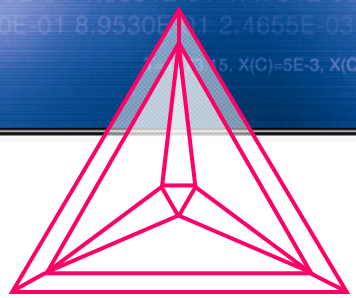


Thermo-Calc Software

CALCULATING THERMODYNAMIC PROPERTIES

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

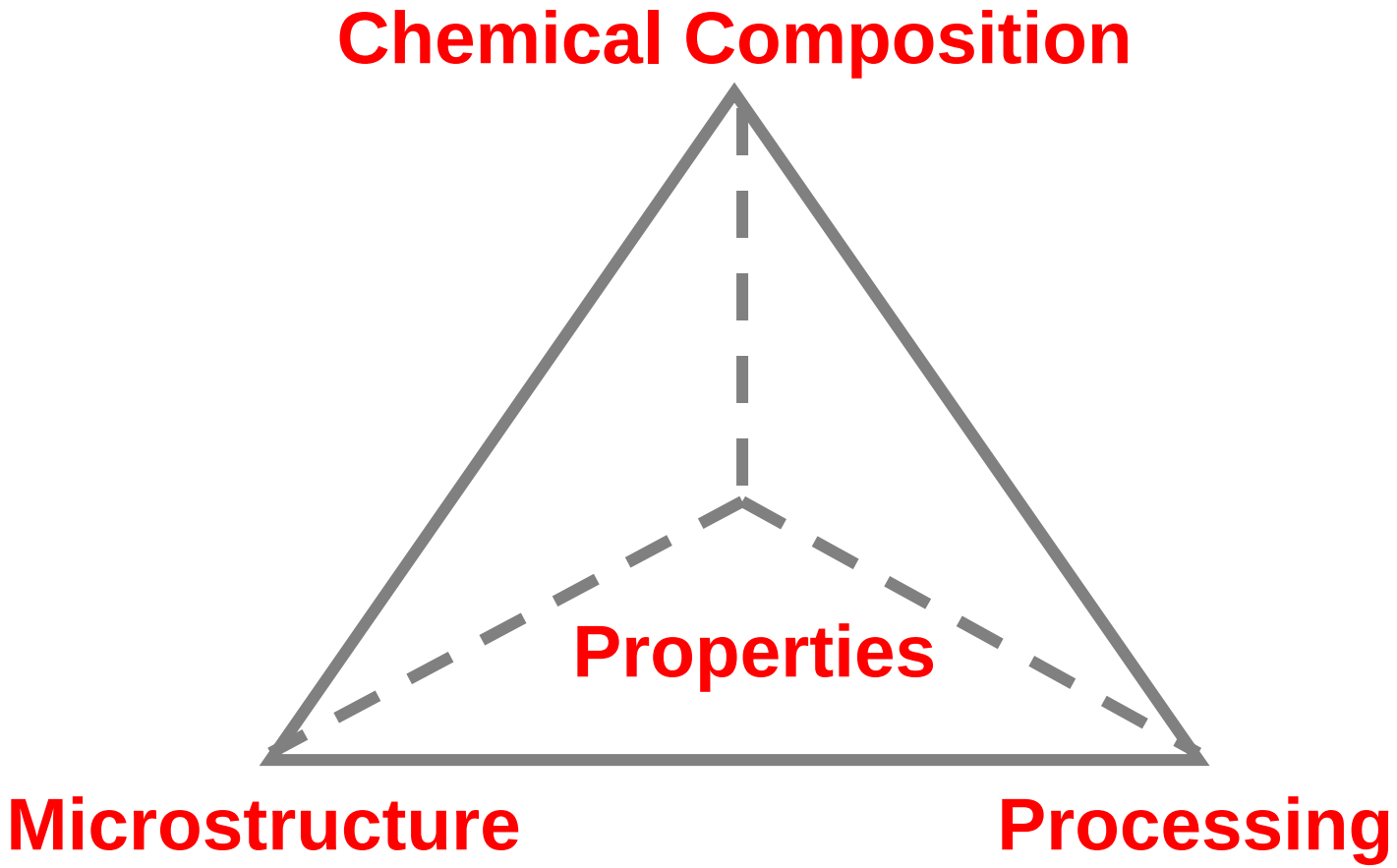
Henrik Strandlund, Xiaogang Lu, Qing Chen

Presented by Paul Mason

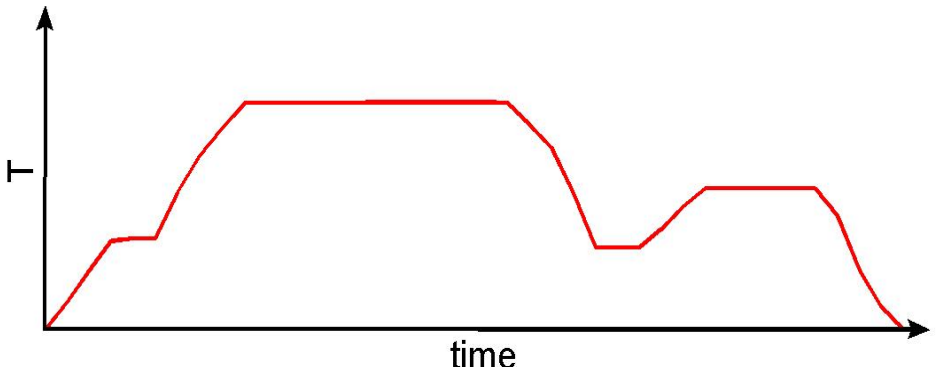
Outline

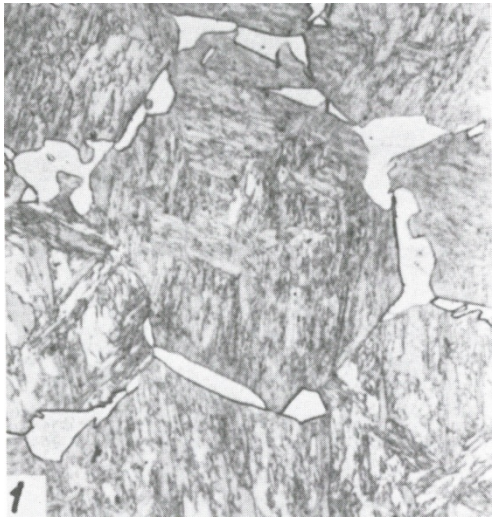
- Background
- Simulations of precipitation
- Models
- New software tool: TC-PRISMA

