RWTH AACHEN UNIVERSITY

Prediction of precipitation kinetics in recycled aluminum alloy with ClaNG

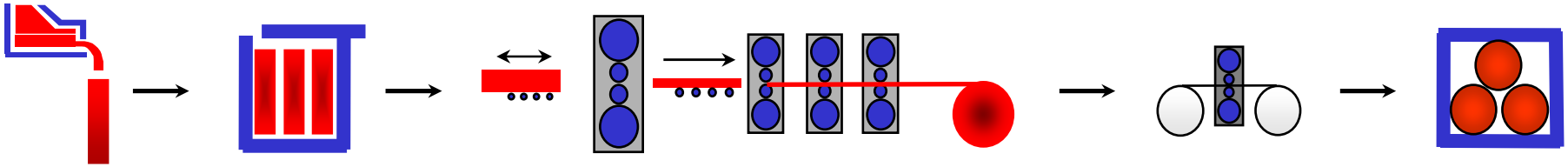
Z. Liu, V. Mohles, G. Gottstein

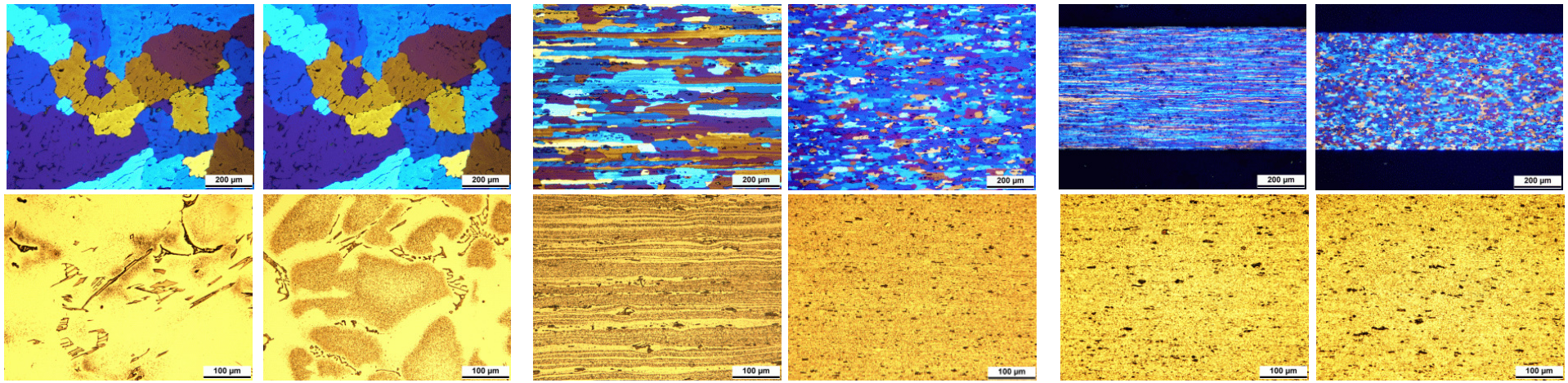
Institut für Metallkunde und Metallphysik

GTT workshop,Herzogenrath, June 03-05, 2009

Aluminum sheet production

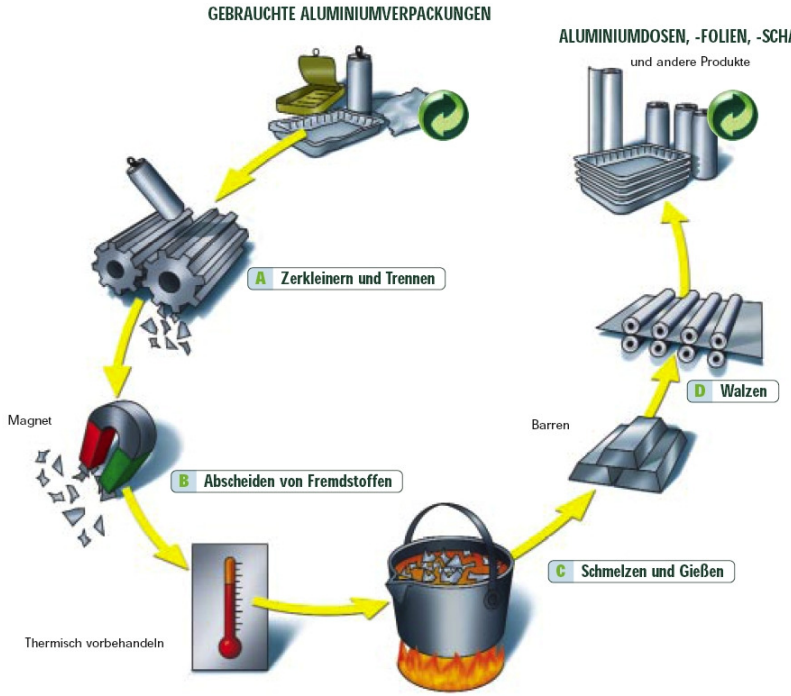
Casting - Homogenization - Hot Rolling - Cold Rolling - Annealing

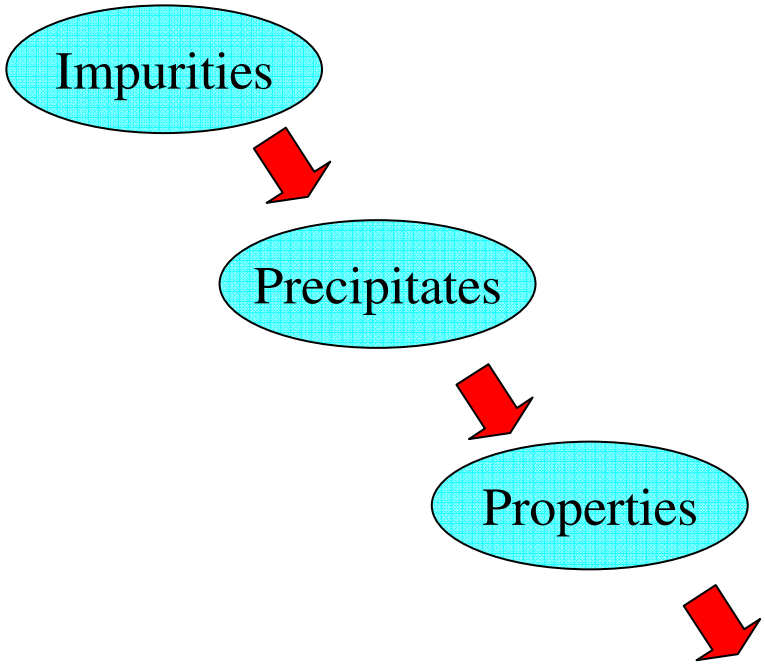




- Mechanical and corrosion properties
- Homogenization: Grain size controlling
- Hot/Cold rolling: interaction with RX or recovery

