

# Computational Thermodynamics Coupled Macro-Microscale Modelling of Industrial Castings

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GOI ESKOLA  
POLITEKNIKOA  
ESCUELA  
POLITÉCNICA  
SUPERIOR



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Commercial casting simulation software solve the heat transfer in the scale of the whole casting.

### Fourier equation

$$\rho \cdot c_p \cdot \frac{\partial T}{\partial t} = K \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + \frac{W}{\rho \cdot c_p}$$

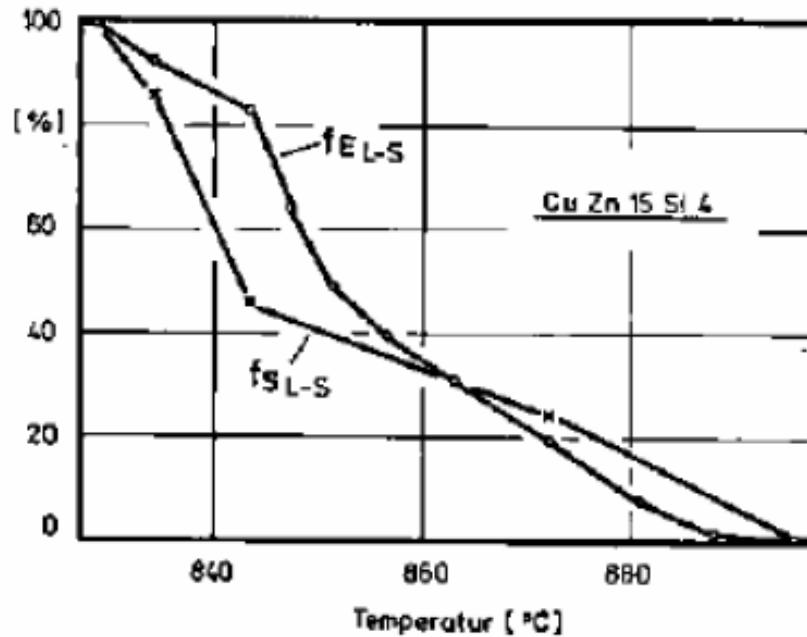
with  $W = L \frac{\partial f_s}{\partial t}$

Demand for:

- Latent Heat data,  $L$
- Latent Heat Release data,  $\frac{\partial f_s}{\partial t}$

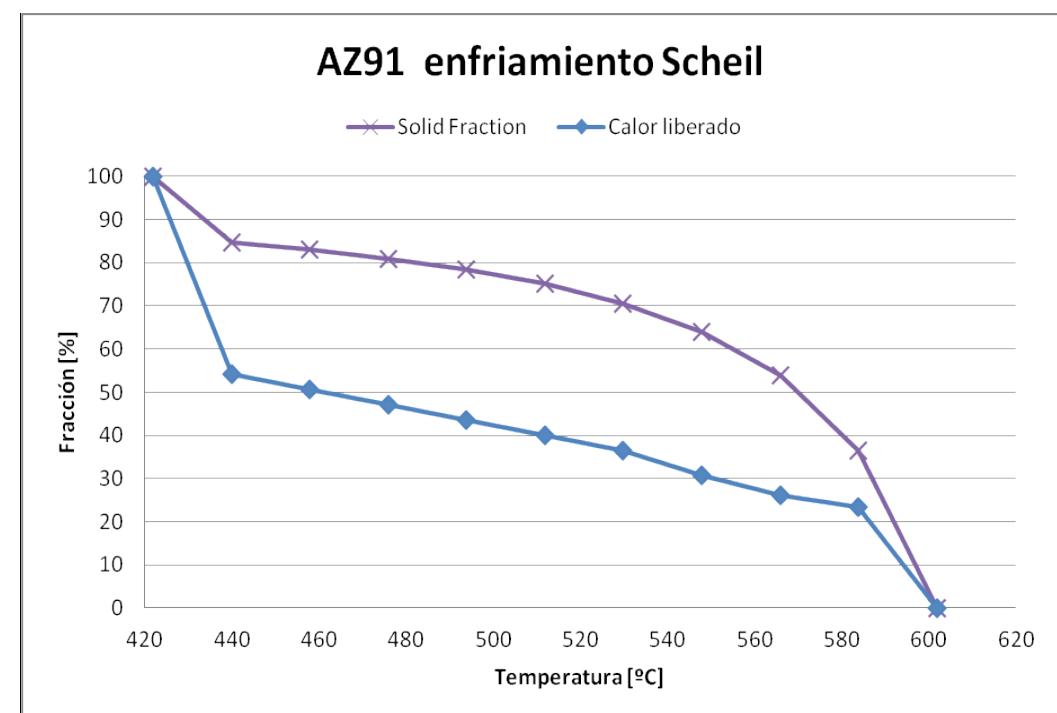
Experimentally obtained **input** data

**Solid Fraction & Latent Heat release assumed to be proportional.**



Solid fraction – Latent heat release  
NOT PROPORTIONAL

K. Weiß. Temperaturfeldberechnung bei Erstarrungsvorgängen unter Berücksichtigung des Einfüllvorganges. Ph.D. thesis, RWTH Aachen, 1986.



- Additionally, **latent heat** amount and release is considered **independent** of the **cooling rate**, but it determines the created microstructure and therefore, the heat released during the solid phase formation.
- Moreover, **invariant liquidus and solidus temperatures** are considered, neglecting cooling rate effect.

**OBJECTIVES:** Improve current casting simulations by,

- 1.) Couple microstructure describing models (microscale) to a commercial casting simulation software (macroscale), WinCast.
- 2.) Couple computational thermodynamics, ChemApp, to the macro-microscale modelling. Treat multicomponent systems.
- 3.) Calculate the latent heat release, phase formation and microsegregation in function of the cooling rate.

## COMMERCIAL SOFTWARE USED

- **WinCast®**: FEM based casting simulation software that solves the heat transfer and energy conservation in the macroscale (the scale of the whole casting).
- **ChemApp®**: programmable subroutines of FactSage that provide multicomponent and multiphase phase equilibrium calculations and the associated energy balances.



