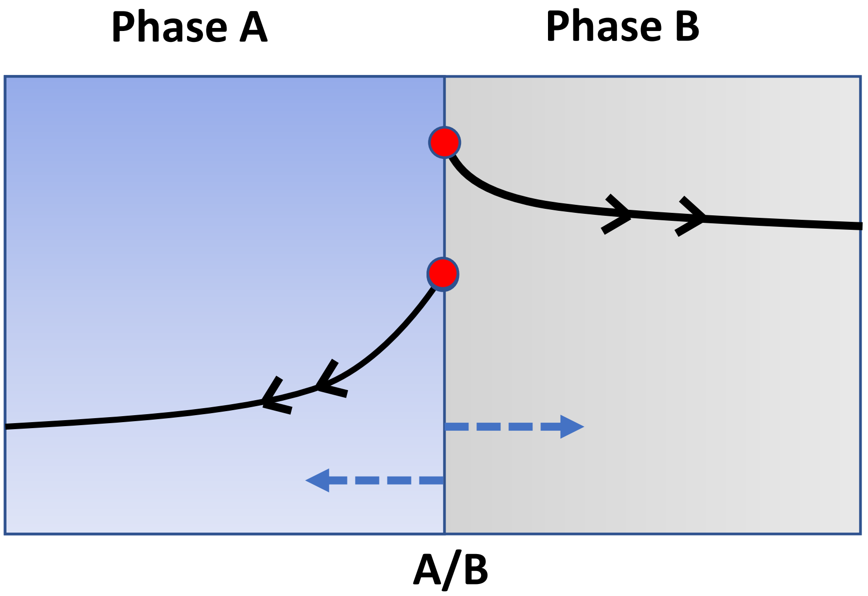
GTT Users meeting
29-30 June 2022

# Modelling of solid-state transformation kinetics in alloys using the ChemApp thermodynamic library: few case studies on commercial alloys

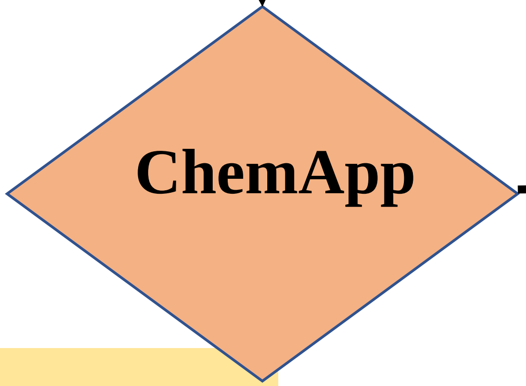
Manas Paliwal
Assistant Professor
Metallurgical and Materials Science
IIT Kharagpur

- *Nishant Kumar * SNU*
- *Ashutosh Kumar and Siddharth Samrah * McGill University*
- *Prof. In-Ho Jung SNU*

# ChemApp for solving phase transformation problems








$$v = \left(\frac{dx}{dt}\right) = \frac{J_k^{R/L} - J_k^{L/R}}{C_k^{R/L} - C_k^{L/R}}$$

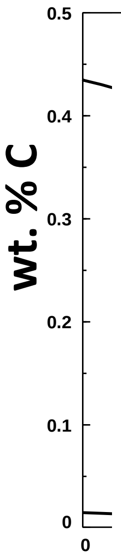
$$J_k = \sum_{j=0}^{n-1} D_{kj}^{n} \frac{\partial C_j}{\partial x}$$