Background

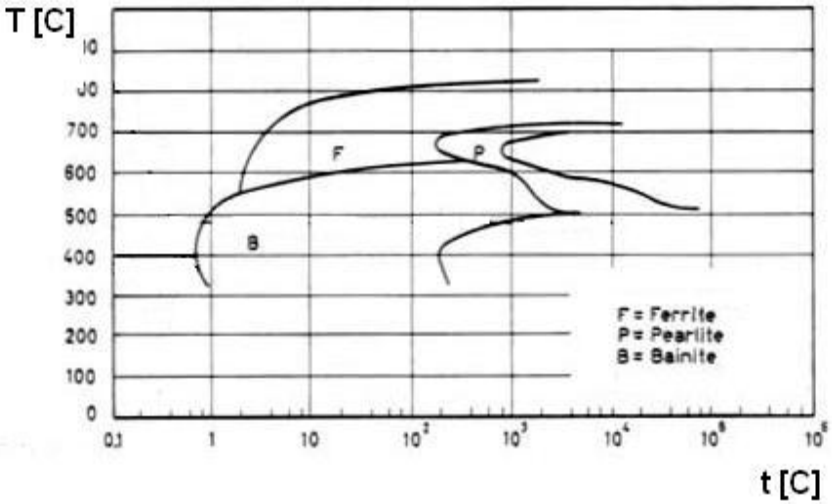

Chemical Composition
Properties
Microstructure
Processing

Industrial Heat treatment





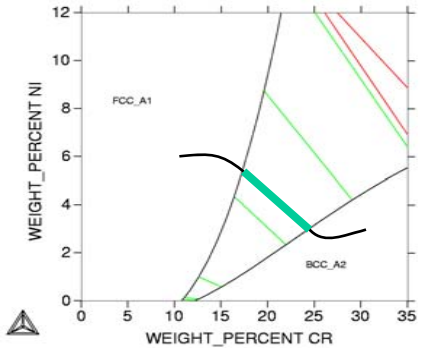
- Optimize processes
- Control the microstructure
- Tailor material properties

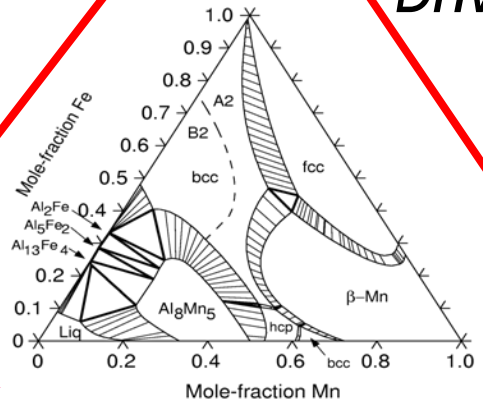


Background

Thermo-Calc Software

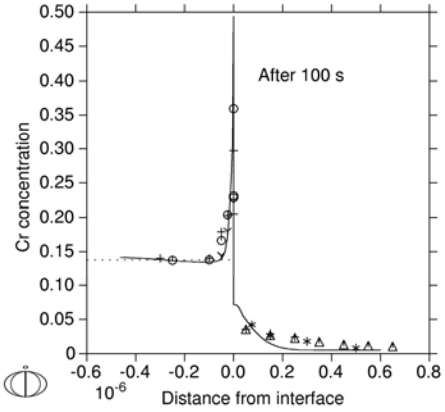
THERMO-CALC





Driving forces

DICTRA



Diffusivities

TC-PRISMA

TTT/CCT

Fractions

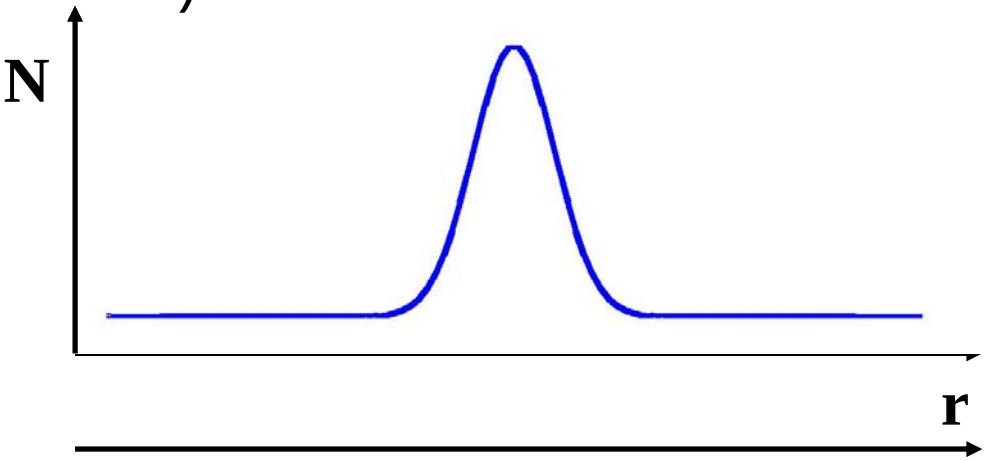
Nucleation

Average quantities

Size distributions

Models: KWN

- 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)

Models: Growth rate (new model)