Aluminum sheet production





Project ClaNG+

- Goal: determine the precipitation kinetics in Al alloys

  ➔ClaNG model

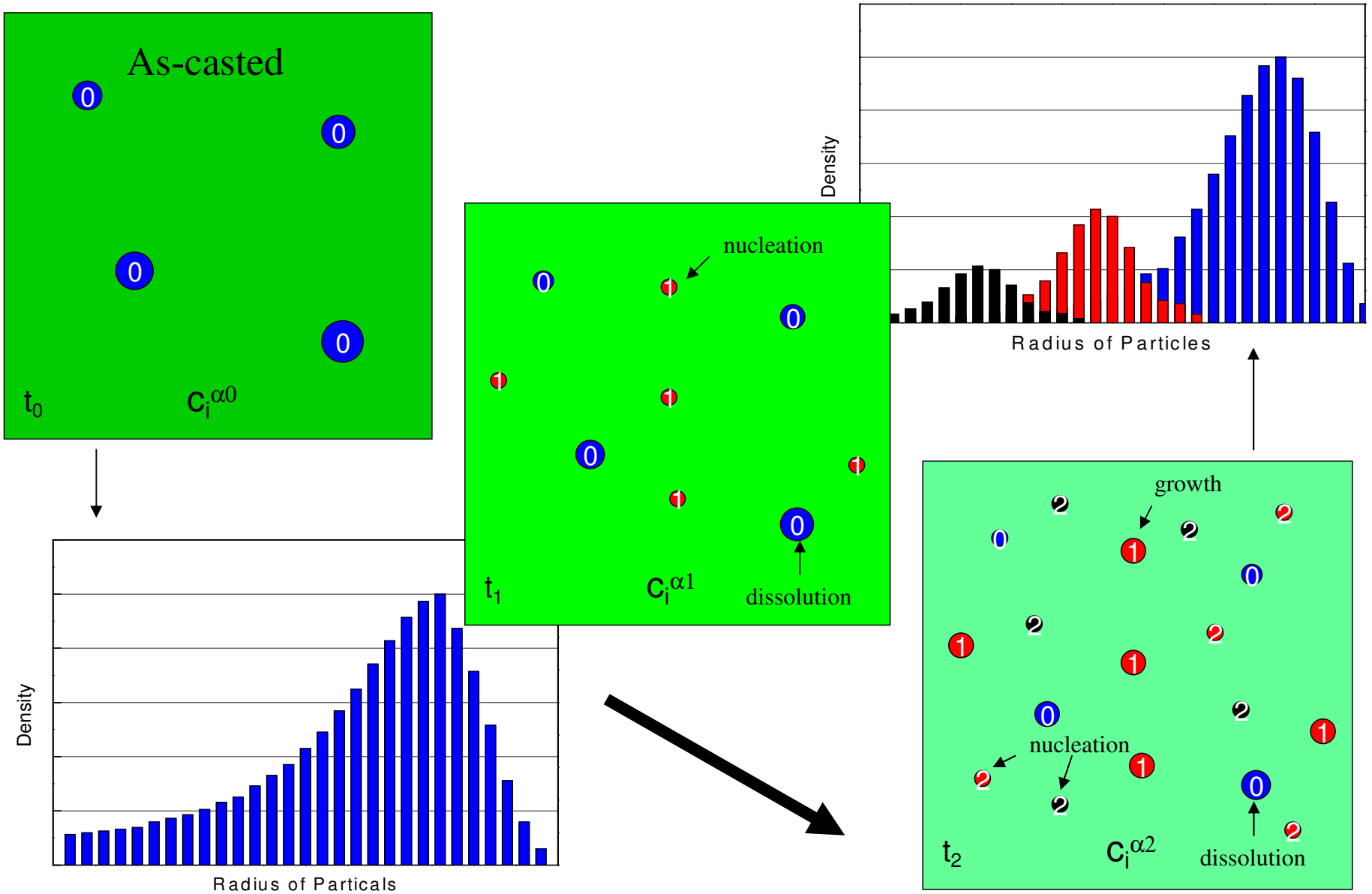
- ✓ Collaboration between
  - Hydro (Aluminum industry)
  - GTT technologies
  - IMM: Institut für Metallkunde und Metallphysik

- ♀ Developed by *M. Schneider*:

  „Modellierung und Validierung zeitabhängiger mikrochemischer Prozesse in Aluminium Knetlegierungen“ RWTH Aachen 2006

- ♀ Modified by *E. Jannot*
- ♀ .....

ClaNG model overview

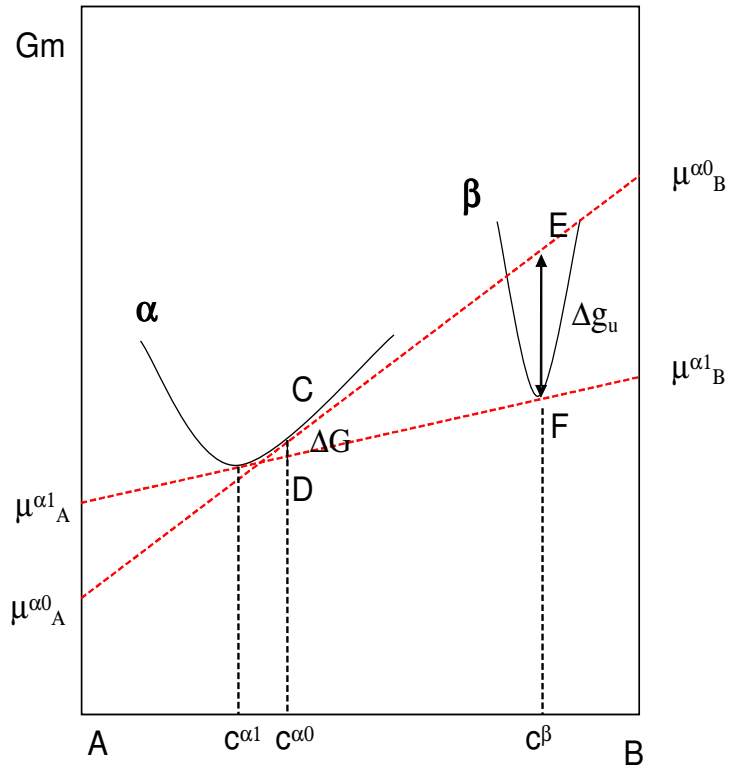


Thermodynamic calculations

- Use ChemApp (GTT):
  - ✓ Set conditions (temperature, concentrations of matrix)
  - ✓ Enter 2 phases: matrix + another phase
  - ✓ Perform equilibrium
    - ➢ Equilibrium concentrations c_i^{α} in the Al matrix α
    - ➢ Equilibrium concentrations c_i^{β} in the phase β
    - ➢ Chemical potentials of the elements

Chemical Driving Force of Nucleation

$$\Delta g_u^{\beta} = \sum_i c_i^{\beta} \cdot (\mu_i^{\alpha 0} - \mu_i^{\alpha 1})$$



Nucleation

- When Δg_u is known, the critical radius r_c can be derived
  - User input = interfacial energy γ

$$r_c = \frac{2\gamma \cdot V_m}{\Delta g_u}$$

- The nucleation rate is given by Becker & Döring theory

$$\dot{N} = N^0 \cdot Z \cdot \beta \cdot \exp\left(-\frac{\Delta G(r_C)}{k_B \cdot T}\right) \cdot \exp\left(\frac{-\tau}{t}\right)$$

HOMOGENEOUS NUCL.

$N^0_{\text{hom}} \approx number\ of\ atoms\ per\ volume (10^{29}\, m^{-3})$

$Volume\ Diffusion : D_{\text{hom}}$

$$\dot{N}_{\text{hom}} = N^0_{\text{hom}} \cdot Z_{\text{hom}} \cdot \beta_{\text{hom}} \cdot \exp\left(-\frac{\Delta G(r_C)}{k_B \cdot T}\right) \cdot \exp\left(\frac{-\tau_{\text{hom}}}{t}\right)$$

HETEROGENEOUS NUCL.

