

Thermo-Calc Software

CALCULATING THERMODYNAMIC PROPERTIES

TC-PRISMA – A Tool for Simulation of Precipitation Reactions in Alloys

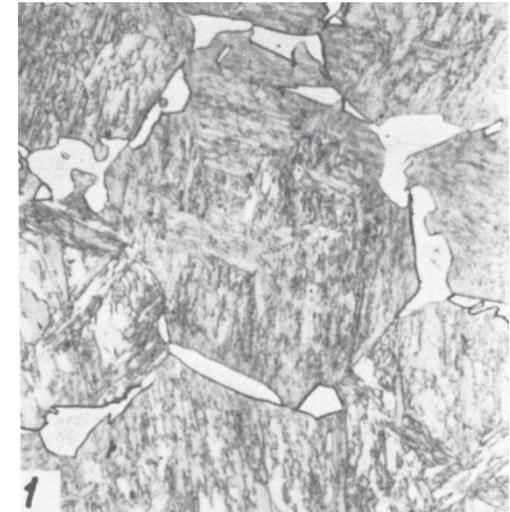
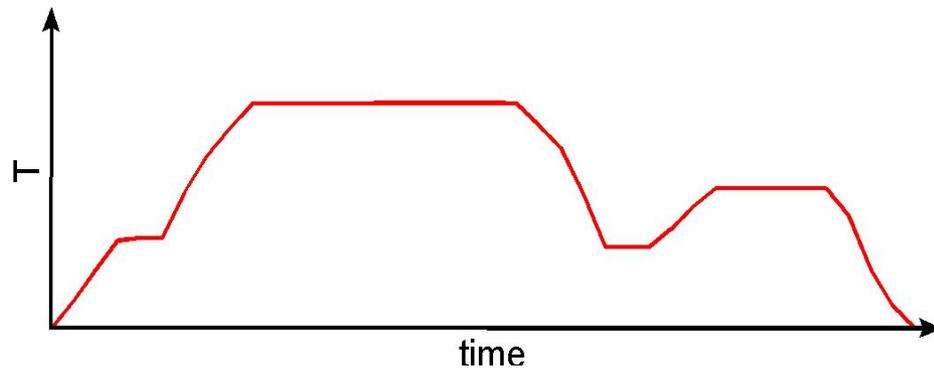
Henrik Strandlund, Xiaogang Lu, Qing Chen

Presented by Paul Mason

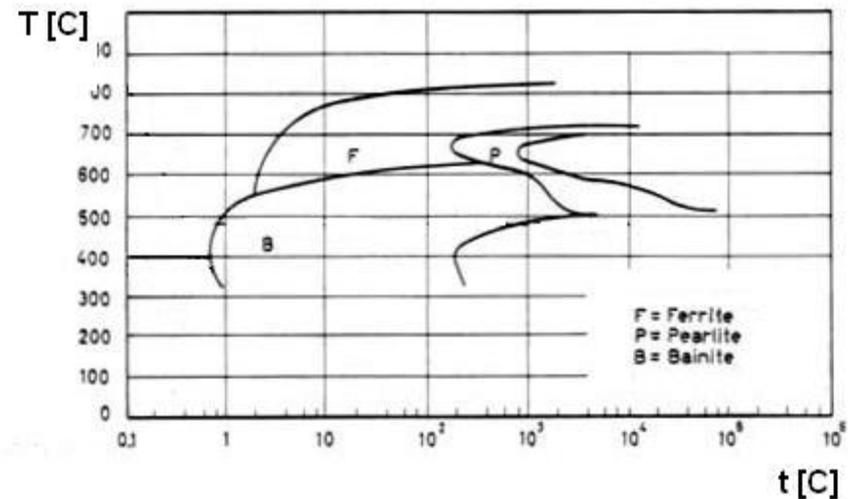


- Background
- Simulations of precipitation
- Models
- New software tool: **TC-PRISMA**

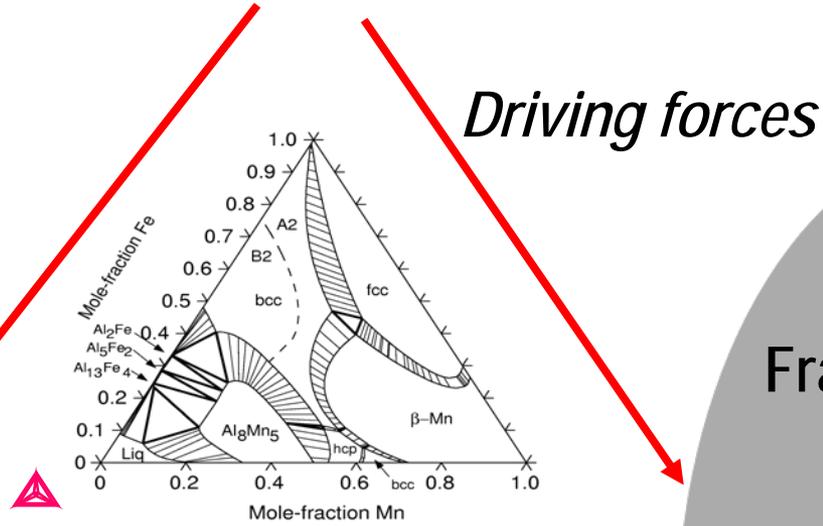
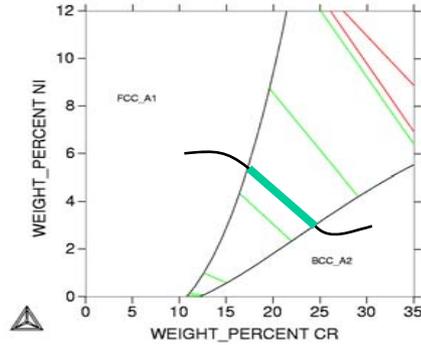
Industrial Heat treatment