**Casting material** → AZ91E Mg alloy

	Al	Zn	Mn	Si	P	Mg
AZ91E	8.48	0.48	0.18	<0.03	<0.02	Balance

Mg-Al-Zn thermodynamic database

**Mould material** → GGG40 grey iron

**Casting method** → Gravity Die casting in permanent mould

Mould temperature: 230 °C

Melt temperature: 730 °C

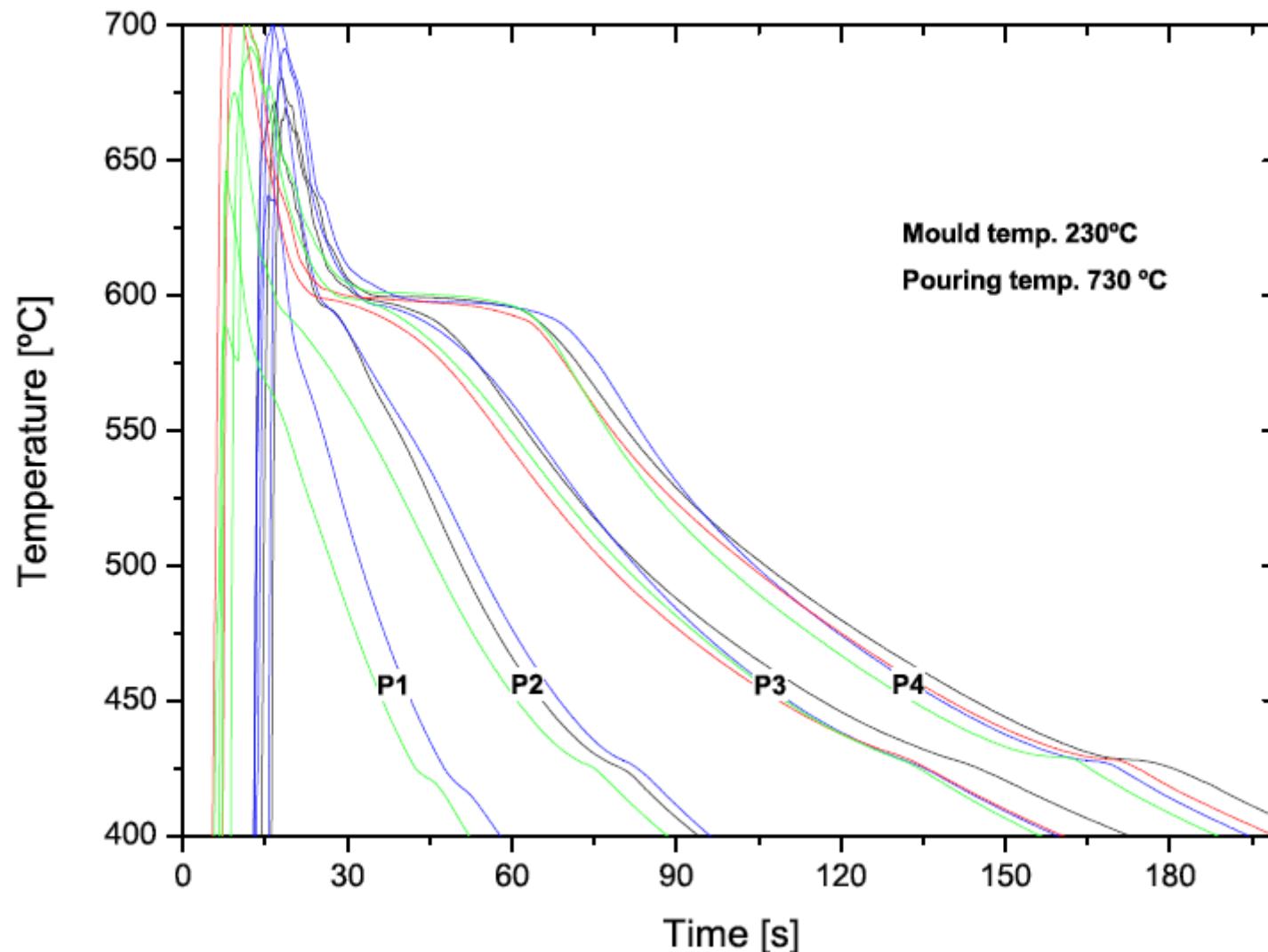
SiC addition for grain refinement

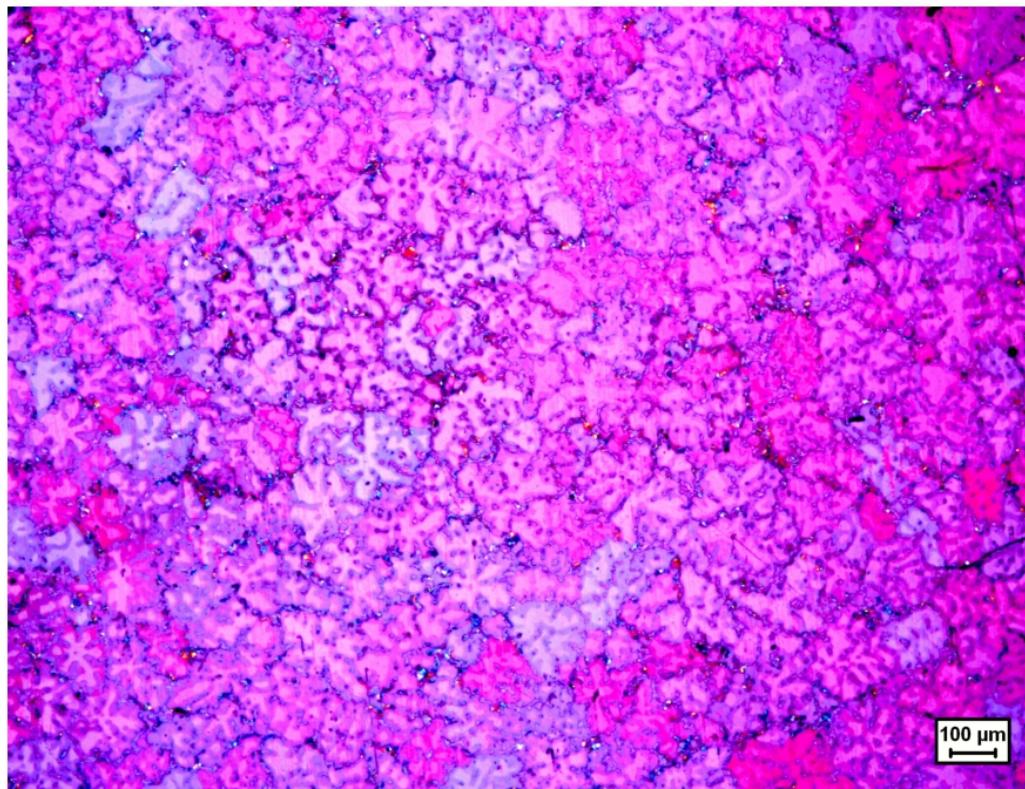
4% SF<sub>6</sub> – CO<sub>2</sub> protective environment

K type thermocouples at middle point  
of each step



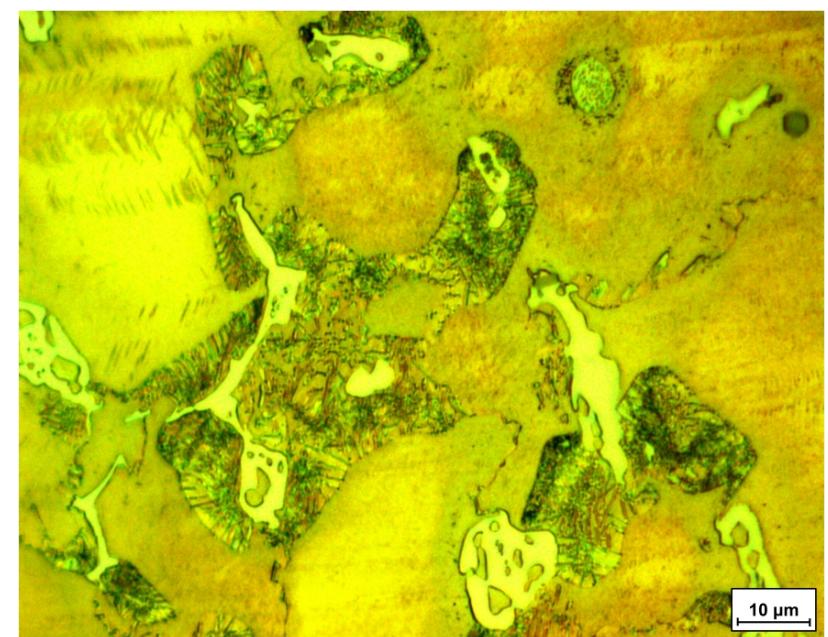
Step widths: 12 mm, 20 mm, 40 mm, 80 mm



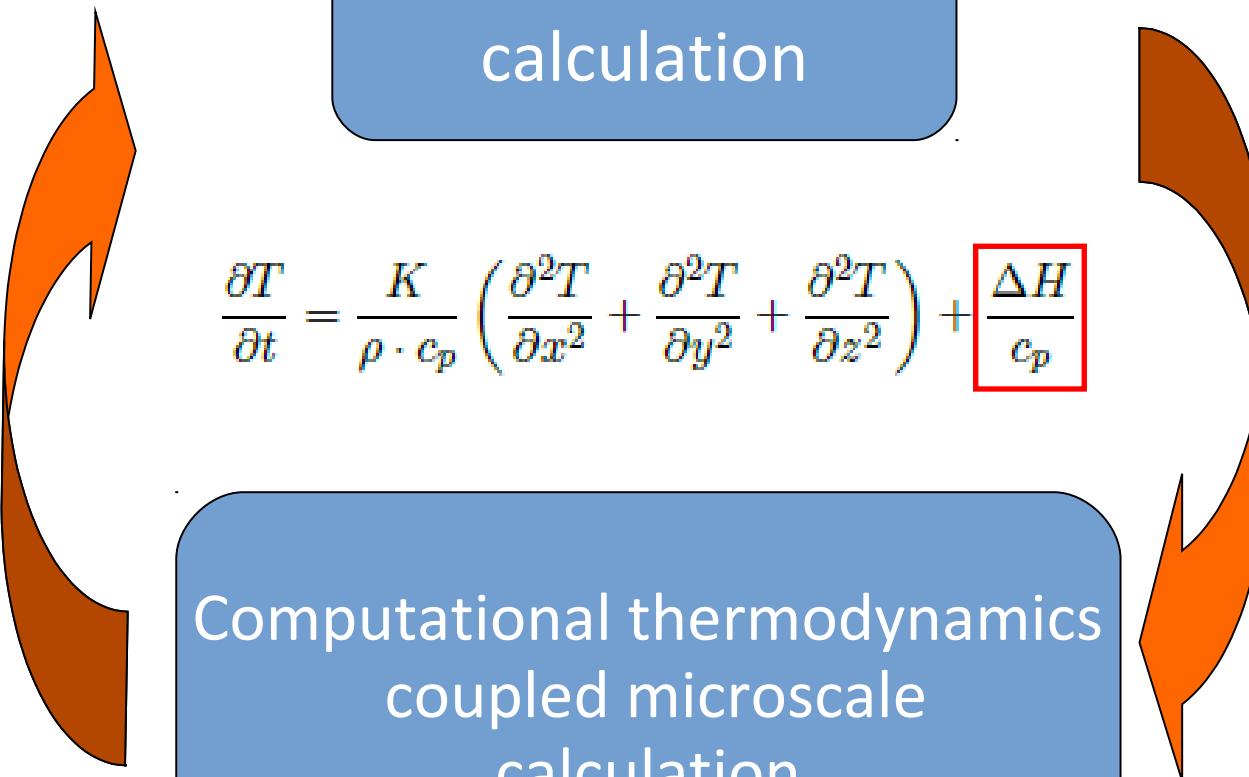


Equiaxed grains  
 $\alpha$ -Mg (HCP\_A3) phase

Semi-divorced eutectic and  
lamellar  $\gamma(\text{Mg}_{17}\text{Al}_{12})$  compound