- 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

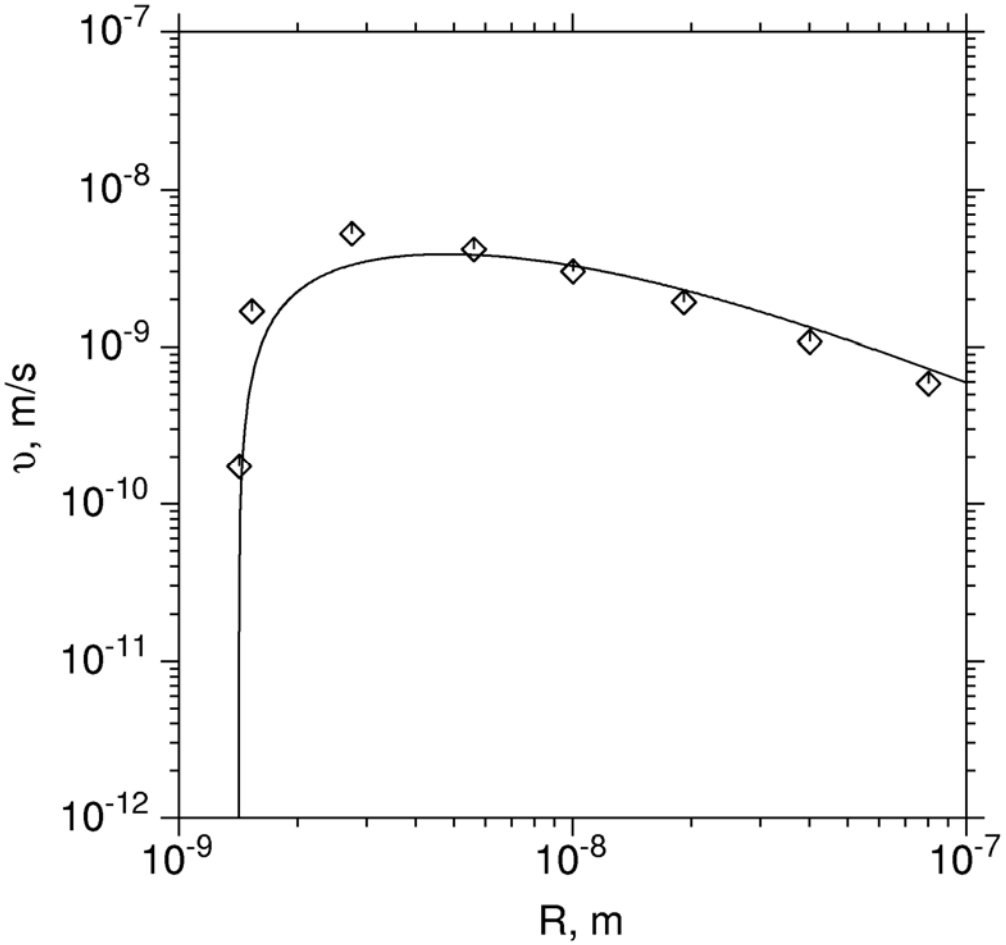
$$v(c_i^P - c_i^I) = c_i^I M_i(\mu_i^M - \mu_i^I)/\xi_i R$$

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

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

Models: Growth rate (new model)

Thermo-Calc Software



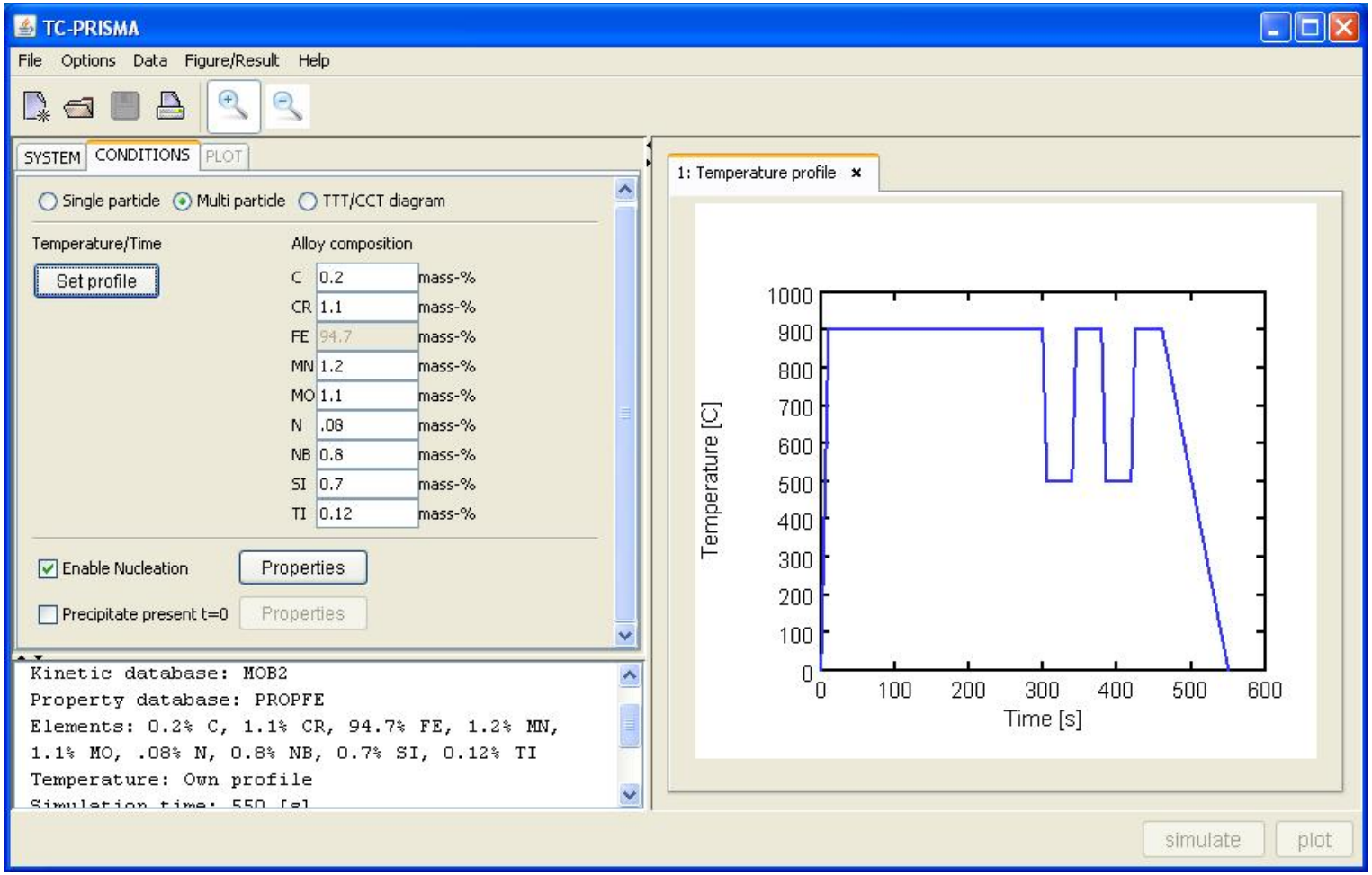
Fe-2%Cr-0.05%C, M23C6 from ferrite, local equilibrium, Cr-diffusion controlled