- Optimize processes
- Control the microstructure
- Tailor material properties

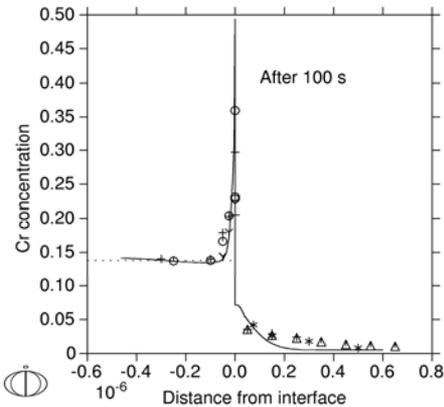


THERMO-CALC



TTT/CCT
Fractions
Nucleation

DICTRA



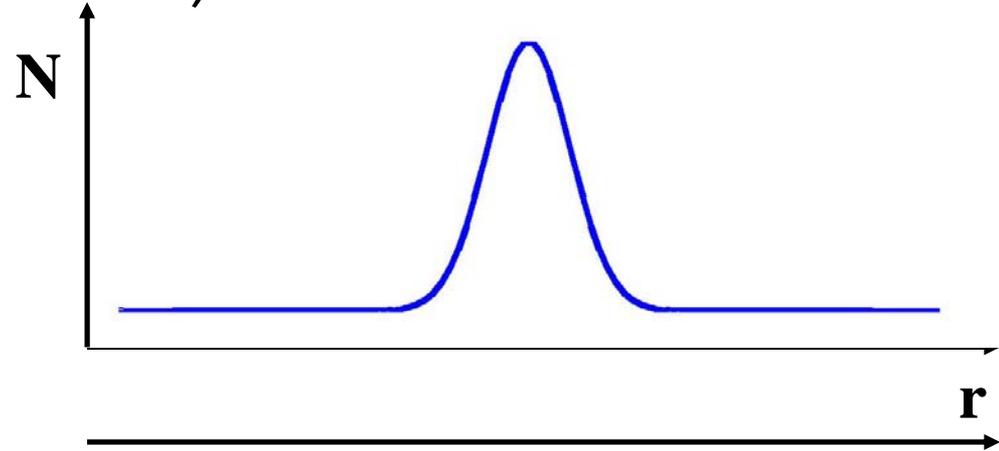
Diffusivities

TC-PRISMA

Average quantities
Size distributions

- Kampmann Wagner (Numerical)

- Nucleation, Growth and Coarsening



- Different size classes

- Temporal evolution of particle size distributions

$$\frac{\partial N_k}{\partial t} = - \frac{\partial (N_k v_k)}{\partial r} + j_k$$

Classical Nucleation Theory

$$j = Z\beta N e^{-\frac{\Delta G}{kT}} e^{-\frac{\tau}{t}}$$

Z – Zeldovich factor

β – atomic attachment rate

N – number of nucleation sites

ΔG – critical driving force for nucleation

τ – Incubation time

Multicomponent effects (e.g. difference in diffusivities) are taken into account in β

Do not consider diffusion inside precipitate (unlike DICTRA)

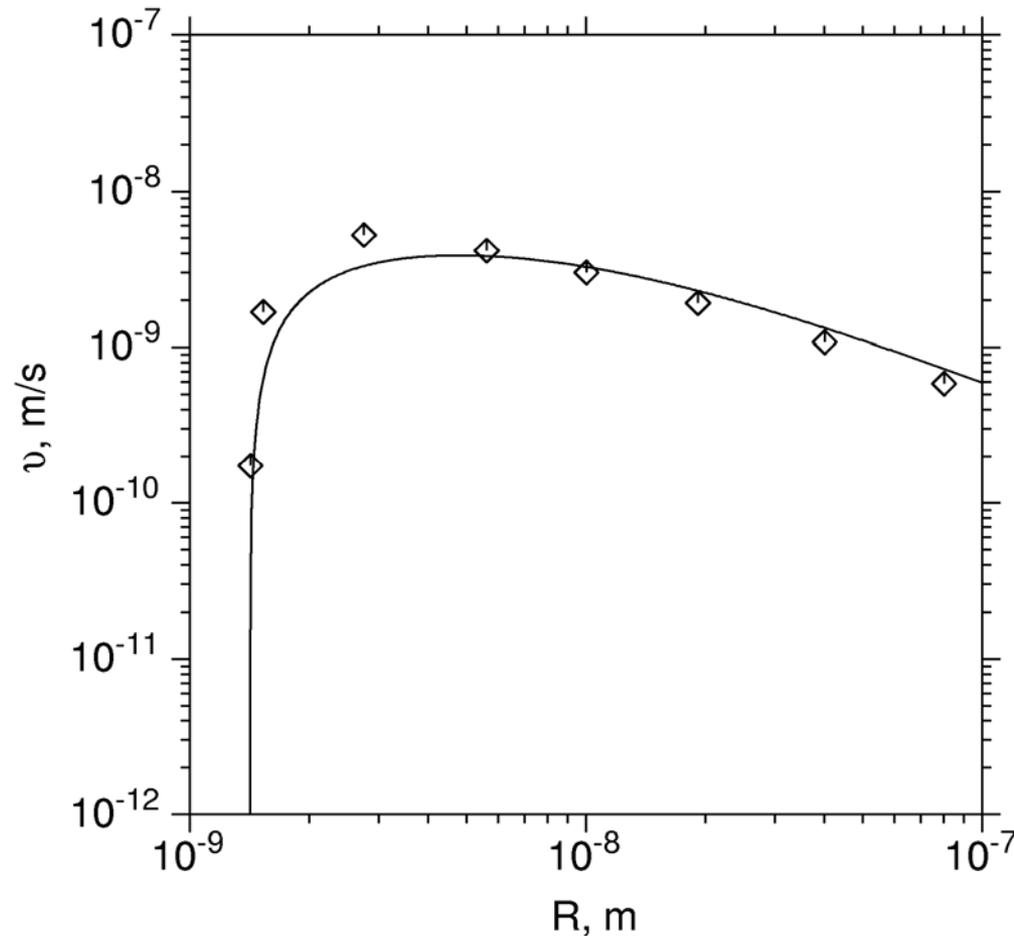
- Want a model capable of treating different growth modes such as **diffusion-controlled, interface-controlled, or mixed mode growth** without detailed solution of composition profile in multi-component matrix phase
- **Large supersaturation, para-equilibrium, and NPLE** can be taken into account

$$v(c_i^P - c_i^I) = c_i^I M_i (\mu_i^M - \mu_i^I) / \xi_i R$$

$$\mu_i^P = \mu_i^I$$

Q. Chen, J. Jeppsson, J. Ågren, Acta Mater. 2008;56:1890

Models: Growth rate (new model)