$N^0_{\text{het}} = \text{funct.}(\rho)$

$Pipe\ diffusion : D_{het}$

$$\dot{N}_{het} = N^0_{het} \cdot Z_{het} \cdot \beta_{het} \cdot \exp\left(-f^{corr}_{het} \cdot \frac{\Delta G(r_C)}{k_B \cdot T}\right) \cdot \exp\left(\frac{-\tau_{het}}{t}\right)$$

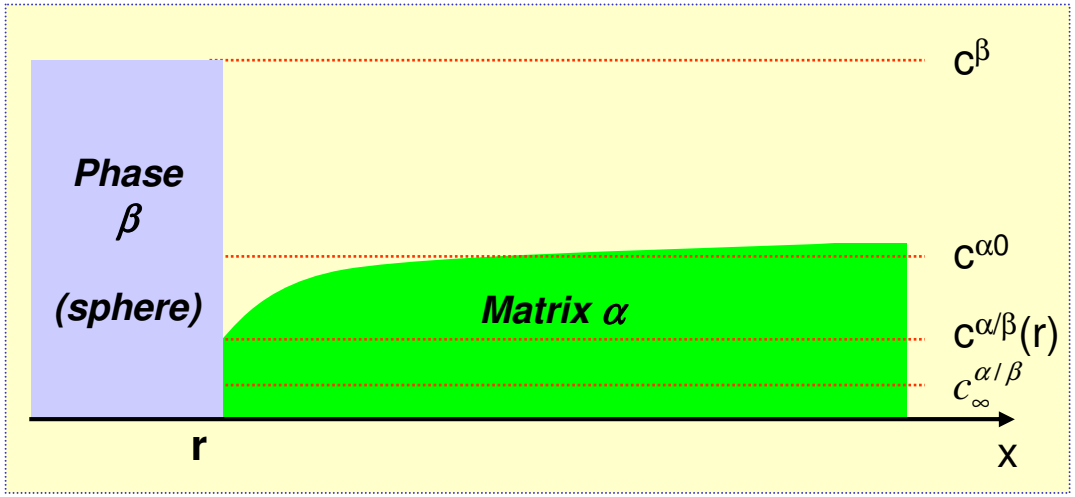
$$\dot{N}_{\text{tot}} = \dot{N}_{\text{hom}} + \dot{N}_{\text{het}}$$

Growth & Coarsening

- Assumption: precipitate growth is controlled by the diffusion in Al alloys. The *slowest diffuser* drives the dance(among the elements contained in the phase)

- Growth and coarseningare considered in a single equation
  - A particle above the critical radius grows
  - A particle below the critical radius dissolves

- The growth law used in ClaNG derives from Zener's formulation
  - All the particles are considered spherical

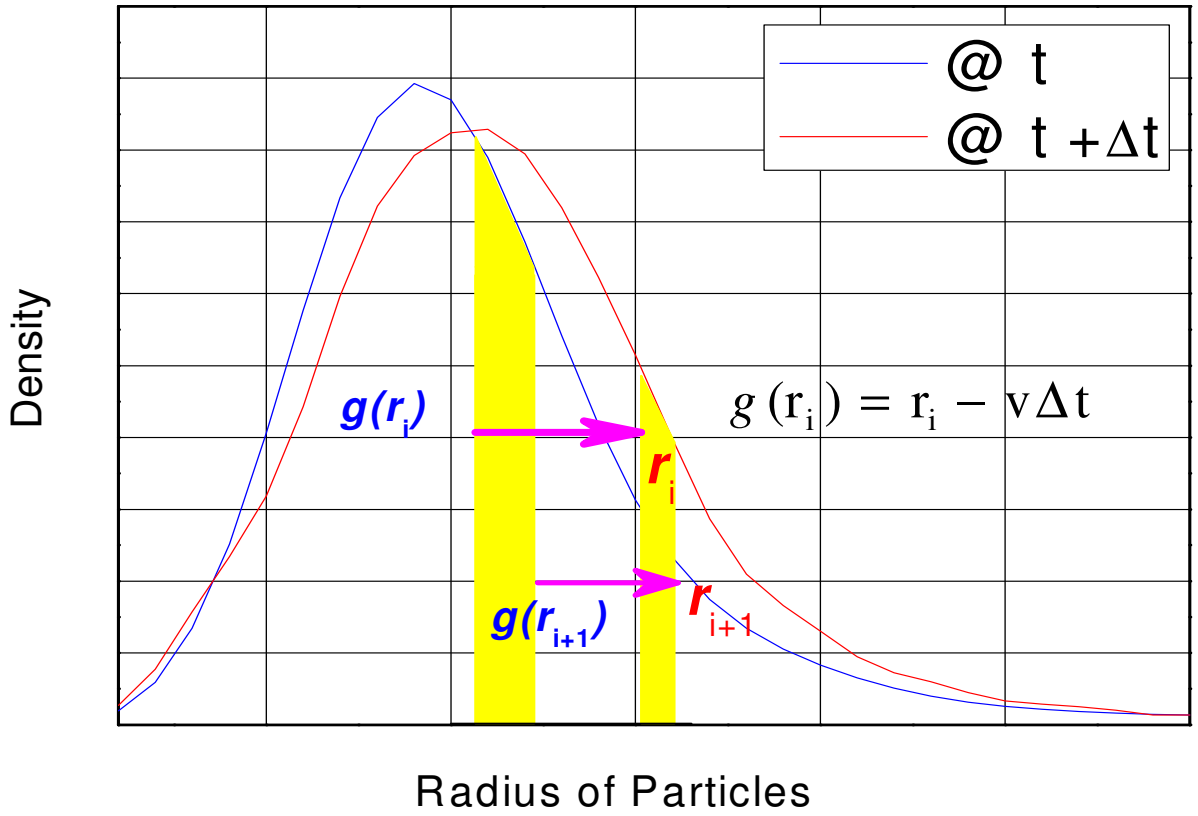


$$v = \frac{dr}{dt} = \frac{c^{\alpha 0} - c^{\alpha/\beta}(r)}{c^{\beta} - c^{\alpha/\beta}(r)} \cdot \frac{D_{slowest}}{r}$$

