VINNOVA DuWelTool

WP2: Thermo-dynamical modelling

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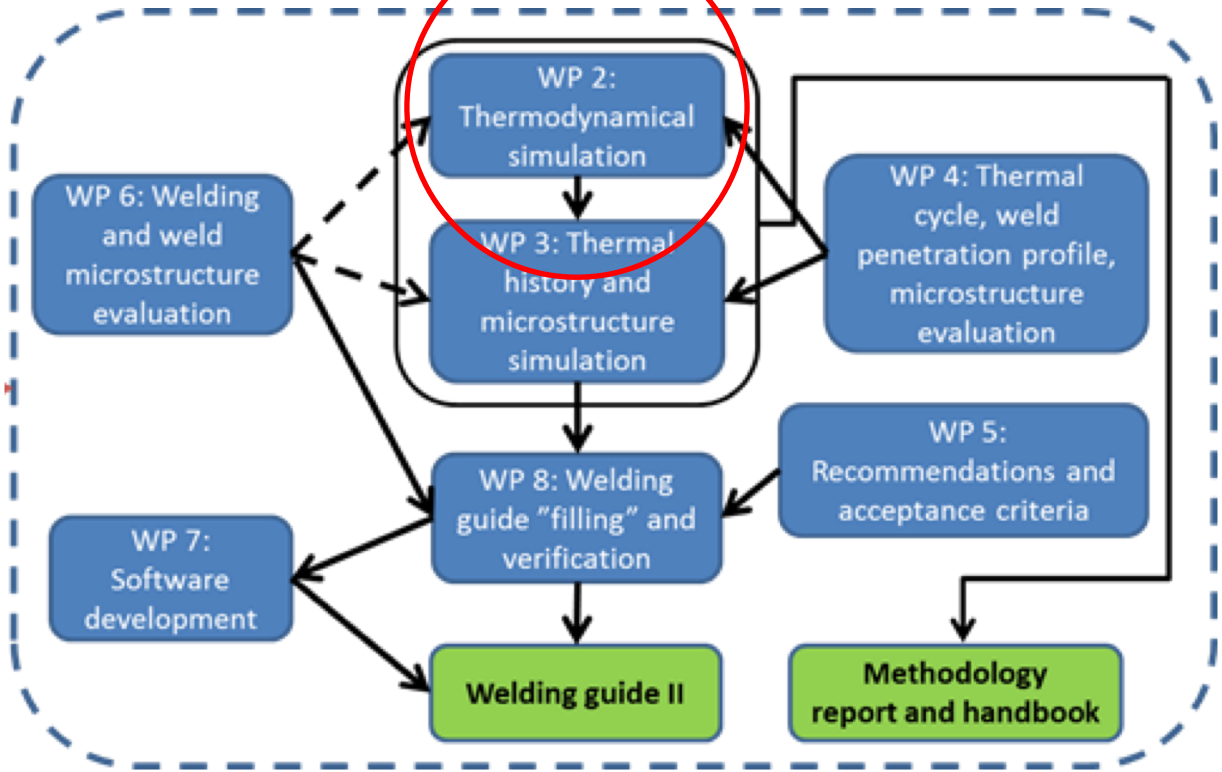
WP2: Thermo-dynamical modelling, WP leader: University West
Purpose: To feed the FEM simulations



Applied simulation models:

Matrix phases:
Liquid → Ferrite + Austenite
Ferrite → Austenite

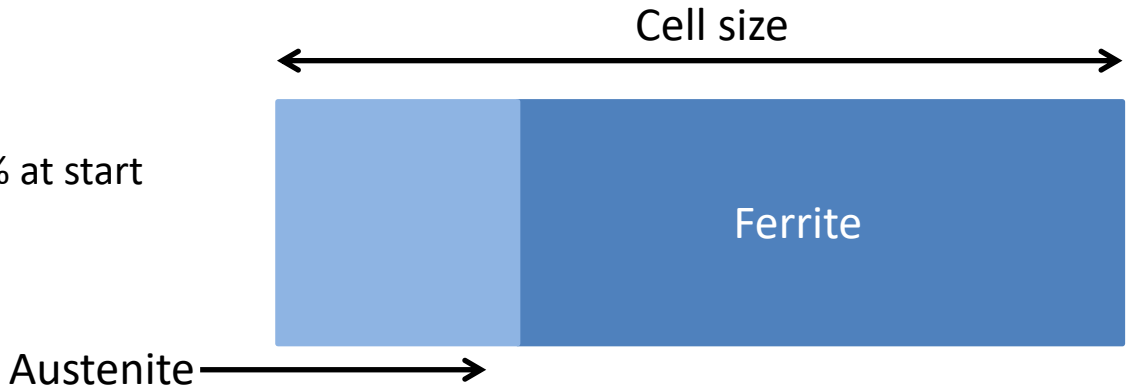
Intermetallic phases:
Ferrite (+Austenite) → Sigma phase or Chi phase
Ferrite → **Sigma phase** or Chi phase + Secondary austenite

Nitrides:
Ferrite → Cr_2N
Ferrite → Austenite + Cr_2N
Ferrite + Cr_2N → Secondary austenite

Advanced nitride matters were left to the SuperAVON project

Set-up 1D kinetic simulation (DICTRA):
- Databases, thermodynamic and kinetic
- Phases
- Chemical composition(s)
- System (cell) size
- Start temperature
- Cooling/heating rate(s)
- Stop temperature

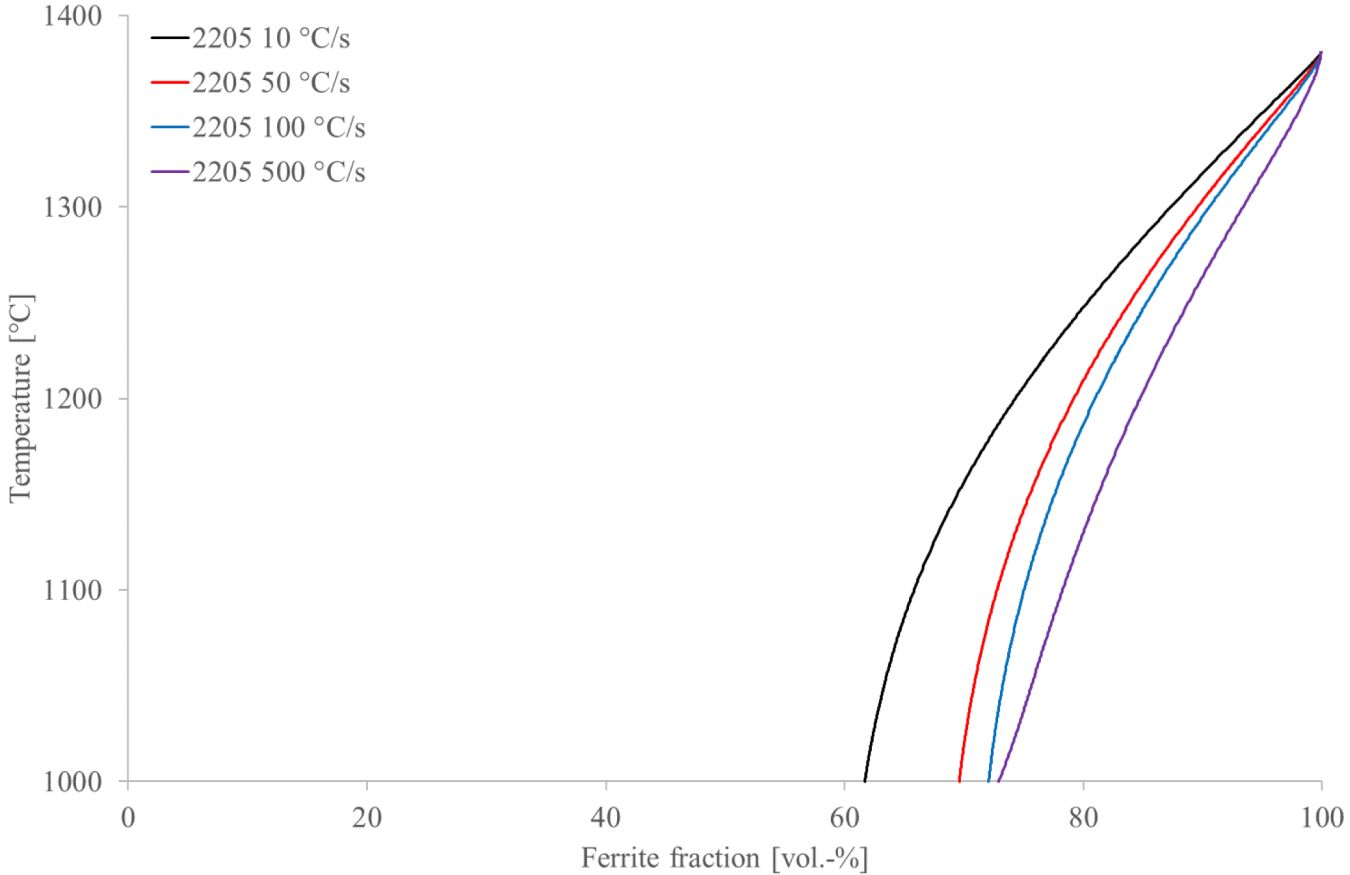
> Ferrite active phase, 100 vol.-% at start
> Austenite as an inactive phase
> Cooling 1600 --> 1000 °C