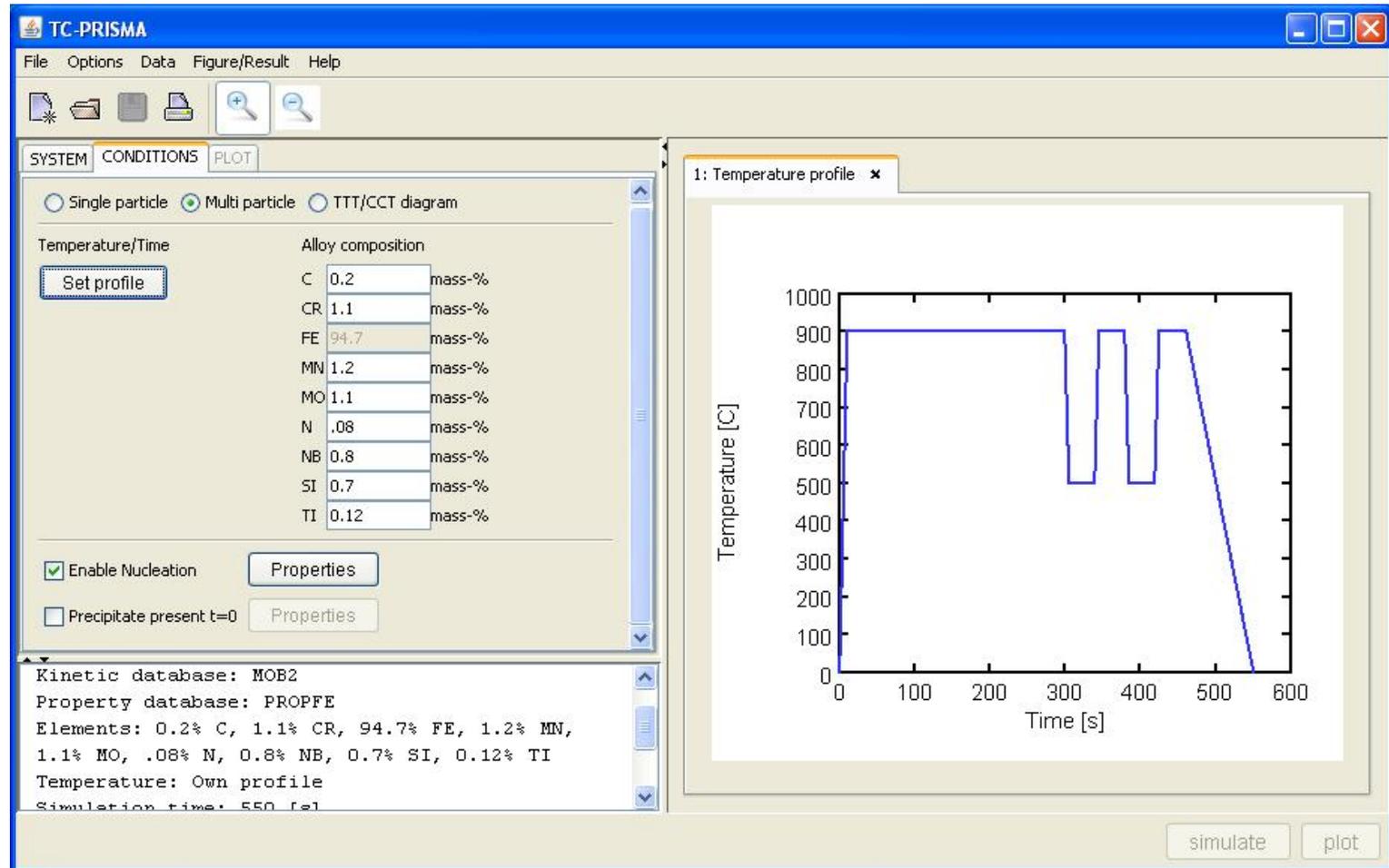


Fe-2%Cr-0.05%C, M₂₃C₆ from ferrite, local equilibrium, Cr-diffusion controlled

Q. Chen, J. Jeppsson, J. Ågren, Acta Mater. 2008;56:1890

TC-PRISMA

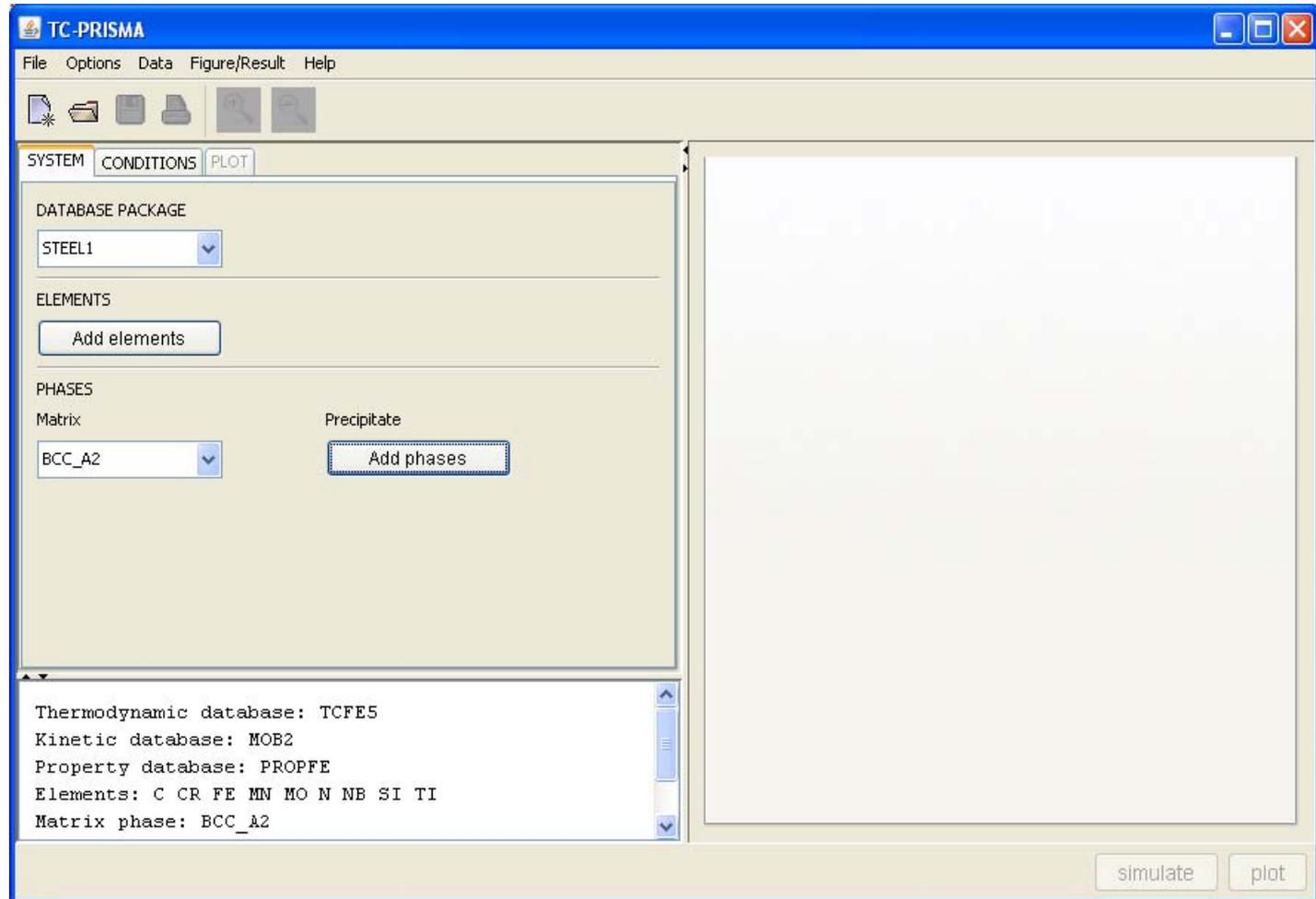
PREcipitation SIMulations in MATERIALS



New software tool: TC-PRISMA

Input data: System

- Databases
- Elements
- Matrix phase
- Precipitates





Input data: Conditions

- Temperature profile
- Composition
- Nucleation properties
- Initial size distribution

Temperature...

