Thermo-Calc Software

Modelling Multicomponent Precipitation Kinetics with CALPHAD-Based Tools

Kaisheng Wu [1], Gustaf Sterner [2], Qing Chen[2], Åke Jansson[2], Paul Mason[1], Johan Bratberg [2] and Anders Engström [2]

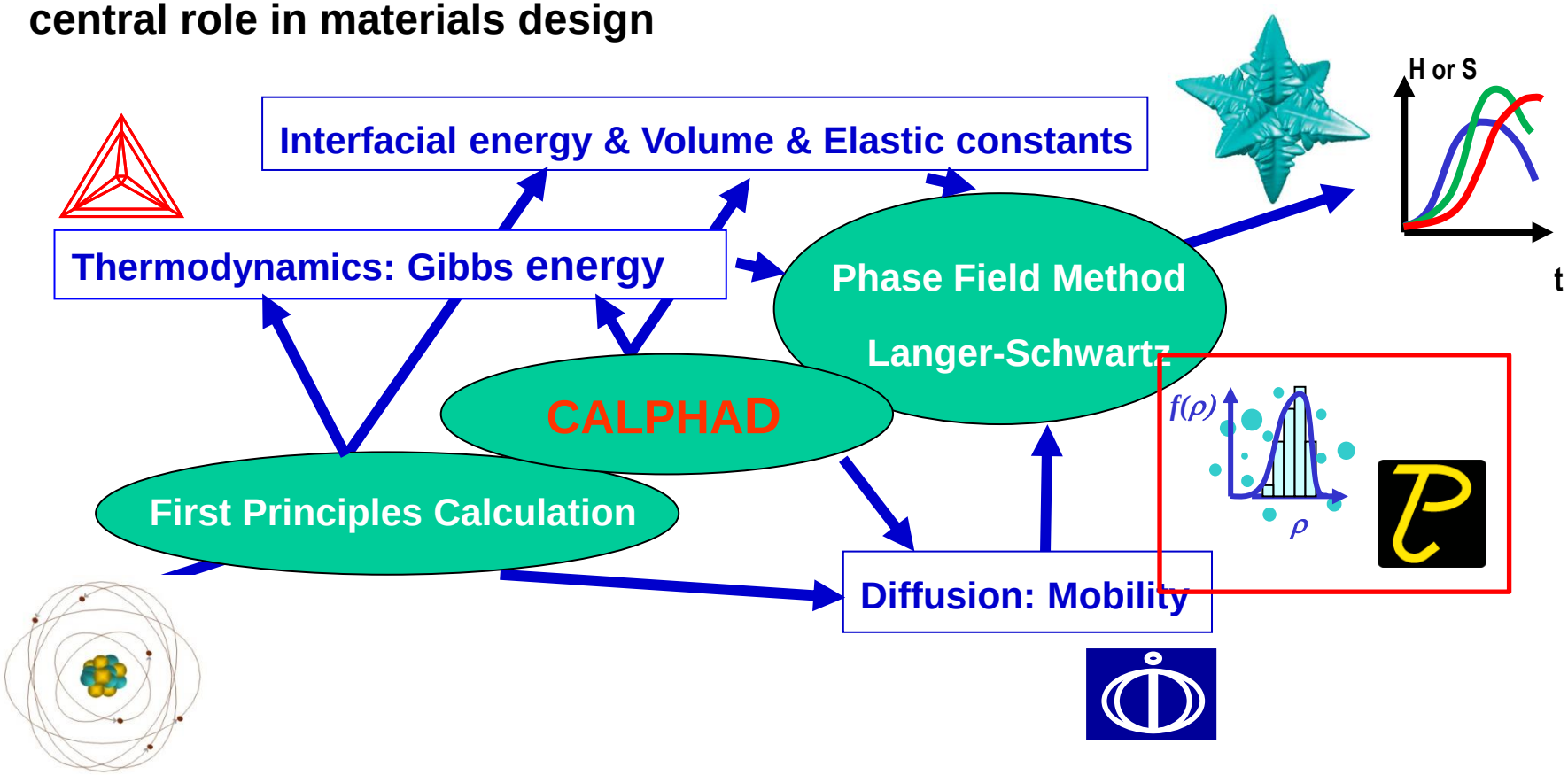
[1]Thermo-Calc Software Inc., [2]Thermo-Calc Software AB

EUROMAT2013, September 8-13, 2013 · Sevilla, Spain

Introduction: CALPHAD

Thermo-Calc Software

CALPHAD method and CALPHAD-based tools play a central role in materials design



CALPHAD-type databases where each phase is described separately using models based on physical principles and model parameters assessed from experimental and ab initio data provide fundamental inputs for predicting microstructure evolution and materials properties.

Introduction: TC-PRISMA

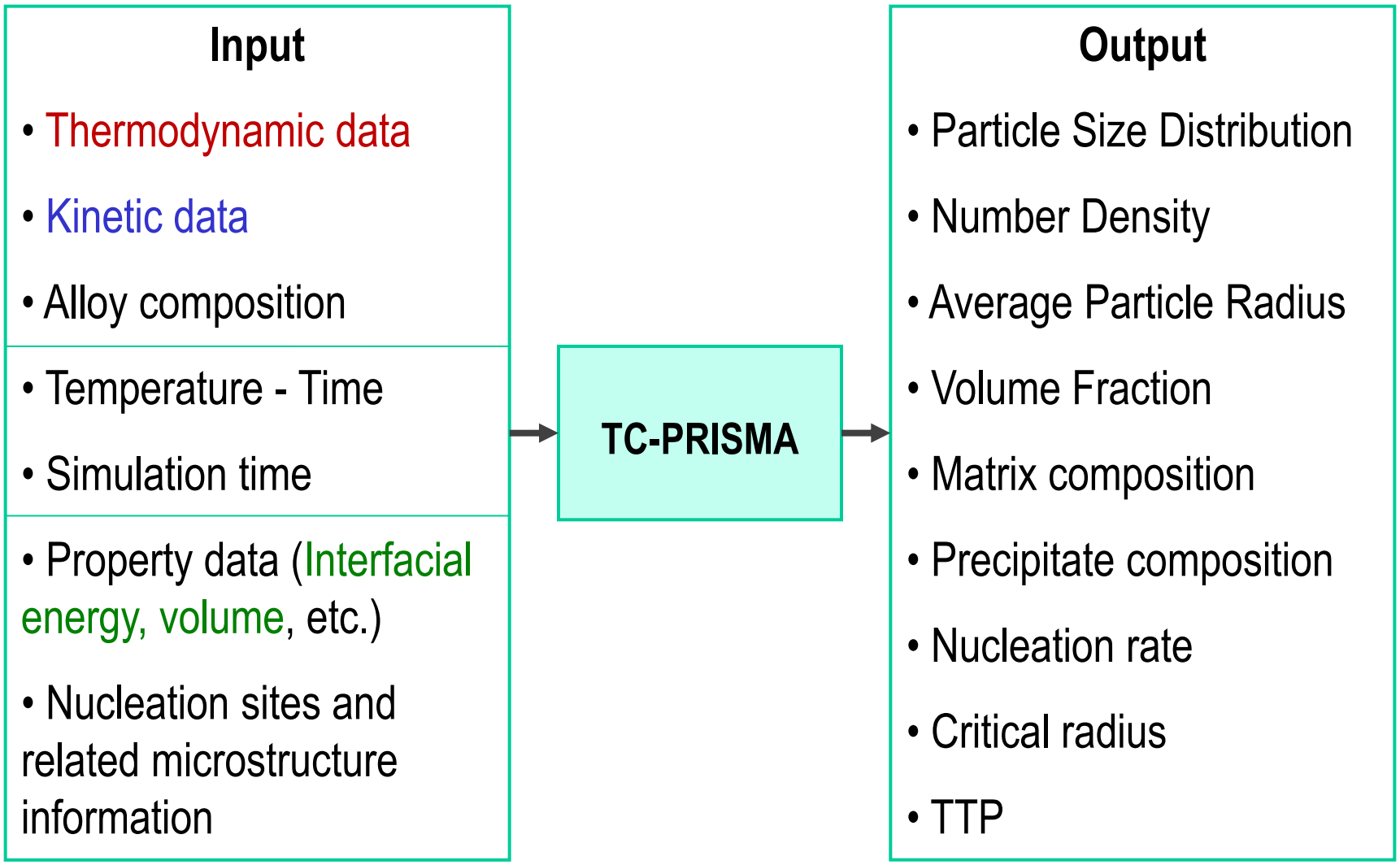
A general computational tool for simulating kinetics of diffusion controlled multi-particle precipitation process in multi-component and multi-phase alloy systems.