Macroscale  
calculation



$\Delta H, c_p, f_l, f_s,$   
 $c_s^*, c_l^*$

$$\frac{\partial T}{\partial t} = \frac{K}{\rho \cdot c_p} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + \frac{\Delta H}{c_p}$$

Temperature  
distribution  
along the casting

Computational thermodynamics  
coupled microscale  
calculation

## Micromodel

- Instantaneous nucleation model based on the experimental results.

$$N_v = 490 \cdot \exp \left( -\frac{1.2}{\Delta T_N} - \frac{0.5}{dT/dt} \right)$$

$$\Delta H_N = H_{liq} - H_N$$

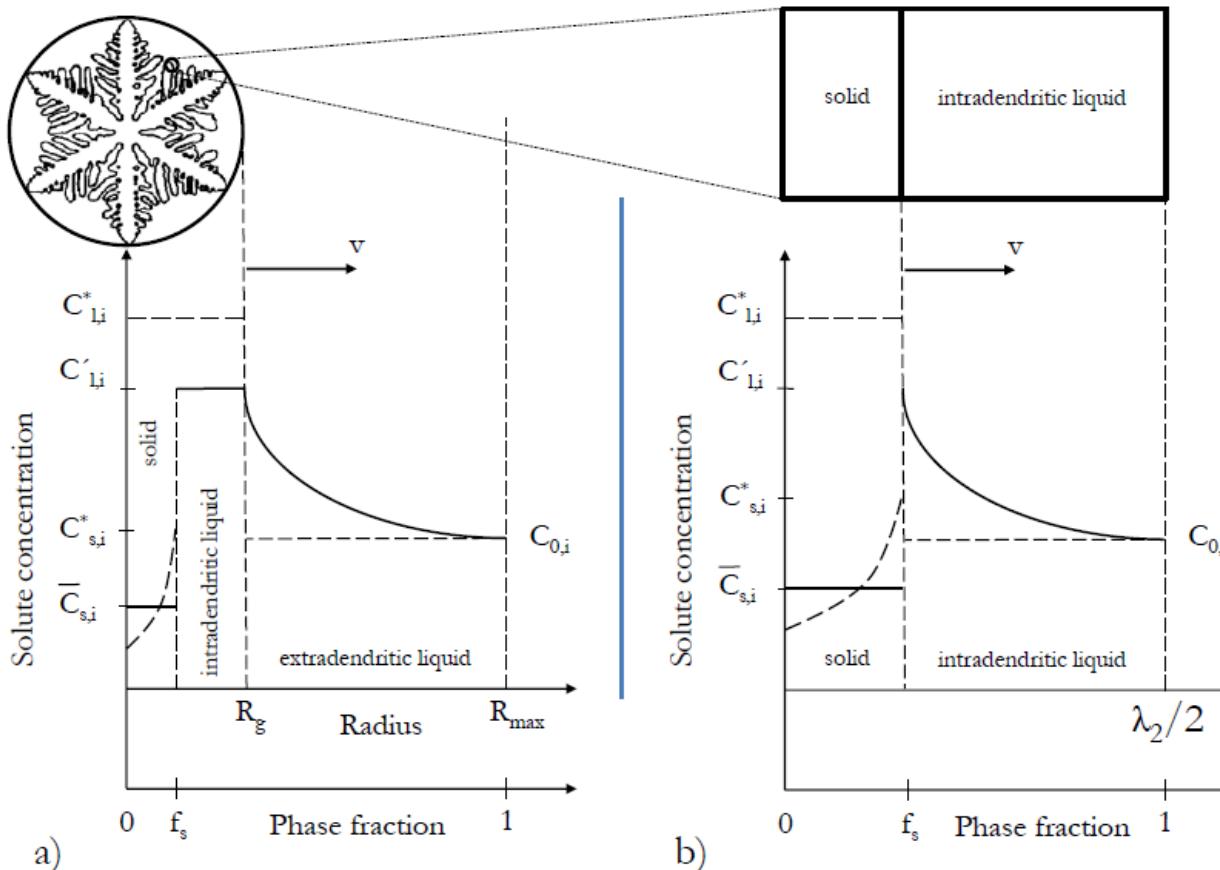
- Equiaxed dendrite growth modelled according to the LGK model.

$$\Delta T = \frac{\Delta H}{c_p} \cdot Iv(Pe_{th}) + \frac{Q_{multi} \cdot Iv(Pe_c)}{(1 - (1 - k_{multi}) \cdot Iv(Pe_c))} + \frac{2\Gamma}{R_d}$$

$$Q_{multi} = \sum m_i \cdot (k_i - 1) \cdot c_{0,i} \quad m_i = \frac{\delta T_L}{\delta c_{0,i}} \quad k_i = \frac{c_{s,i}^*}{c_{l,i}^*} \quad k_{multi} = \frac{\sum c_{s,i}^*}{\sum c_{l,i}^*}$$

## Micromodel

- Solute diffusion in liquid phase and no diffusion in solid phase.



Solute flux analysis

$$\frac{c'_{l,i}(x, t) - c_{0,i}}{c^*_{l,i} - c_{0,i}} = 1 - erf\left(\frac{x}{2\sqrt{D_i \cdot t}}\right)$$

Diffusion length scale ( $x$ )  
 $f(\text{impingement})$

## Micromodel

- Thermodynamic equilibrium calculations at the solid-liquid interface provide

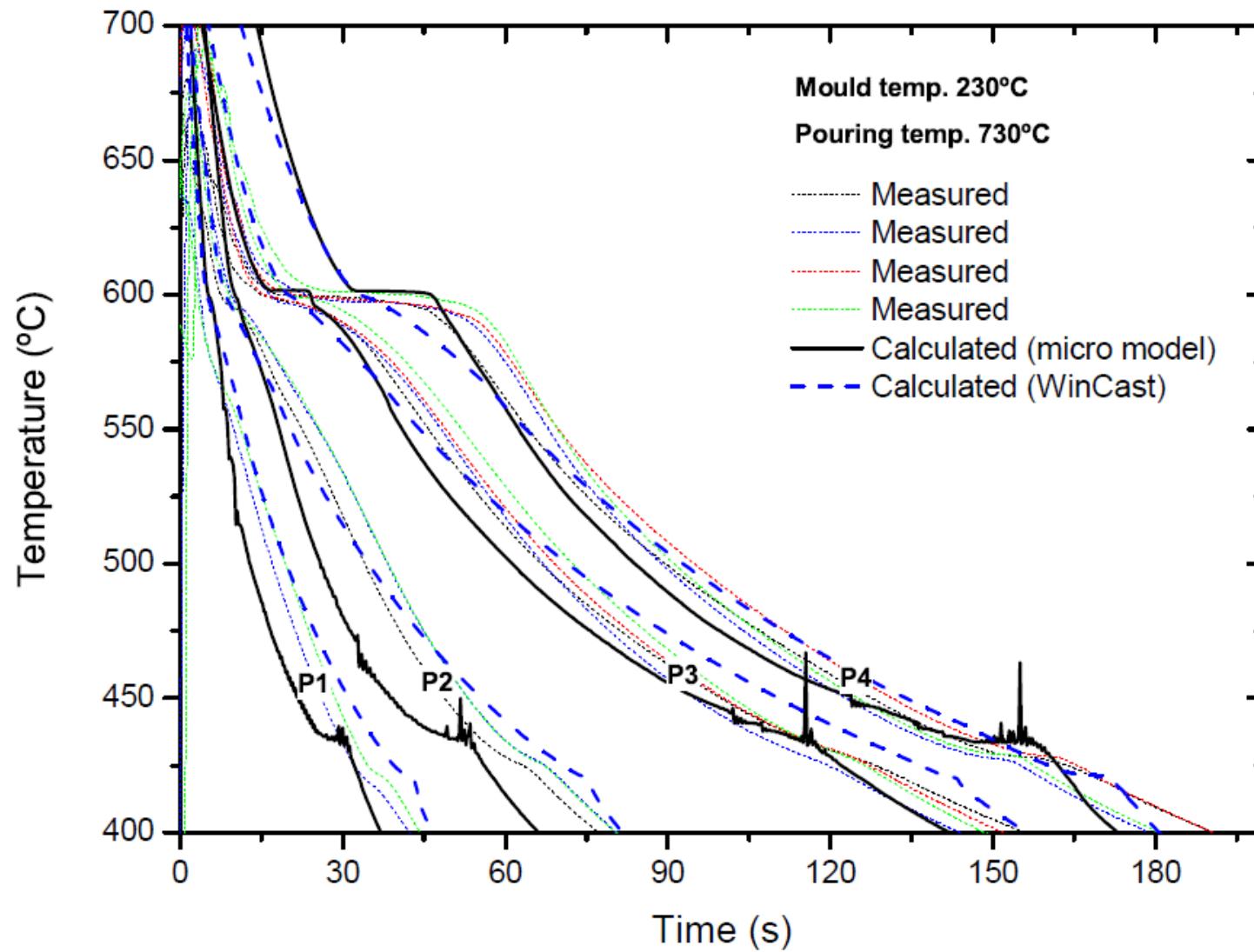
$$f_s^\phi = f_s^{0,\phi} + \Delta f_s^\phi$$

