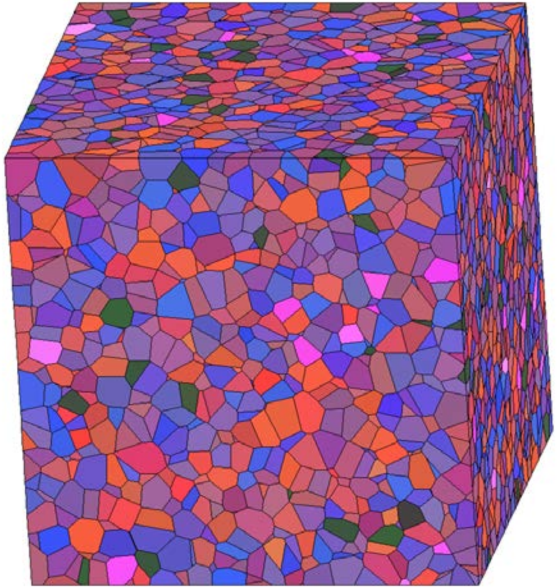
Remark: Because in 3D there are more grains than in a cross section, most orientations are assigned to more than 1 grain

**) TI = Texture Index [see Sidor J, e.a.: Acta Materialia, 2008]*

3D texture generation from 2D EBSD

Using 2D EBSD data



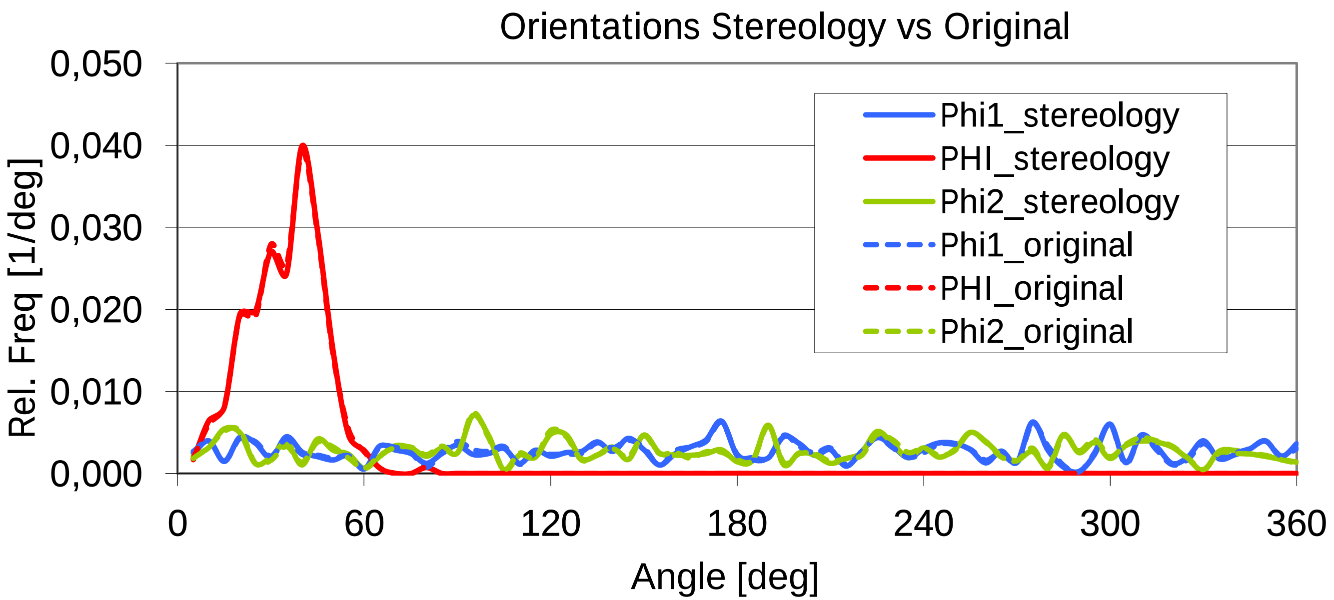


*EBSD of hot rolled sample representation of *.ang file 845 grains can be seen.*

Based on grainfile of hot rolled sample a 3D artificial microstructure has been constructed
Dimensions: 400 x 400 x 400 microns
14,000 grains have been used to get the same amount of grains than in a cross section.