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

Thermo-Calc Software

TC-PRISMA

PRecIpitation Simulations in MAterials



New software tool: TC-PRISMA

Thermo-Calc Software

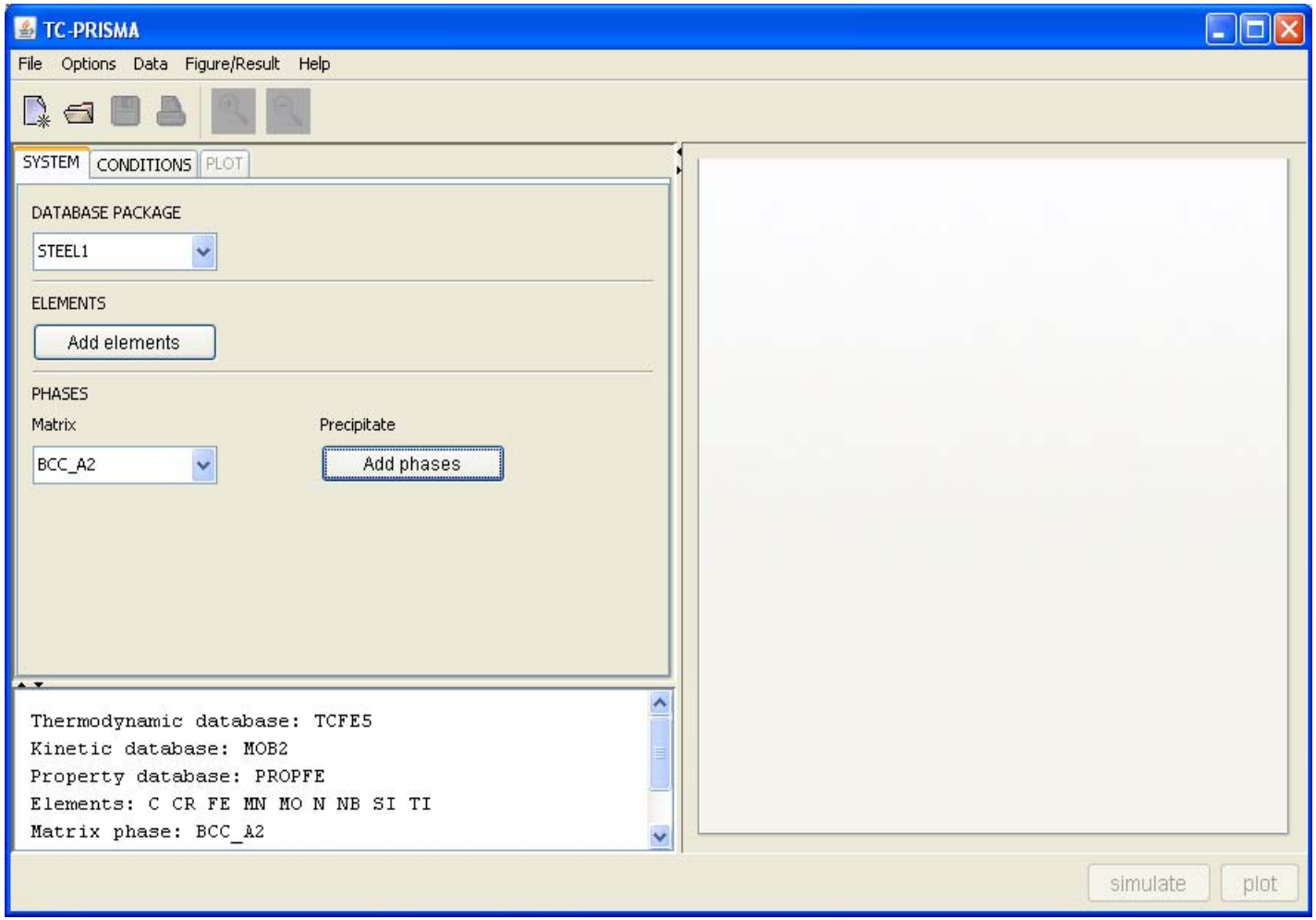
Input data: System

-Databases

-Elements

-Matrix phase

-Precipitates



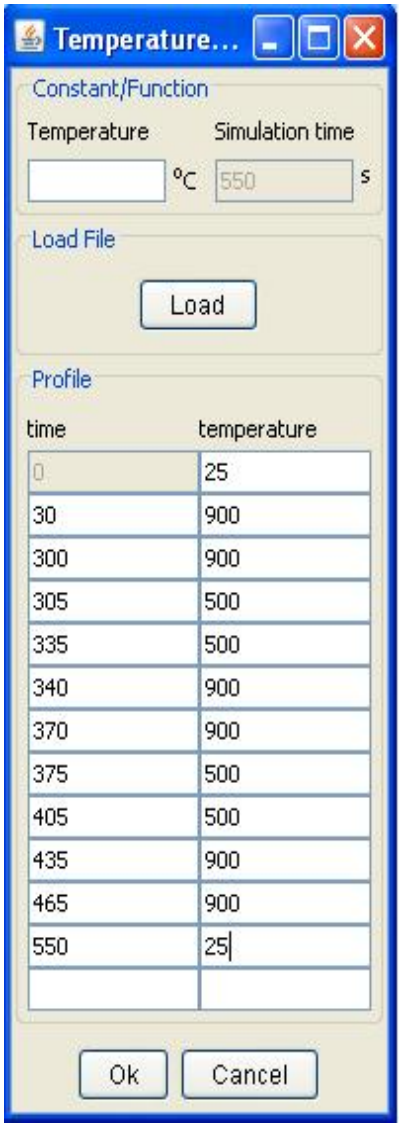
Input data: Conditions