$c^{\alpha/\beta}(r)$ is Gibbs-Thomson concentration at the interface

Phase Evolution_*Size*

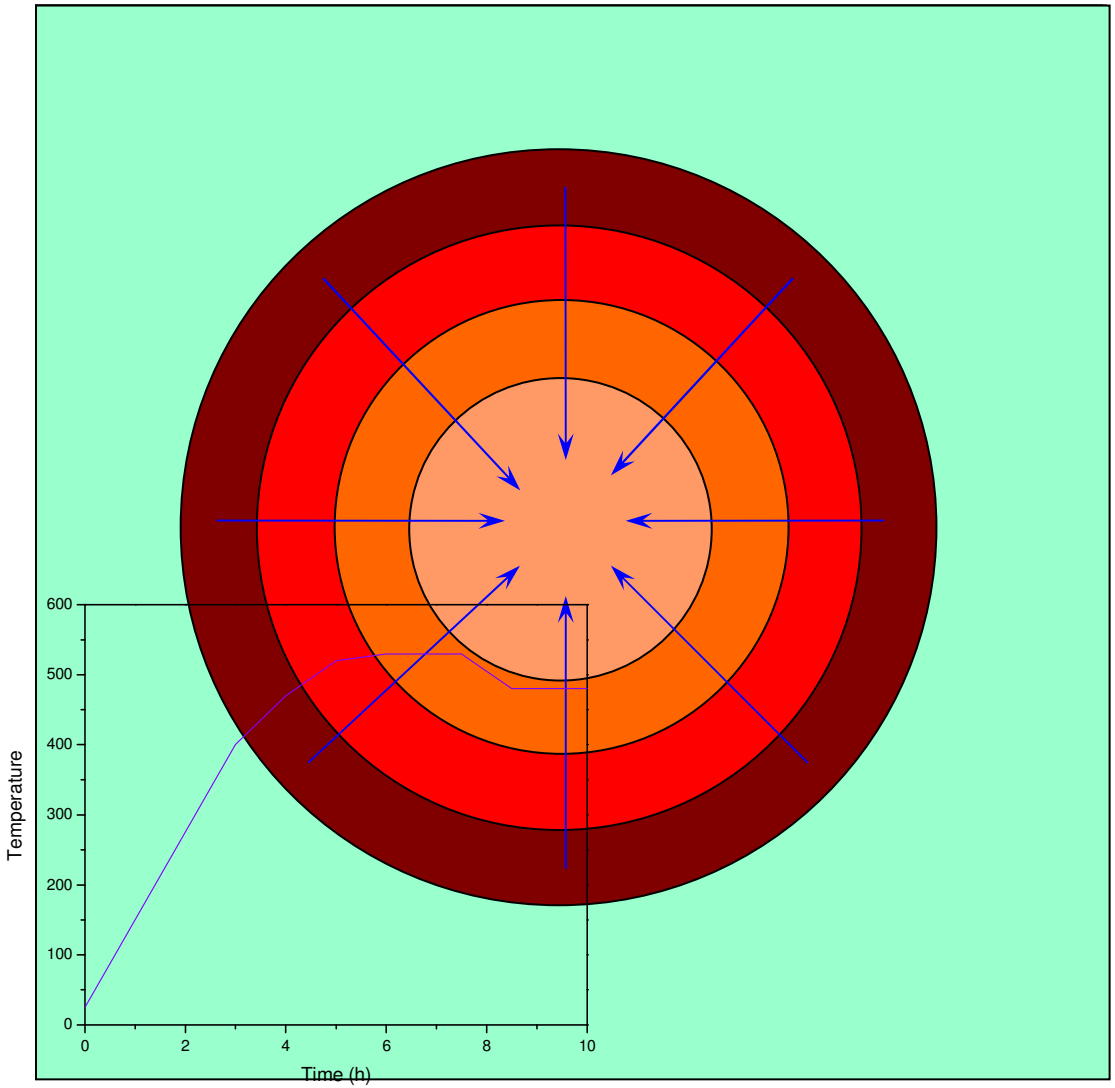
- Discretization in radius classes



$$N_i(t+\Delta t) = N_i(t) + \int_{g(r_i)}^{r_i} f(r,t)\cdot dr - \int_{g(r_{i+1})}^{r_{i+1}} f(r,t)\cdot dr \quad \left(+ \dot{N}_i^{nucl}\,\Delta t\right)$$

Runge-Kutta method

Phase Evolution_*Composition*



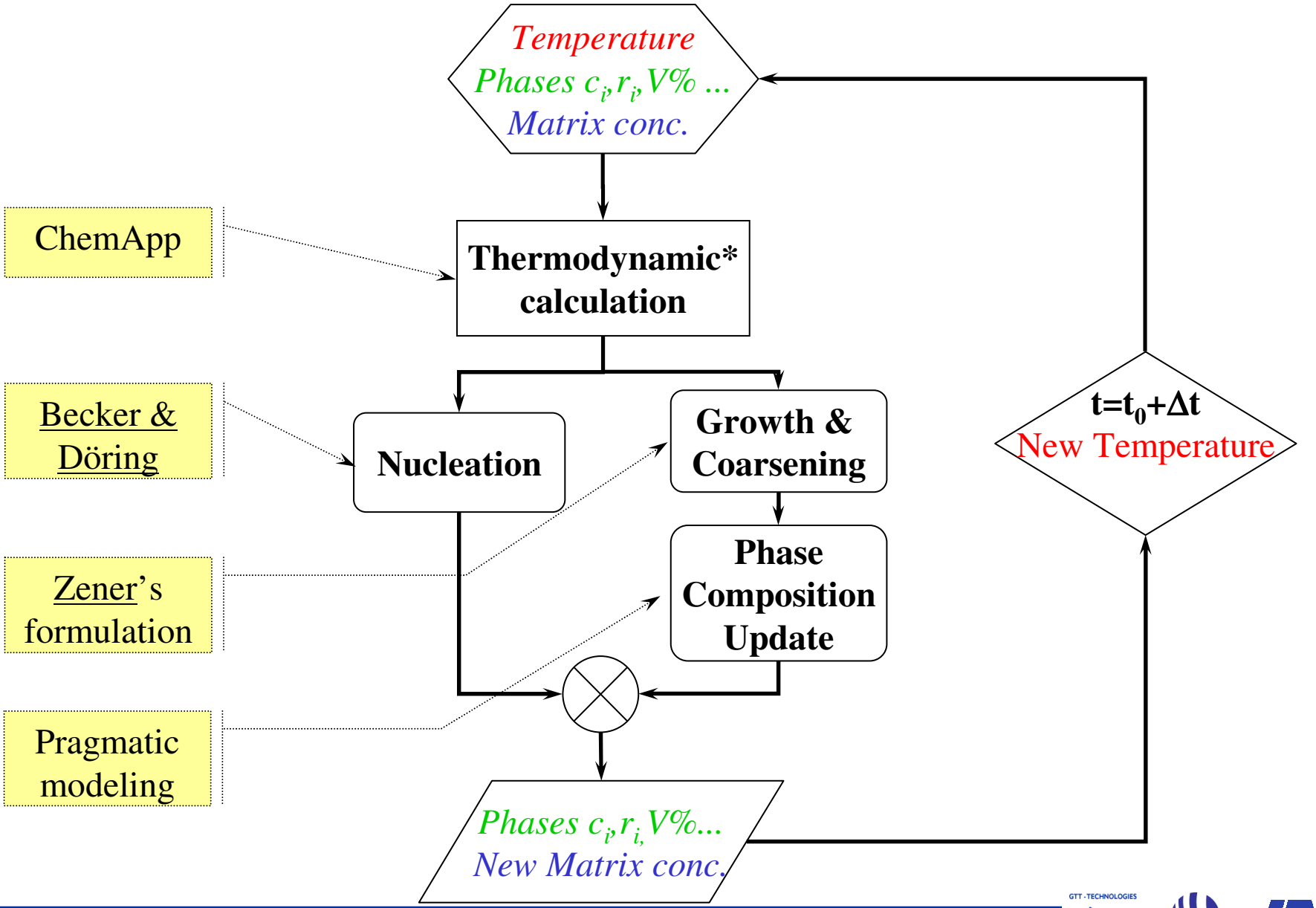
- During heat treatment, the phase equilibrium composition changes
- Diffusion in precipitates does the work

☹ Diffusion coefficient D_p in the phase is generally unknown

✓ Pragmatic modeling: use of an empirical factor to level diffusion

✓ $D_p = f_{corr} D_{bulk}$

Short Review



Prediction Quality of ClaNG

- Alloy AA3014
  - M.Schneider *„Modellierung und Validierung zeitabhängiger mikrochemischer Prozesse in Aluminium Knetlegierungen“ RWTH Aachen 2006*
- Alloy AA5182
  - *A. Knoll „Untersuchungen zur Entwicklung der Mikrochemie während der Homogenisierung von Aluminiumwalzlegierungen“*

Simulation of AA3014

Composition of alloy AA3014	
Element	wt%
Mg	1.0964
Mn	0.8425
Fe	0.4691
Si	0.1713
Ti	0.0182
Cu	0.1762
Cr	0.0084
Zn	0.0176
Al	…

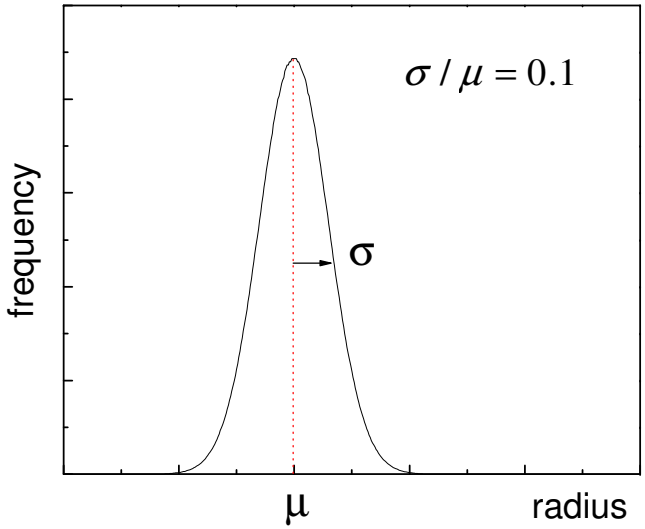
➢ *AlTT* database(8 Elements)

Pre-existed Phases:

