MODELLING OF SIGMA PHASE FORMATION DURING ISOTHERMAL AGING OF A SUPERDUPLEX STAINLESS STEEL

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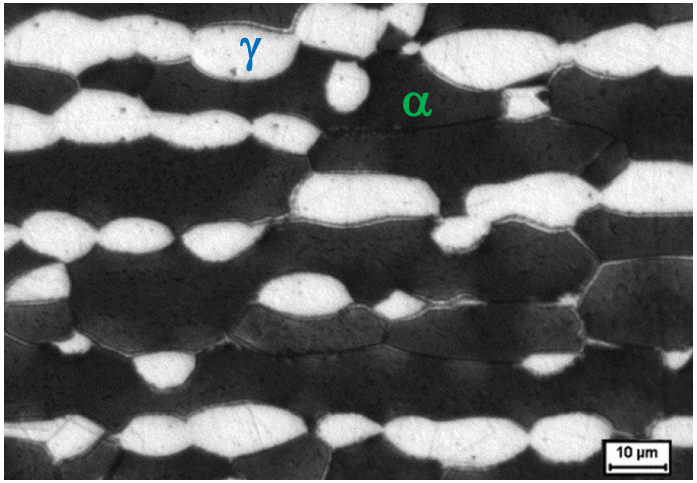
Duplex Stainless Steels (DSS)

Equal amounts of ferrite (α, BCC) and austenite (γ, FCC)

- Corrosion resistance, mechanical strength, toughness
- PREN = [(%Cr) + 3.3(%Mo) + 16(%N)]

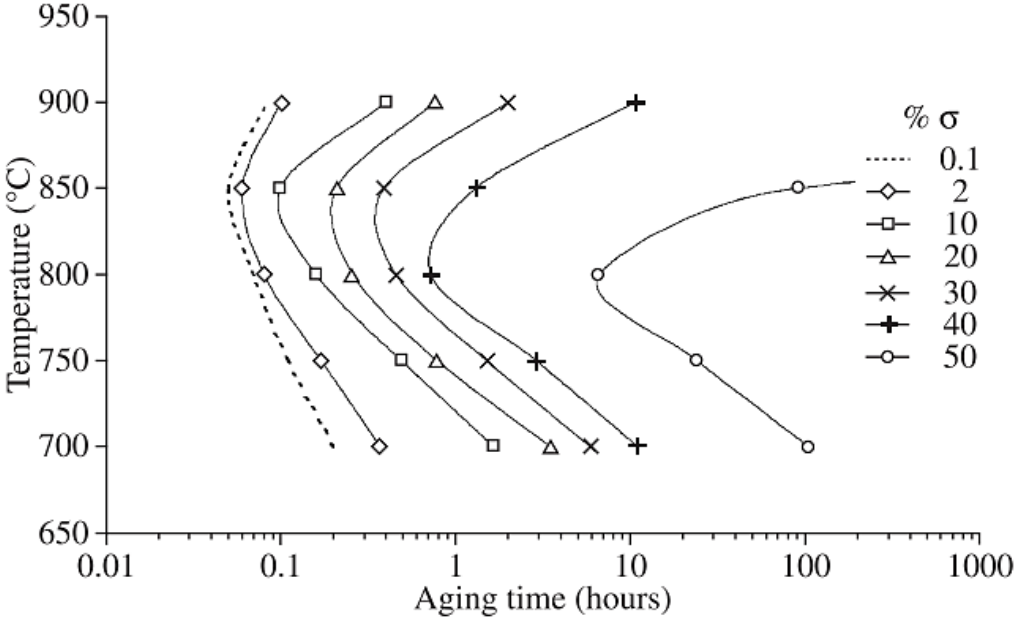
PREN	classification
<30	Lean duplex
30<PREN<40	Standard duplex
40<PREN<50	**Superduplex**
>50	Hyperduplex



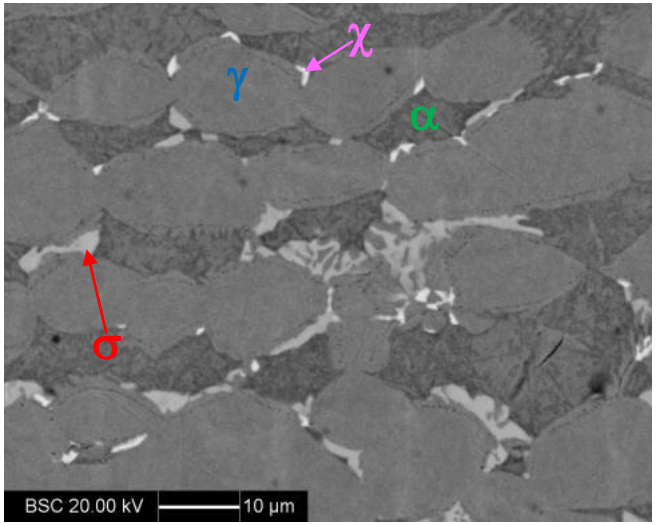
D. C. dos Santos, R. Magnabosco, C. Moura-Neto, *Influence of sigma phase formation on pitting corrosion of an aged UNS S31803 duplex stainless steel*. Corrosion, v. 69, p. 900-911, 2013.

Metastable structure of ferrite (α, BCC) and austenite (γ, FCC) in the solution-treated condition