3D texture generation from 2D EBSD

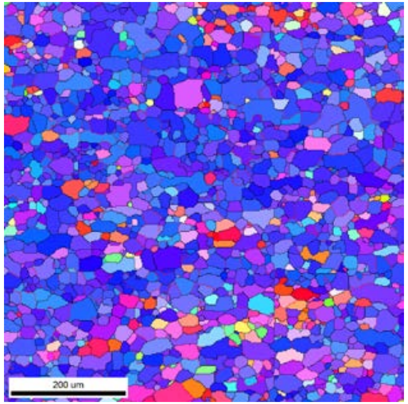
How good is it?



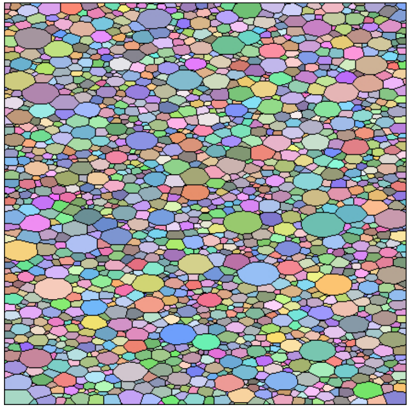
Original: EBSD grain file data
Stereology are 3D data from microstructure model

Laguerre Voronoi

user defined size distribution



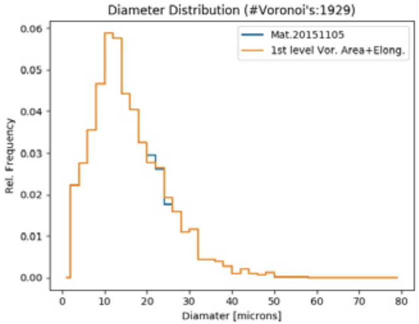
EBSD IPF image from IF steel grade



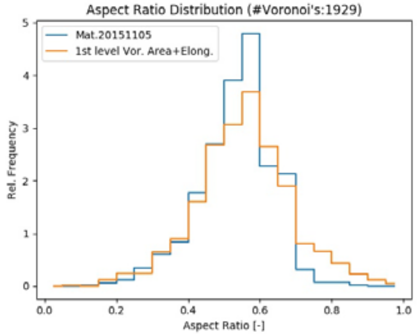
Laguerre Voronoi

Laguerre Voronoi: 1929 cells, with specified weights and average elongation 1.74:1

- Diameters: fits measurement perfect
- Aspect ratios: in-line with real material, but grain morphology is still different



Eq. diameter distribution: EBSD versus Laguerre Voronoi



Aspect ratio distribution : EBSD versus Laguerre Voronoi

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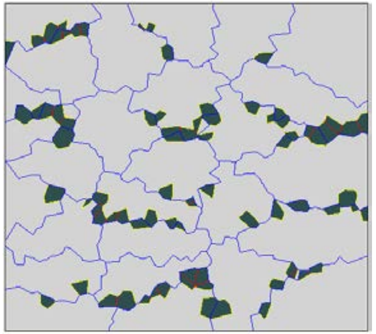
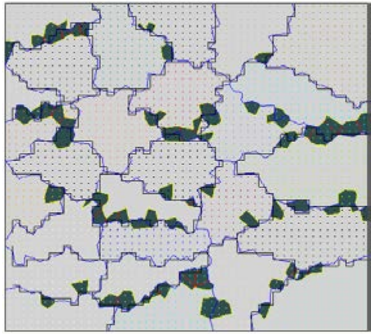
Connection to FFT Spectral Solver crystal plasticity code