TC-PRISMA is based on Langer-Schwartz theory [1], and it adopts Kampmann-Wagner numerical (KWN) method [2] to compute the concurrent nucleation, growth, and coarsening of dispersed phase(s).

[1] Langer J, Schwartz A. Phys. Rev. A 1980;21:948-958.
[2] Wagner R, Kampmann R. Homogeneous Second Phase Precipitation. In: Haasen P, editor. Materials Science and Technology: A Comprehensive Treatment. Weinheim: Wiley-VCH, 1991. p. 213.

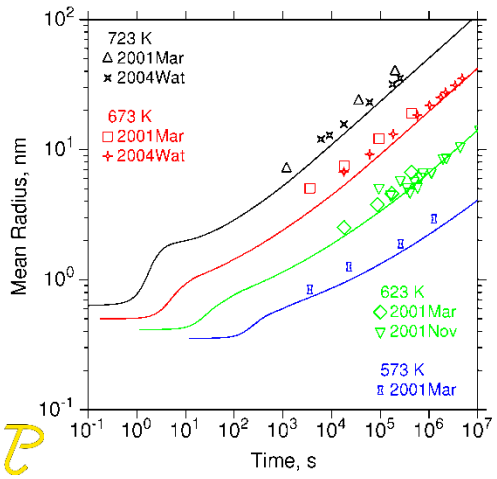
Introduction: In and Output

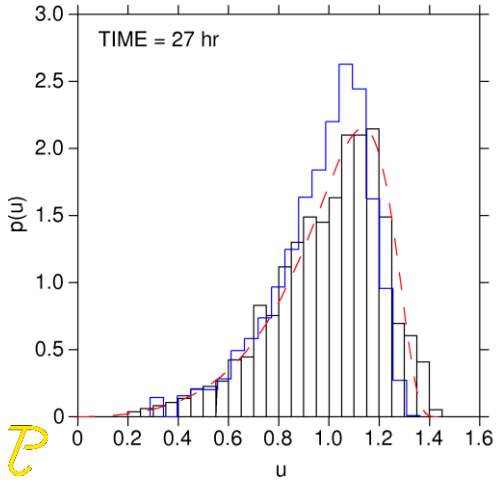
Thermo-Calc Software

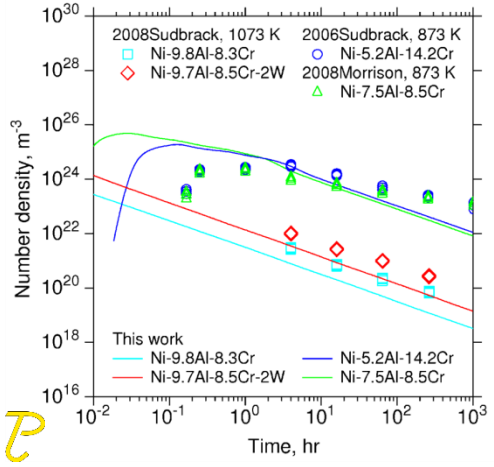


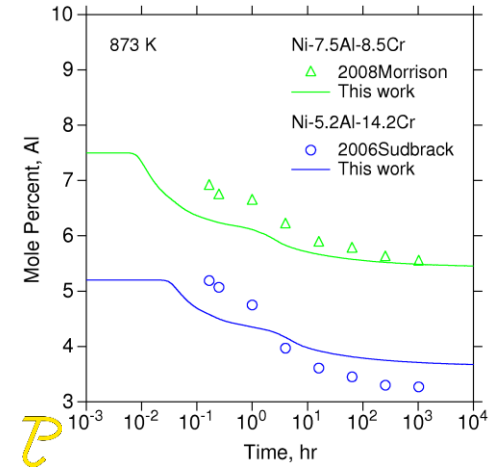
Introduction: Example of results

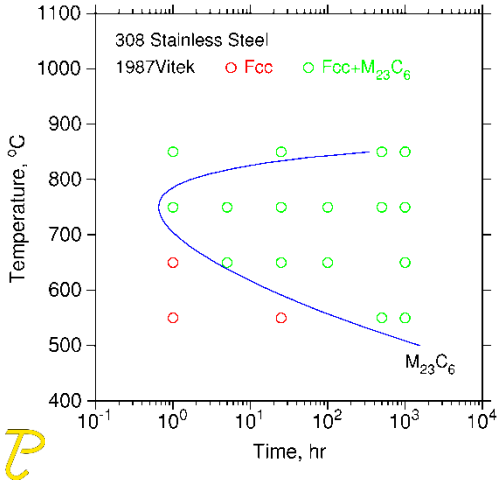
Thermo-Calc Software

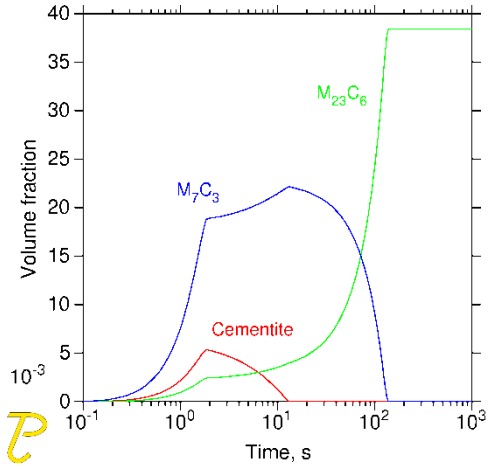










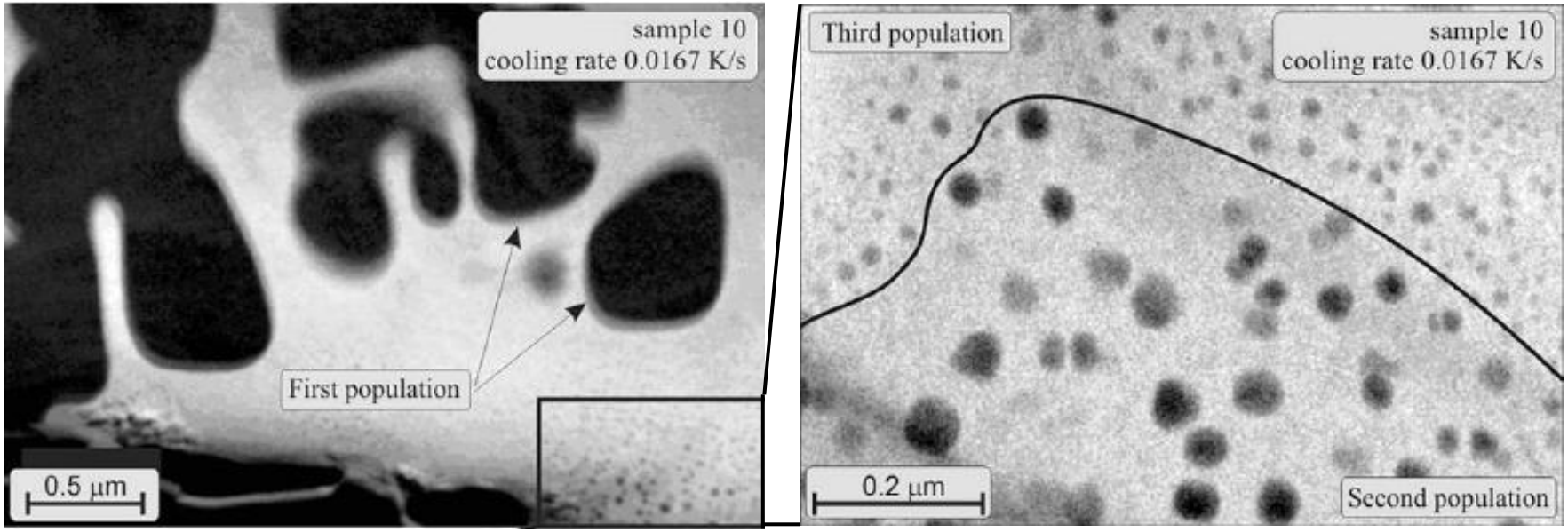


All above simulations made under isothermal conditions.