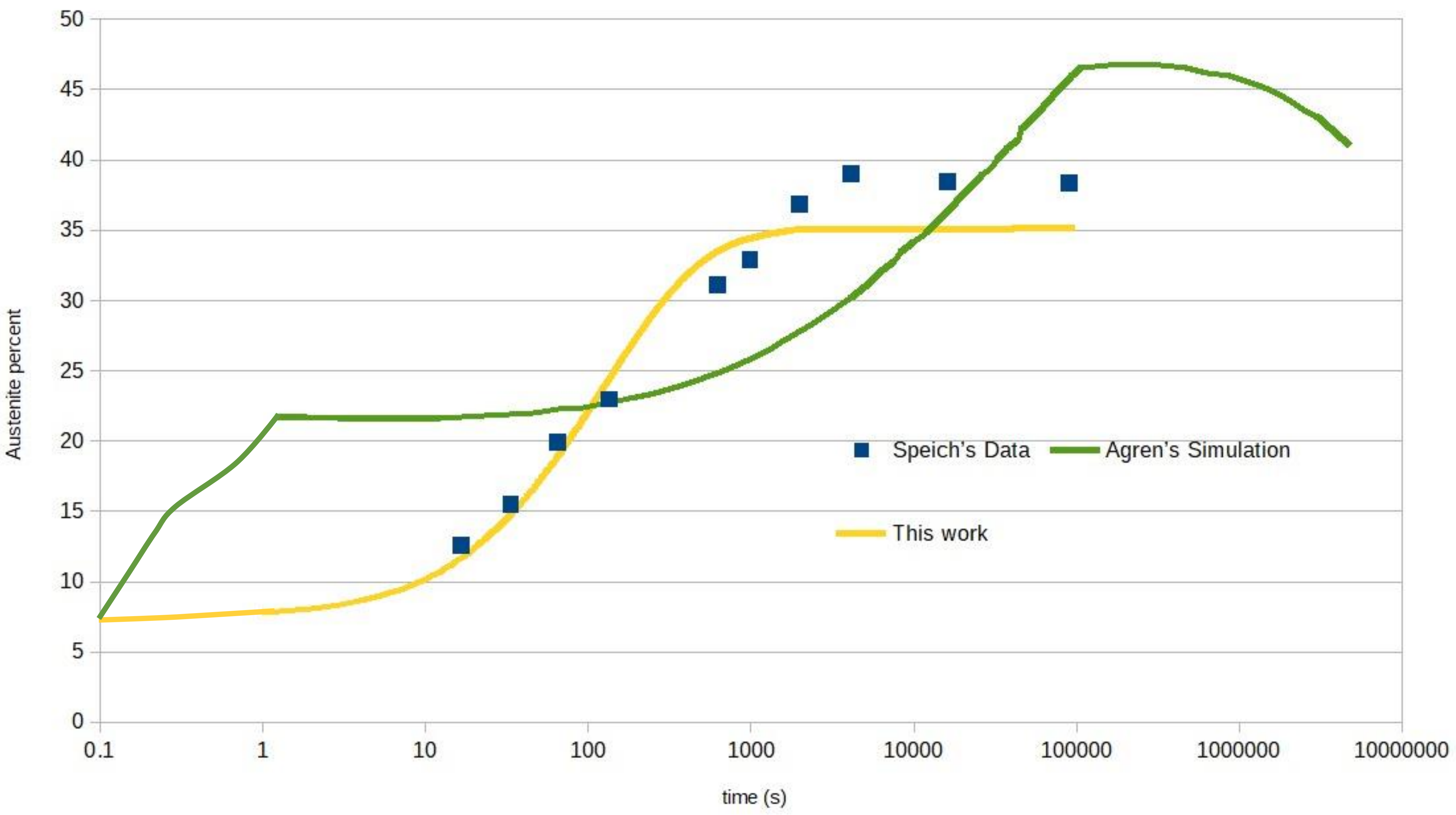
$$D_{kj}^{n} = \sum_{i=0}^{n} (\delta_{ik} - c_k) c_i M_i \left(\frac{\partial \mu_i}{\partial c_j} - \frac{\partial \mu_i}{\partial c_n}\right)$$

$$\frac{\partial C_k}{\partial t} = \nabla . \left(D_{kj}^{n} \nabla C_k\right)$$

* Solidification calculations
*Phase dissolution or growth
*Solute redistribution
*Precipitation calculations