Sigma phase (σ) formation between ~ 600-950°C



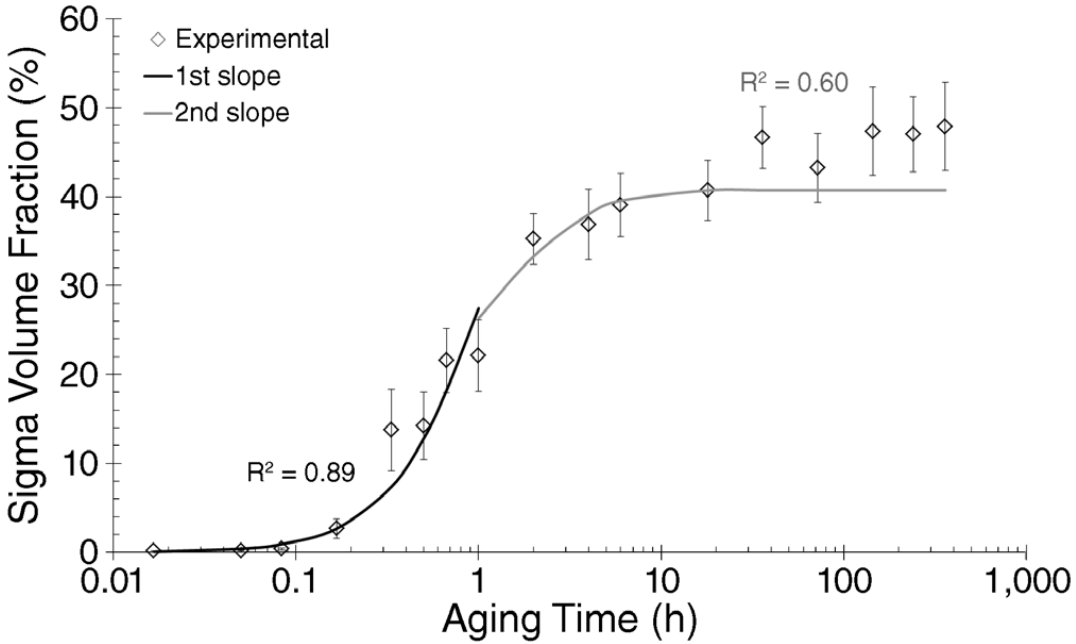
R. Magnabosco, *Kinetics of sigma phase formation in a Duplex Stainless Steel.* Materials Research, v. 12, p. 321-327, 2009.



UNS S31803 30min@850°C

D. C. Santos, R. Magnabosco. *Influence of intermetallic phase content and microstructure on pitting potential of a duplex stainless steel.* EUROCORR 2014, Pisa. Conference Proceedings.

Sigma phase (σ) formation @ 850°C



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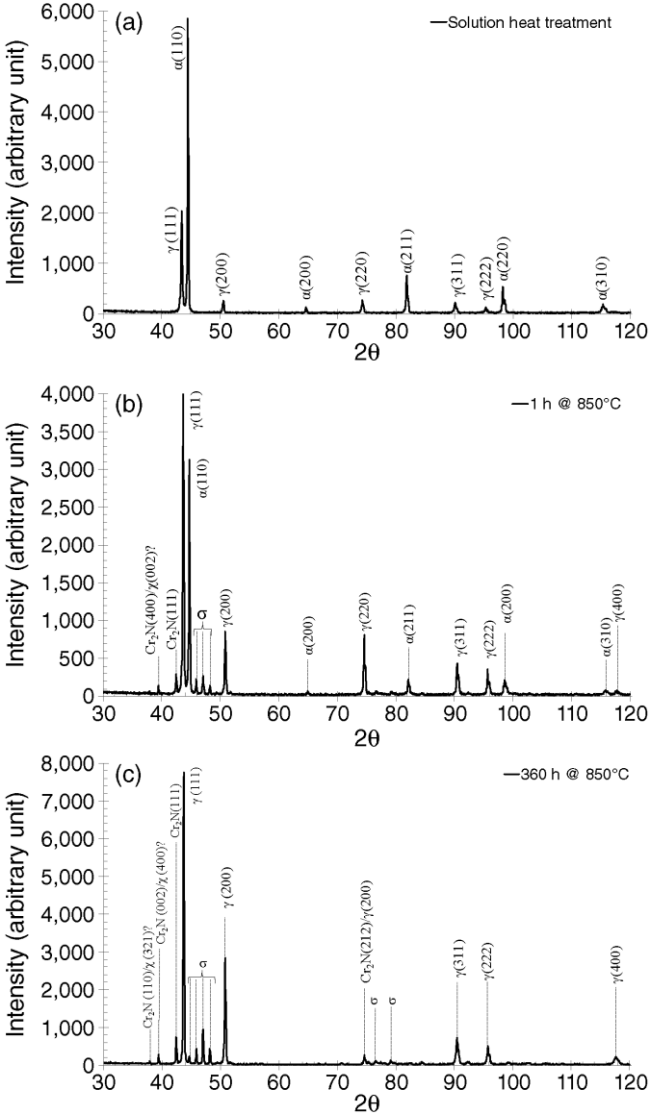
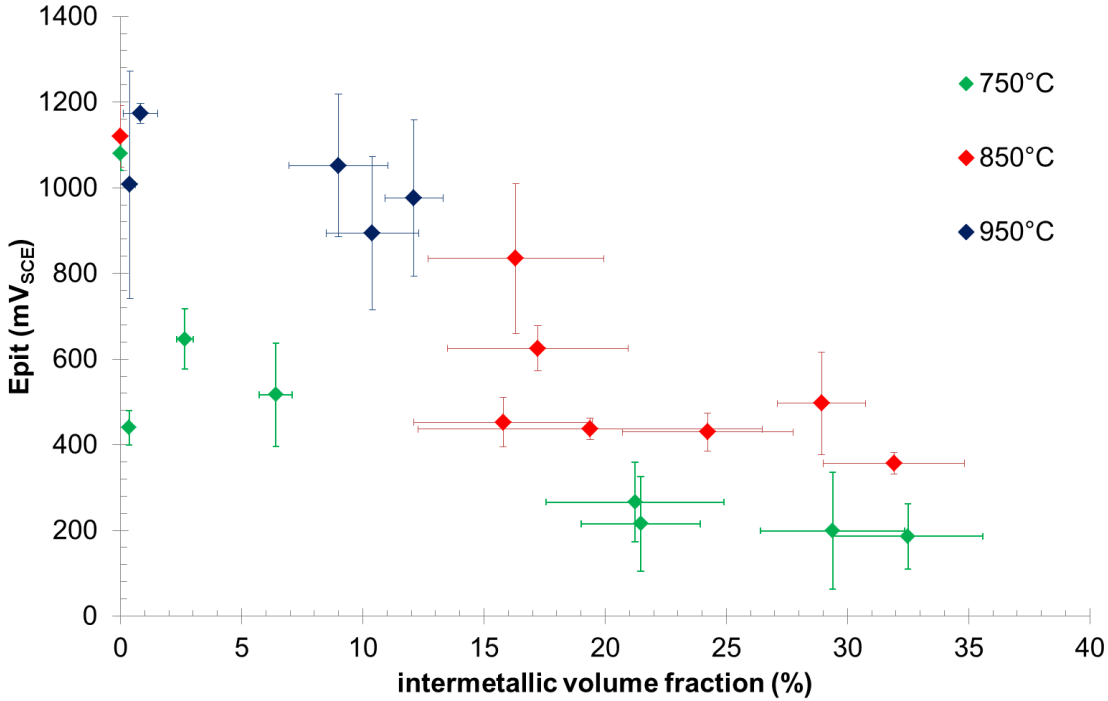