Non-Isothermal Conditions

Thermo-Calc Software

γ/γ' Microstructure in U720 Li



Continuous cooling at 0.0167 K/s

R. Radis et al., Acta Materialia, 57(2009)5739-5747

Ni-8Al-8Cr and Ni-10Al-10Cr

Thermo-Calc Software

J Mater Sci (2013) 48:825–831
DOI 10.1007/s10853-012-6802-7

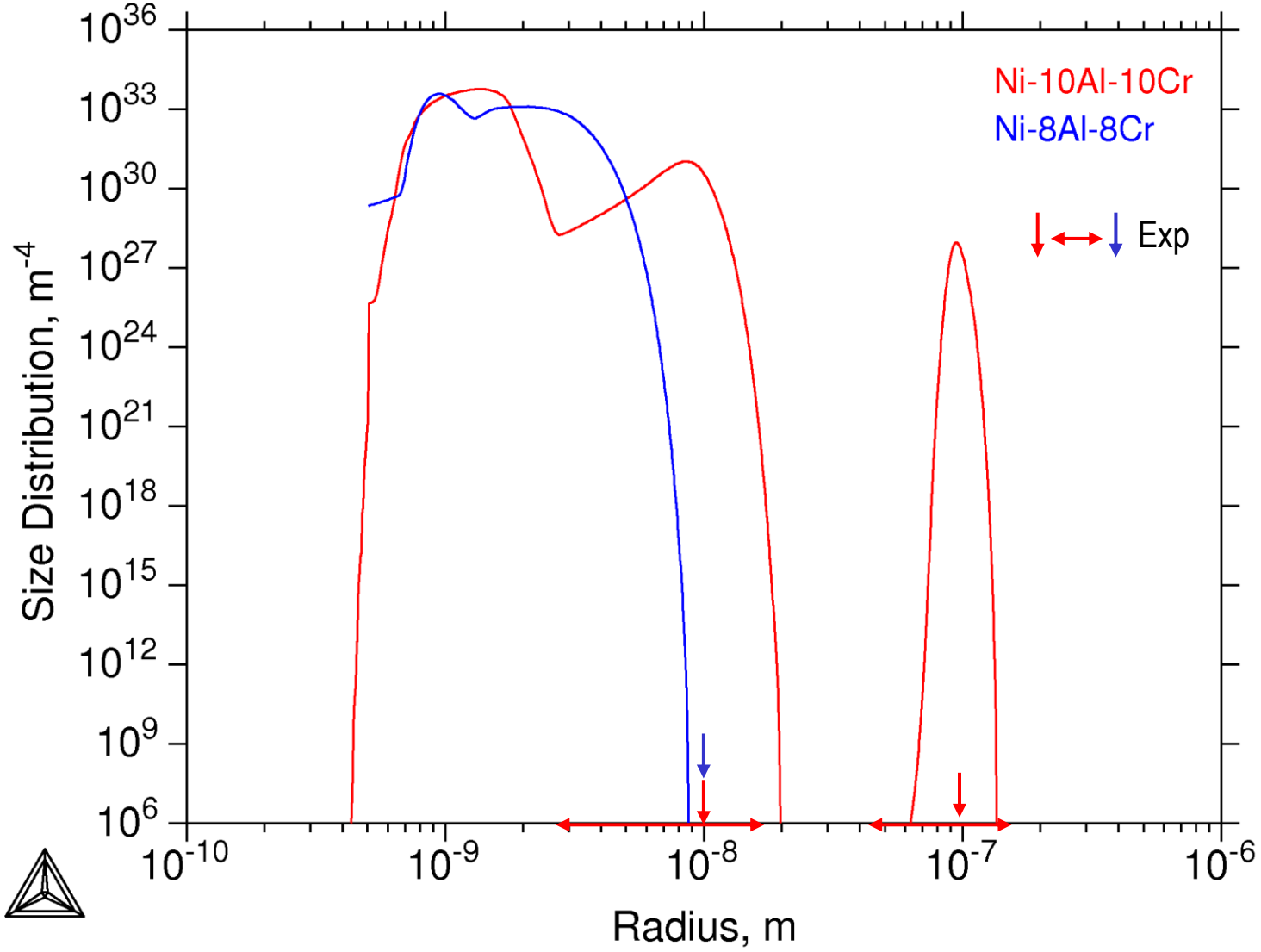
Influence of composition on monomodal versus multimodal γ' precipitation in Ni–Al–Cr alloys

T. Rojhirunsakool · S. Meher · J. Y. Hwang · S. Nag · J. Tiley · R. Banerjee

Abstract This study investigates the influence of alloy composition on γ' precipitation in Ni–8Al–8Cr and Ni–10Al–10Cr at.% during continuous cooling from a supersolvus temperature. When subjected to the same cooling rate, Ni–8Al–8Cr develops a monomodal population, whereas Ni–10Al–10Cr develops a multimodal (primarily bimodal) population of γ' precipitates. The bimodal γ' precipitate size distribution in Ni–10Al–10Cr alloy can be attributed to two successive nucleation bursts during continuous cooling while the monomodal γ' size distribution in Ni–8Al–8Cr results from a single nucleation burst followed by a longer time—wider temperature window for nucleation resulting in a larger number density of precipitates. Three-dimensional atom