# Ferrite to Austenite Growth: Fe-1.5 Mn-0.06 C system



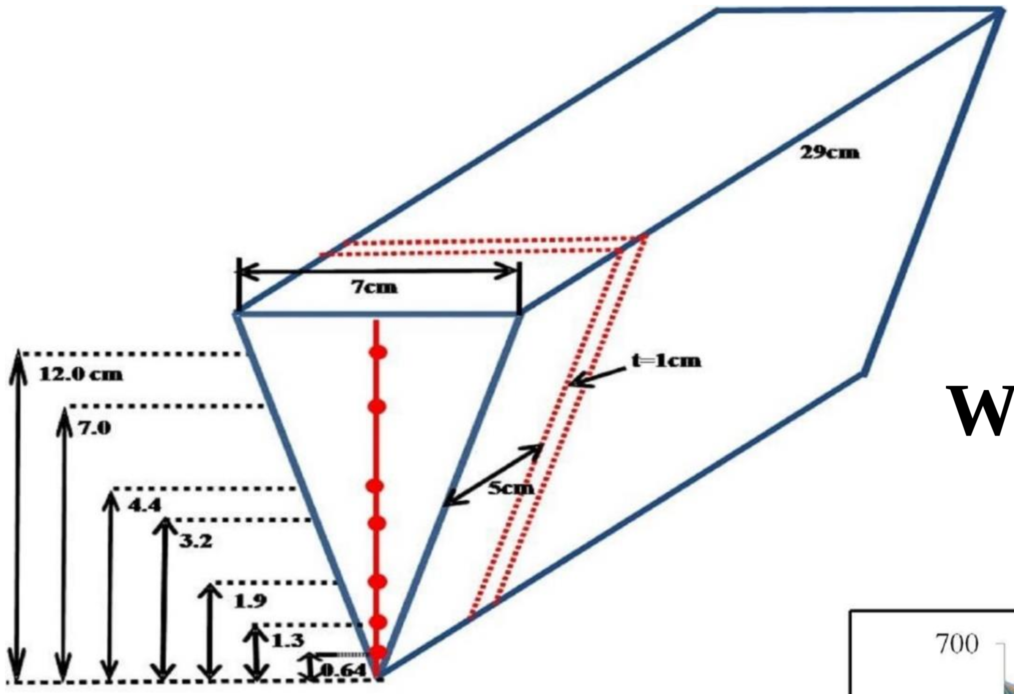




In

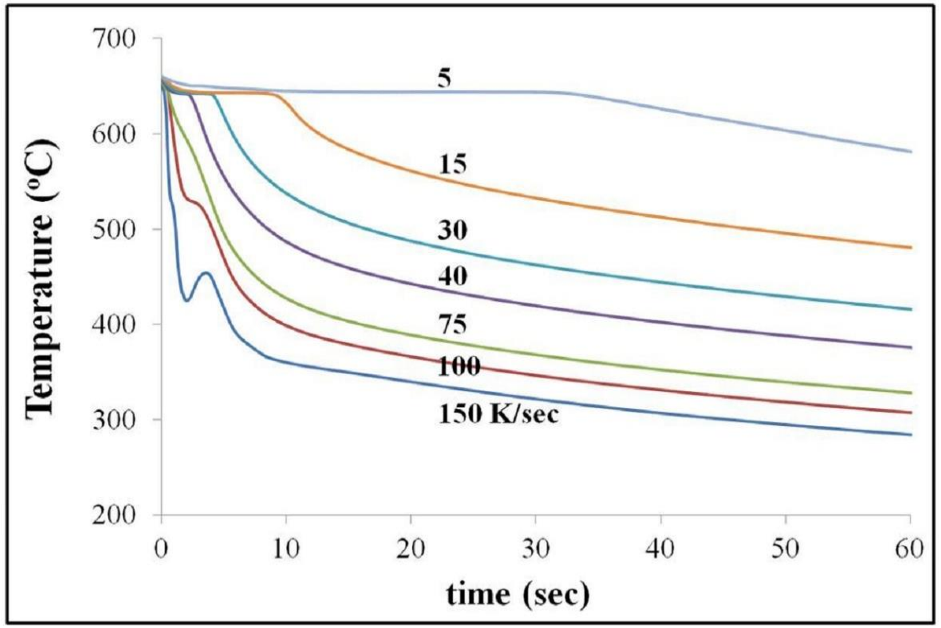
nanganese

Speich e

# Mg- 6 wt. % Sn – 1 wt. % Al: As-cast




Water cooled Cu mold



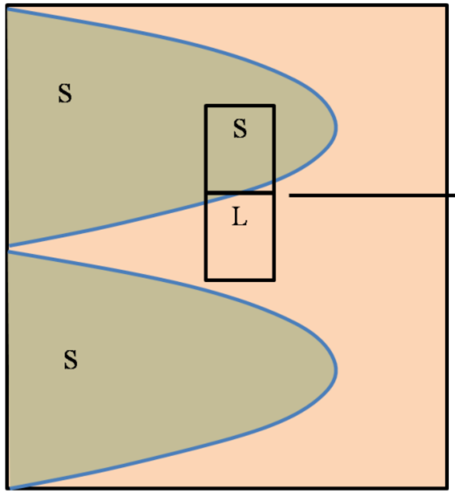
# Solidification model

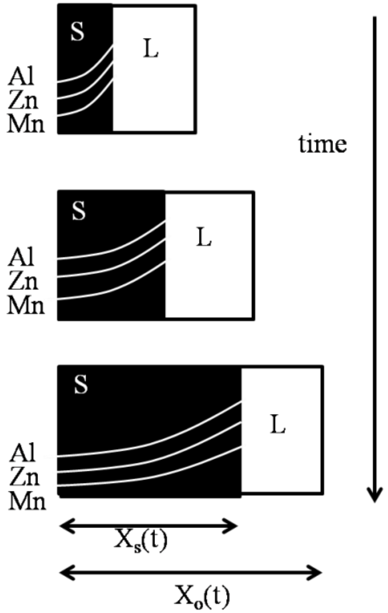
## Morphology

**Kurz, Giovanola and Trivedi (KGT model)**

Kurz W, Giovanola B, Trivedi R. Acta Metall. 1986:34:823

## Microsegregation




**Solute balance**

$$\int_0^{Xsi} C_{si}dx + \int_{Xsi}^{Xo} C_{li}dx = X_o C_{oi}$$

**Coarsening**[2]

$$X_o(t)^3 - X_o(0)^3 = \int_o^t M_i dt$$

**Backdiffusuion**

$$\frac{\partial C_{si}}{\partial t} = D_{si}\frac{\partial^2 C_{si}}{\partial x^2}$$