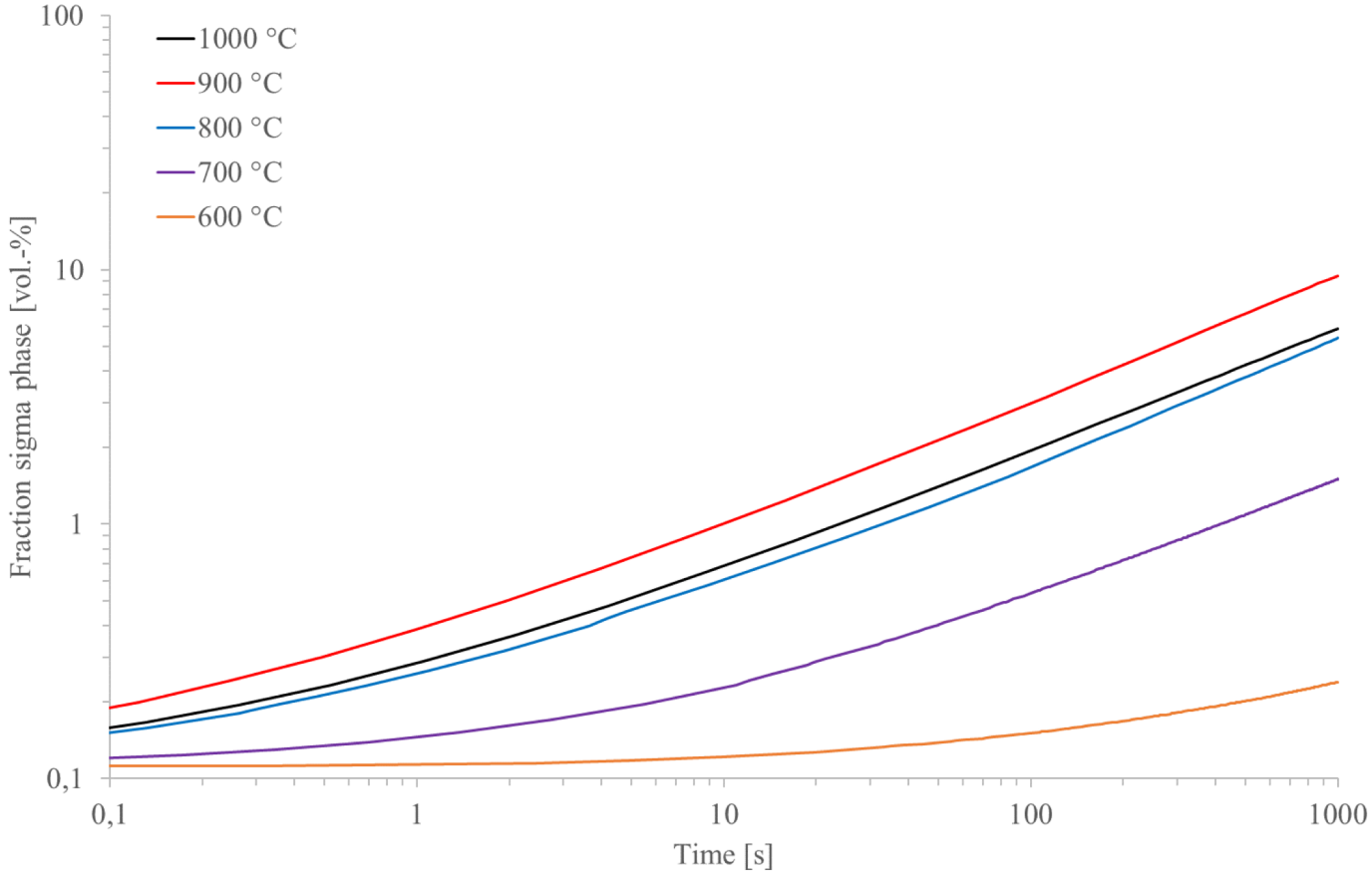
Software:
Thermo-Calc and DICTRA with databases TCFE8 (thermodynamics) and MOBFE3 (mobilities)