$$\overline{c}_{s,i}^\phi = \frac{c_{s,i}^{0,\phi} \cdot f_s^{0,\phi} + c_{s,i}^\phi \cdot \Delta f_s^\phi}{f_s^\phi}$$

$$\Delta H = \Sigma \Delta H_\phi = \Sigma [\Delta H_\phi(t) - \Delta H_\phi(t - \Delta t)]$$

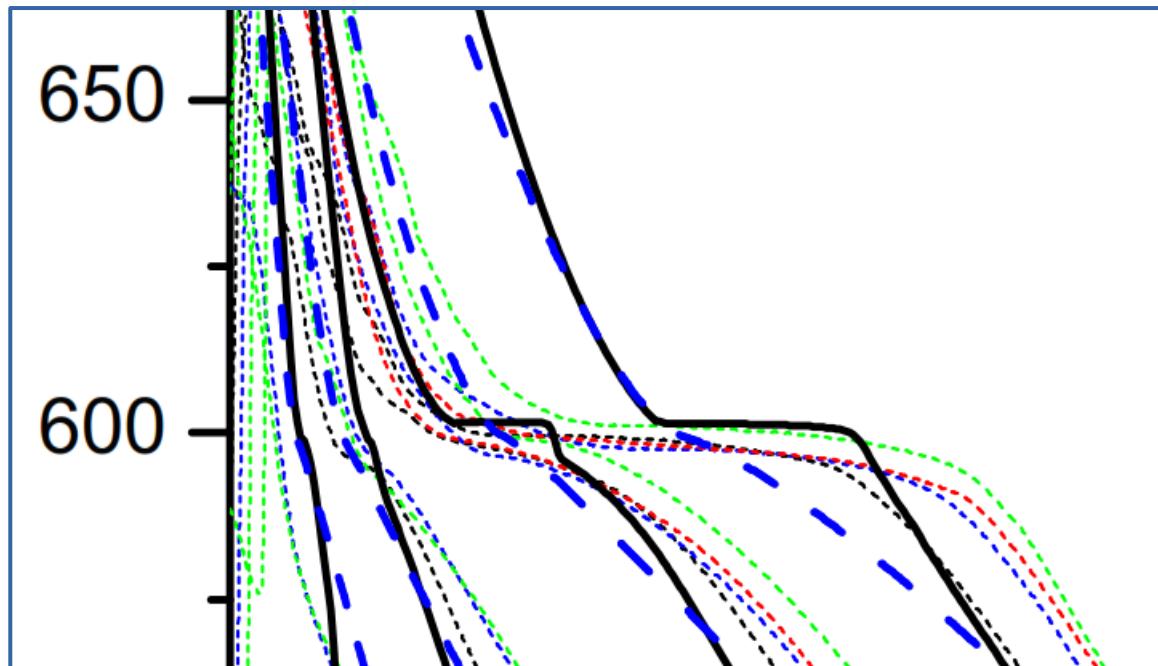
# RESULTS

## Temperature-time curves



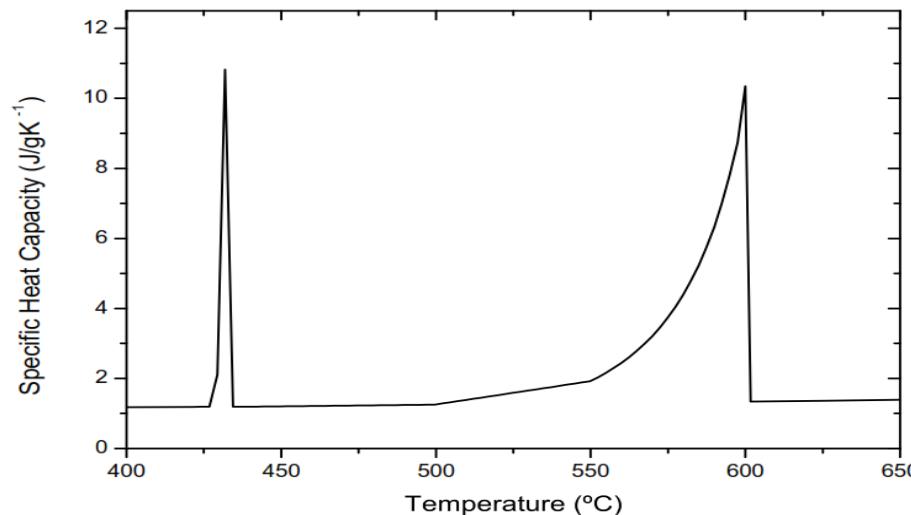
# RESULTS

## Temperature-time curves

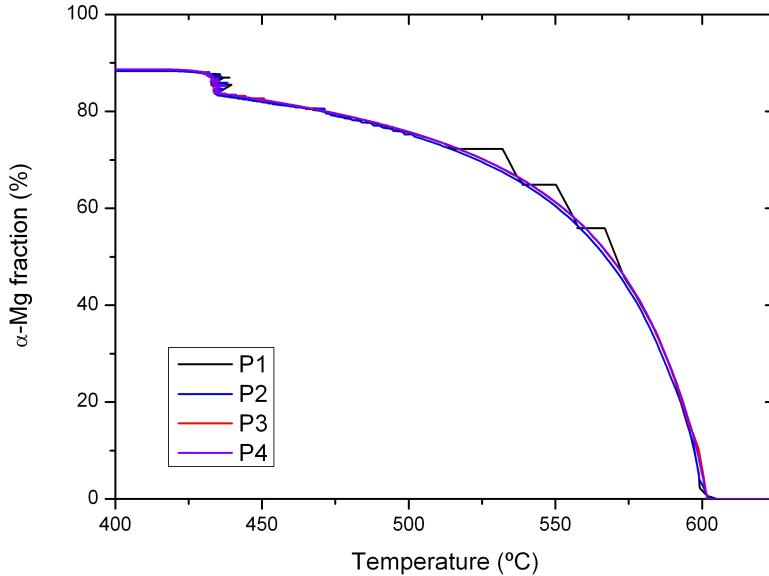
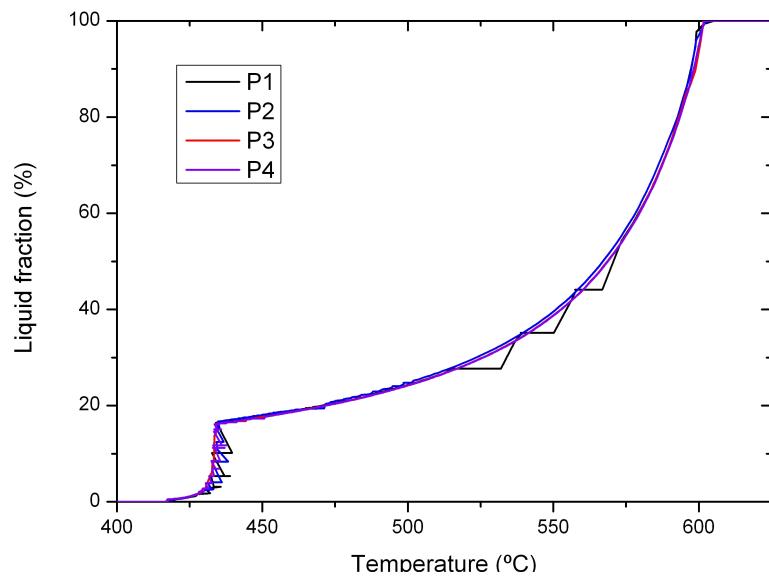