Formation of Cr and Mo depleted zones around sigma phase compromises corrosion resistance



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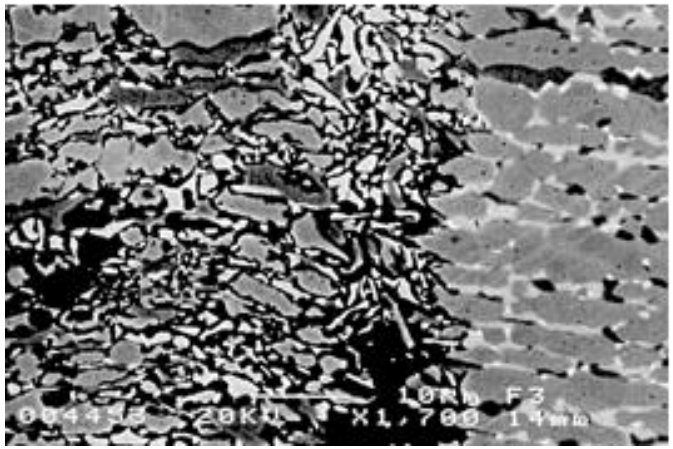
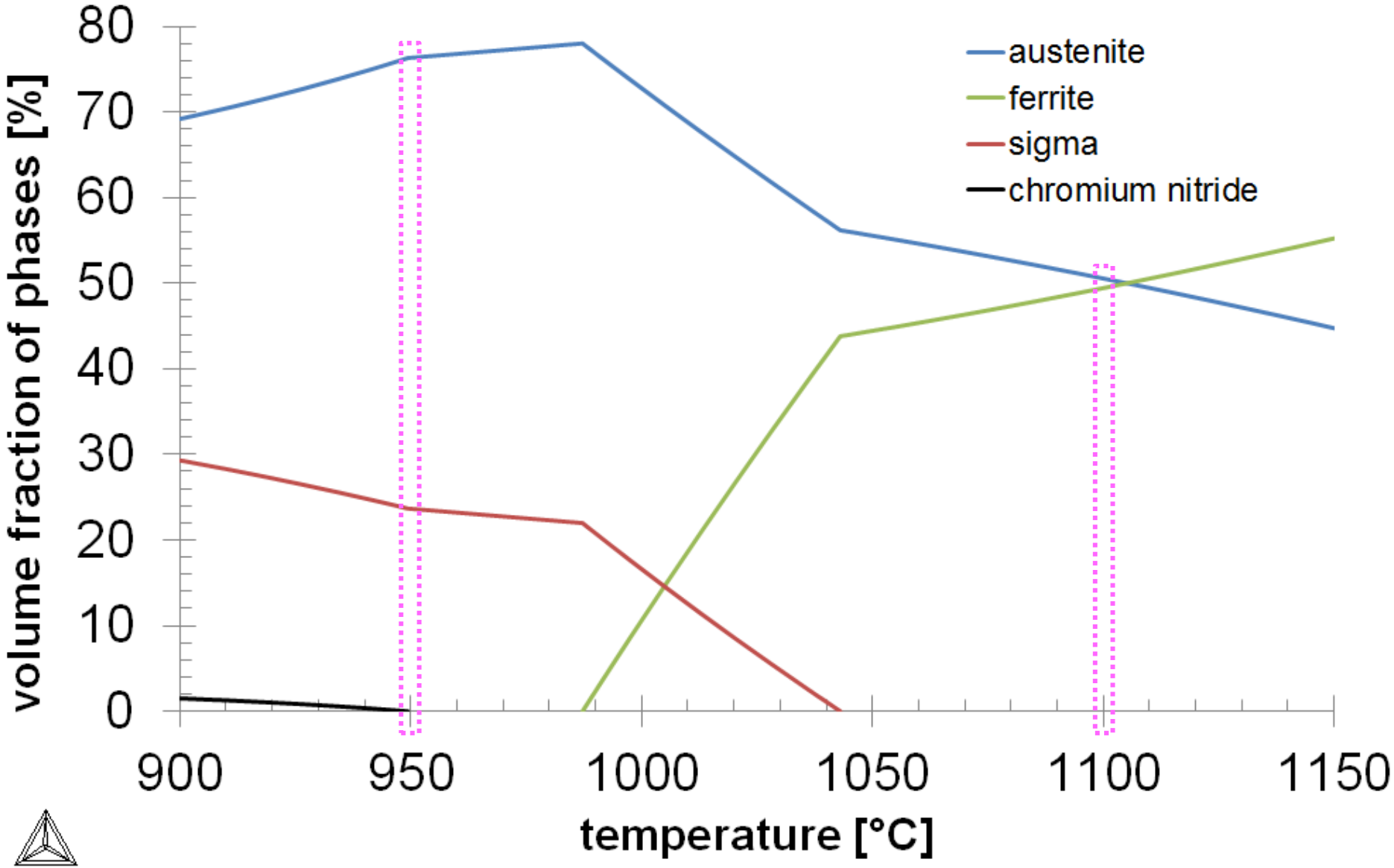


UNS S31803 30min@850°C

R. Magnabosco, N. Alonso-Falleiros. *Pit Morphology and Its Relation to Microstructure of 850°C Aged Duplex Stainless Steel.* Corrosion, v. 61, n.2, p. 130, 2005.

This work is a first approach on the simulation aided by Thermo-Calc® and DiCTra® of sigma phase formation in a superduplex stainless steel solution treated at 1100 °C and isothermal aged at 950°C, considering the heterogeneous nucleation of sigma and its growth over ferrite.