Voronoi based microstructure



Rectangular grid
User defined resolution

- Voronoi model generates directly input files for DAMASK *) code
- Phenomenological material model based on Schmids law

$$\dot{\gamma} = \dot{\gamma}_0 \left|\frac{\tau_s}{\tau_c}\right| sgn(\tau_c)$$

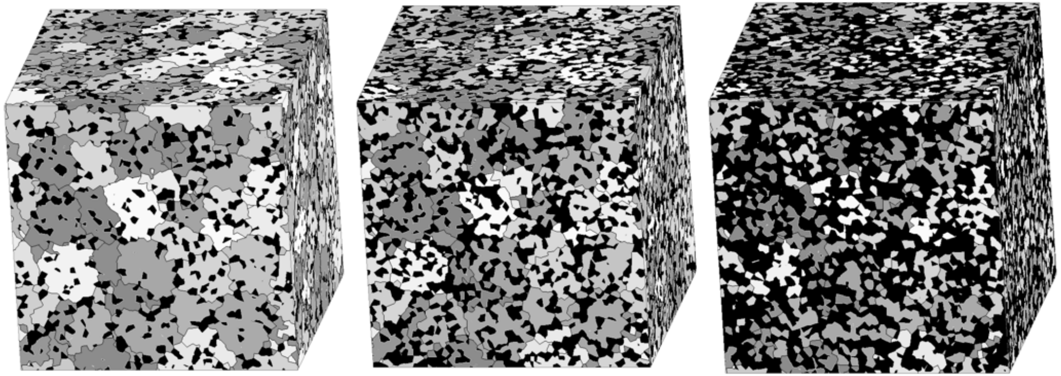
$\dot{\gamma}_0$, τ_s , τ_c Reference shear rate, saturation stress, critical resolved shear stress

$$\dot{\tau}_c = q_{\alpha\beta} h_0 \left(1 - \frac{\tau_c}{\tau_s}\right)^a \left|\dot{\gamma}\right|$$

$q_{\alpha\beta}$, h_0, a Slip hardening parameters

*) [Düsseldorf Advanced MAterial Simulation Kit for studying crystal plasticity, MPI für Eisenforschung]

Microstructure built with Voronoi based algorithm



V_M= 19.8 %　　V_M= 39.9 %　　V_M= 60 %

Artificial Dual Phase microstructures constructed with the multi-level Voronoi generator

- Different volume fraction of martensite (V_M).
- Grey levels indicate Euler angle orientations of ferrite grains.

Crystal plasticity (CP) parameters

```
Nslip              12  0  0  0       # per family
Ntwin               0  0  0  0       # per family
c11                233.3e9
c12                135.5e9
c44                118.0e9
gdot0_slip           0.001
n_slip              20
tau0_slip            88.0e6 0 0 0      # per family
tausat_slip          205.0e6 0 0 0      # per family
gdot0_twin           0.001
n_twin              100
tau0_twin            31.0e6 0 0 0      # per family
s_pr               0       # push-up factor for slip saturation due to twinning
twin_b              0
twin_c              0
twin_d              0
twin_e              0
h0_slipslip          495.0e6
h0_sliptwin           0
h0_twinslip           0
h0_twintwin           0
interaction_slipslip    1 1 1.4 1.4 1.4 1.4
interaction_sliptwin    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
interaction_twinslip    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
interaction_twintwin    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
w0_slip              1.0
atol_resistance        1
```

Crystal plasticity parameters of BCC Ferrite

```
Nslip              12  0  0  0            # per family
Ntwin               0  0  0  0            # per family
c11                417.4e9
c12                242.4e9
c44                211.1e9
gdot0_slip           0.001
n_slip              20
tau0_slip            575.00e6 0 0 0          # per family
tausat_slip          1280.0e6 0 0 0          # per family
gdot0_twin           0.001
n_twin              100
tau0_twin            31.0e6 0 0 0          # per family
s_pr               0                # push-up factor for slip saturation due to twinning
twin_b              0
twin_c              0
twin_d              0
twin_e              0
h0_slipslip          53500.0e6     # 35000.0e6
h0_sliptwin           0
h0_twinslip           0
h0_twintwin           0
interaction_slipslip    1 1 1.4 1.4 1.4 1.4
interaction_sliptwin    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
interaction_twinslip    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
interaction_twintwin    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
w0_slip                        1.0
atol_resistance        1
```