-Temperature profile

-Composition

-Nucleation properties

-Initial size distribution

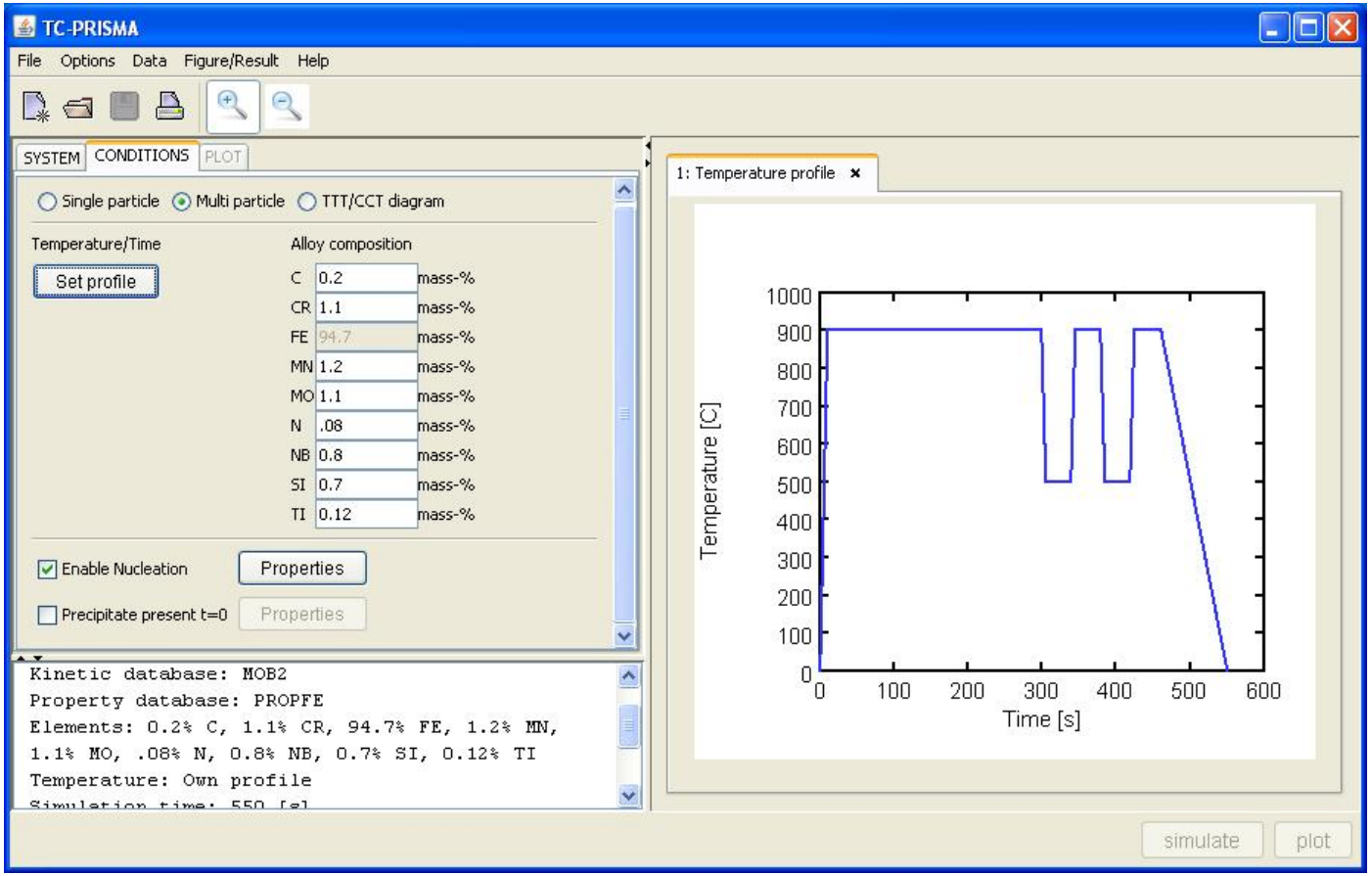


New software tool: TC-PRISMA

Thermo-Calc Software

Input data: Conditions

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



Input data: Conditions

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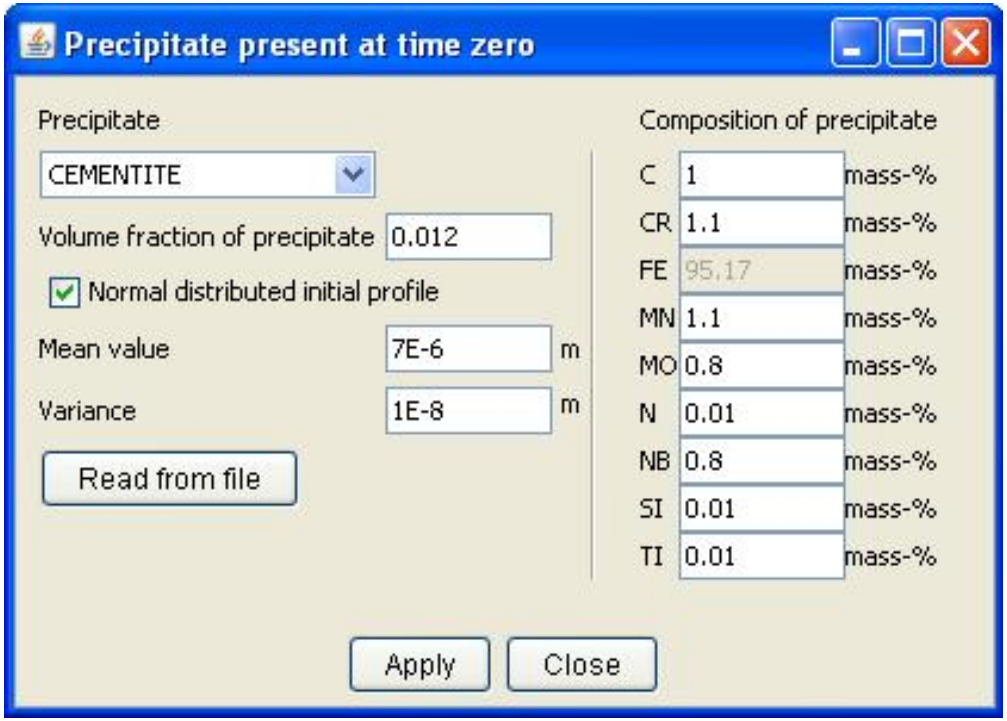