Difficulties reproducing the nucleation undercooling

$$\Delta T_n \uparrow \quad \Delta H_n \uparrow \quad c_p \downarrow$$

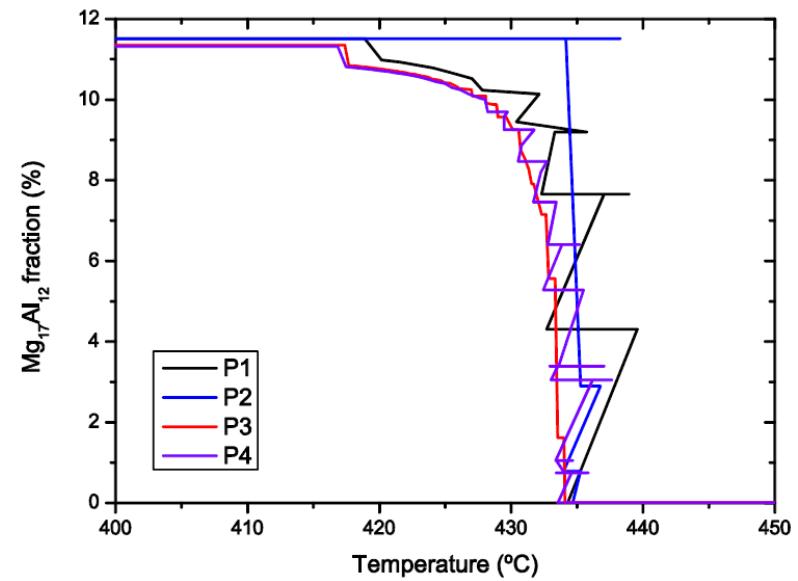


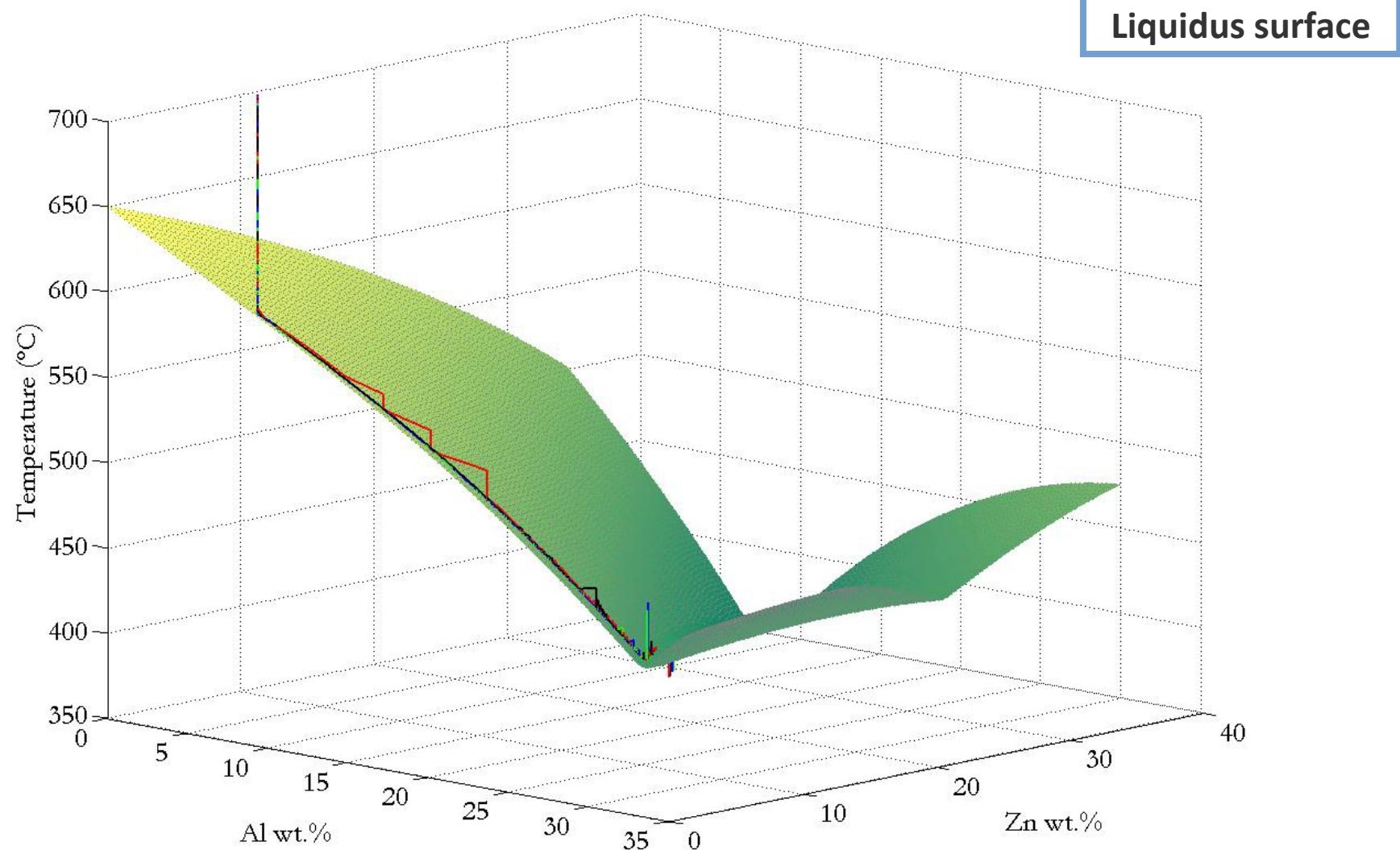
“False” recalescence effect

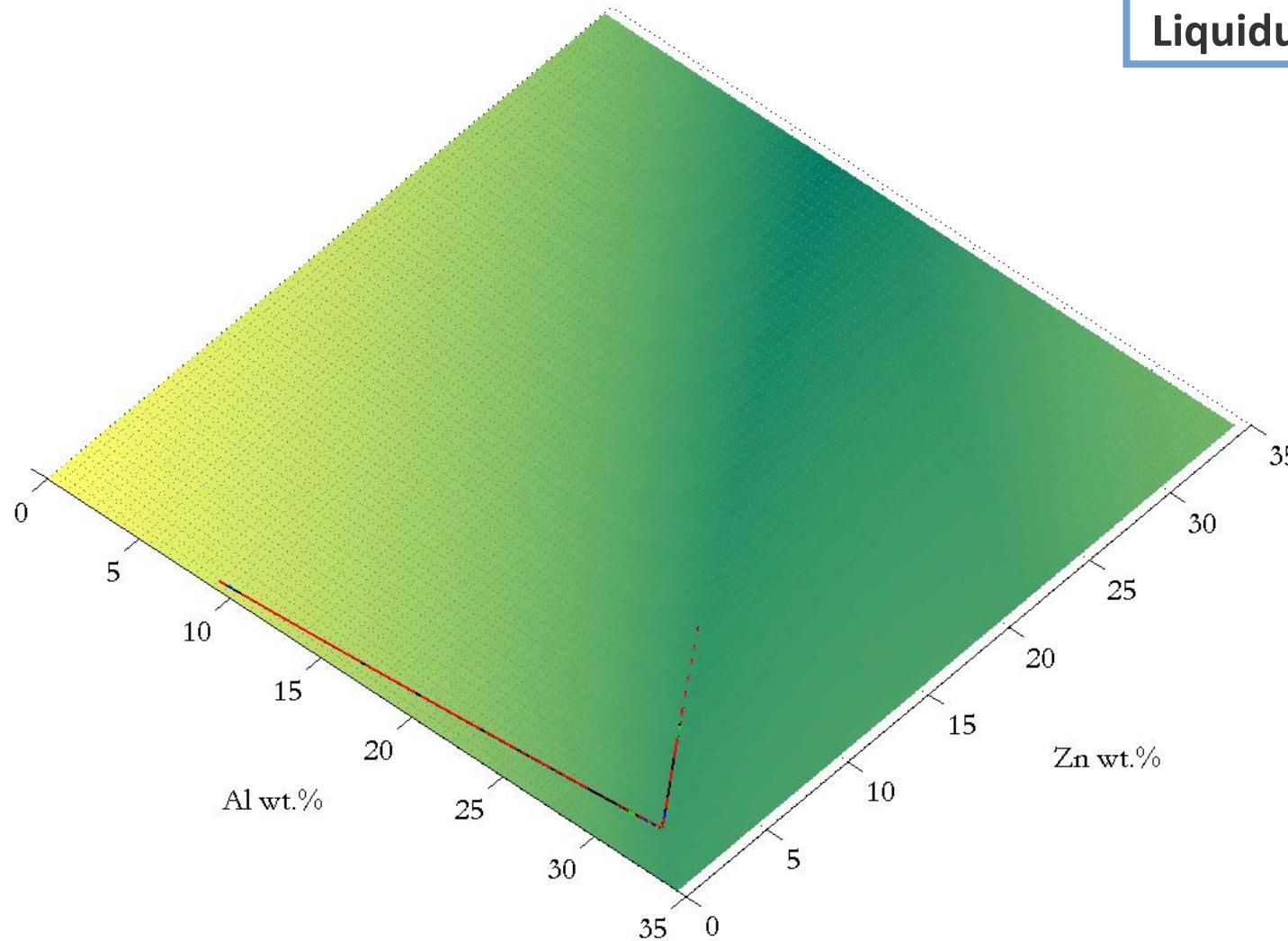


### Solidified phases

- 88.5 %  $\alpha(\text{Mg})$  [HCP\_A3]
- 11.5%  $\gamma(\text{Mg}_{17}\text{Al}_{12})$