**Local thermodynamic eqb.**

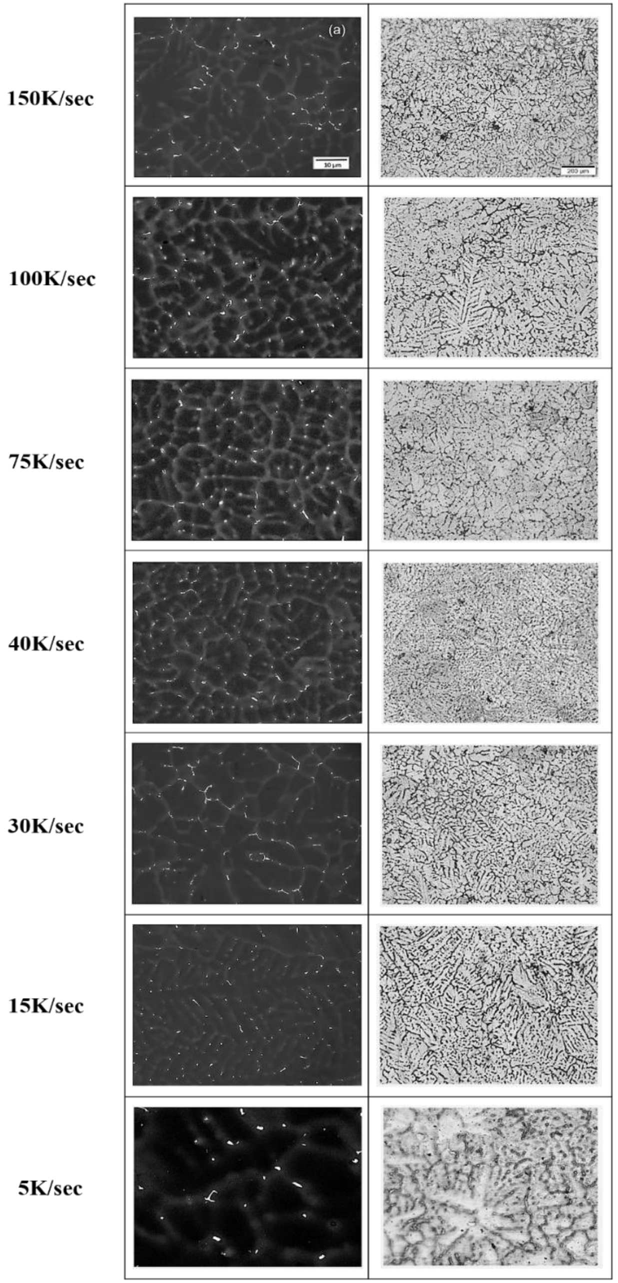
$$C_{si} = k_i C_{li}$$

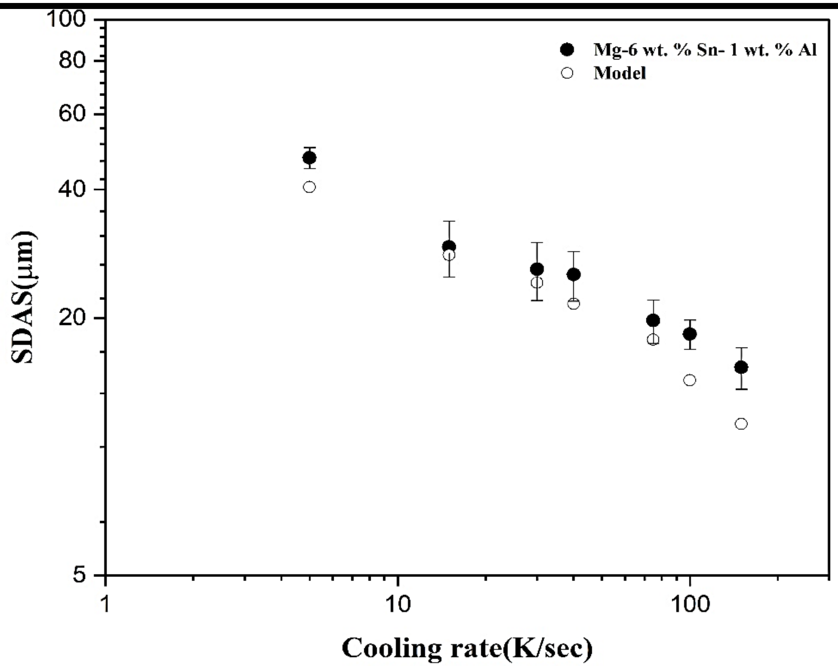

[4]. M. Paliwal and I.-H Jung, Acta Mat. 61 (2013) 4848-4860.
[5]. M. Paliwal, D.-H Kang, E. Esaadiqi and I.-H Jung Metall. Trans. 45A (2014) 3308-3320
[6]. M. Paliwal and I.-H Jung, J. Cryst. Growth, 394 (2014) 28-38.