Ni-8Al-8Cr and Ni-10Al-10Cr

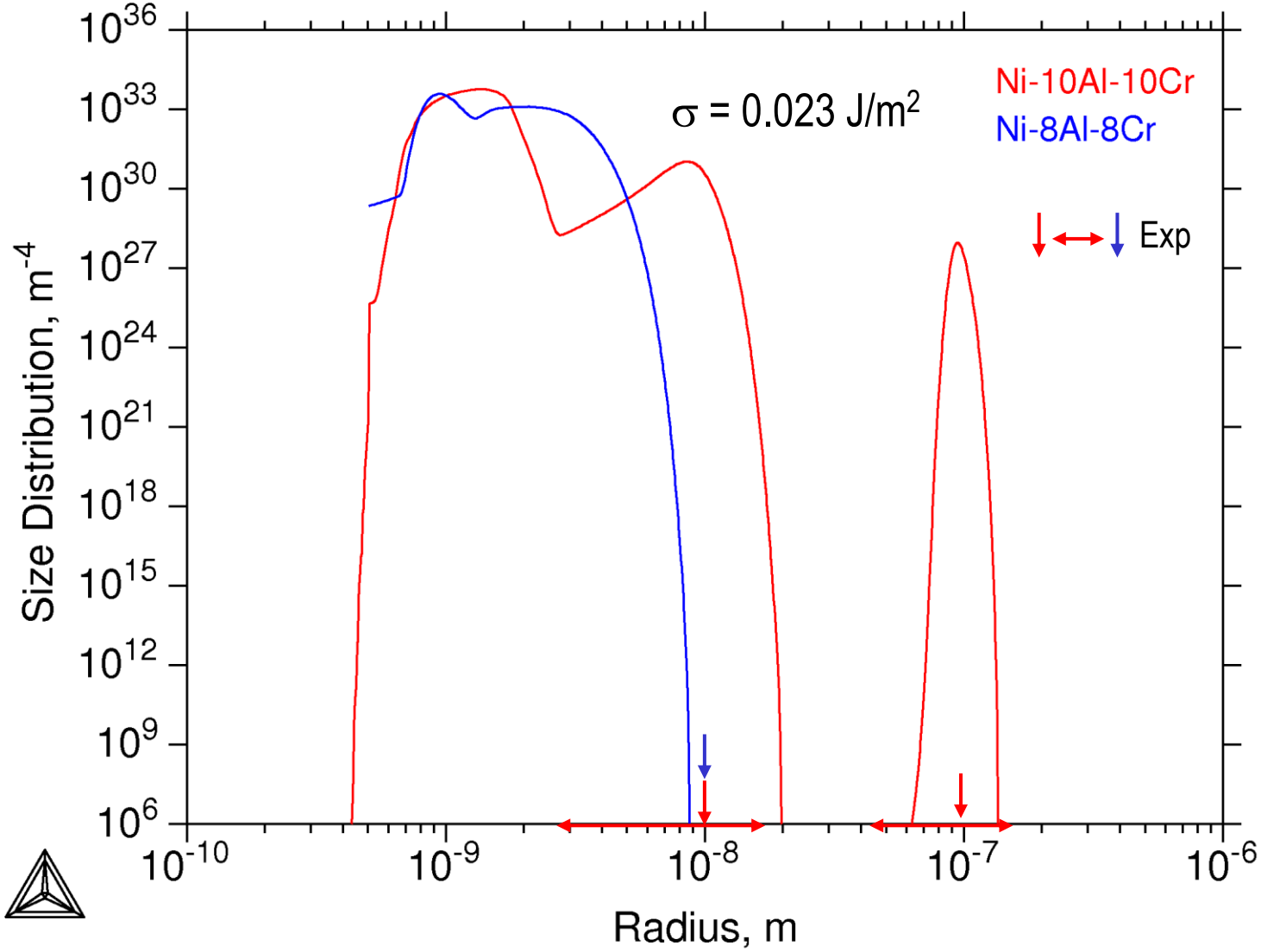
Thermo-Calc Software



Continuous cooling from 1150 to 380 °C with a cooling rate of 14 °C/min.

Ni-8Al-8Cr and Ni-10Al-10Cr

Thermo-Calc Software

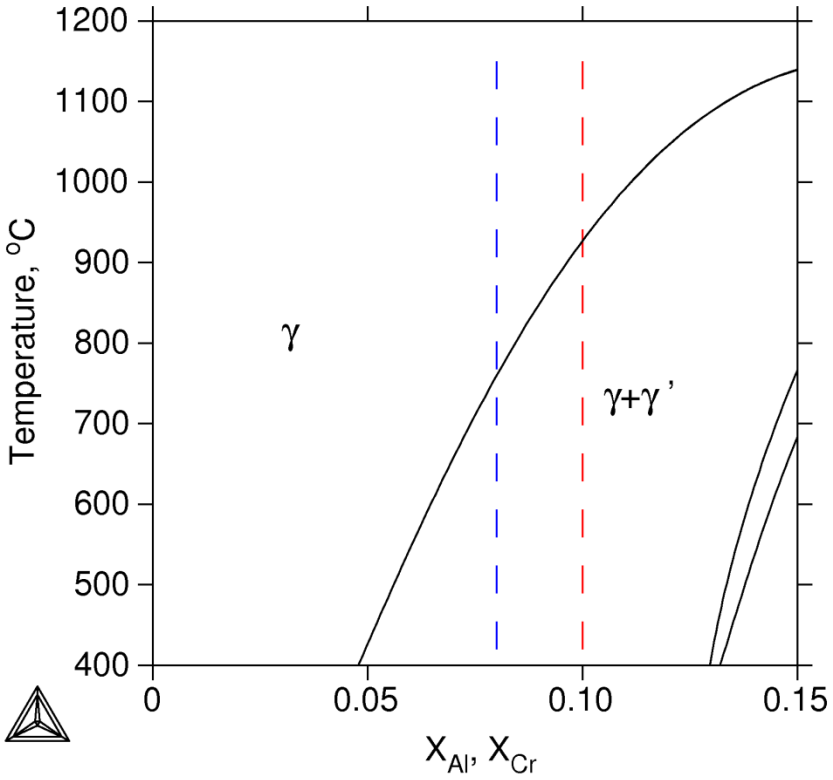


Ni-8Al-8Cr have larger misfit between γ and γ′ compared to Ni-10Al-10Cr.

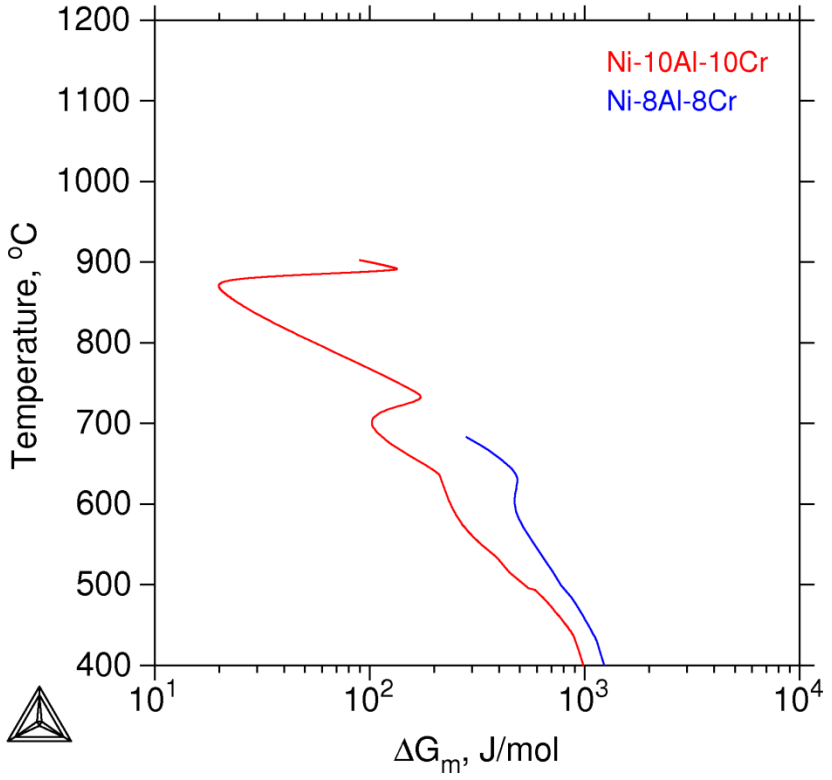
This will give an elastic energy contribution which has not been considered in the simulation.