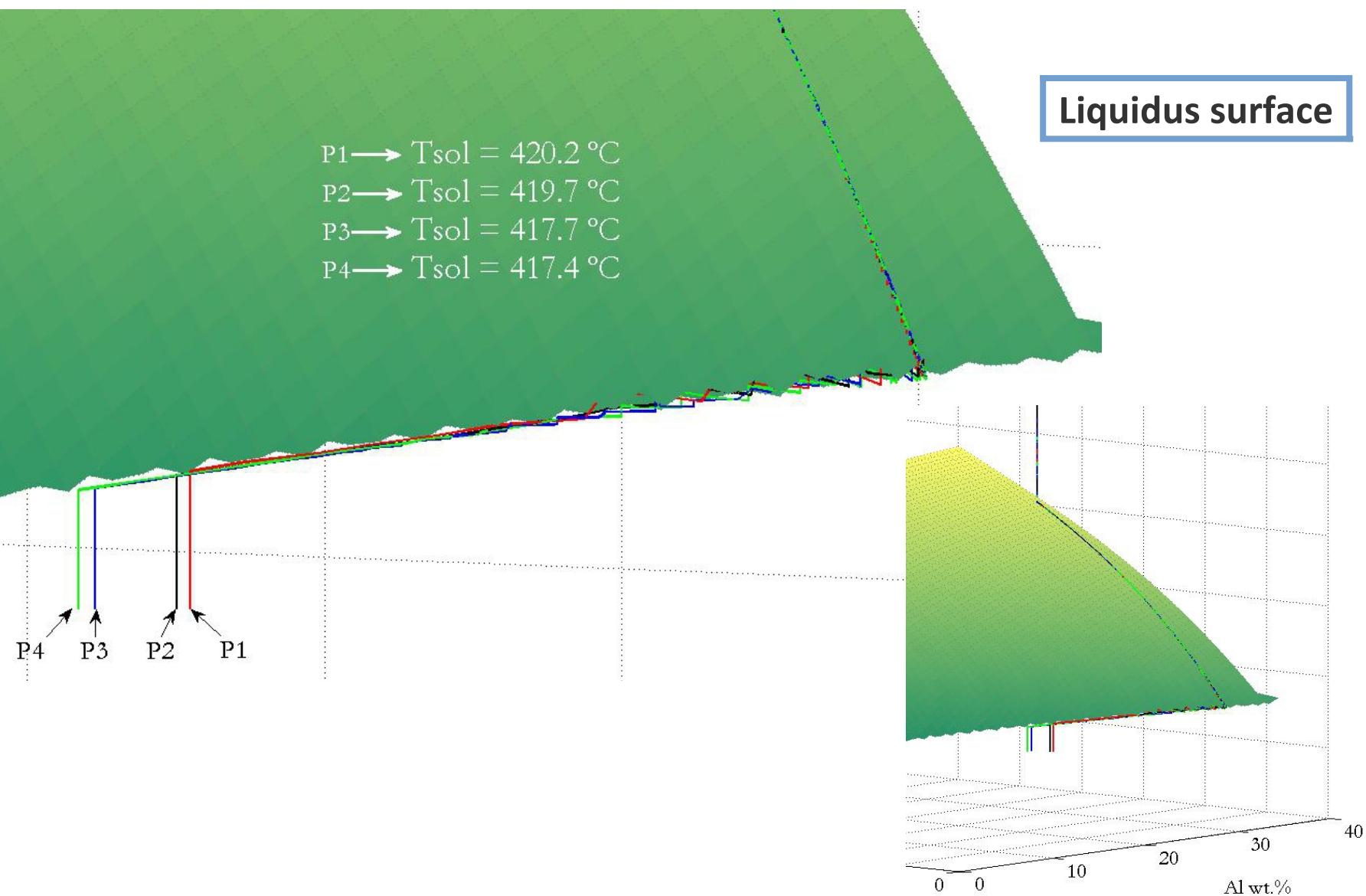


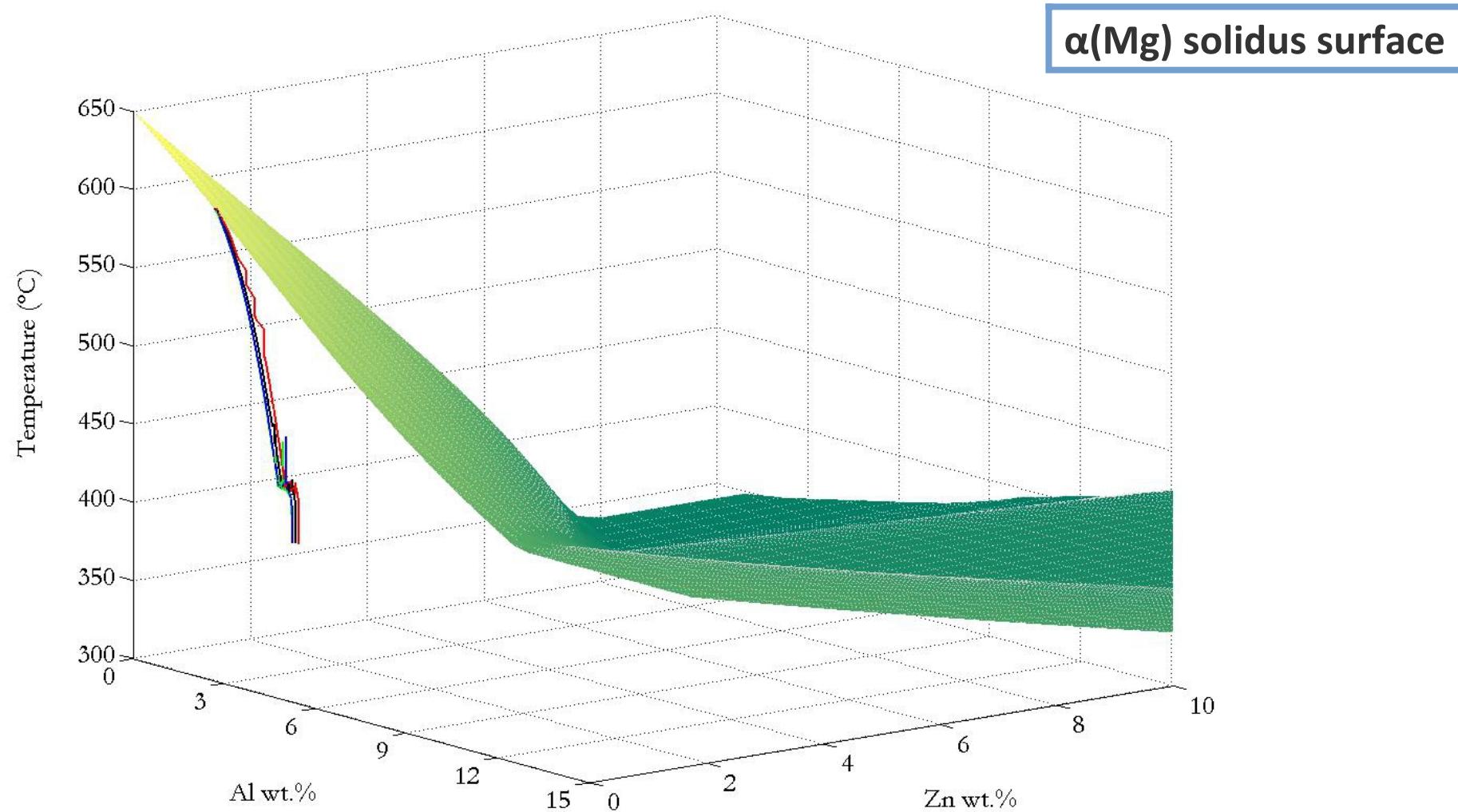


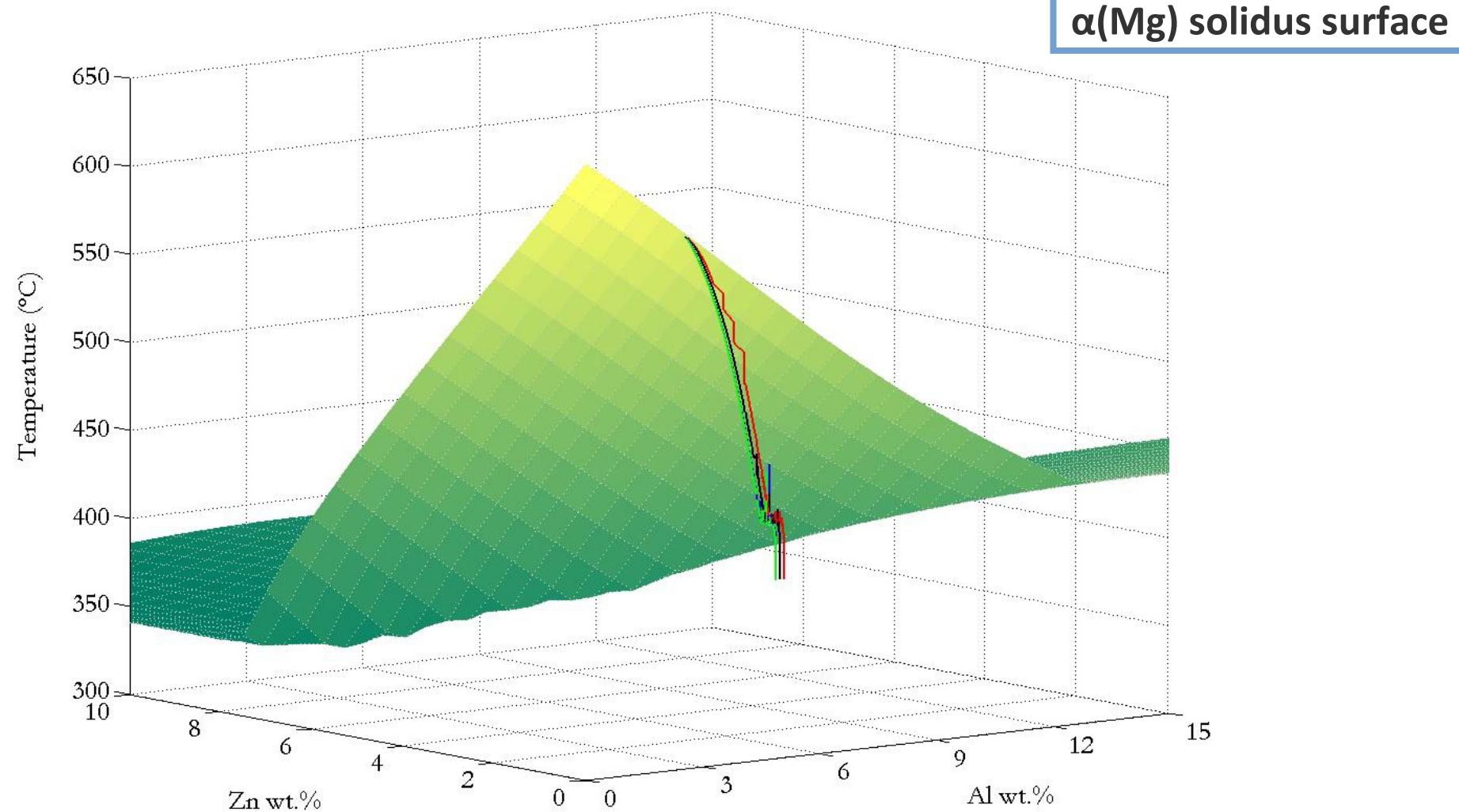


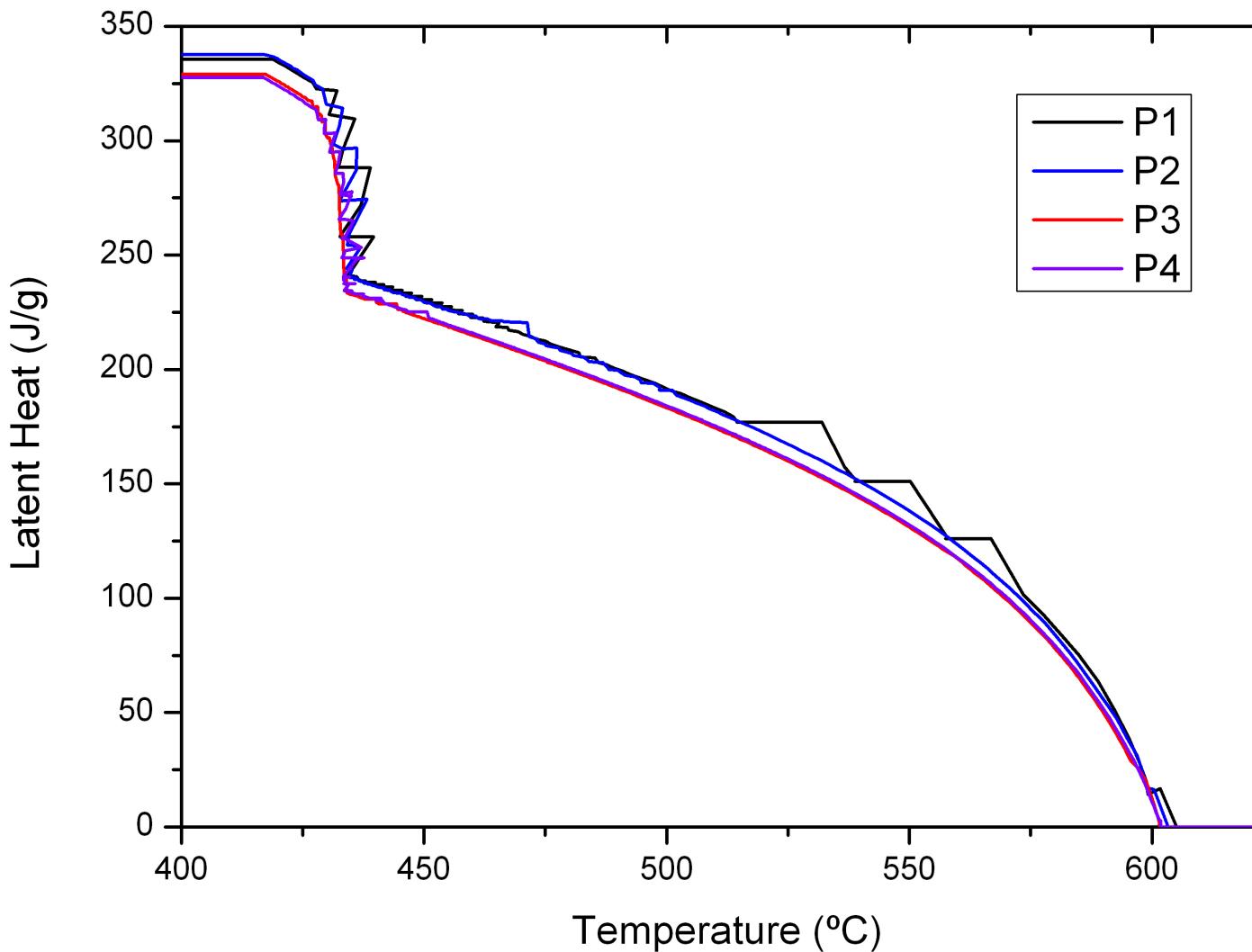
# RESULTS

## Phase Distribution







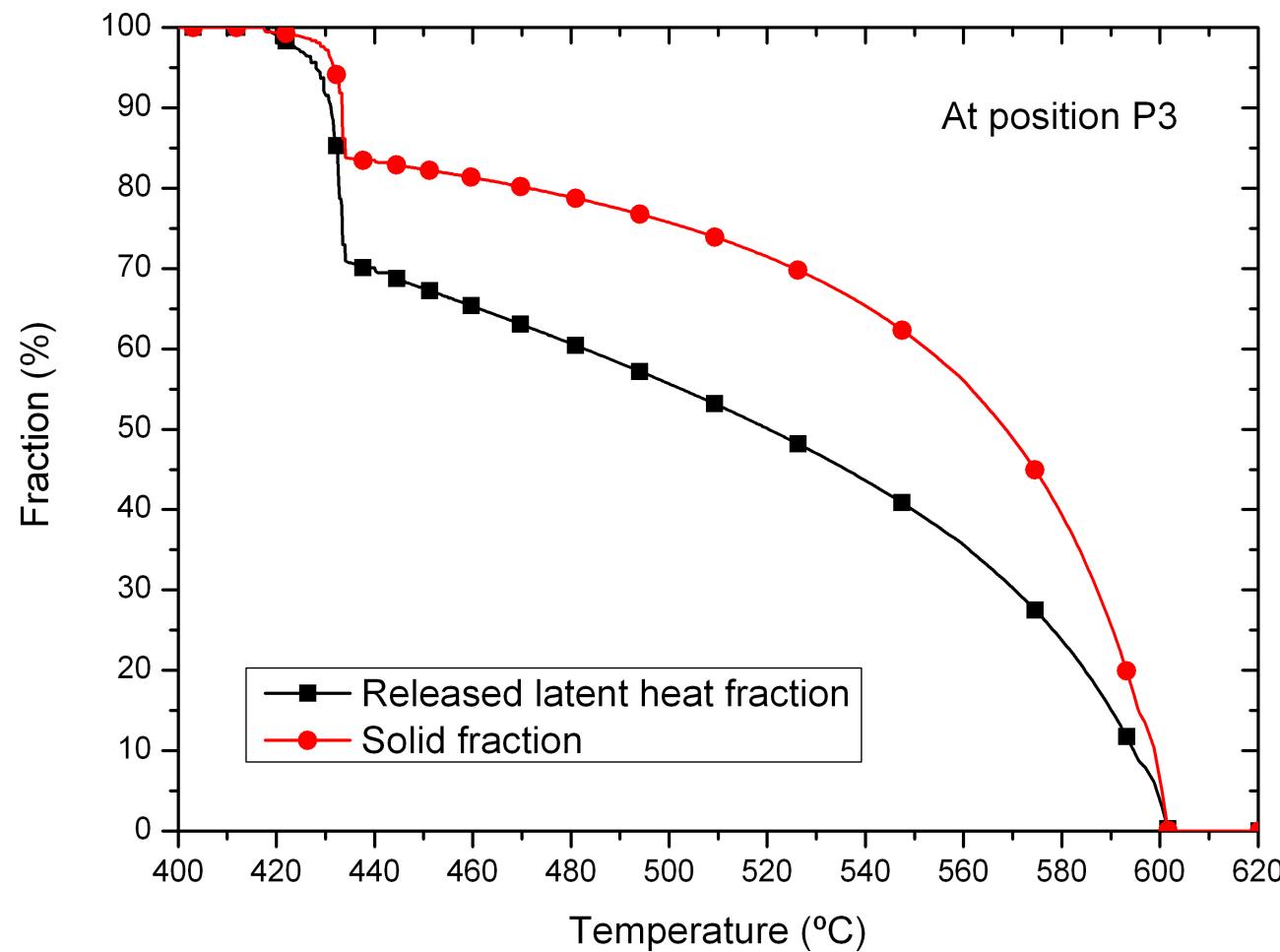


Total Latent Heat  
 $327 \text{ J/g} \div 337 \text{ J/g}$

No remarkable  
cooling rate effect

# RESULTS

## Latent Heat release vs Solid fraction



Remaining liquid before eutectic transformation → 15%

Latent heat released during eutectic transformation → 30%