Materials:

	Mn	Cr	Ni	Mo	N
LDX 2101	5.0	21.5	1.5	-	0.22
2304	-	23.0	4.8	0.3	0.10
2205	-	22.0	5.5	3.0	0.17
2507	-	25.0	7.0	4.0	0.27
23 7 NL	-	23.0	7.5	0.3	0.14
22 9 3 NL	-	22.5	9.0	3.0	0.18
25 9 4 NL	-	25.0	9.5	3.5	0.25



Results: 2205 single pass α → γ



Results: 2507 α → σ

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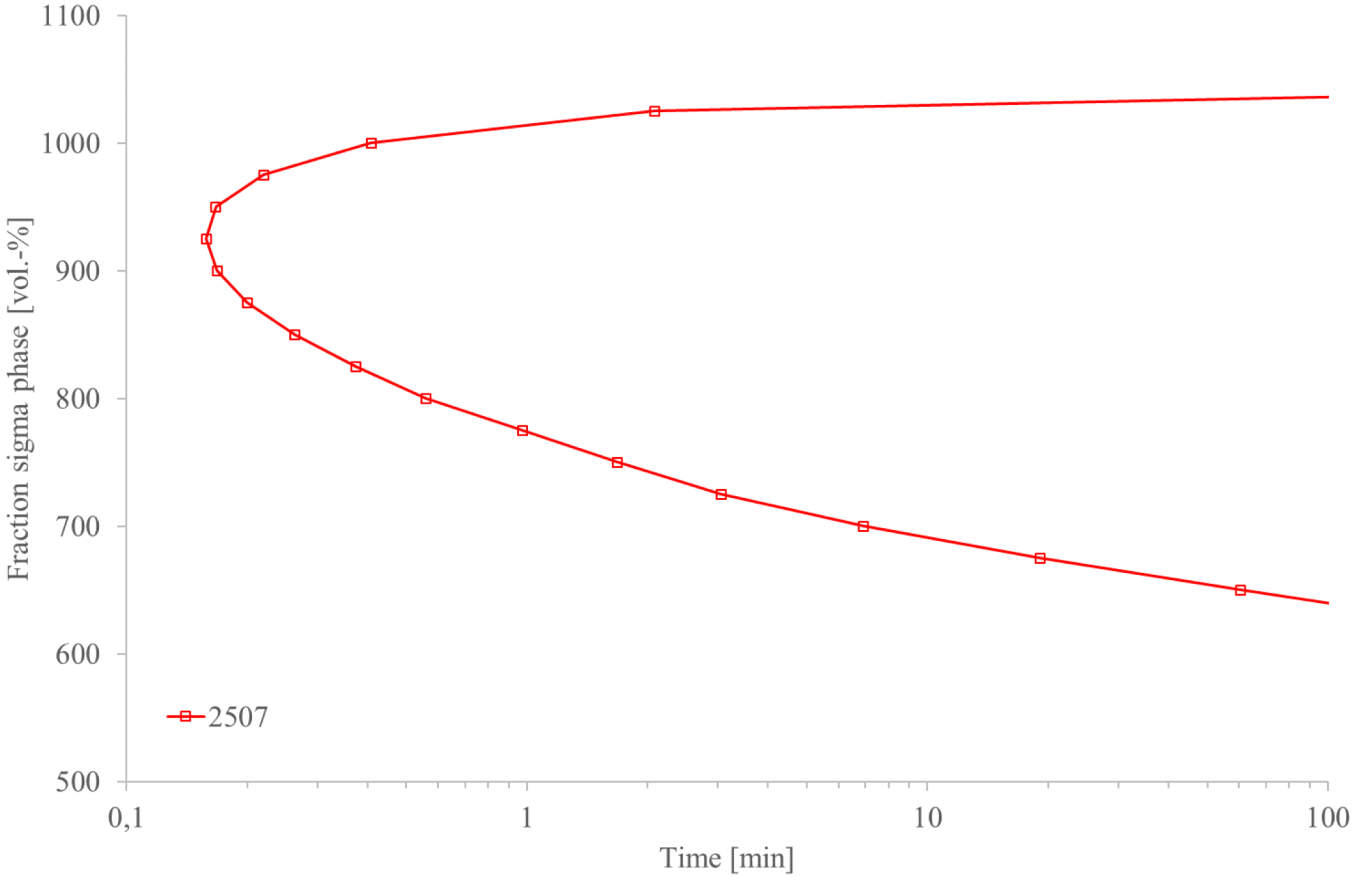
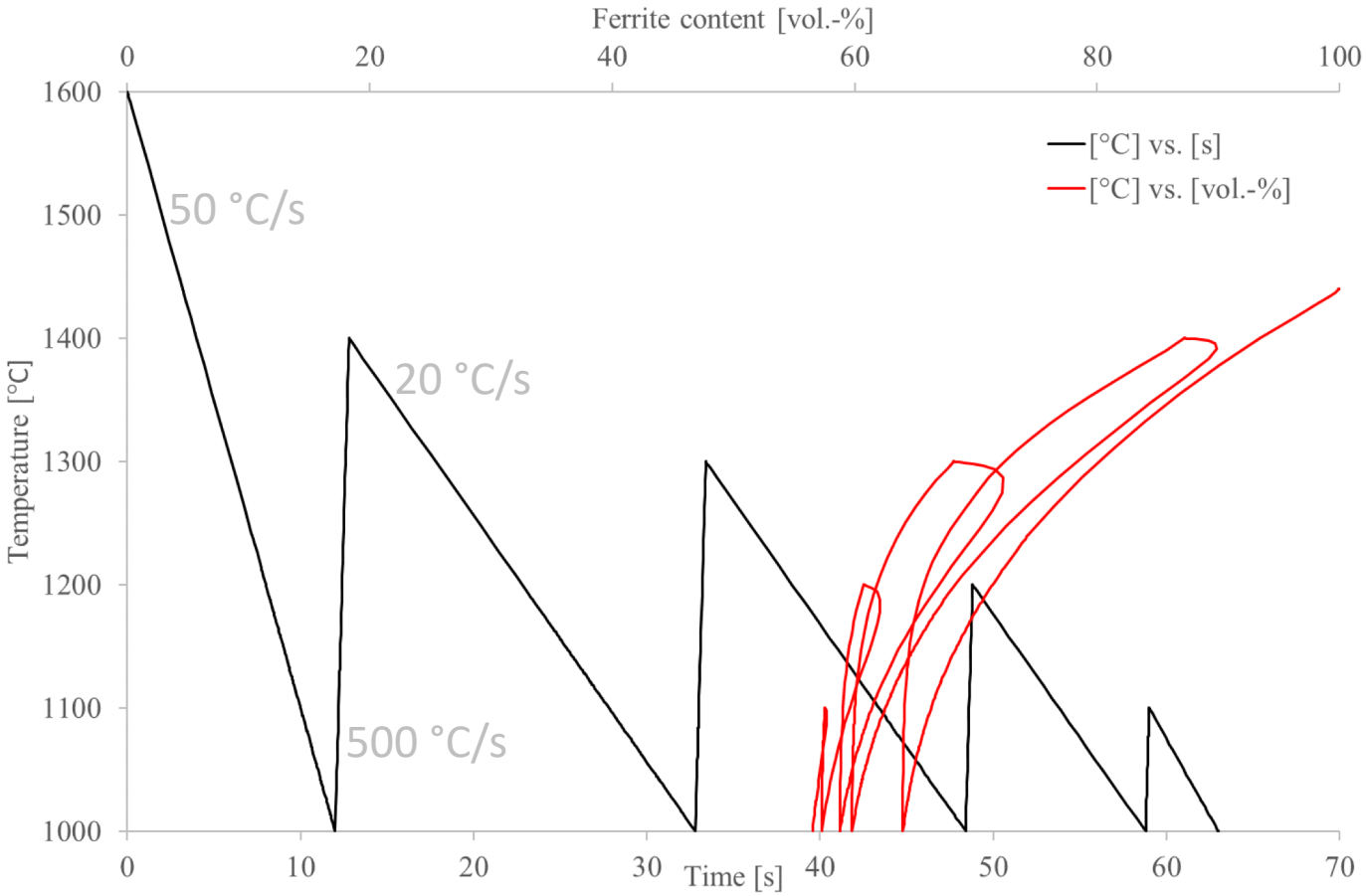