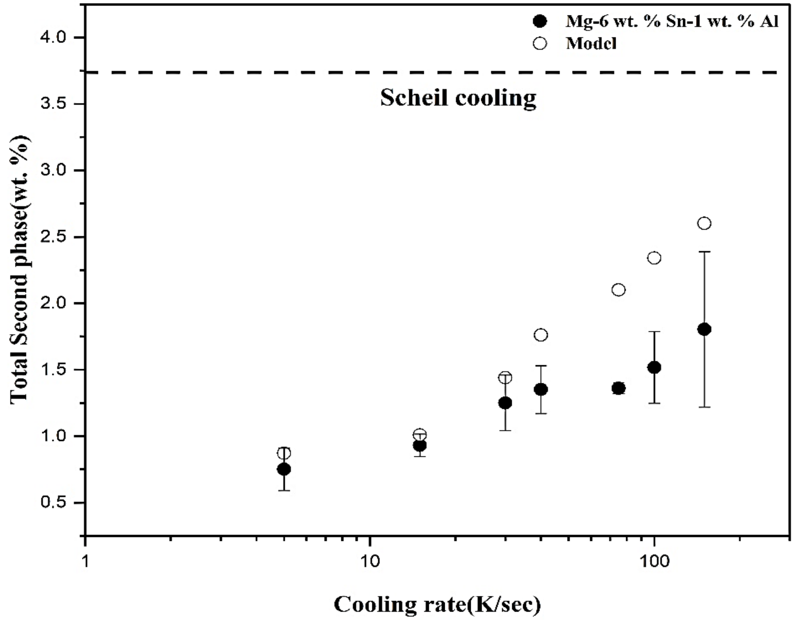



[2] Roosz et al. Mat. Sci. Tech. 1986:2:1149

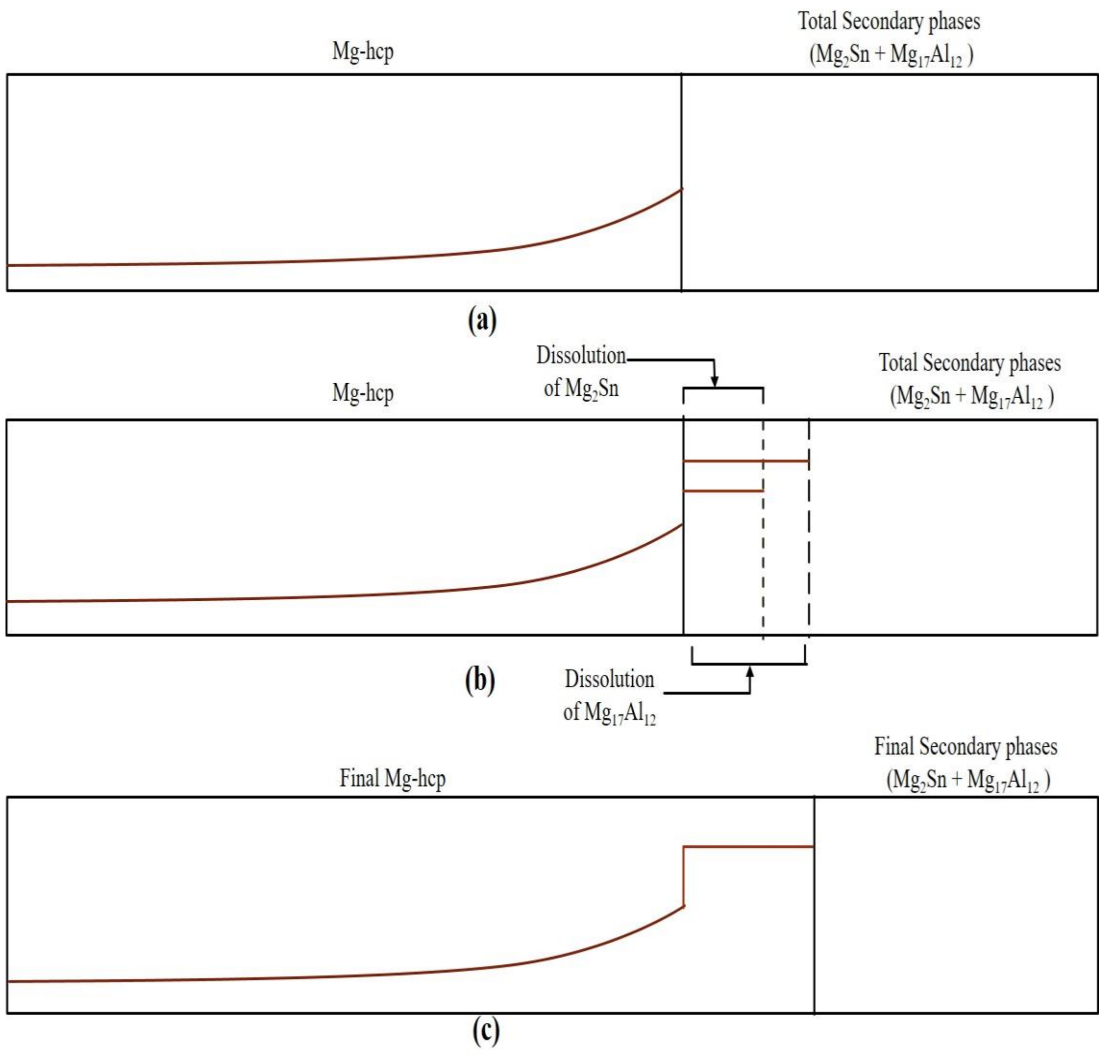