Ni-8Al-8Cr and Ni-10Al-10Cr

Thermo-Calc Software



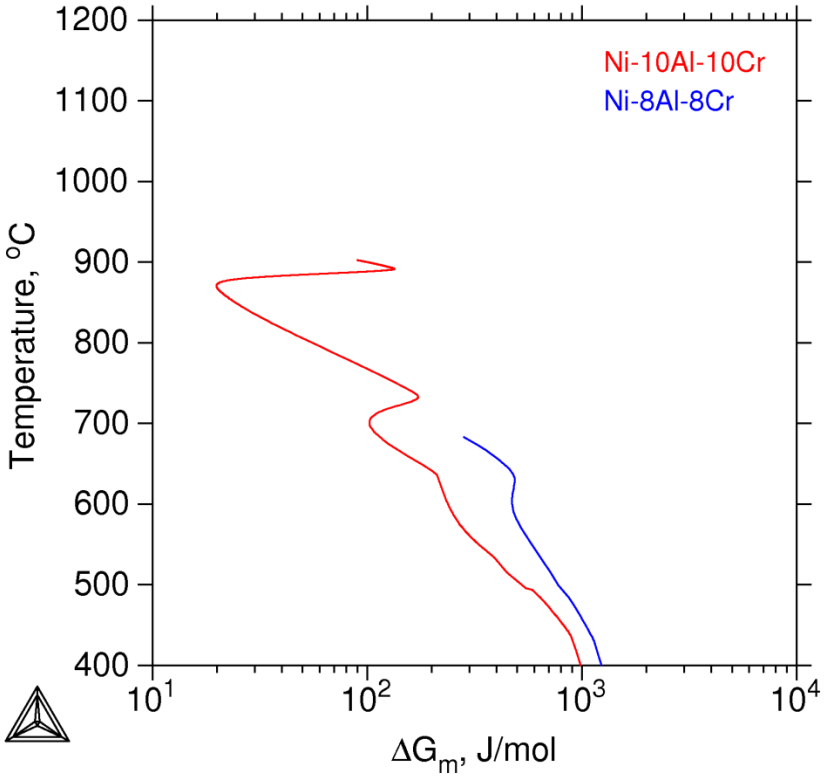
Vertical Section Ni-xAl-xCr



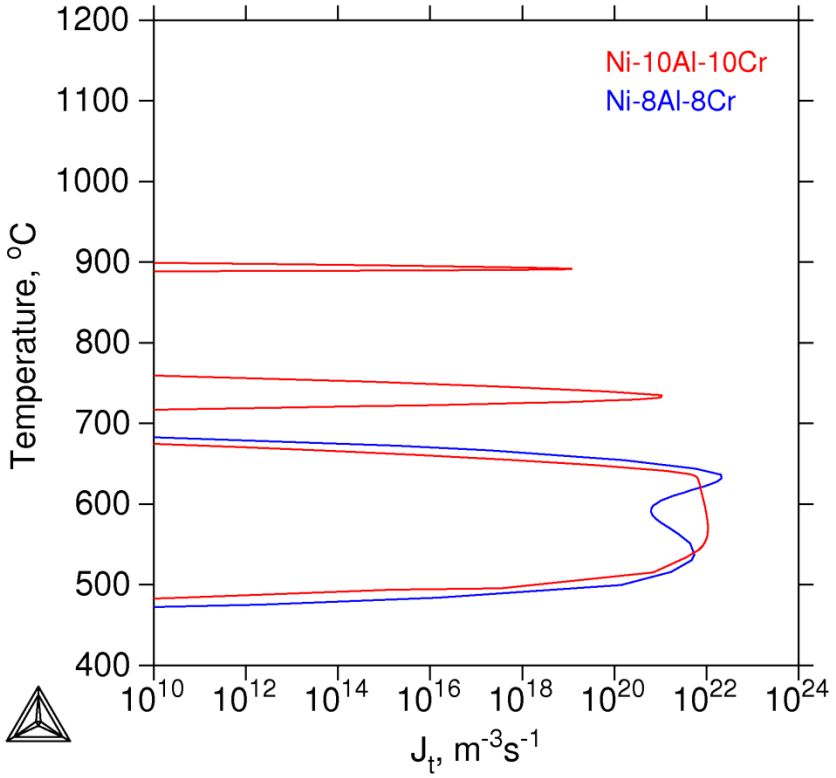
Thermodynamic driving force

Ni-8Al-8Cr and Ni-10Al-10Cr

Thermo-Calc Software



Thermodynamic driving force



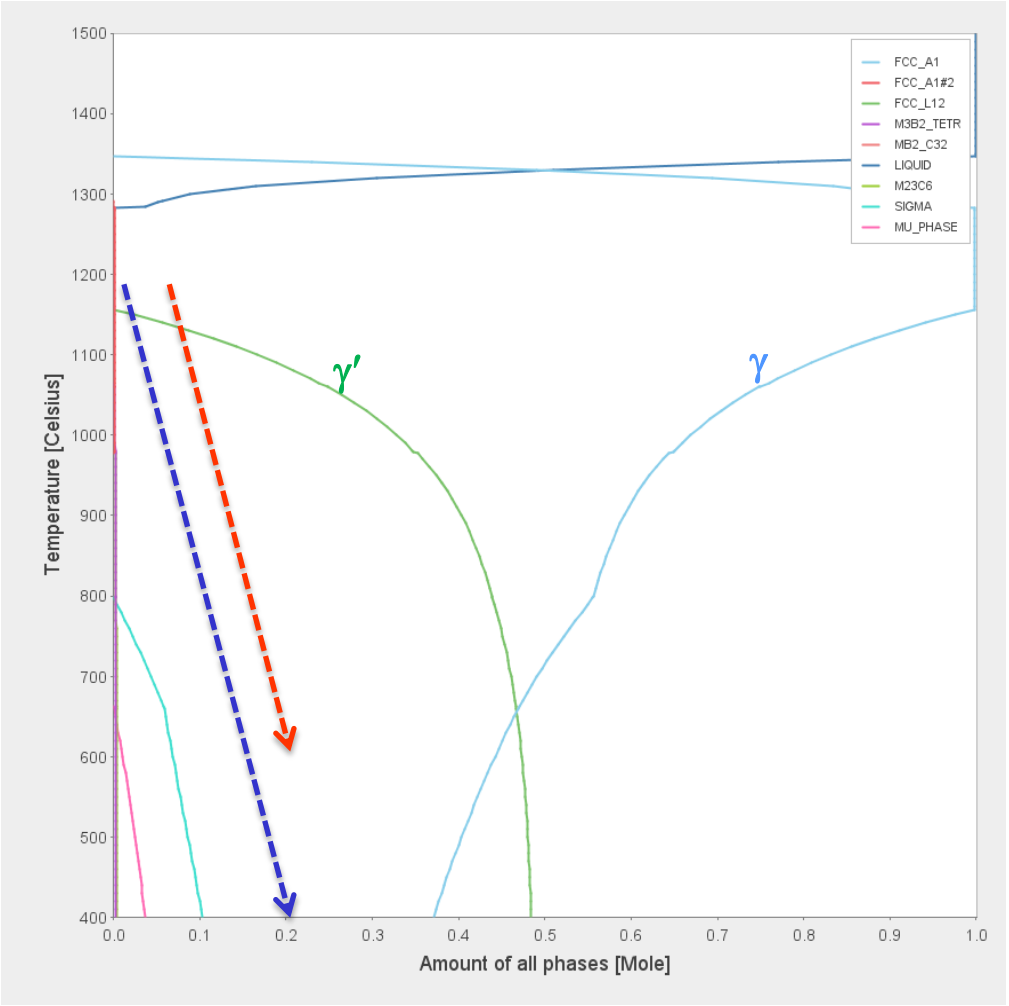
Nucleation rate

U720Li

Thermo-Calc Software

Precipitation Kinetics during Continuous Cooling

wt.%	1*	2**
Al	2.53	2.46
B	0.014	
C	0.014	0.025
Co	14.43	14.75
Cr	15.92	16.35
Fe	0.09	0.06
Mo	2.96	3.02
Ti	4.96	4.99
W	1.26	1.3
Zr		0.035
Ni	Bal	Bal