Crystal plasticity parameters of BCC Martensite

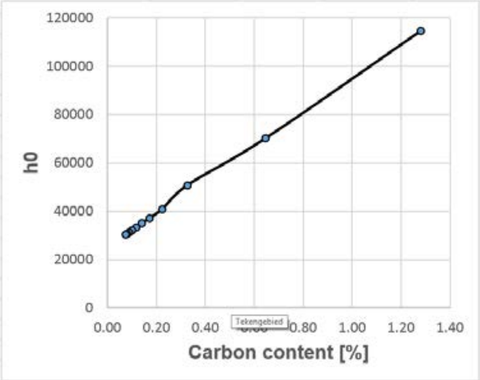
Simulations with Fourier Spectral code of DAMASK using phenopowerlaw for plasticity and Hooke law for elasticity
Parameters taken from reference DP600 [thesis Diehl]

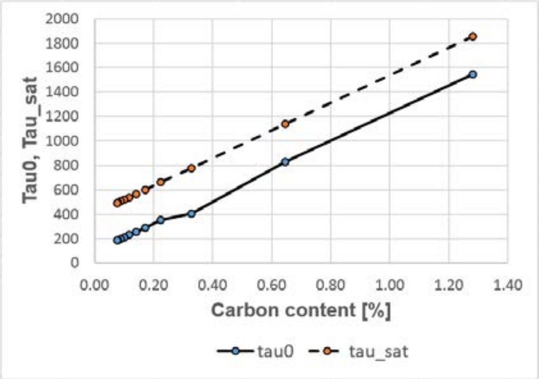
Crystal plasticity parameters: optimization procedure

$$min\left\{\sum\left[\sigma(h_0, \tau_0, \tau_s, \varepsilon_{SP}) - \sigma_{SP}\right]^2\right\}$$

ε_{SP} : Strain vector of exp. curve

σ_{SP} : Stress vector of exp. curve

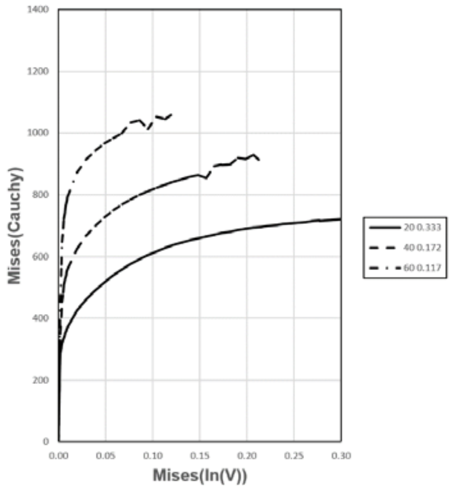


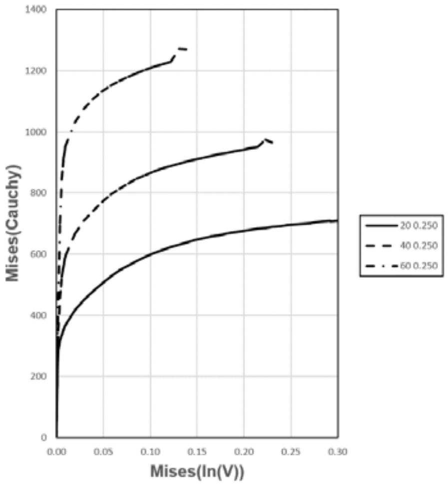


Relation of crystal plasticity parameters (in MPa) with carbon content of martensite. On the left hardening parameter h_0. On the right the critical resolved shear stress τ_c and the saturation stress τ_s

*) *[Rodriquez R: Mechanical behaviour of steels with mixed microstructures (2004)]*