… reasons for 1100 °C and 950 °C …



EXPERIMENTAL PROCEDURES

Element	wt.%
Cr	**24.95**
Ni	**6.91**
Mo	**3.79**
N	**0.26**
Mn	0.43
C	0.015
Si	0.26
Cu	0.083
Fe	balance

PREN = 41.6

UNS S32750
superduplex stainless steel

- Solution treated 30 min @ 1100 °C
- Isothermically aged between 300 s and 14400 s @ 950 °C

- Sigma content → quantitative stereology of BSC images (σ, Mo-rich, appears brighter); analysed area of ~ 0.224 mm² per specimen

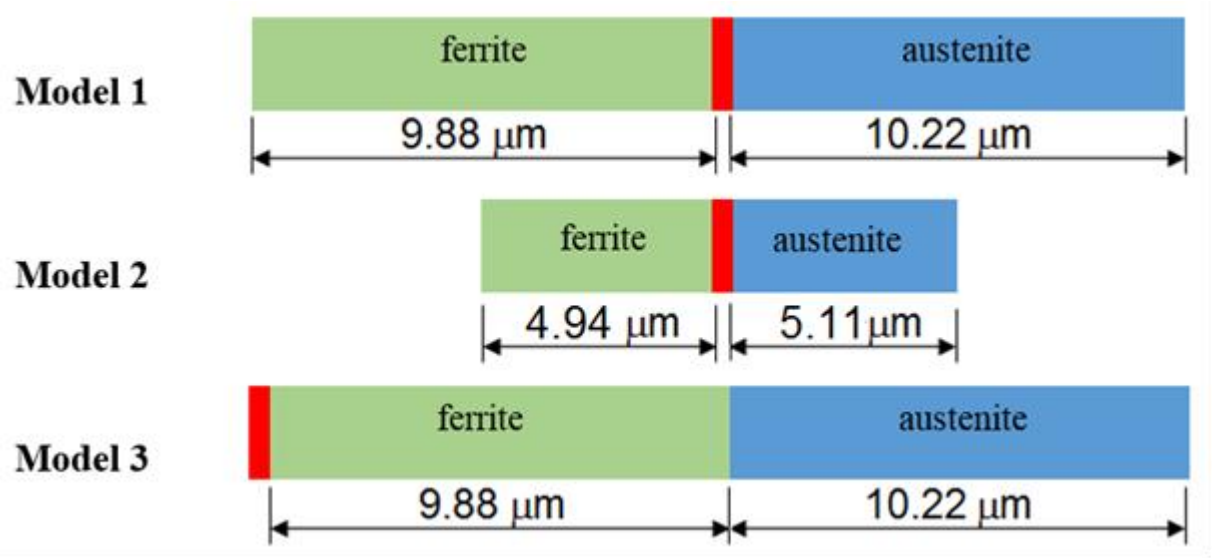
EQUILIBRIUM COMPUTER SIMULATIONS

- Thermo-Calc® software, TCFE6 database.
- Chemical composition and volumetric fractions of ferrite and austenite in equilibrium at 1,100°C
- Only considered the presence of Fe, Cr, Ni, Mo and N to simplify the simulation.

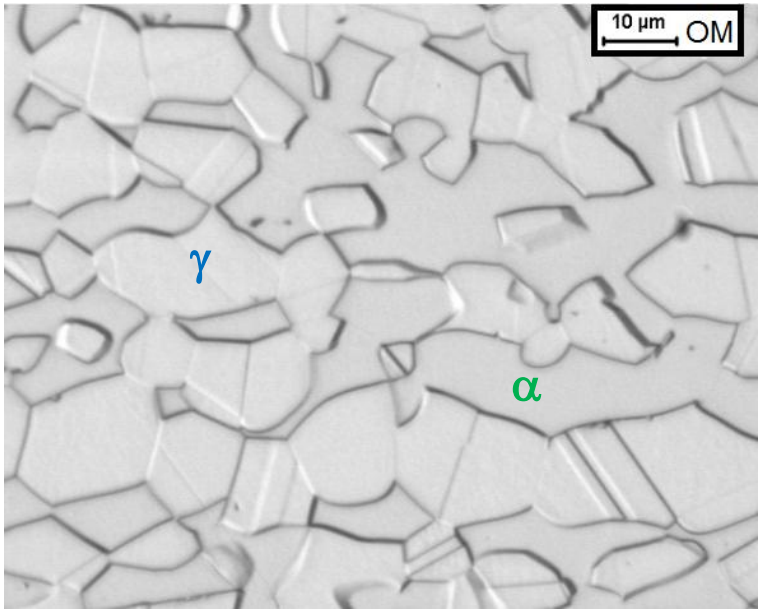
	chemical composition [wt.%]		
Element	Steel	ferrite @ 1100°C (49.4 v%)	austenite @ 1100°C (50.6 v%)
Cr	24.95	26.50	23.43
Ni	6.91	5.26	8.51
Mo	3.79	4.65	2.95
N	0.26	0.04	0.47

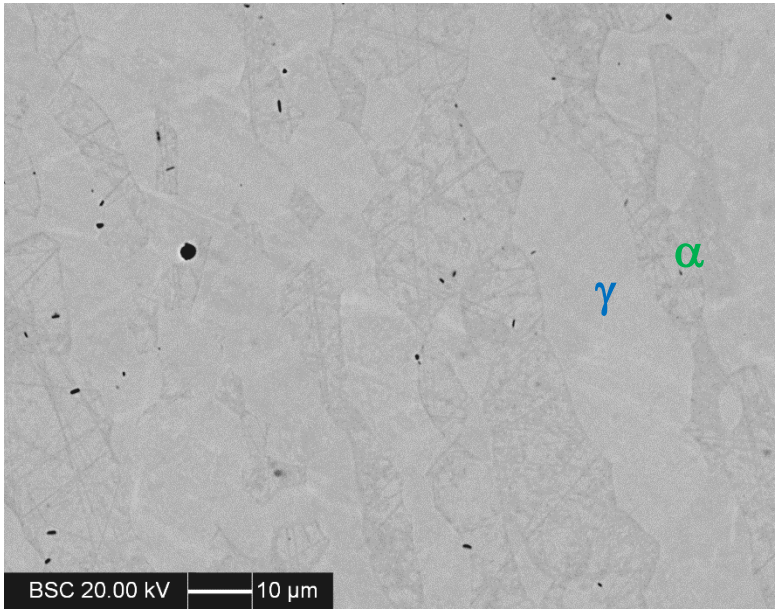
KINETICS COMPUTER SIMULATIONS

- DiCTra® software
- Thermodynamic database: TCFE6
- Diffusional data: MOB2
- Sigma phase (inactive in the beginning of the simulation) is nucleated at ferrite boundaries, with a unidirectional resulting diffusion flux.