Alpha ($Al_{12}(Mn,Fe)_3Si_2$) $r=2\mu m$

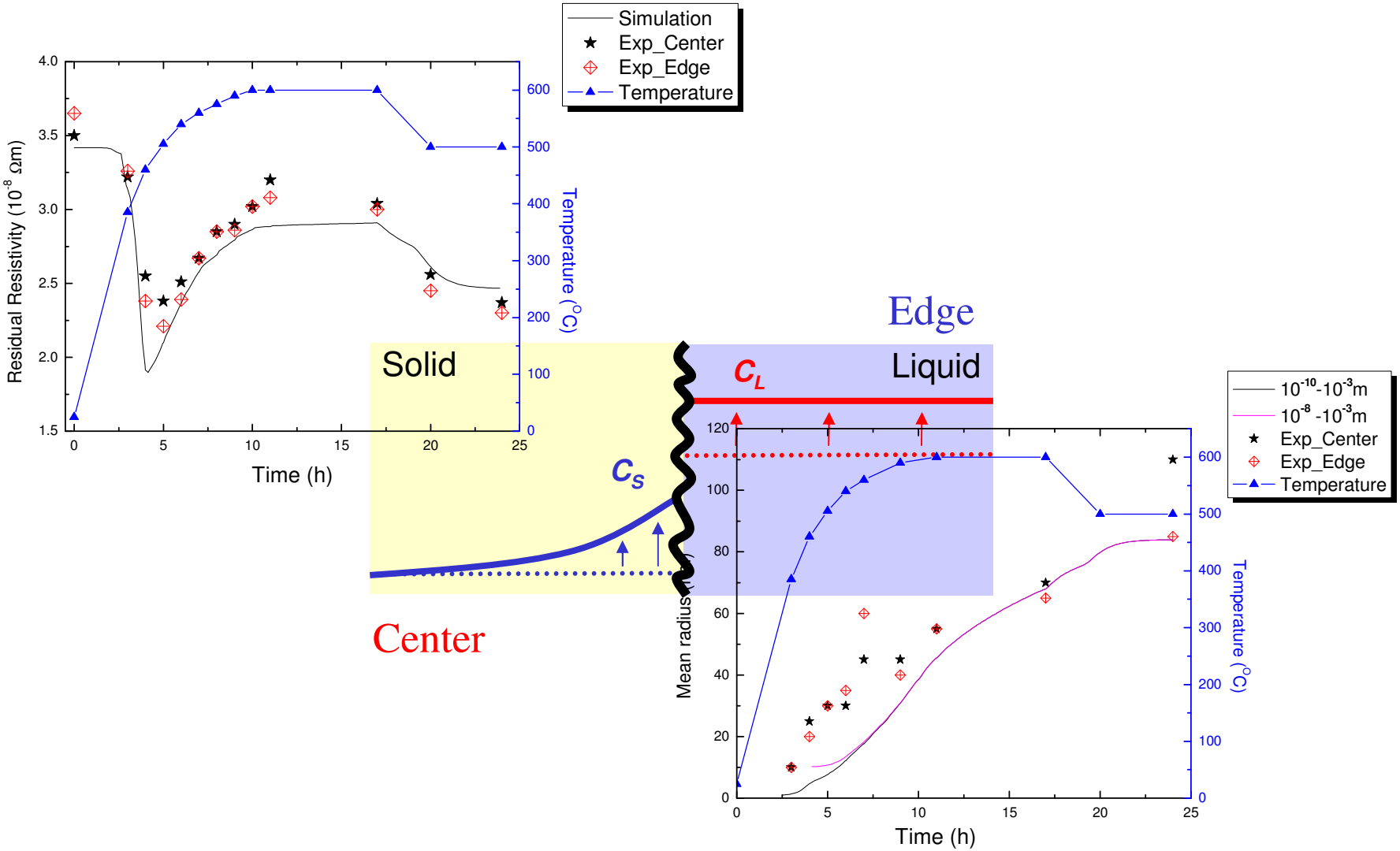
Mg_2Si $r=30nm$

follow Gauss distribution



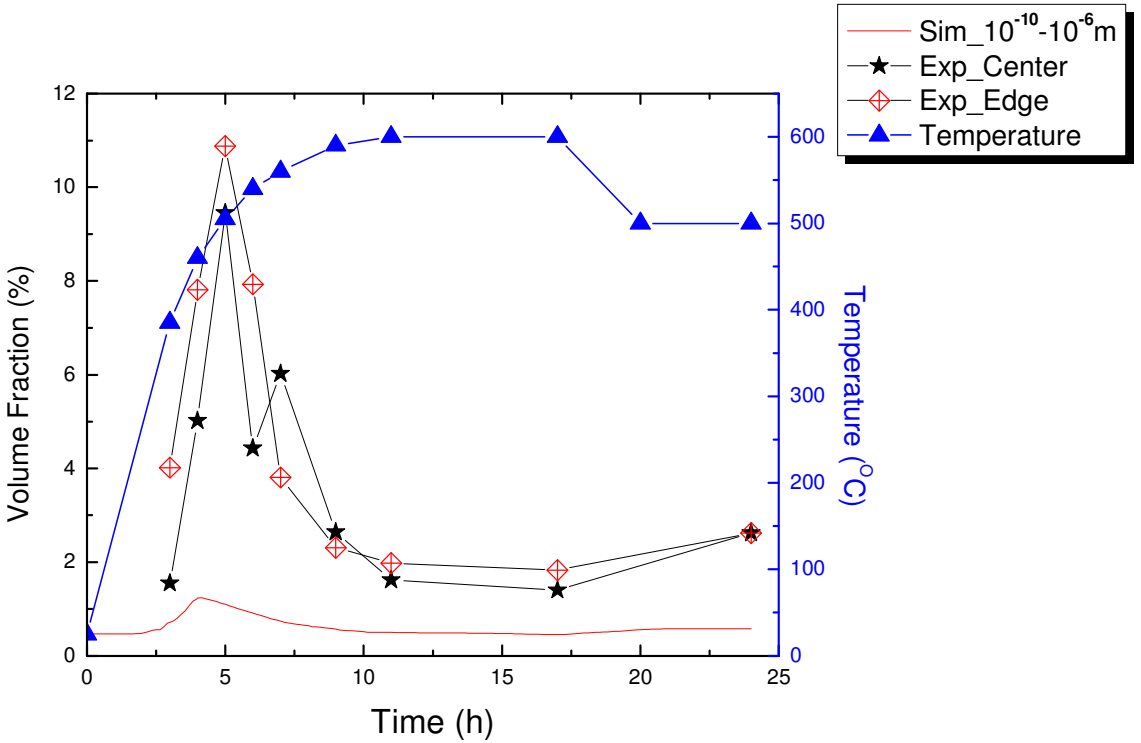
$$f_r = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{(r-\mu)^2}{2\sigma^2})$$

AA3014_Residual Resist&Mean Radius



AA3014_Volume Fraction

Volume Fraction of Dispersoides



Reason: etching of the dispersoides

Simulation of AA5182

Composition of alloy AA5182	
Element	wt%
Mg	4.200
Mn	0.330
Fe	0.250
Si	0.052
Ti	0.021
Cu	0.014
Cr	0.001
Zn	0.003
Al	…

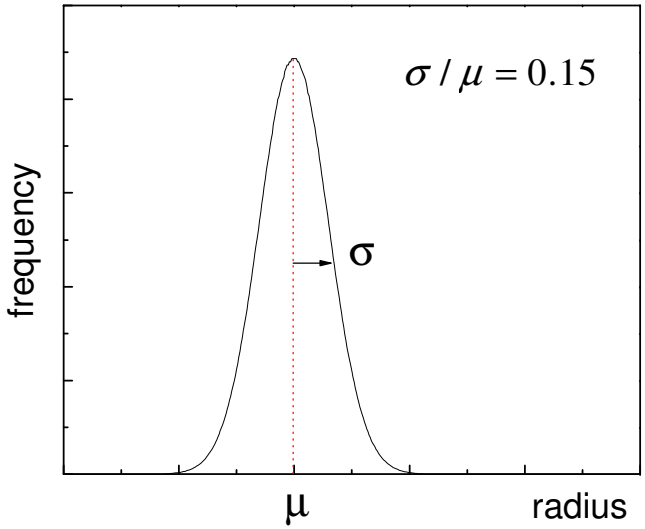
➢ *AlTT* database(8 Elements)