- Macro-microscale modelling coupled to Calphad modelling improves the simulation of castings:
  - Multicomponent systems. No more binary systems.
  - Improved temperature-time descriptions.
  - Grain growth and impingement can be modelled.
  - Latent Heat release calculation in function of cooling rate.
  - Latent Heat release – Solid Fraction relationship uncoupled. Not proportionals.
  - Phase distribution and their composition calculated.

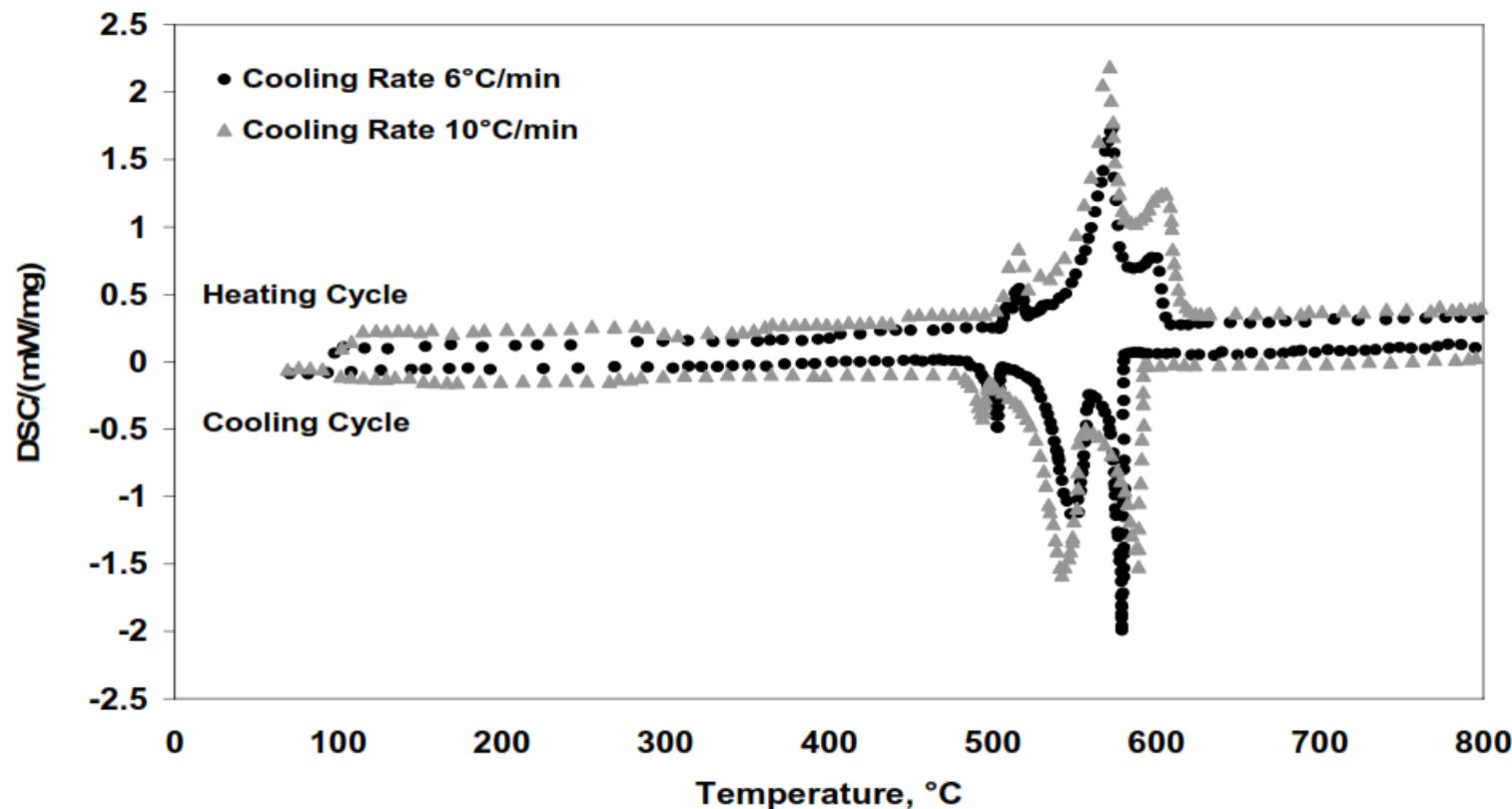
### FUTURE WORK

- Reduce calculation time.
- Improve nucleation description: nucleation undercooling,  $c_p$  description  $f(dT/dt)$
- Improve eutectic transformation description.

Danke für Ihre Aufmerksamkeit !!

Thank you for your attention !!

Eskerrik asko zuen arretagatik !!



*DSC curves for the 3XX aluminum alloys with 7wt% Si and 4wt% Cu for two heating and cooling rates.*

M. B. Djurdjevic *et al.*, *The Effect of Chemistry and Cooling Rate on the Latent Heat Released During the Solidification of the 3XX Series of Aluminum Alloys*, Materials Science Forum, Vols. 539-543 (2007) pp 299-304.