- Databases: TTNI8+MOBNI1

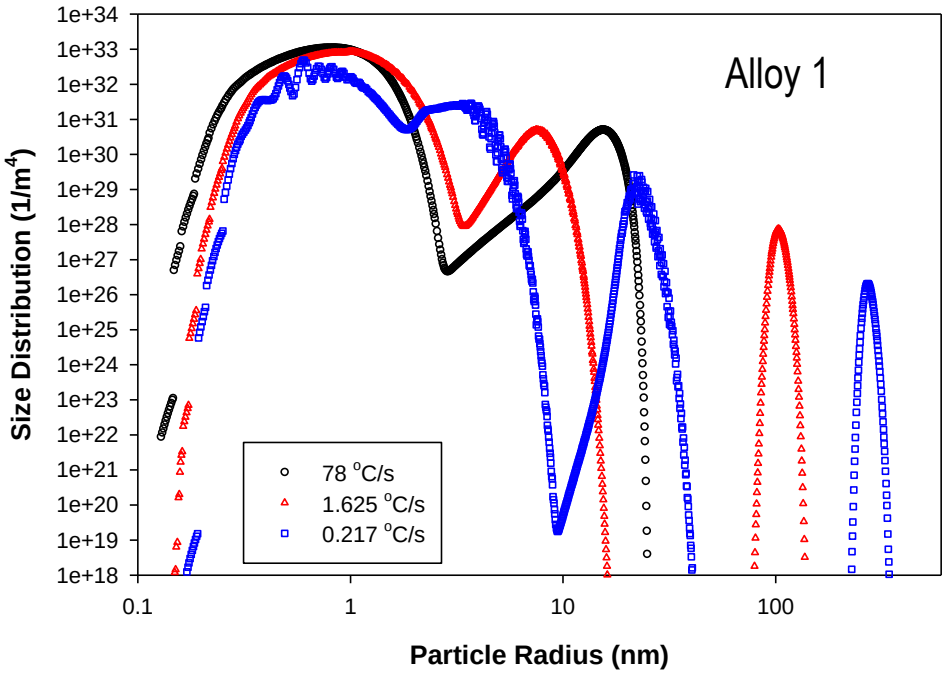
* Radis et al., *Superalloys* 2008

** Mao et al., *Metall. Mater. Trans. A, 32A(10) 2441(2001)*

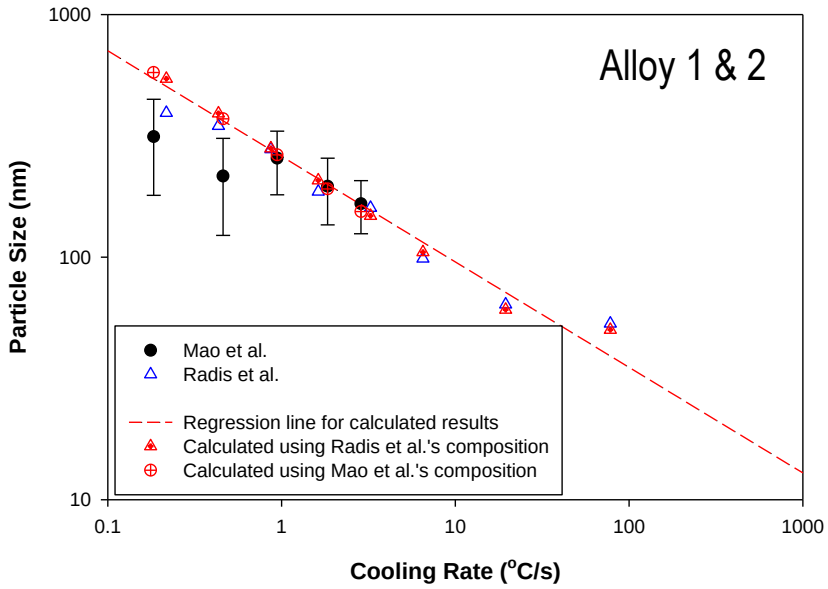
U720Li : Cooling Rate Effect

Thermo-Calc Software

Size Distribution



Mean Particle Size



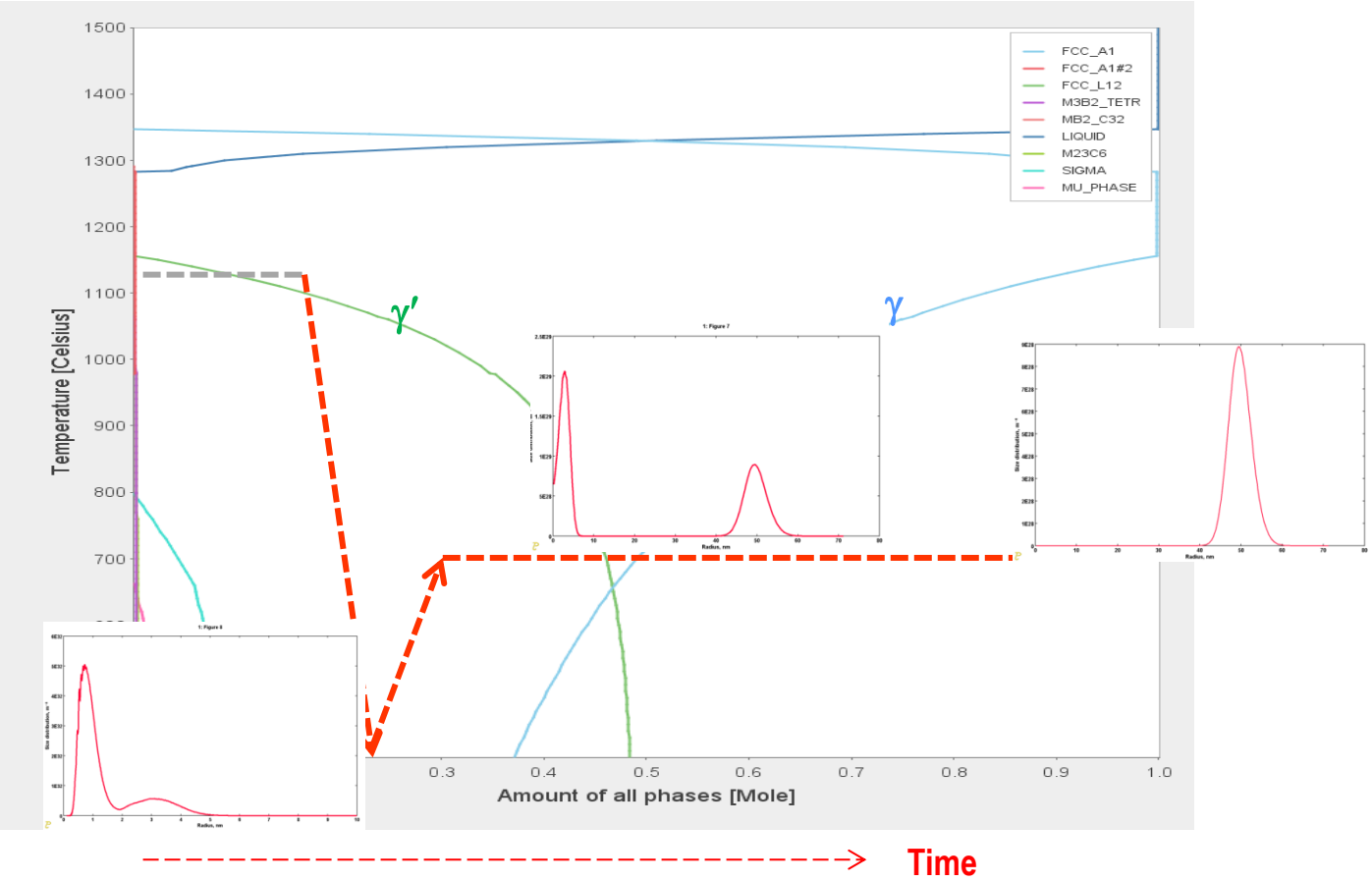
σ = 0.025 J/m^2

U720Li

Thermo-Calc Software

Secondary/Tertiary γ′ during Cooling + Aging

	wt.%*
Al	2.51
B	0.014
C	0.011
Co	14.66
Cr	16.14
Mo	2.98
Si	0.05
Ti	5.08
W	1.23
Ni	Bal