Influence of C content on CP parameters Martensite





Comparison of simulated flow curves (in MPa) of DP steel grades with 20%, 40%, 60% martensite. Left: Martensite properties corrected for different carbon content. Right: Without this correction

**) [Thomser C: Modelling the mechanical properties of multiphase steels based on microstructures, proc. IDDRG2007]*

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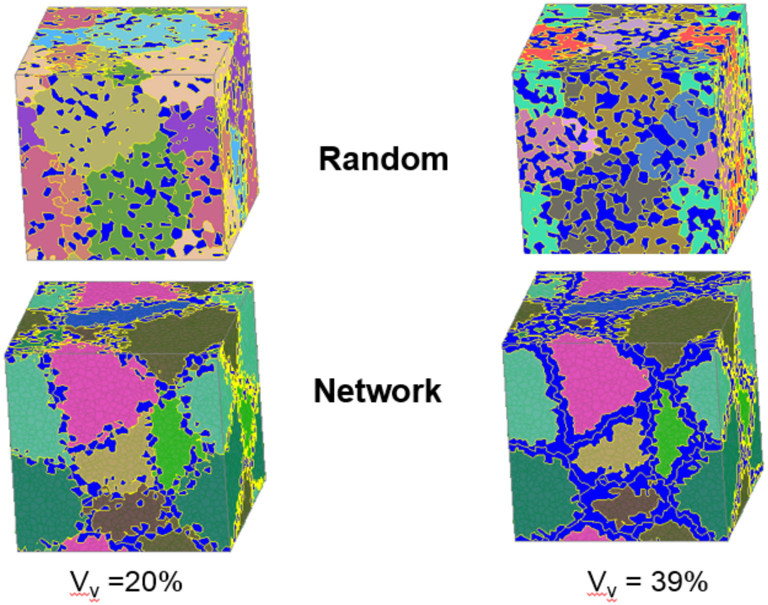
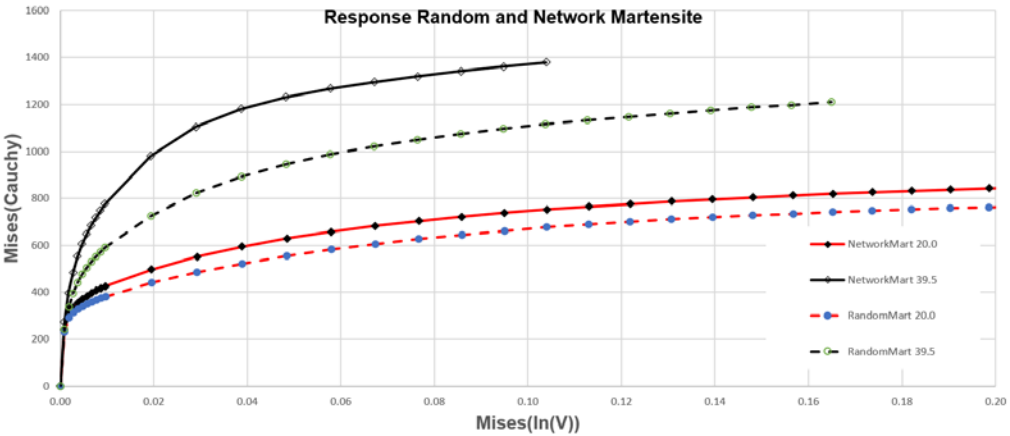
Closed network configuration



Parametric study of the influence of the spatial distribution of martensite particles (blue) in Dual Phase microstructures for two different volume fractions of martensite (20% and 39%)

Closed network configuration



Comparison of hardening response (in MPa) between Dual Phase microstructures with randomly distributed martensite and martensite in a network at ferrite grain boundaries.

→ Closed network gives a higher hardening response.