Constant/Function

Temperature Simulation time

°C s

Load File

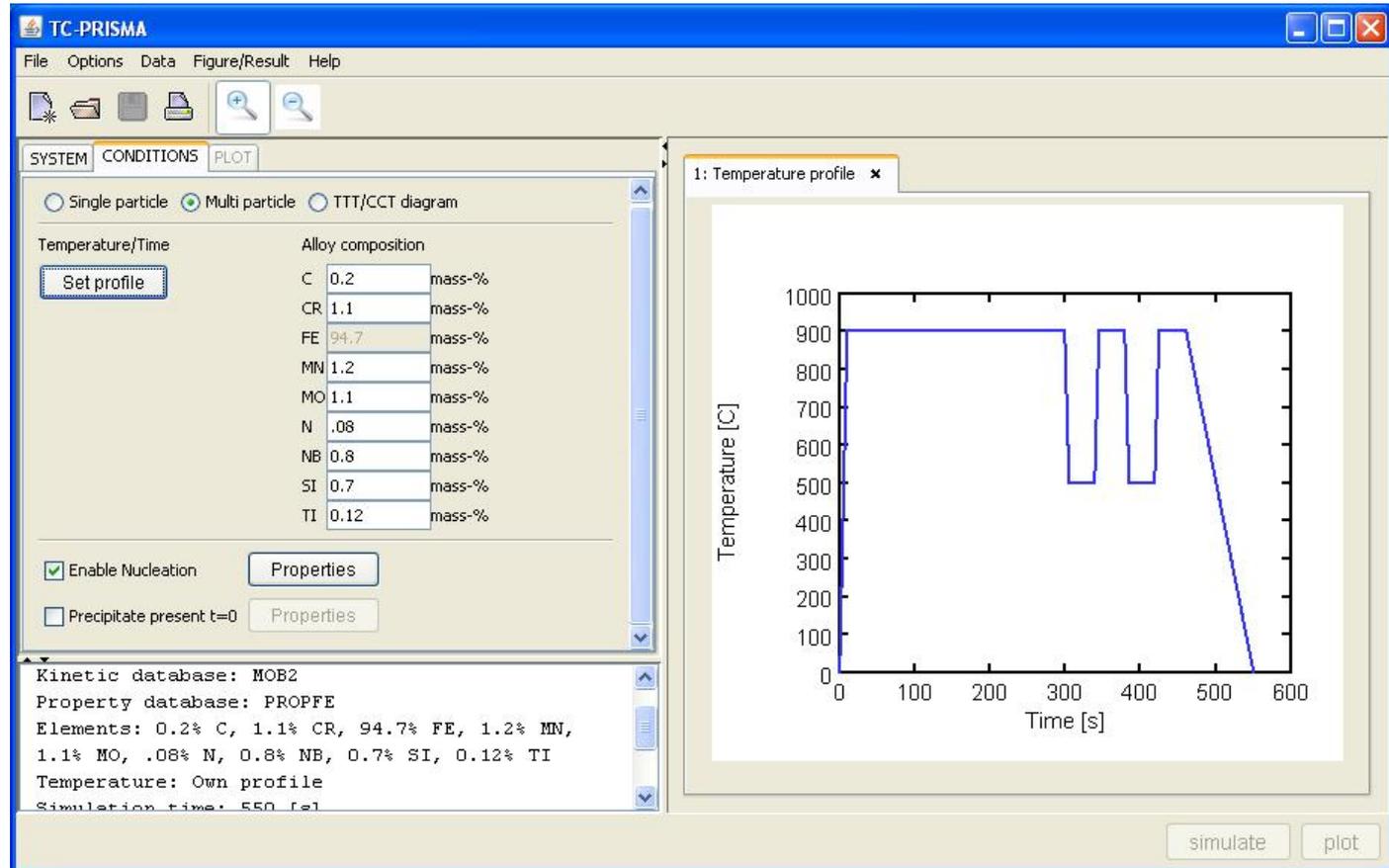
Profile

time	temperature
0	25
30	900
300	900
305	500
335	500
340	900
370	900
375	500
405	500
435	900
465	900
550	25

New software tool: TC-PRISMA

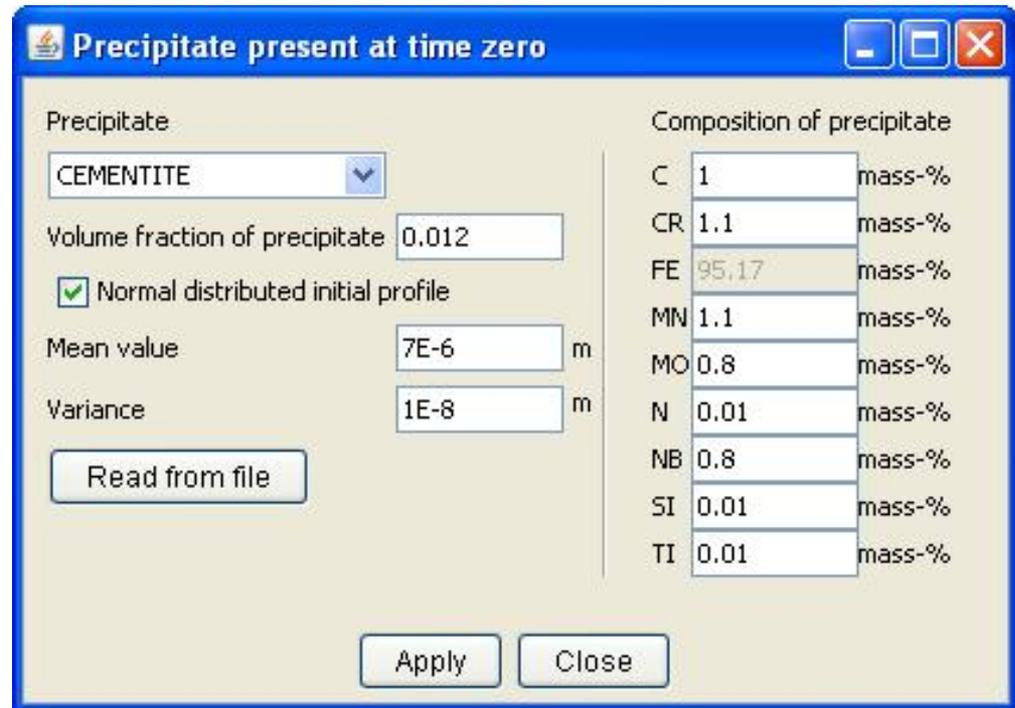
Input data: Conditions

- Temperature profile
- Composition
- Nucleation properties
- Initial size distribution