Input data: Conditions

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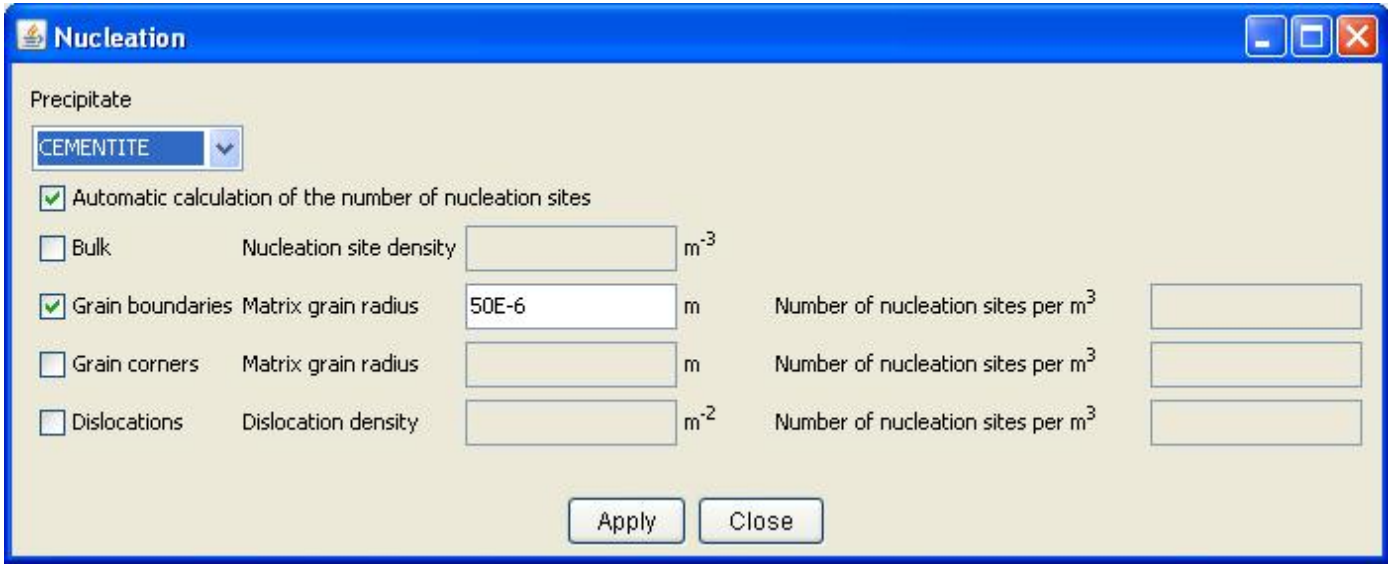
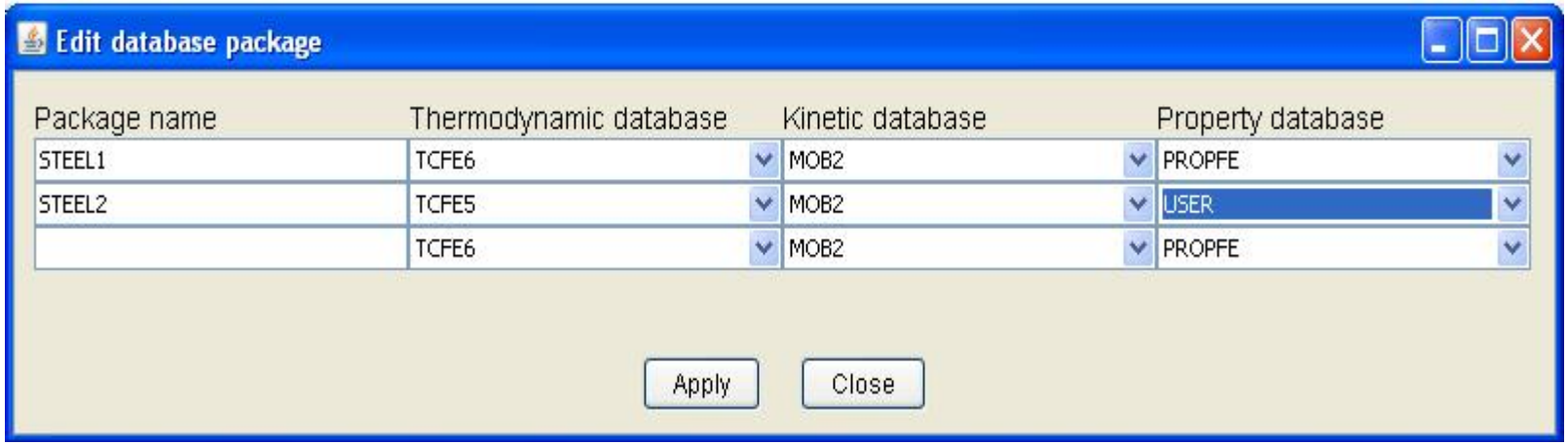


New software tool: TC-PRISMA

Thermo-Calc Software

Input data: Data

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



New software tool: TC-PRISMA

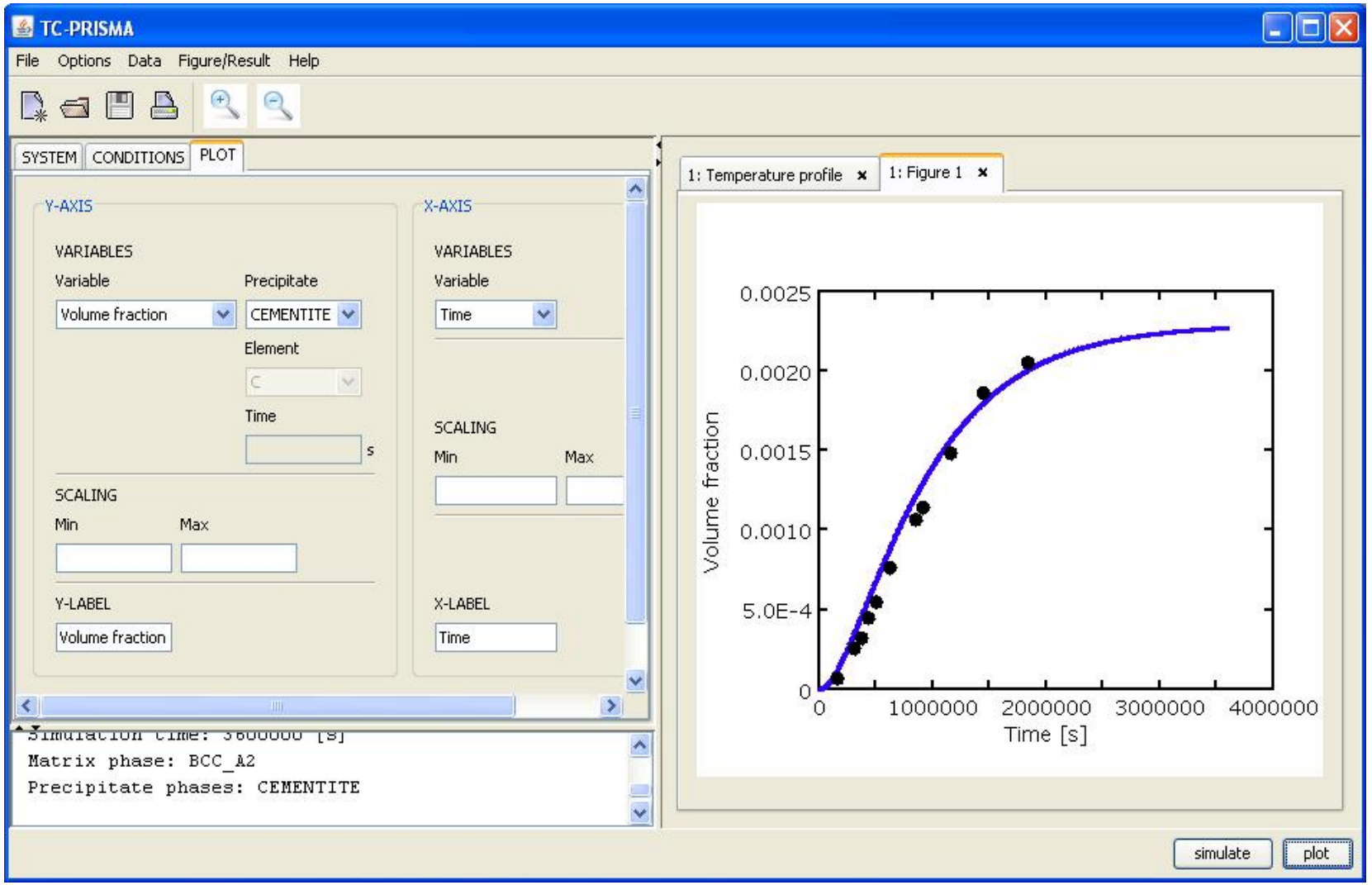
Calculates:

- 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

Thermo-Calc Software

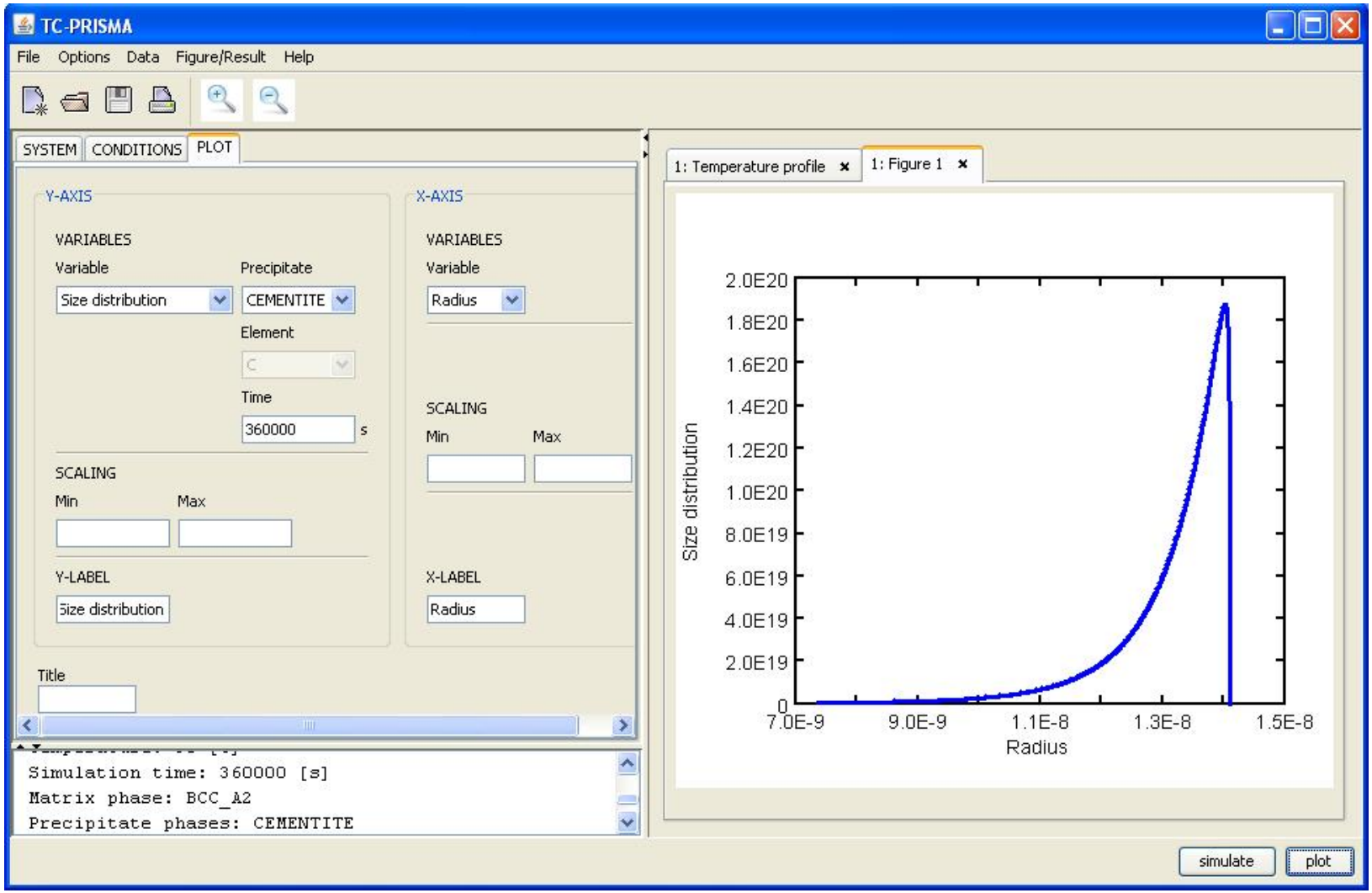
Calculation of volume fraction of cementite for low alloyed steel at 311K compared to experimental data