→ Effect is larger for higher volume fractions

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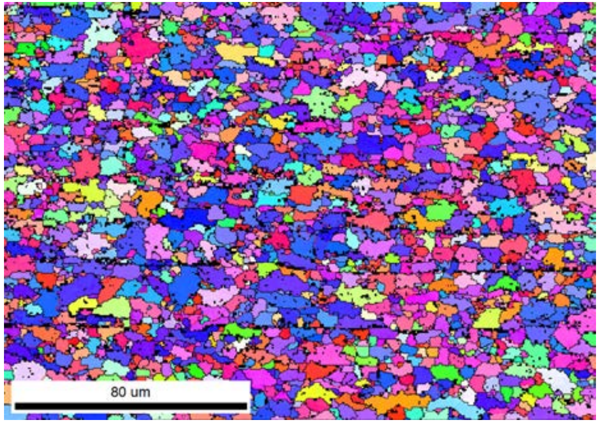
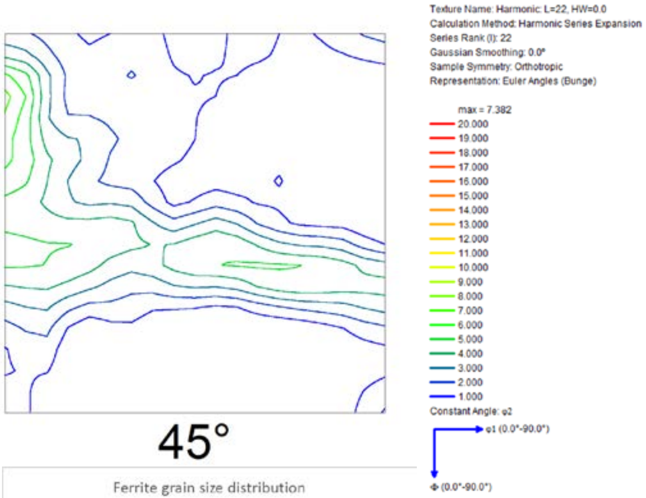
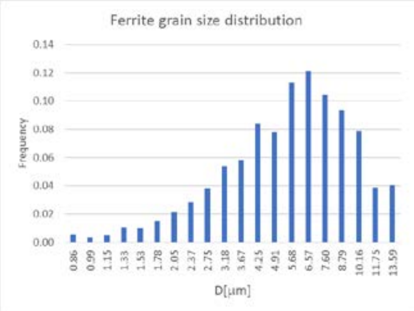
EBSD input from DP600



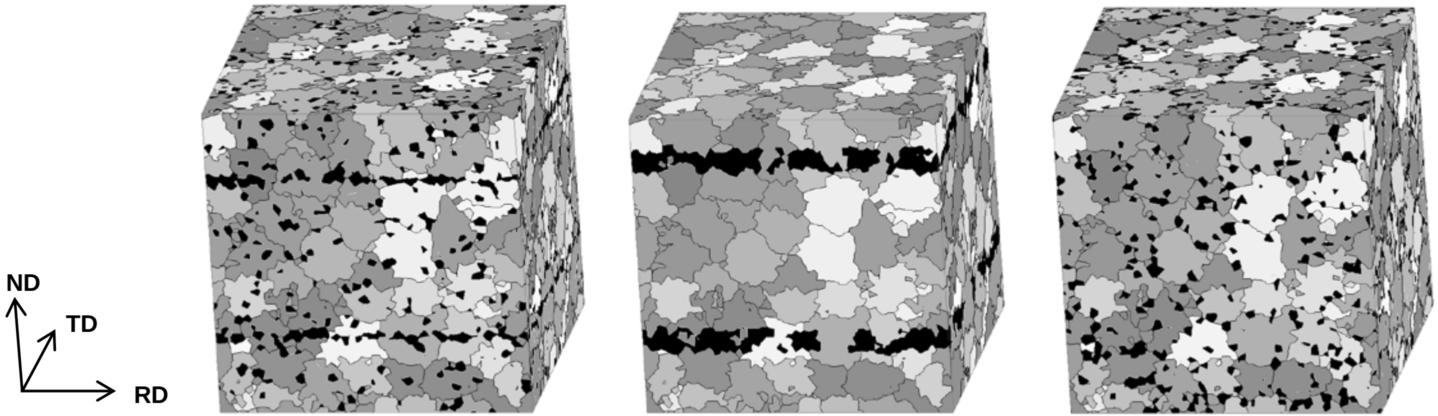
Inverse Pole Figure (above)
Sample dimensions: 204μm x144μm
ODF Ferrite (above right)
Ferrite grain size distribution (right)