Input data: Conditions

- Temperature profile
- Composition
- Nucleation properties
- Initial size distribution



Precipitate present at time zero

Precipitate

CEMENTITE

Volume fraction of precipitate 0.012

Normal distributed initial profile

Mean value 7E-6 m

Variance 1E-8 m

Read from file

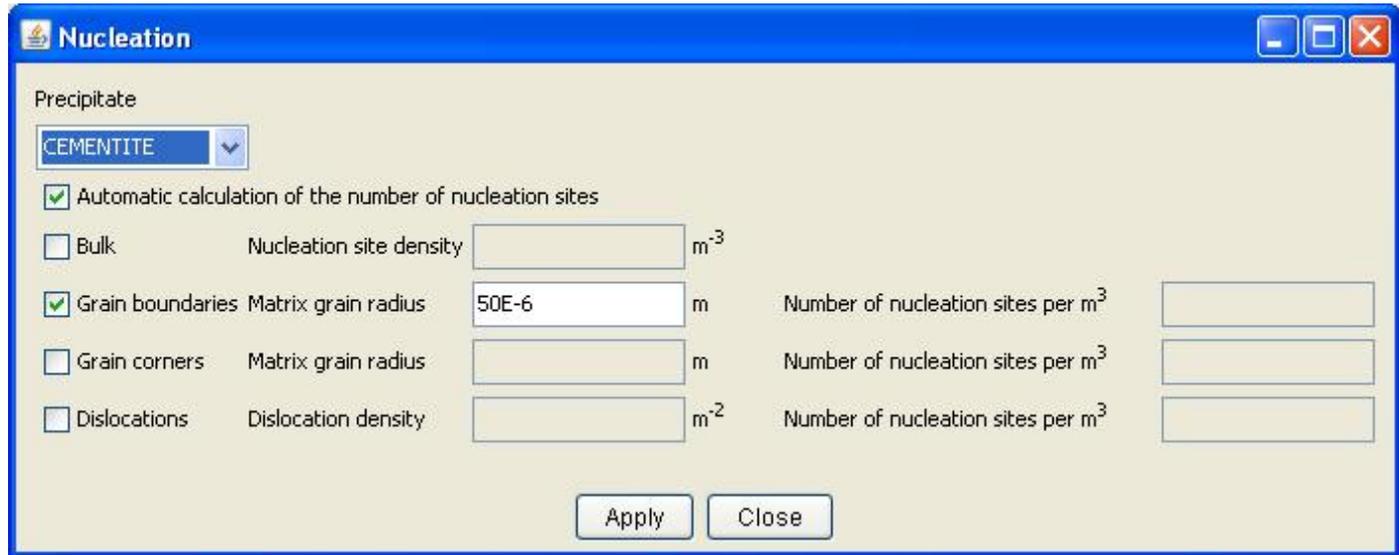
Composition of precipitate

C	1	mass-%
CR	1.1	mass-%
FE	95.17	mass-%
MN	1.1	mass-%
MO	0.8	mass-%
N	0.01	mass-%
NB	0.8	mass-%
SI	0.01	mass-%
TI	0.01	mass-%

Apply Close

Input data: Conditions

- Temperature profile
- Composition
- Nucleation properties
- Initial size distribution



Nucleation

Precipitate
CEMENTITE

Automatic calculation of the number of nucleation sites

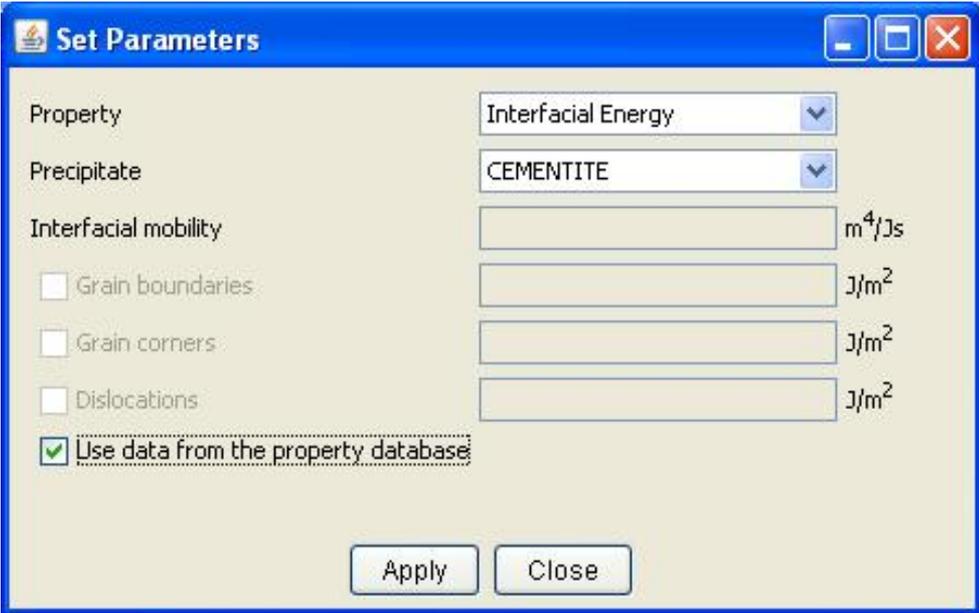
<input type="checkbox"/> Bulk	Nucleation site density	<input type="text"/>	m ⁻³		
<input checked="" type="checkbox"/> Grain boundaries	Matrix grain radius	<input type="text" value="50E-6"/>	m	Number of nucleation sites per m ³	<input type="text"/>
<input type="checkbox"/> Grain corners	Matrix grain radius	<input type="text"/>	m	Number of nucleation sites per m ³	<input type="text"/>
<input type="checkbox"/> Dislocations	Dislocation density	<input type="text"/>	m ⁻²	Number of nucleation sites per m ³	<input type="text"/>