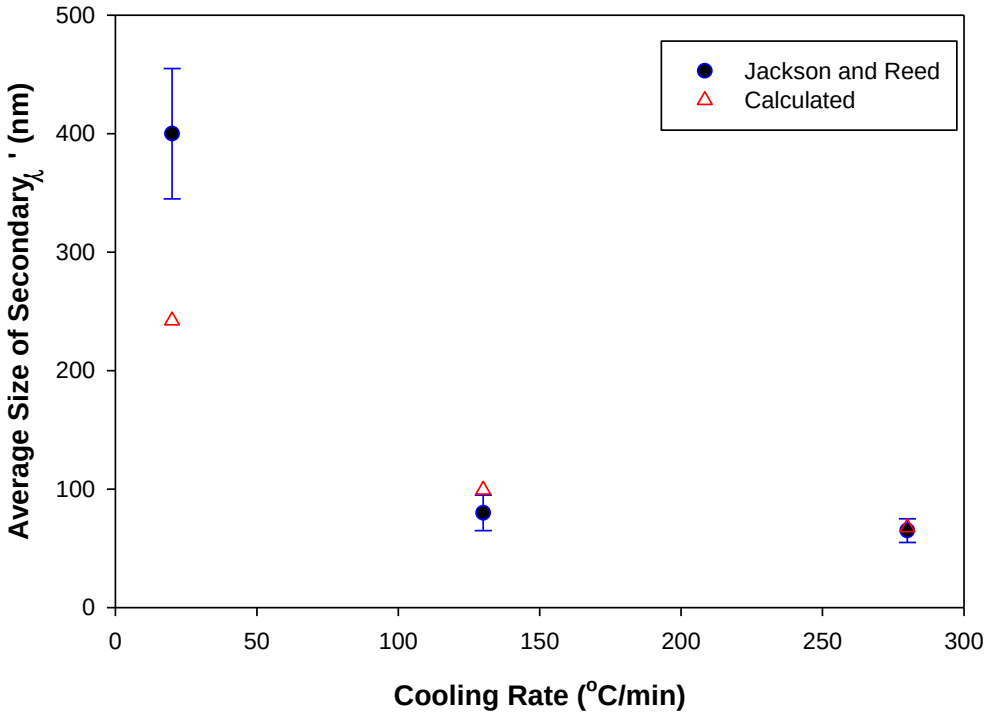
- No primary γ′ is considered, but γ matrix concentration is adjusted due to primary γ′ formation at 1105°C (based on equilibrium calculation)
- Heat Treatment: cooling from 1105°C to 400 °C, followed by aging at 700°C for 24hrs

* M.P.Jackson and R.C.Reed, Mater. Sci. Eng. A259(1999)85-97

U720Li

Thermo-Calc Software

Secondary γ′ Size After Cooling + Aging



σ = 0.025 J/m^2

- Simulations are good for large to intermediate cooling rate (> 1°C/s)
- Future model improvements include multiple nucleation sites, mean field deviation, loss of coherency, interfacial energy variation, interface mobility, morphology change ….

Estimation of interfacial energy

Thermo-Calc Software

- Classic or non-classic thermodynamics
- Atomistic modeling - molecular dynamics and Monte Carlo method
- First principles

Distribution of Al-Li α/δ' interfacial energy value found in literature

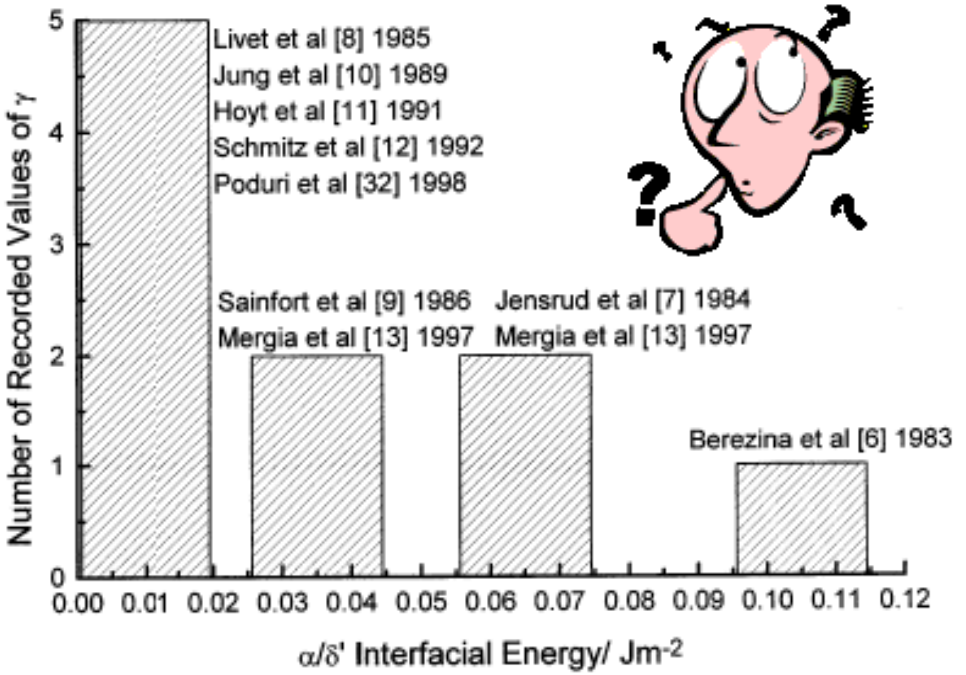


Fig. 1. Values of the α/δ' interfacial energy that have been measured over the period 1983–1998.

1999Noble, Mater Sci Engr, A266, 80-85

Our first approximation

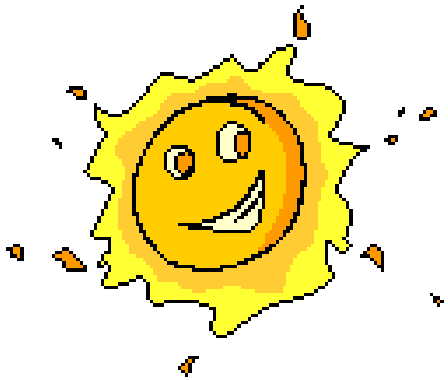
Thermo-Calc Software

For a binary matrix and precipitate of the same structure that can be described by a regular solution model*

$$\sigma_c = \frac{N_s Z_s}{N_A Z_l} \Delta E_{sol} \qquad \Delta E_{sol} = \Omega \left(X_P - X_M \right)^2$$

- Misciblity gap of non-regular solution phase
- Matrix and precipitate of different structure
- Multicomponent system

$$\Delta E_{sol} \; ?$$



* Based on Becker R. Ann Phys 1938;424:128

Some example results

Thermo-Calc Software

System	Phases	Estimation (J/m^2)	Literature (J/m^2)
Al-Li	α/δ'	0.011	0.004 to 0.115
Cu-Ti	Cu/Cu4Ti	0.035	0.067, 0.031
Ni-Al-Cr	γ/γ'	0.022	0.023
Co-W-C	Co/WC	0.68	0.44 to 1.09

Used in Current Calculations

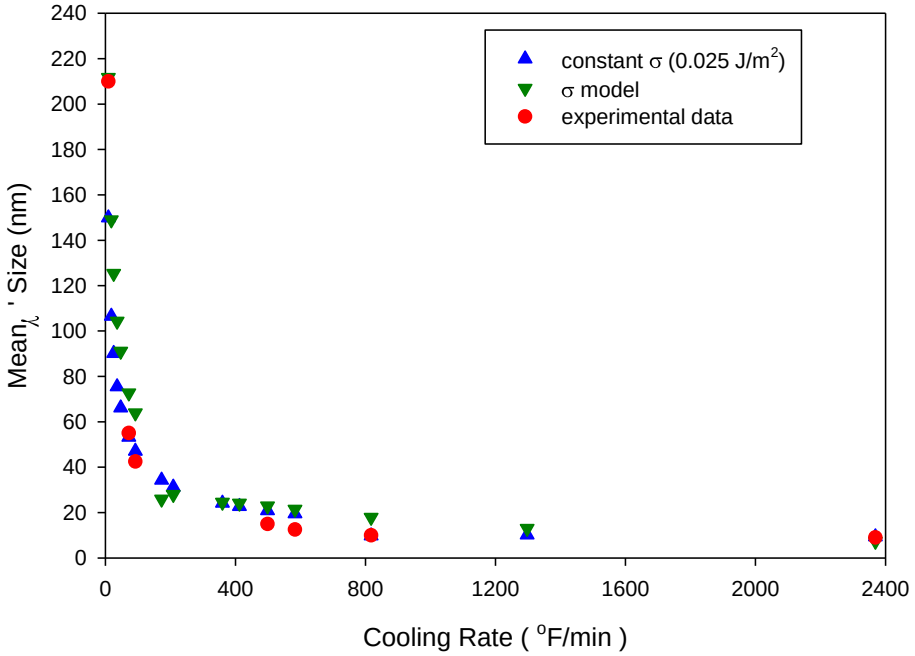
System	Phases	Estimation (J/m^2)	Used (J/m^2)
Ni-Al-Cr	γ/γ'	0.022	0.023
Ni-Superalloys(Bulk)	γ/γ'	0.03~ 0.06	0.025
Ni-Superalloys(GB)	γ/γ'	~ 0.06	0.06