	D_F [μm]	D_M [μm]
Weighted average	6.259	1.045





Microstructure models

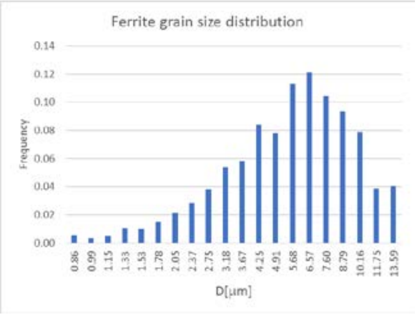


Model 1 Model 2 Model 3

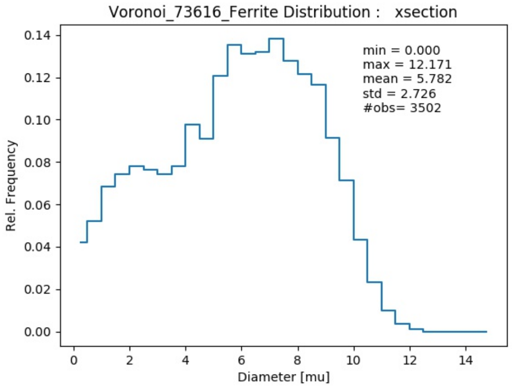
Periodic RVE's (dimensions 50x50x50μm), Grey colors indicate different crystal orientations
Identical volume fractions of martensite V_M = 11.9 %

- Model 1: Realistic: martensite particles random and in bands
- Model 2: 100% banded distribution of martensite particles
- Model 3: 100% random distribution of martensite particles

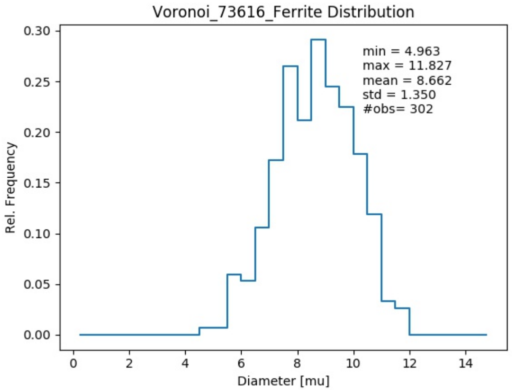
Ferrite grain size statistics



2D EBSD



Cross section from RVE

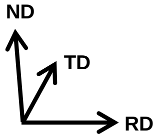


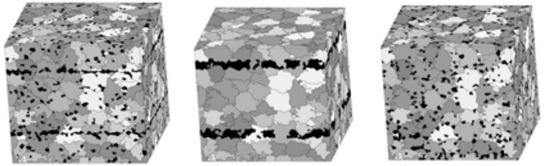
RVE 3D size distribution

Shape of 3D distribution differs from 2D
In 2D mean Ferrite grain D = 5.8 μm
In 3D mean Ferrite grain D = 8.7 μm