Pre-existed Phases:

Al_3Fe Al_3Ti

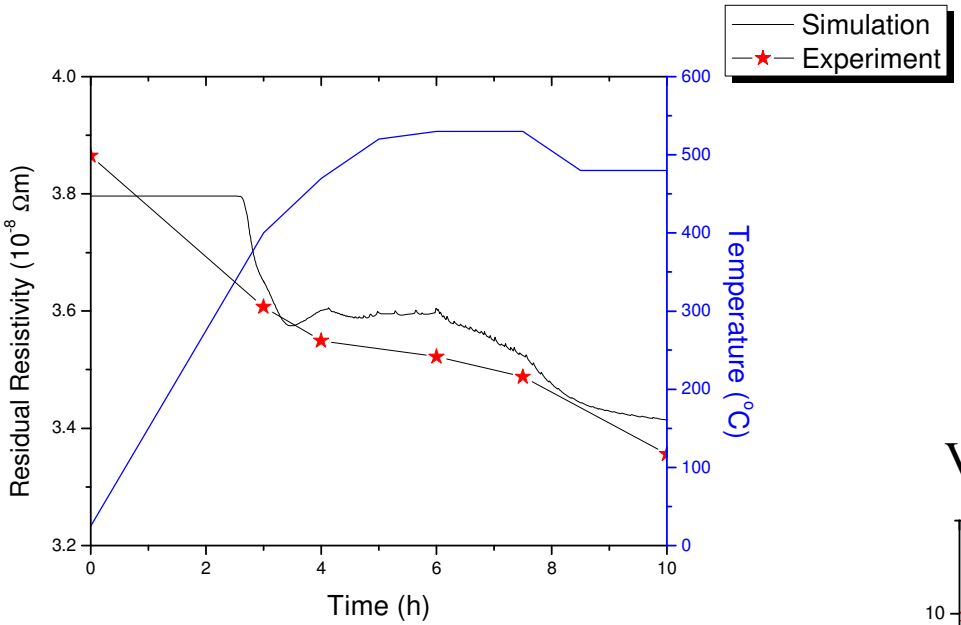
Al_6Mn Mg_2Si

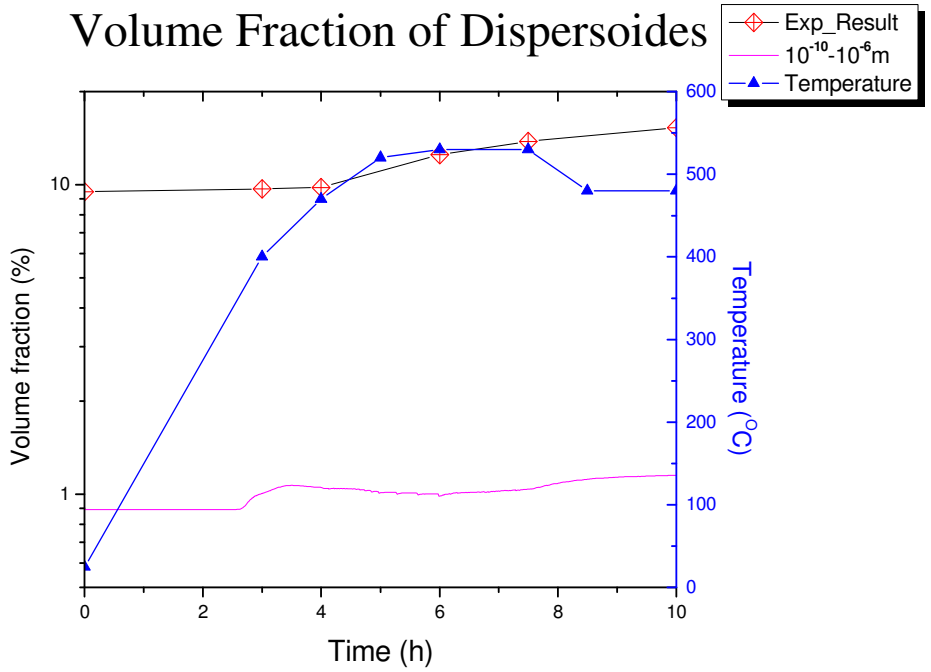
follow Gauss distribution



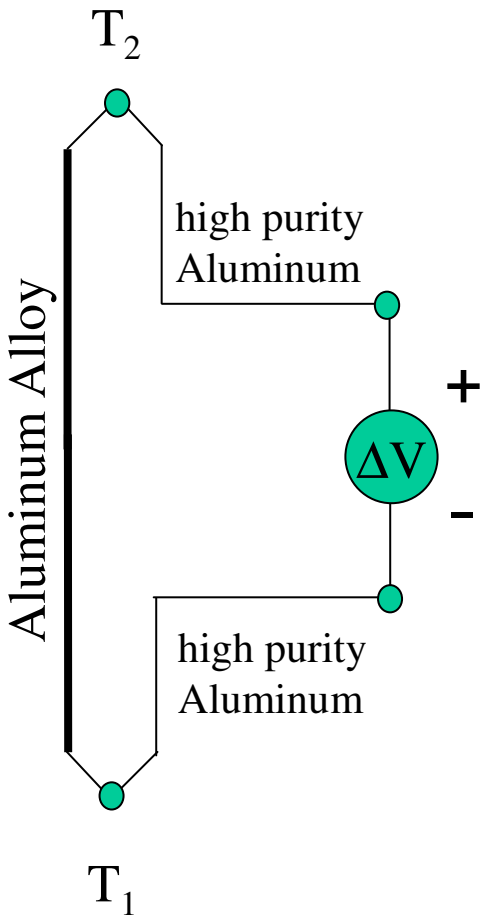
$$f_r = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{(r-\mu)^2}{2\sigma^2})$$