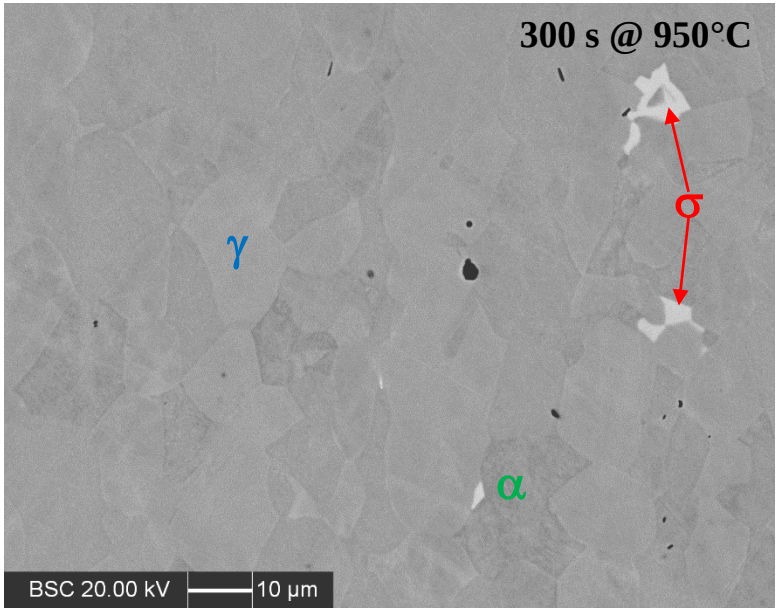


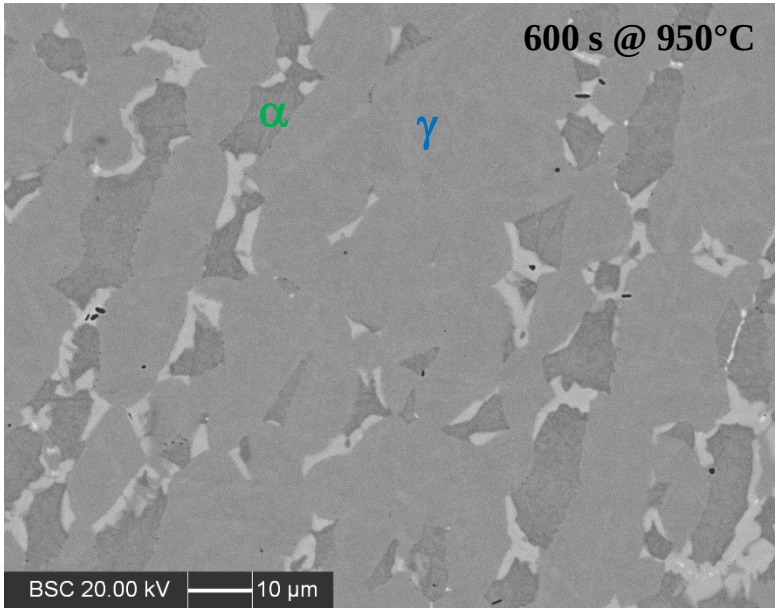
RESULTS AND DISCUSSION

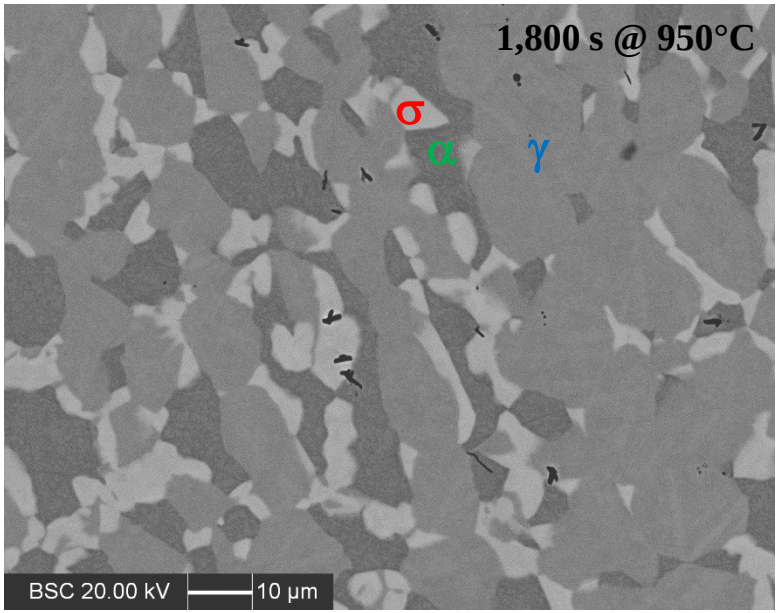


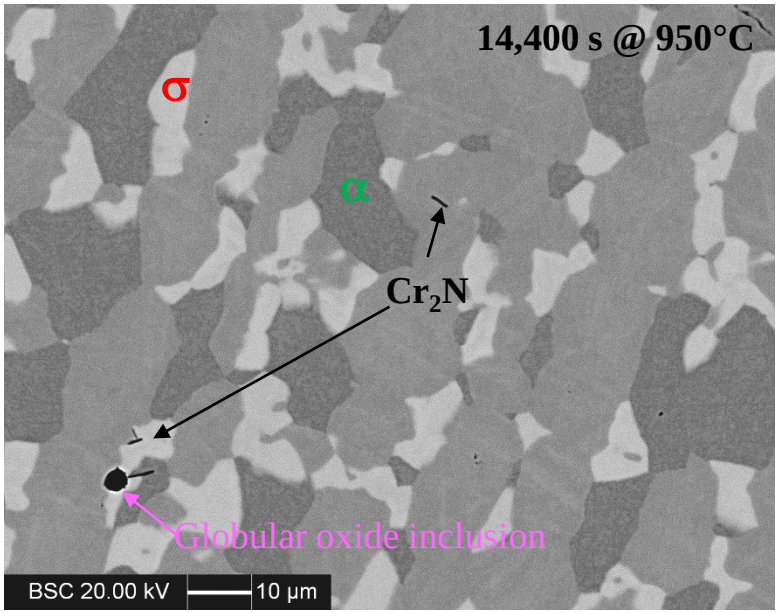


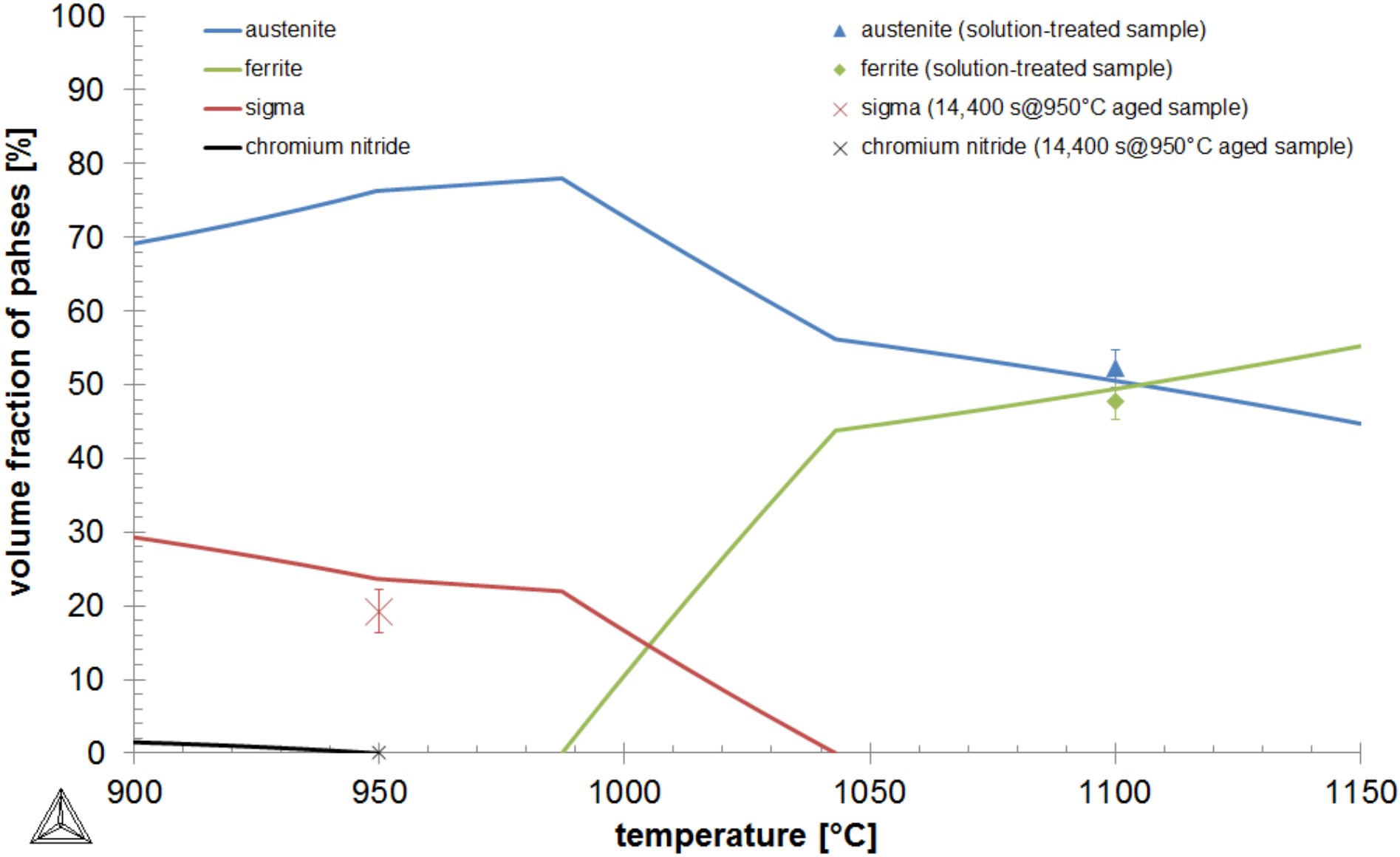
Solution treated 30 min @ 1100 °C

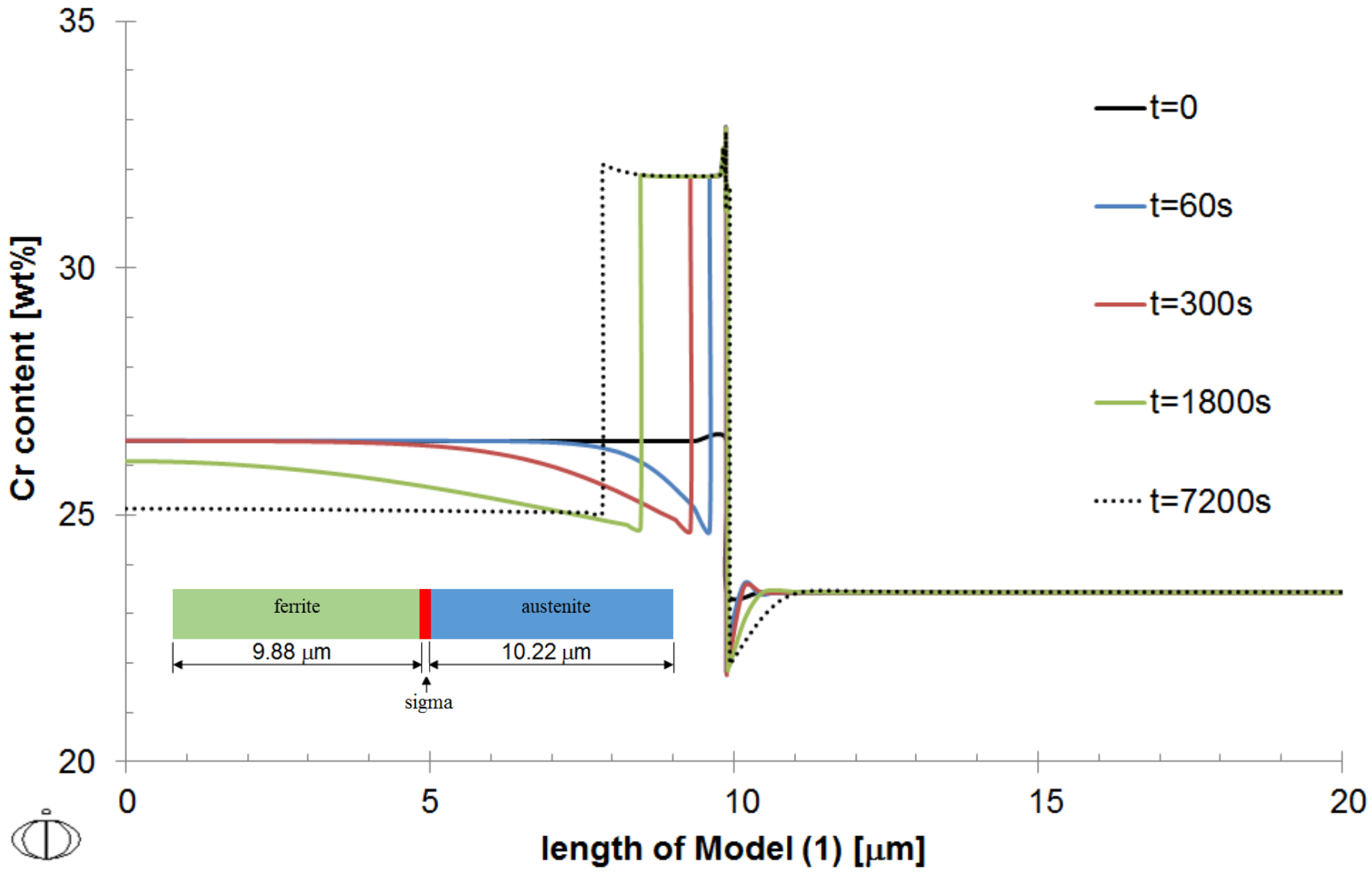

300 s @ 950°C
γ
σ
α
BSC 20.00 kV
10 µm

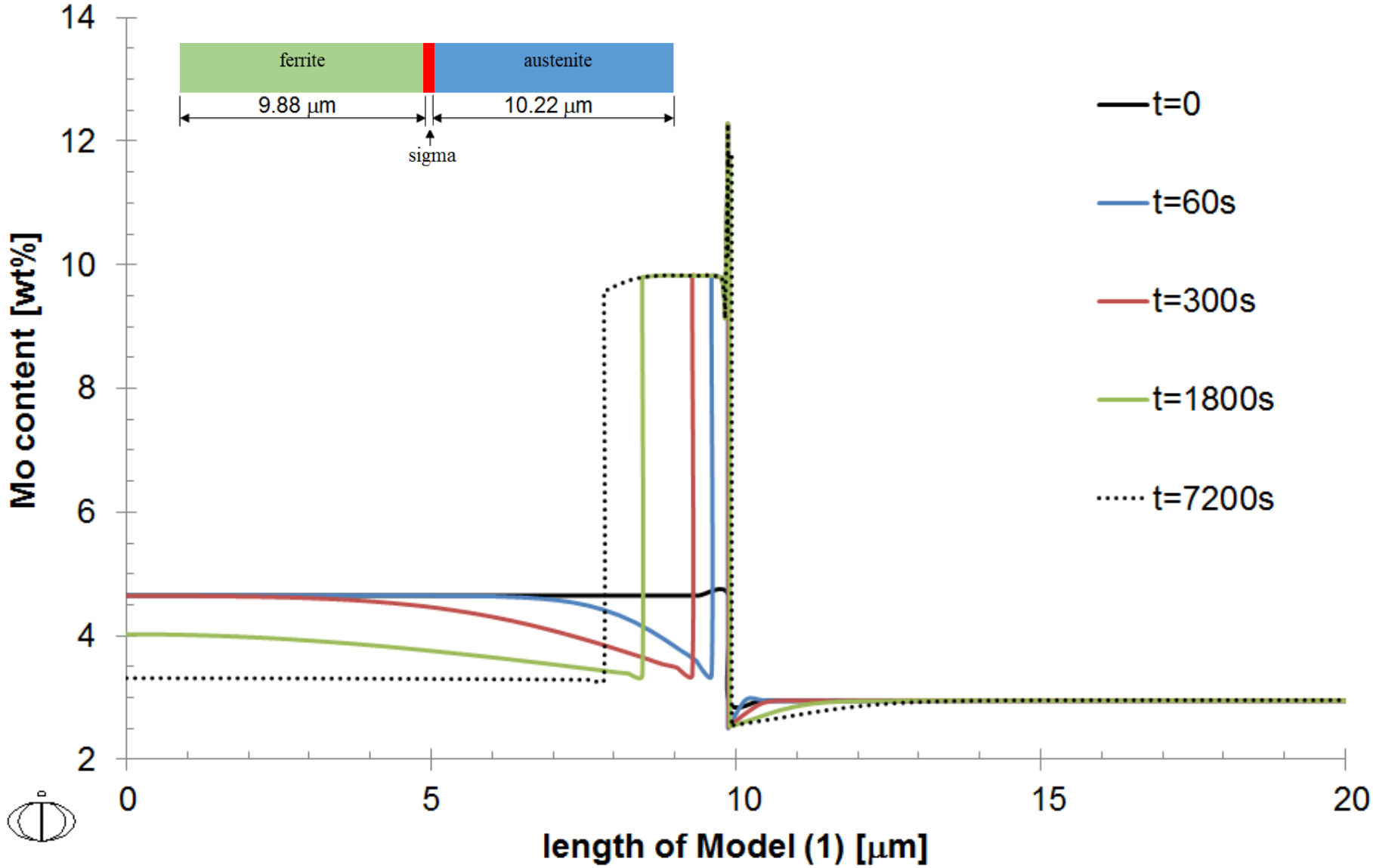

600 s @ 950°C
α
γ
BSC 20.00 kV
10 µm

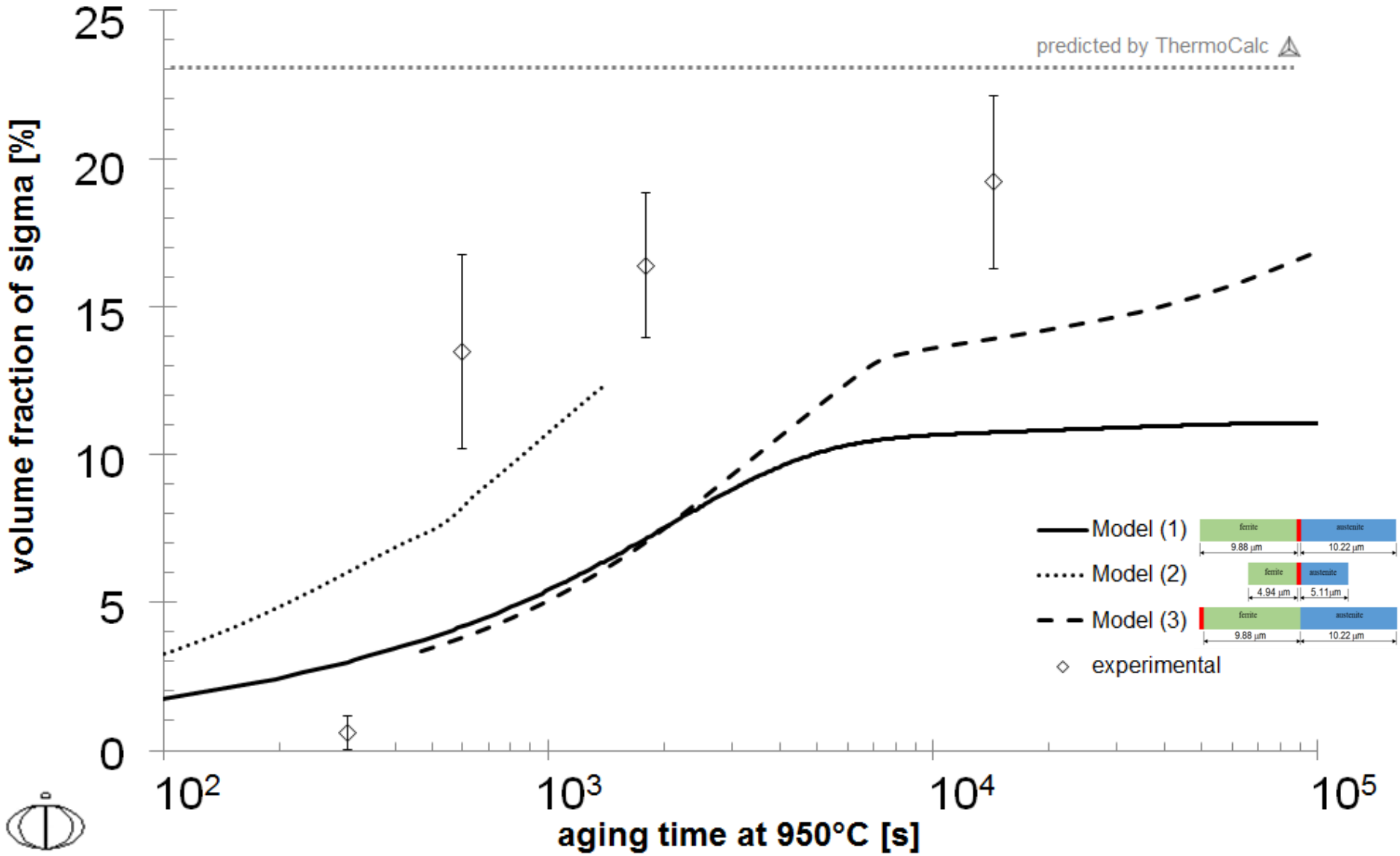

1,800 s @ 950°C
σ
α
γ
BSC 20.00 kV
10 µm


14,400 s @ 950°C
σ
α
Cr_2N
Globular oxide inclusion
BSC 20.00 kV
10 µm


100
90
80
70
60
50
40
30
20
10
0
volume fraction of pahses [%]
austenite
ferrite
sigma
chromium nitride