Uni-axial tensile Response curves

Uni-axial tensile tests at
0º , 90º and 45º to RD





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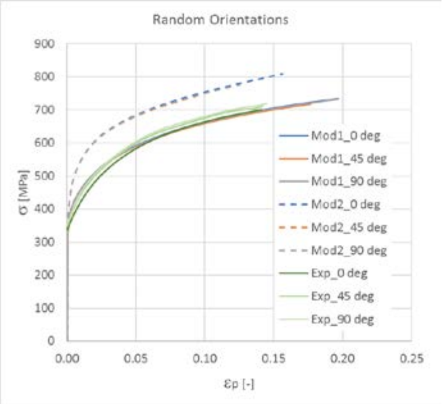
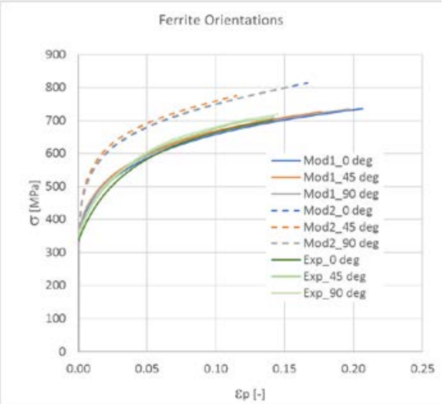
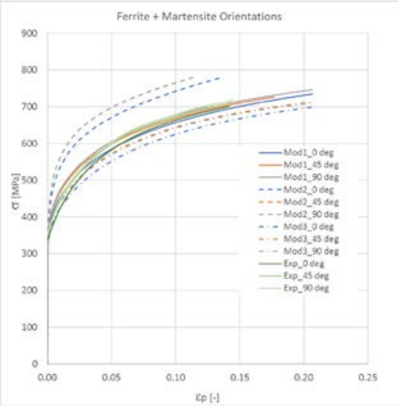


F, M: random orientations



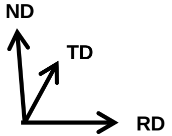
F: EBSD orientations
M: random orientations



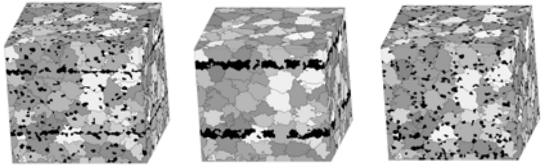
F: EBSD orientations
M: EBSD Martensite orientations

→ Microstructures with martensite in bands gives a higher response
→ Orientations of martensite particles influence the response in different directions in case of non-random ODF's

Predicted versus experimental R-values



Uni-axial tensile tests at
0º , 90º and 45º to RD



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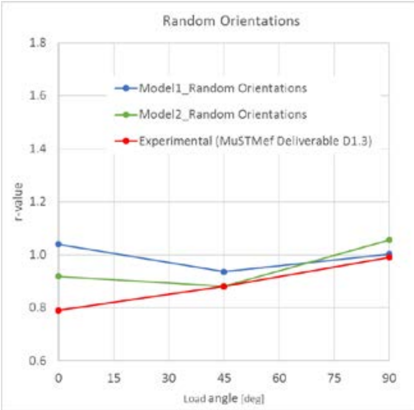
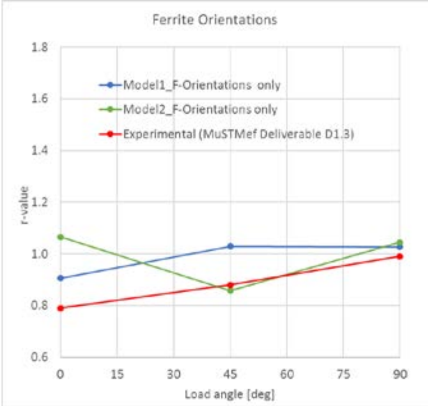
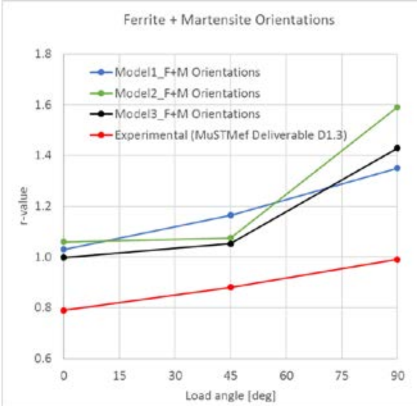


F, M: random orientations



F: EBSD orientations
M: Random orientations



F: EBSD orientations
M: EBSD Martensite orientations

→ **Realistic model** predicts trend of experimental R-value most accurate, if orientations of ferrite and martensite have been taken into account! Values are however constant 0.2 too high.

Thank you!
Do you have any questions?

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Tata Steel

Department R&D Applications & Engineering

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