AA5182_Residual Resist&Volume Fraction

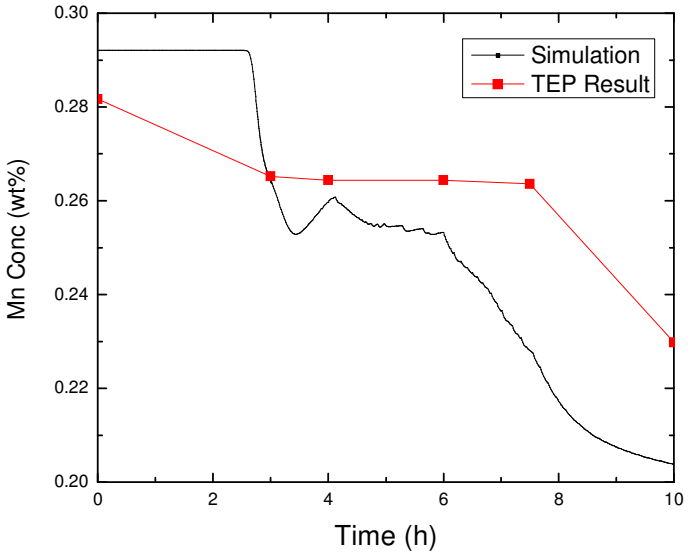


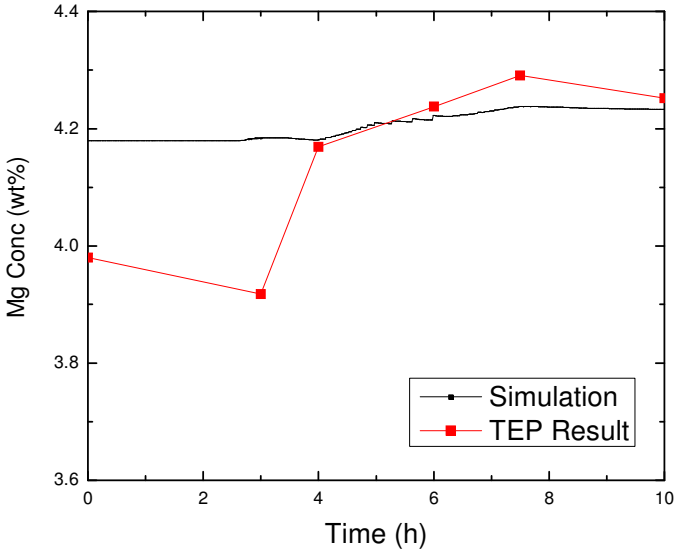


AA5182_Thermo Electrical Power

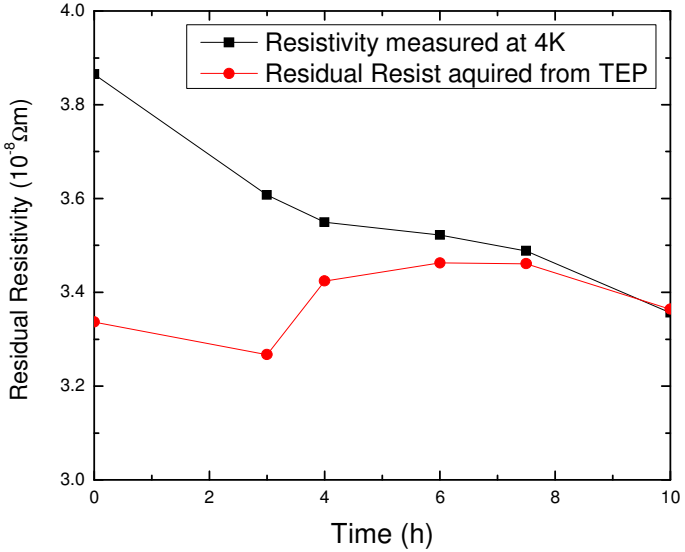


TEP



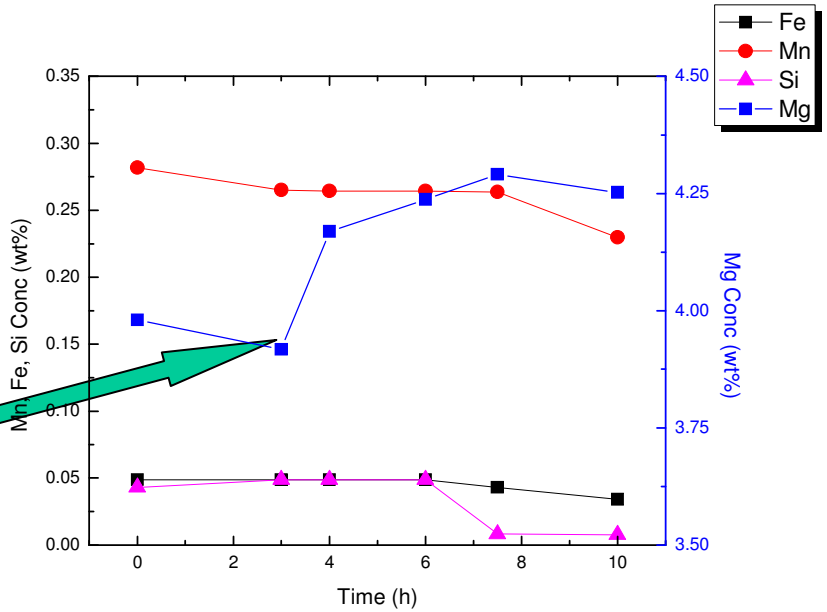


AA5182_Thermo Electrical Power



one of them is incorrect

Inhomogeneity of Alloy



Prediction Quality of ClaNG

☺ Residual Resistivity, mean radius, matrix composition (TEP) match very well with each other.

☹ Volume fraction of dispersoides measured by experiment is too high,due to experiment method

✓ Prediction of ClaNG is correct.

Simulation of AA5182

Composition of alloy AA5182	
Element	wt%
Mg	4.200
Mn	0.330
Fe	0.250
Si	0.052
Ti	0.021
Cu	0.014
Cr	0.001
Zn	0.003
Al	…

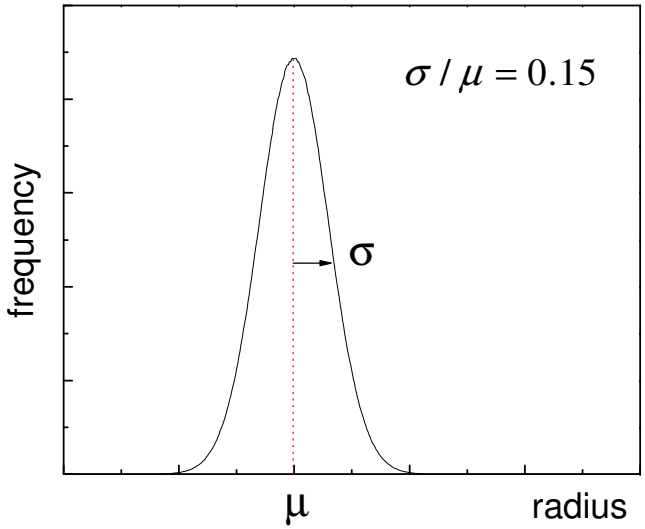
➢ *AlTT* database(8 Elements)

Pre-existed Phases:

Al_3Fe Al_3Ti

Al_6Mn Mg_2Si

follow Gaus distribution



$$f_r = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{(r-\mu)^2}{2\sigma^2})$$