austenite (solution-treated sample)
ferrite (solution-treated sample)
sigma (14,400 s@950°C aged sample)
chromium nitride (14,400 s@950°C aged sample)
900
950
1000
1050
1100
1150
temperature [°C]


35
30
25
20
Cr content [wt%]
0
5
10
15
20
length of Model (1) [μm]
t=0
t=60s
t=300s
t=1800s
t=7200s
ferrite
austenite
9.88 μm
10.22 μm
sigma


ferrite
austenite
9.88 µm
10.22 µm
sigma
t=0
t=60s
t=300s
t=1800s
t=7200s
Mo content [wt%]
length of Model (1) [µm]
14
12
10
8
6
4
2
0
5
10
15
20


predicted by ThermoCalc
volume fraction of sigma [%]
25
20
15
10
5
0
10^2
10^3
10^4
10^5
aging time at 950°C [s]
Model (1)
ferrite
austenite
9.88 µm
10.22 µm
Model (2)
ferrite
austenite
4.94 µm
5.11µm
Model (3)
ferrite
austenite
9.88 µm
10.22 µm
experimental

CONCLUSIONS

The thermodynamic equilibrium of a superduplex stainless steel was modelled through computer simulation using Thermo-Calc software and TCFE6 thermodynamic database, and they were validated experimentally.

CONCLUSIONS

Despite the fact that DiCTra models can qualitatively describe the phenomenon of sigma growth from ferrite and the associated composition gradients expected in ferrite and austenite around the formed sigma phase, none of the three studied models were capable of describe the evolution of the sigma volume fraction through aging time at 950°C.

CONCLUSIONS

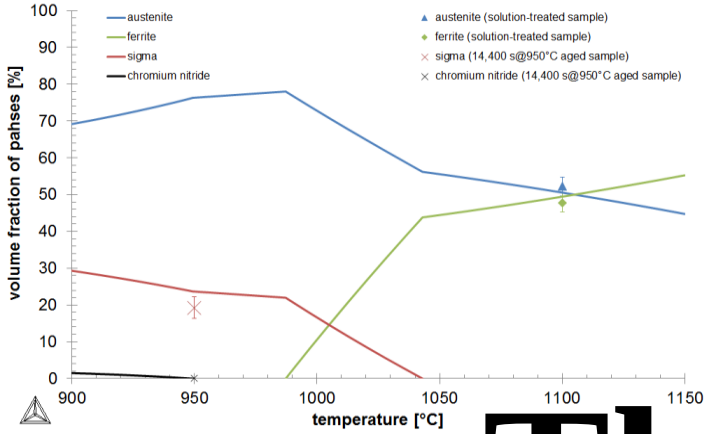
The studied models only consider unidimensional diffusion flux for the growth of a single heterogeneously nucleated sigma phase, and this can be a reason for the poor description of the sigma phase content through aging time.

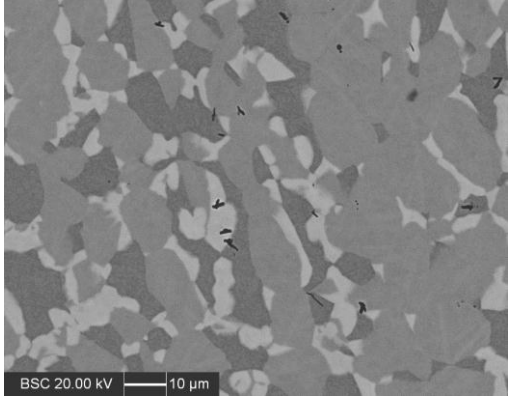
FUTURE WORKS:

Models that consider the sigma phase growth not only restricted to one-dimensional diffusion, as those that enable radial growth or spherical particles.

Models to assess the occurrence of eutectoid decomposition of ferrite in austenite and sigma.

Models to evaluate the effect of different rates of nucleation, as the ones possible by Prisma® software.





Thank you!

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