Apply Close

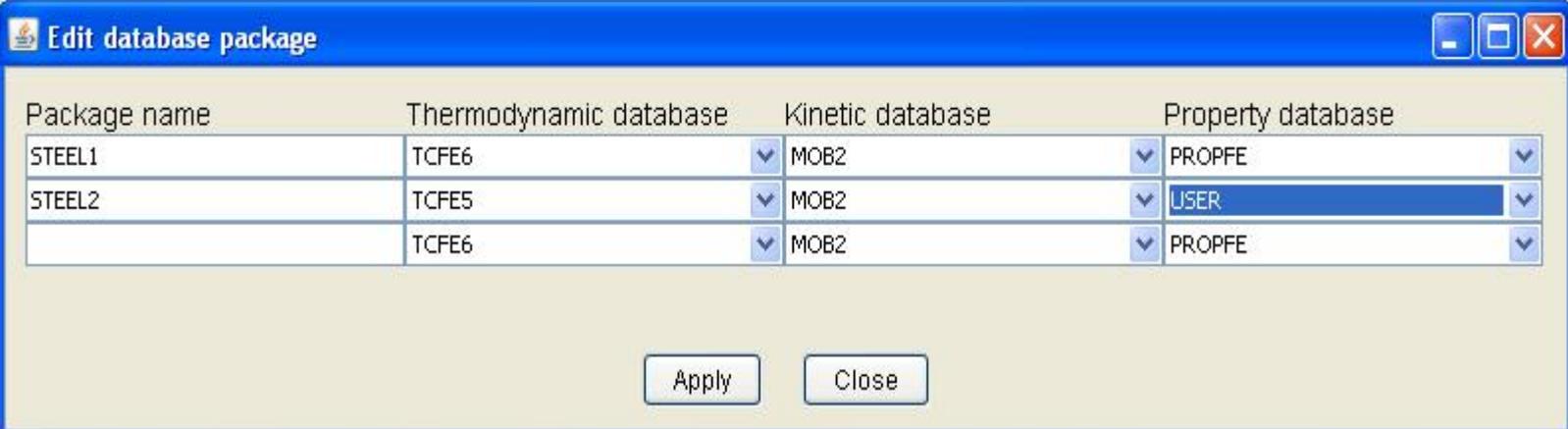
New software tool: TC-PRISMA

Input data: Data

- Interfacial energies
- Molar Volumes
- Interface mobilities
- Poission Ratio
- Bulk Modulus
- Diffusional mobilities
- Thermodynamic Data



The 'Set Parameters' dialog box is used to configure simulation parameters. It features several dropdown menus and checkboxes. The 'Property' dropdown is set to 'Interfacial Energy', and the 'Precipitate' dropdown is set to 'CEMENTITE'. The 'Interfacial mobility' field is empty, with units of m^4/Js . There are three checkboxes for 'Grain boundaries', 'Grain corners', and 'Dislocations', all of which are currently unchecked. The 'Use data from the property database' checkbox is checked. At the bottom, there are 'Apply' and 'Close' buttons.



The 'Edit database package' dialog box displays a table with columns for 'Package name', 'Thermodynamic database', 'Kinetic database', and 'Property database'. The table contains three rows of data. The 'STEEL2' row has 'USER' selected in the 'Property database' column. At the bottom, there are 'Apply' and 'Close' buttons.

Package name	Thermodynamic database	Kinetic database	Property database
STEEL1	TCFE6	MOB2	PROPF6
STEEL2	TCFE5	MOB2	USER
	TCFE6	MOB2	PROPF6

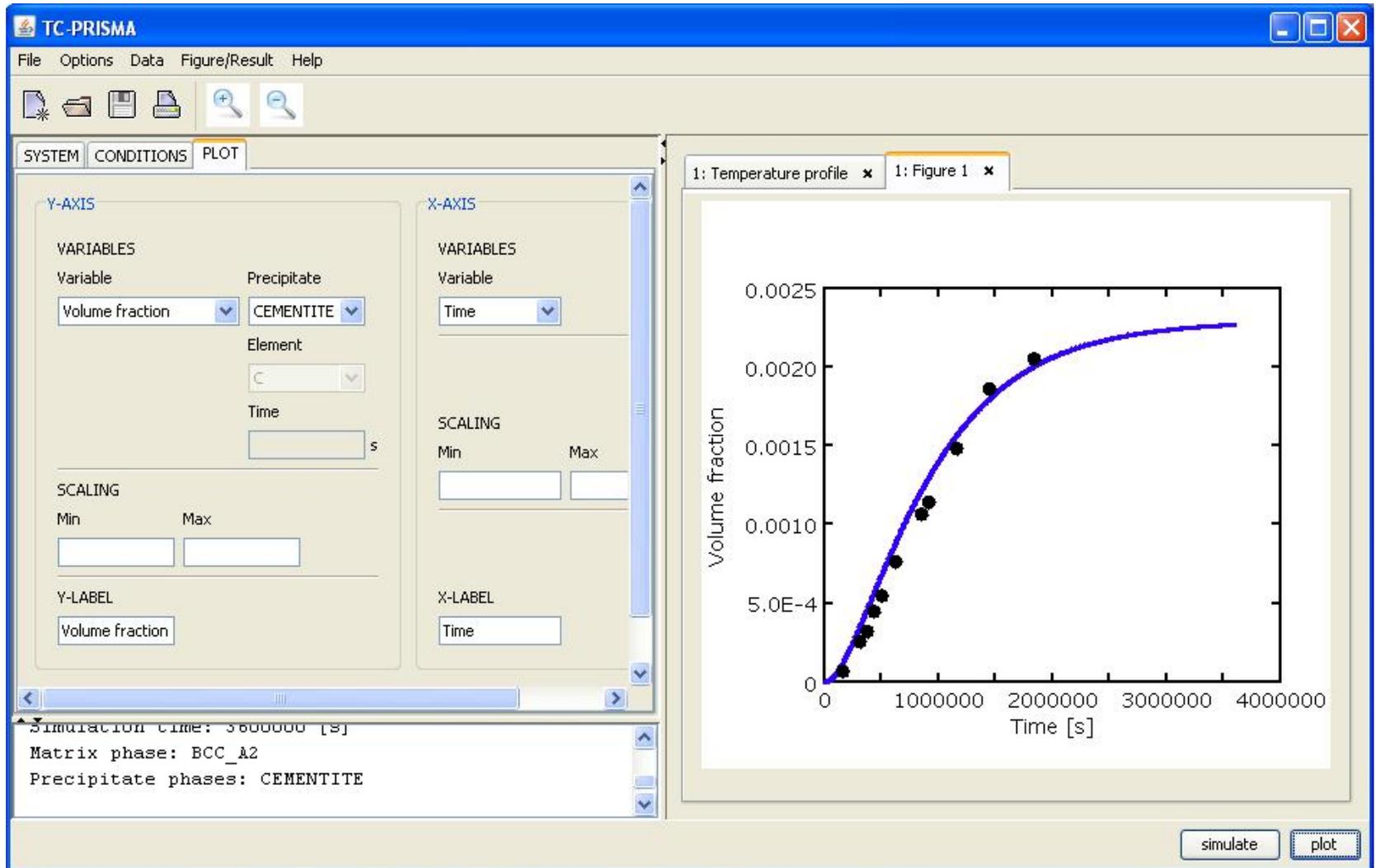


Calculates:

- TTT/CCT diagrams
- Temporal evolution of particles distributions
- Average particle radius as a function of time
- Phase fractions
- Average composition in precipitates and matrix
- Interfacial compositions for each particle size
- Nucleation rate
- Growth rate for each particle size
- Critical radius as a function of time
- User defined functions

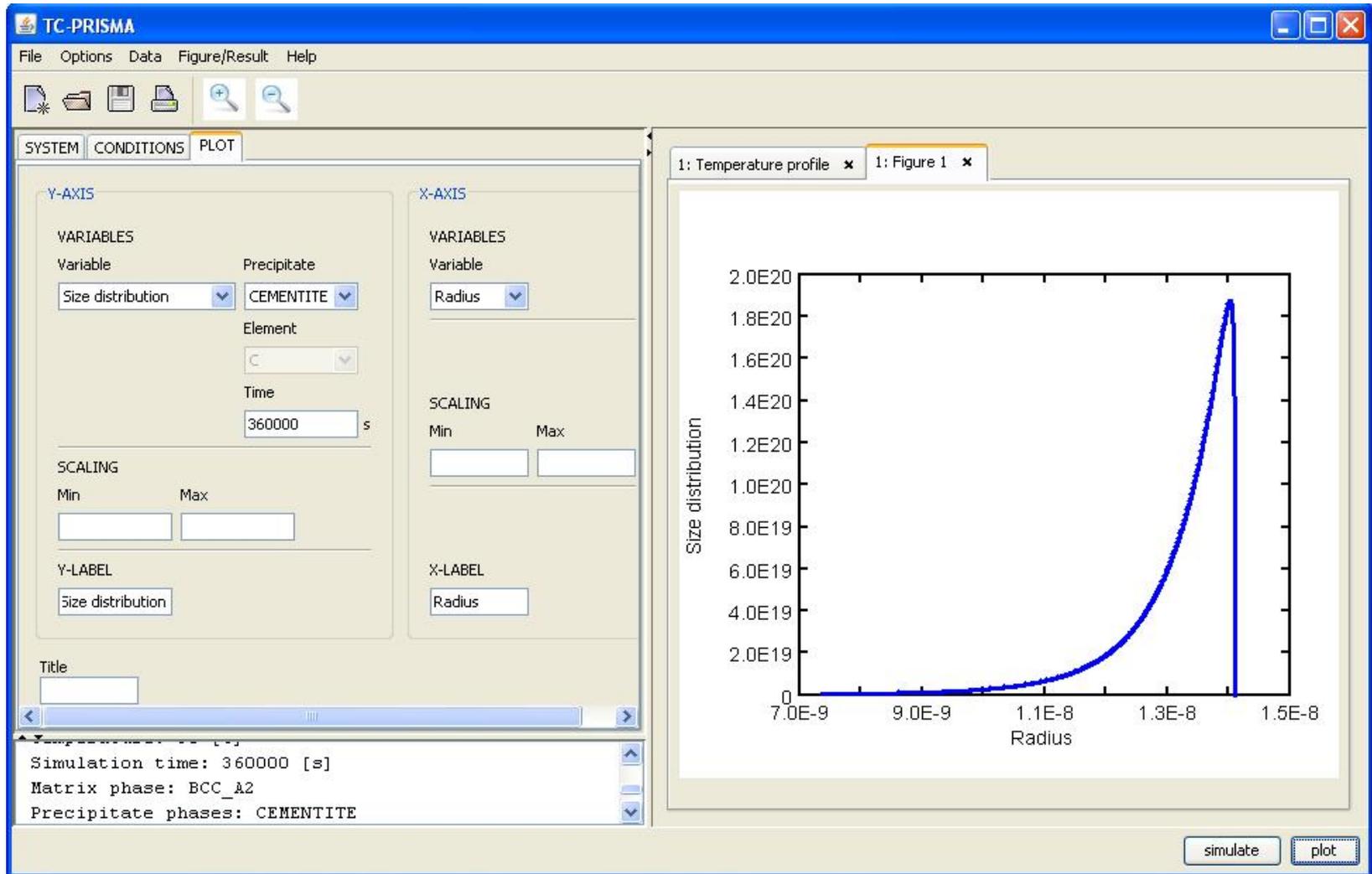
Precipitation of cementite

Calculation of volume fraction of cementite for low alloyed steel at 311K compared to experimental data



Precipitation of cementite

Calculation of size distribution of cementite particles for low alloyed steel at 311K after 100 hours