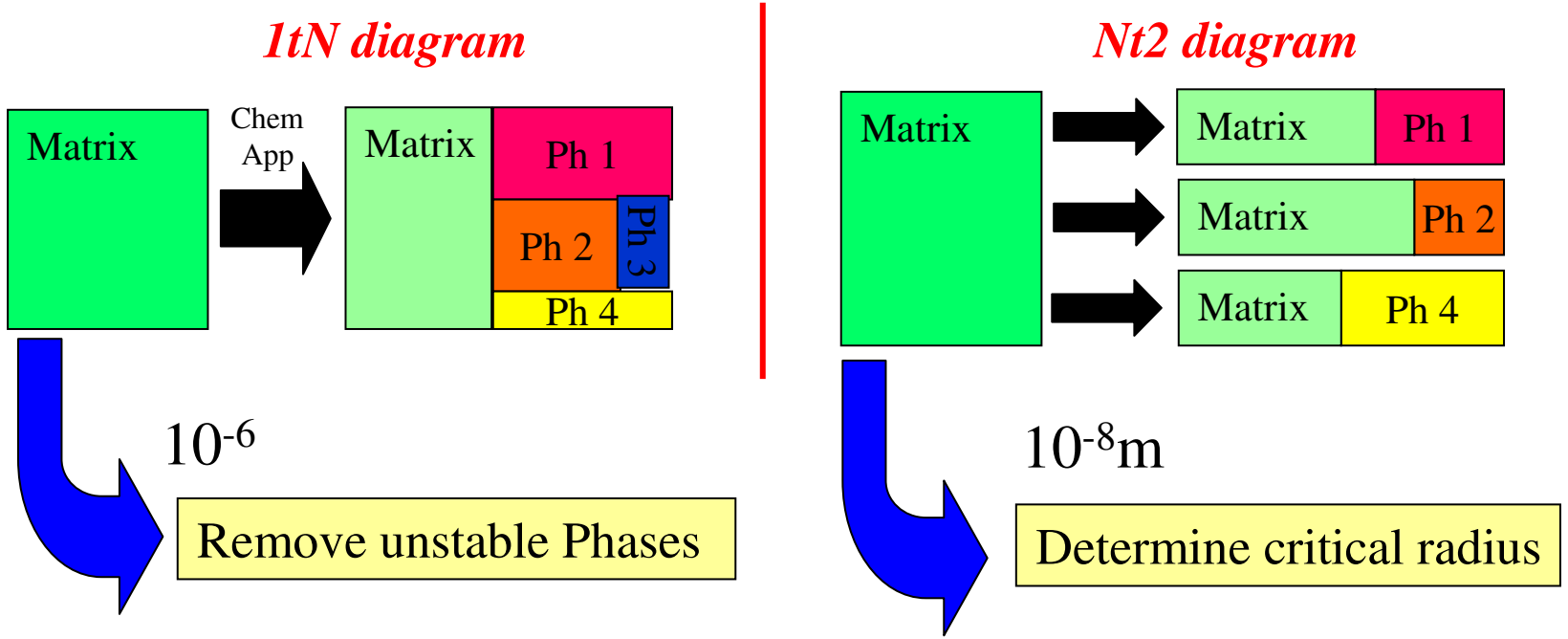
Database Extension

- Original database contains 8 Elts and 27 Phases
- New database contains 15 Elts and 42 Phases

Elt	Al	B	C	Cr	Cu	Fe	Mg	Mn	Ni	Si	Sr	Ti	V	Zn	Zr
TTal15	●	●	●	●	●	●	●	●	●	●	●	●	●	●	●
TTal8	●			●	●	●	●	●		●		●			

Optimization of the computation

- ✓ The phase diagram for the considered alloy is first calculated before starting a ClaNG calculation
- ✓ Two types of phase diagrams calculation



Only left phases ➡ ClaNG

AlTT8 Vs AlTT15

Input composition of Databank AlTT8

Element	wt%
Mg	4.200
Mn	0.330
Fe	0.250
Si	0.052
Ti	0.021
Cu	0.014
Cr	0.001
Zn	0.003
Al	...

Input composition of Databank AlTT15

Element	wt%	Element	wt%
Mg	4.200	B	1e-4
Mn	0.330	C	1e-6
Fe	0.250	Ni	1e-4
Si	0.052	Sr	1e-4
Ti	0.021	V	1e-4
Cu	0.014	Zr	5e-4
Cr	0.001		
Zn	0.003		
Al	...		

Phases in Database AlTT8

```
2009.05.28  15:32:16  MESSAGE:   1tN Diagram in File Thermodyn_1tN.txt
2009.05.28  15:32:17  MESSAGE:   Nt2 Diagram in File Thermodyn_Nt2.txt
2009.05.28  15:32:20  MESSAGE:   The Phase [ 2] = [AL2CU]          with VolFrac =   0.015 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [ 3] = [AL3FE]          with VolFrac =   1.132 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [ 5] = [AL3TI]          with VolFrac =   0.302 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [ 6] = [AL6MN]          with VolFrac =   2.011 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [ 7] = [AL7CR]          with VolFrac =   2.122 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [ 8] = [ALMG_BETA]      with VolFrac =  11.045 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [ 9] = [ALPHA]          with VolFrac =   1.147 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [10] = [E_ALCRMGMN]                   with VolFrac =   1.867 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [11] = [FCC_A1]         with VolFrac = 100.000 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [12] = [MGZN2#1]        with VolFrac =   0.028 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [14] = [T_ALCUMGZN]                  with VolFrac =   8.488 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [15] = [Al13Cr4Si4]      with VolFrac =   0.003 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [16] = [Al20Cu2Mn3]      with VolFrac =   0.074 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [17] = [Al3Fe<AL3NI>]    with VolFrac =   0.482 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [18] = [Al5Cu2Mg8Si6]    with VolFrac =   0.062 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [19] = [Al7Cu2Fe]        with VolFrac =   0.030 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [20] = [Al8FeMg3Si6]     with VolFrac =   0.150 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [21] = [Al9Fe2<AL9FENI>]                with VolFrac =   0.663 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [22] = [Al71Fe19Si1<AFS_ALPHA>]       with VolFrac =   0.499 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [23] = [Al692Fe154Si154<AFS_BT>]      with VolFrac =   0.324 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [25] = [Mg2Si]          with VolFrac =   0.150 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [26] = [Si<SILICON>]    with VolFrac =   0.050 Perc. is considered
2009.05.28  15:32:20  MESSAGE:   The Phase [27] = [Al2CuMg<S>]     with VolFrac =   0.024 Perc. is considered
2009.05.28  15:32:20  MESSAGE:
2009.05.28  15:32:20  MESSAGE:   The Phase [ 1] = [LIQUID]         with VolFrac =   0.175 Perc. is not considered
2009.05.28  15:32:20  MESSAGE:
2009.05.28  15:32:20  MESSAGE:   The Phase [ 4] = [AL3NI2]         has a too low VolFrac =   0.000 Perc.
2009.05.28  15:32:20  MESSAGE:   The Phase [13] = [MGZN2#2]        has a too low VolFrac =   0.000 Perc.
2009.05.28  15:32:20  MESSAGE:   The Phase [24] = [Ti<MC>]         has a too low VolFrac =   0.000 Perc.
2009.05.28  15:32:20  MESSAGE:
```

Considered Phases:23/27

Removed Phases:4 /27

Phases in Database AlTT15

```
2009.05.29  08:52:05   MESSAGE:
***  Phase Diagram for the given alloy  between 25.0 DegC and 530.0 DegC  for a min. VolFrac of 1.0E-05  ***
2009.05.29  08:52:05   MESSAGE:        1tN Diagram in File Thermodyn_1tN.txt
2009.05.29  08:52:08   MESSAGE:        Nt2 Diagram in File Thermodyn_Nt2.txt
2009.05.29  08:52:22   MESSAGE:        The Phase [ 2] = [AL3FE]      with VolFrac =   1.156 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [ 3] = [AL3MG2]   with VolFrac =  10.983 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [ 4] = [AL3NI]      with VolFrac =   0.483 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [ 6] = [AL3TI]      with VolFrac =   0.273 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [ 8] = [AL6MN]     with VolFrac =   2.011 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [ 9] = [AL7CR]      with VolFrac =   2.124 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [10] = [AL9FENI]  with VolFrac =   0.664 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [11] = [ALPHA]     with VolFrac =   1.662 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [12] = [E_ALCRMGMN]          with VolFrac =   1.869 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [13] = [FCC_A1]    with VolFrac = 100.000 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [17] = [MGZN2]     with VolFrac =   0.029 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [18] = [T_ALCUMGZN]          with VolFrac =   8.196 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [19] = [Al13Cr4Si4]          with VolFrac =   0.003 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [20] = [Al20Cu2Mn3]          with VolFrac =   0.074 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [21] = [Al2Si2Sr]   with VolFrac =   0.080 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [23] = [Al4Sr]      with VolFrac =   0.080 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [24] = [Al5Cu2Mg8Si6]        with VolFrac =   0.062 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [25] = [Al7Cu2Fe] with VolFrac =   0.030 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [27] = [Al8FeMg3Si6]         with VolFrac =   2.173 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [29] = [<ALFESI_ALPHA>]      with VolFrac =   0.635 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [30] = [<ALFESI_BETA>]       with VolFrac =   0.784 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [31] = [Mg2Si]      with VolFrac =   2.880 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [33] = [Al2CuMg]  with VolFrac =   0.024 Perc. is considered
2009.05.29  08:52:22   MESSAGE:        The Phase [35] = [Si<SILICON>]         with VolFrac =   0.960 Perc. is considered
```

Considered Phases:24/42

Phases in Database AlTT15

Removed Phases:16/42


iM
Thanks very much for your attention !!!
?
?
?