Precipitation of cementite

Thermo-Calc Software

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

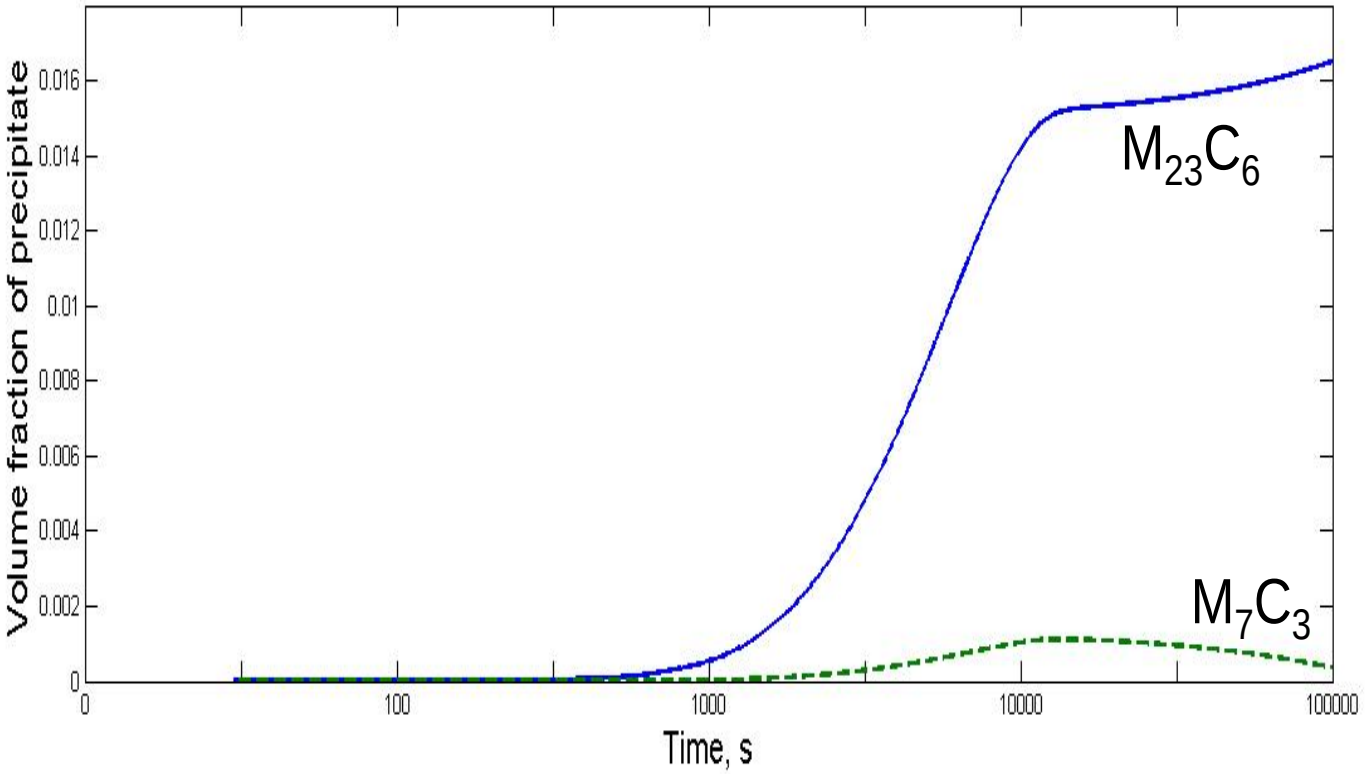


Precipitation of $M_{23}C_6$ and M_7C_3

Thermo-Calc Software

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

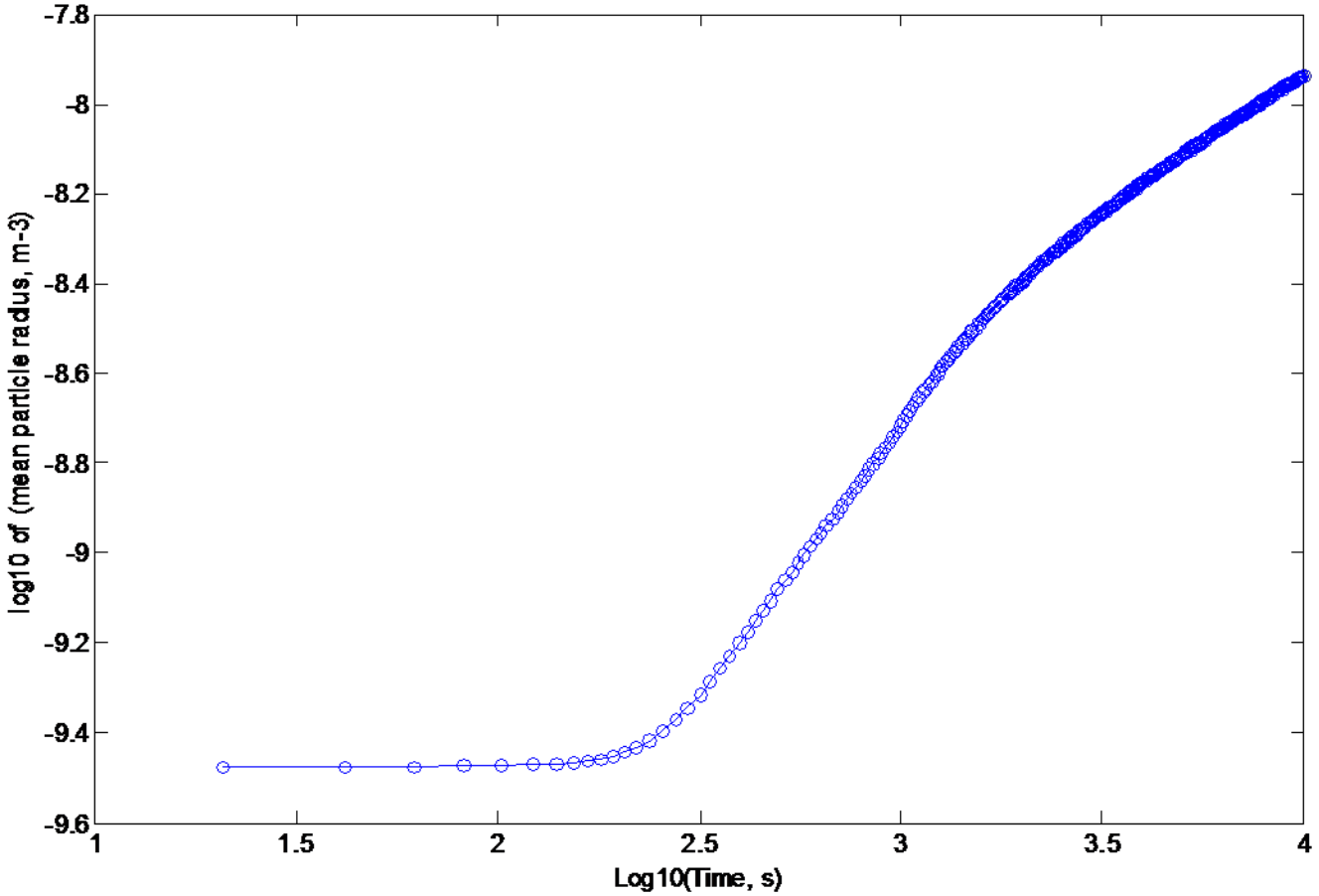
Metastable M_7C_3 forms at the beginning and desolves



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

Summary

- 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