Results: 2507 α → σ (1 %)



Results: 2507 multipass α → γ

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In this WP a large number of simulations were carried out using computational thermodynamics and the Thermo-Calc and DICTRA software:
- Austenite precipitation during cooling
- Sigma phase precipitation during cooling and during isothermal conditions
- Nitride and secondary austenite precipitation

Multipass simulations:
- Austenite precipitation/growth/dissolution
- Sigma phase precipitation/growth/dissolution

---> Delivered to the FEM simulations for further processing

Extent of work carried out:

~ 161 .TCM files, macros for Thermo-Calc (finishes within minutes)

~ 988 .DCM files, macros for DICTRA (finishes within hours)

Conclusions:

Thermo-Calc Software AB:
https://www.thermocalc.com/

S. Wessman, M. Selleby: Evaluation of Austenite Reformation in Duplex Stainless Steel Weld Metal using Computational Thermodynamics, Welding in the World 58 (2014) 2 217-224.

S. Wessman, R. Pettersson: Application of computational thermodynamics to predict growth of intermetallic phases in superduplex stainless steels, Steel Research International 86 (2015) 1339-1349.

M. A. Valiente Bermejo, S. Wessman: Computational thermodynamics in ferrite content prediction of austenitic stainless steel weldments, Welding in the World 63 (2019) 627–635.

S. Wessman: On the use of computational thermodynamics for predicting the precipitation and growth of secondary phases in stainless steels, European Stainless Steel Conference & Expo Duplex 2019, Sept. 30 - Oct. 2 (2019), Vienna, Austria.