- Interfacial energy shows composition and temperature independence
- Estimated value seems better for grain boundary precipitation in multi-component alloys
- Further developments include diffusiveness of interface, incoherency, size effect, grain boundary energy…

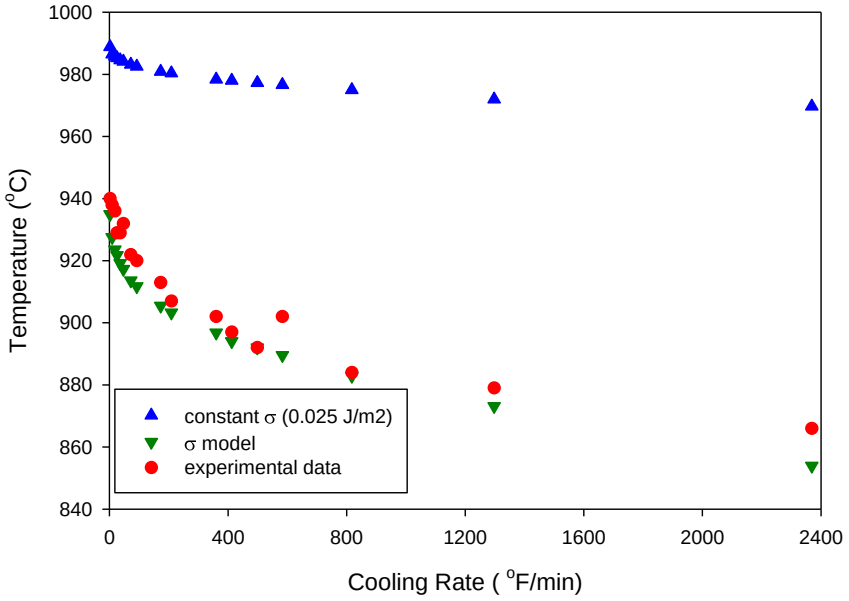
Alloy 282

Thermo-Calc Software

Mean Particle Size (Bulk)



CCT Starting Temperature



	Al	Co	Cr	Fe	Mo	Ti	Ni
wt.%	1.5	10.0	19.0	1.5	8.5	2.1	Bal.

- Databases: TCNI5+MOBNI2

* Experimental data from B. Alexandrov et al., "Continuous heating and cooling transformation diagram in Ni-base superalloy 282", TMS 2011

Summary

- A non-isothermal model has been developed in TC-PRISMA and has been successfully applied to simulate multi-modal particle size distribution of γ' precipitates in Ni-base superalloys
- More GUI outputs have been provided to facilitate separate analyses of particle size distribution, mean size, volume fraction, and number density
- A model has been implemented to estimate the interfacial energy between matrix and precipitate phases

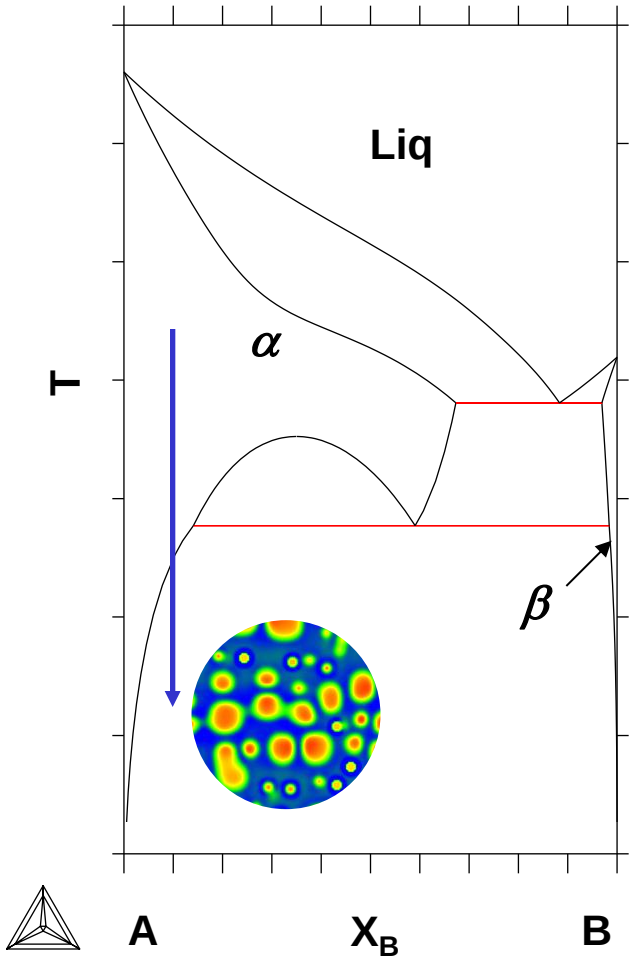
Thermo-Calc Software

Thank You!

Theory: Conservation laws

Thermo-Calc Software

LS (Langer-Schwartz) and KWN (Kampmann and Wagner Numerical) Approach



Continuity equation

$$\frac{\partial f(R,t)}{\partial t} = -\frac{\partial}{\partial R}\left[\upsilon(R,t) f(R,t)\right] + j(R,t)$$

$$C_0^{\alpha} = C^{\alpha} + \left(C^{\beta} - C^{\alpha}\right)\int_0^{\infty} \frac{4\pi}{3} f(R,t) R^3 dR$$

Mass balance

$$N = \int_0^{\infty} f(R,t)dR \qquad \overline{R} = \frac{1}{N}\int_0^{\infty} f(R,t)RdR$$

$$\phi = \int_0^{\infty} \frac{4\pi}{3} f(R,t)R^3 dR$$

Models: Multicomponent Nucleation

Thermo-Calc Software

Classic Nucleation Theory

Grain size, dislocation density, etc

$$J(t) = J_S \exp\left(-\frac{\tau}{t}\right) \qquad J_s = Z\beta^* N \exp\left(\frac{-\Delta G^*}{kT}\right)$$

Interfacial energy Volume

$$Z = \left\{\frac{-1}{2\pi kT}\left(\frac{\partial^2 \Delta G_n}{\partial n^2}\right)_{n^*}\right\}^{1/2} \qquad \Delta G^* = \frac{16\pi\sigma^3 V_m^2}{3\Delta G_m^2}$$

$$\beta^* = \frac{4\pi r^{*2}}{a^4}\left[\sum_{i=1}^{n}\frac{\left(X_i^{\beta/\alpha} - X_i^{\alpha/\beta}\right)^2}{X_i^{\alpha/\beta} D_i}\right]^{-1} \qquad \tau = \frac{1}{2Z^2\beta^*}$$

Models: Multicomponent Growth Rate

Thermo-Calc Software

Q. Chen, J. Jeppsson, J. Ågren, Acta Mater. 56(2008)1890-1896

Advanced – Analytical Flux-balance Approximation

$$\mu_i^{\alpha/\beta} = \mu_i^{\beta/\alpha} + \frac{2\sigma V_m^{\beta}}{r}$$

Cross diffusion

high supersaturation

$$\upsilon\left(c_i^{\beta/\alpha} - c_i^{\alpha/\beta}\right) = c_i^{\alpha/\beta} M_i \left(\mu_i^{\alpha} - \mu_i^{\alpha/\beta}\right) / \xi_i r$$

Simplified – Pseudo-steady state Approximation

$$\upsilon = \frac{K}{r}\left(\Delta G_m - \frac{2\sigma V_m}{r}\right)$$

Pseudo-binary dilute solution Approximation

$$\upsilon = \frac{X^{\alpha} - X^{\alpha/\beta}}{X^{\beta} - X^{\alpha/\beta}} \frac{D}{r} \qquad \frac{X^{\alpha/\beta}}{X_e^{\alpha}} = \exp\left(\frac{1 - X_e^{\alpha}}{X^{\beta} - X_e^{\alpha}} \frac{2\sigma V_m^{\beta}}{RTr}\right)$$