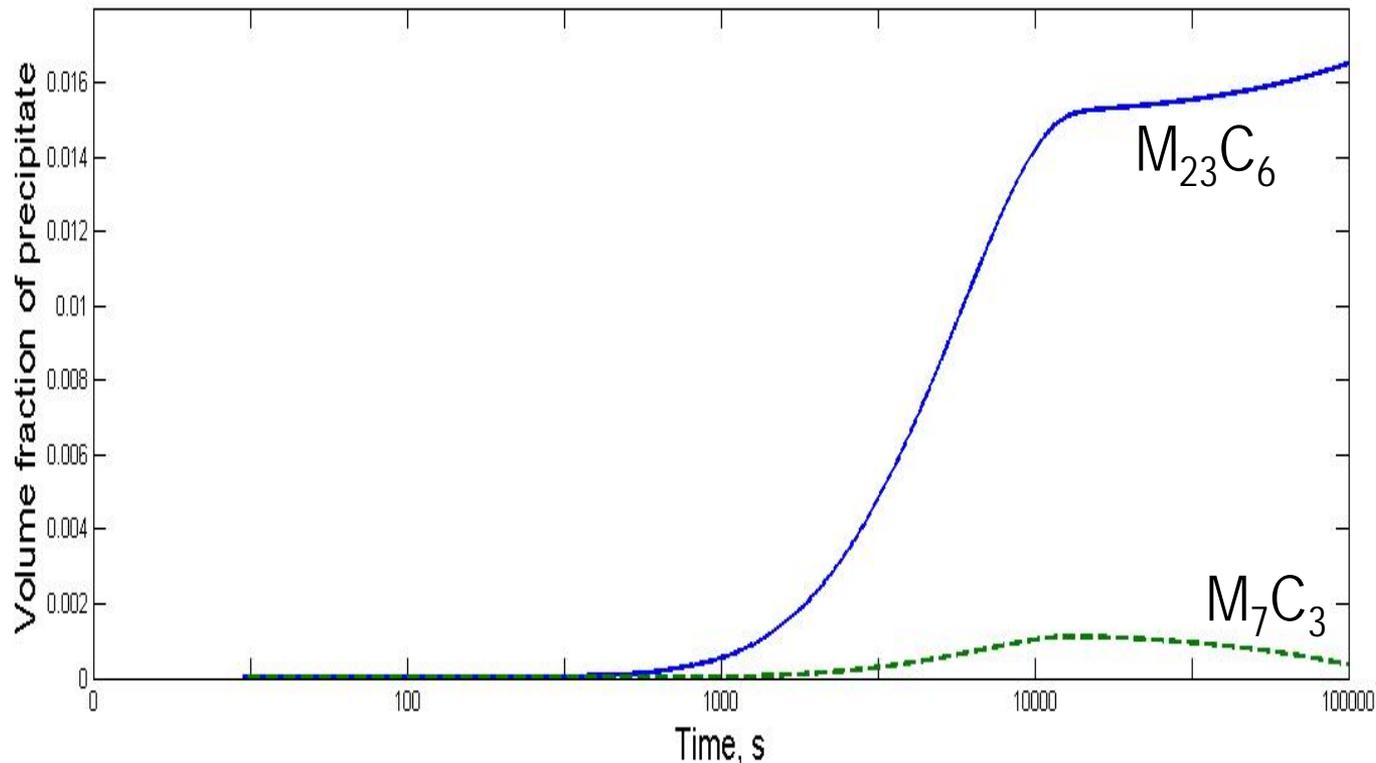


Precipitation of $M_{23}C_6$ and M_7C_3



Precipitation of $M_{23}C_6$ from ferrite in Fe-12%Cr-0.1%C at 1053K

Metastable M_7C_3 forms at the beginning and desolves

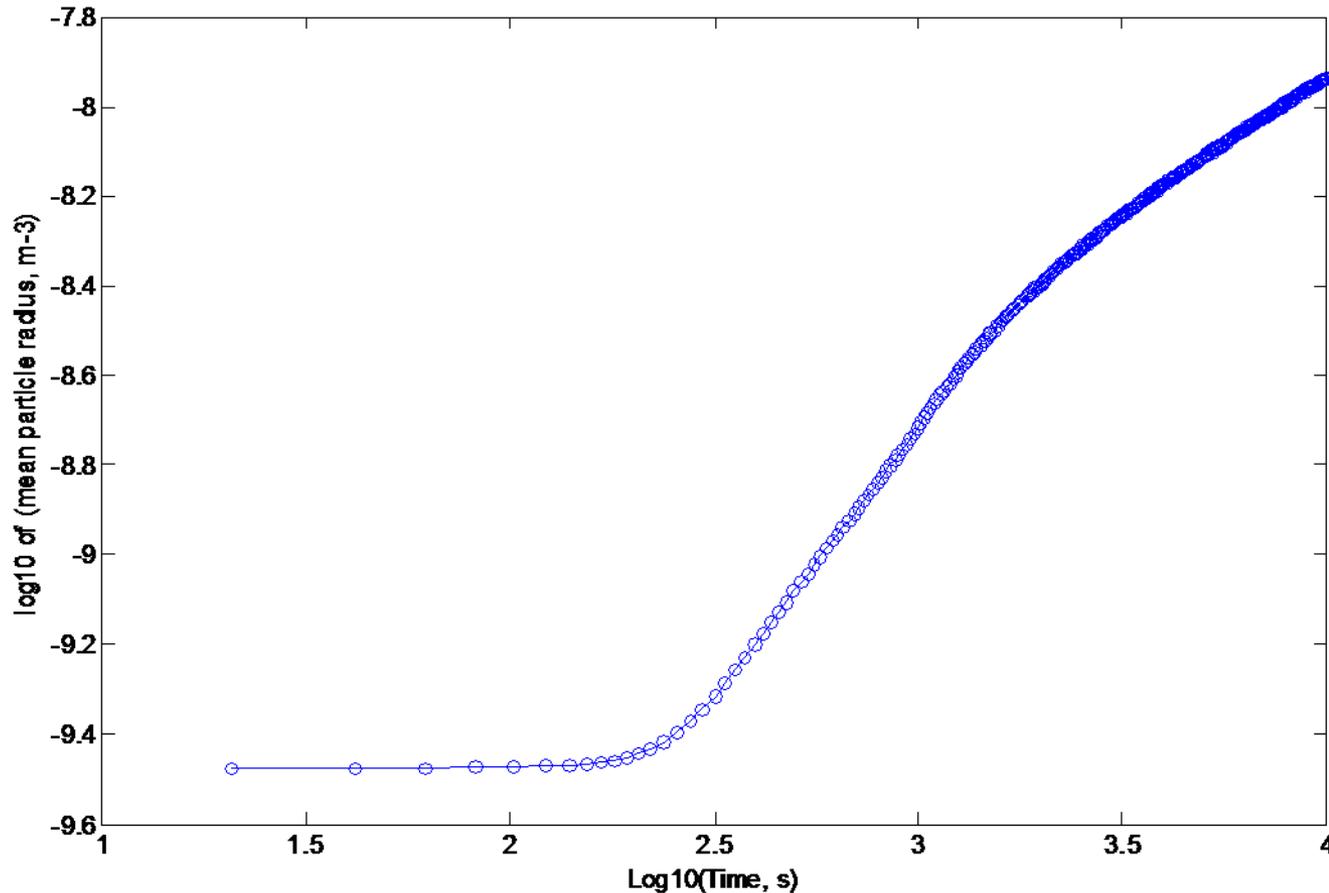


Similar calc by Inden and Schneider using DICTRA took days/hrs.
This calc in TC-PRISMA on a timescale of minutes (and includes larger no. of particles).

Precipitation of $M_{23}C_6$ from austenite



Thermo-Calc Software



Precipitation of $M_{23}C_6$ from austenite at 923 K in steel AISI316.

Composition (wt%): Fe-0.05C-16Cr-1.5Mn-2.3Mo-11Ni-0.6Si.

Benchmark calc: Takes approx. 30 minutes



- A new software tool for simulation of precipitation reactions in multicomponent, multiphase alloys, TC-PRISMA, is being developed by Thermo-Calc Software
- The KWN approach is taken, but a completely new model for the growth rate is applied
- Classical nucleation theory, but multicomponent effects are taken into account
- A new database containing interfacial energies for steels is under development