# Mg- 6 wt. % Sn – 1 wt. % Al: As-cast

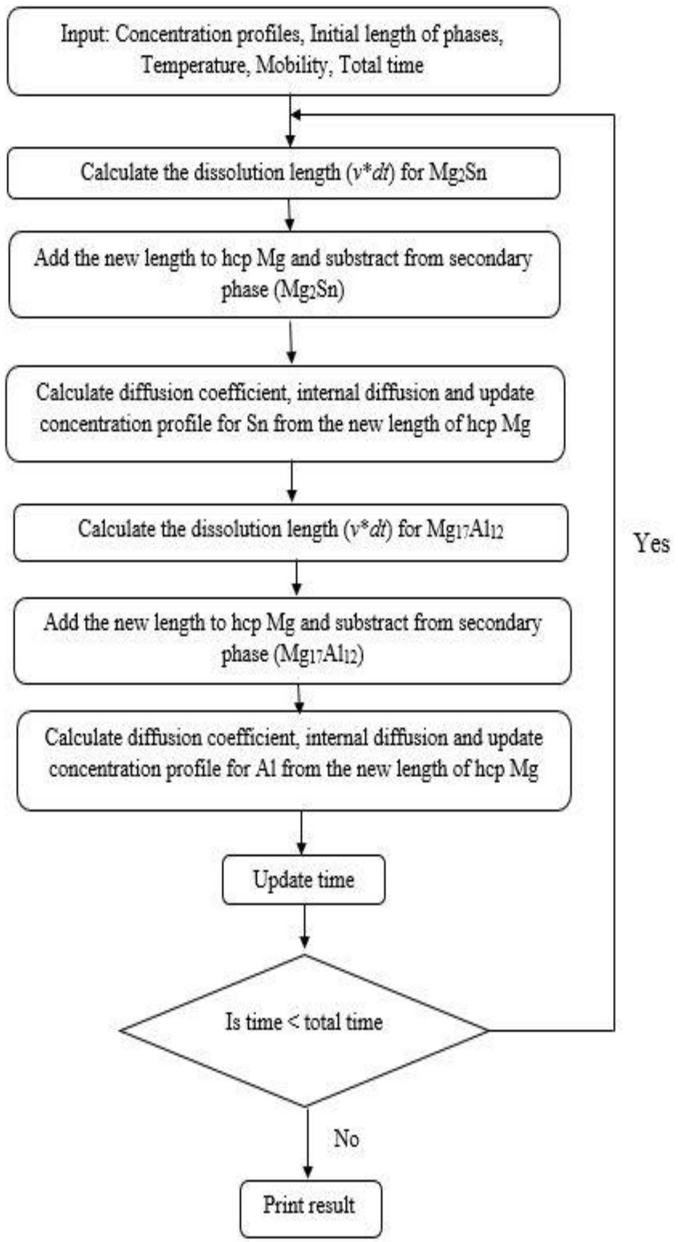


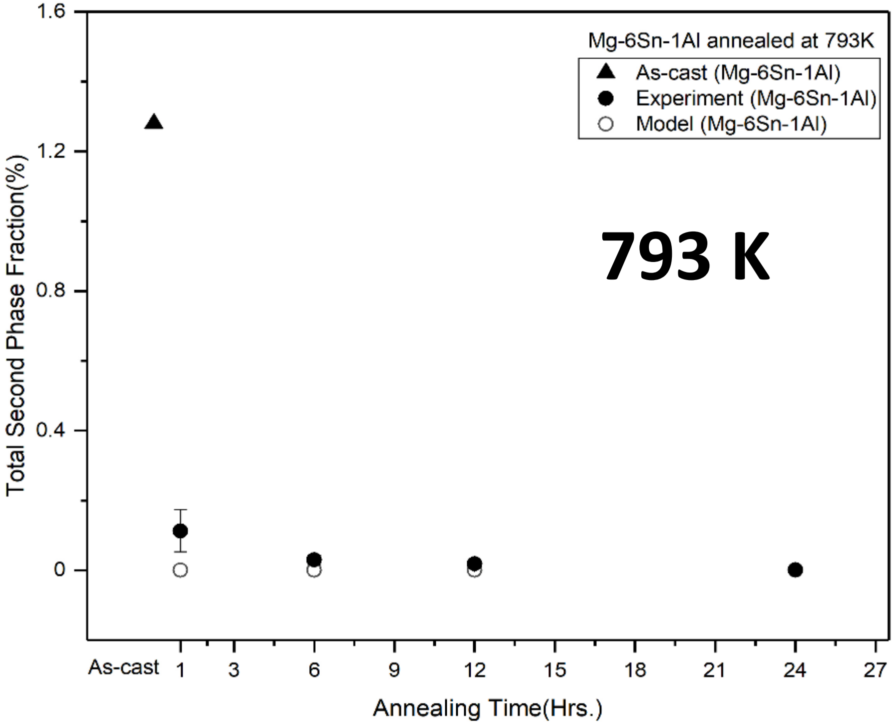



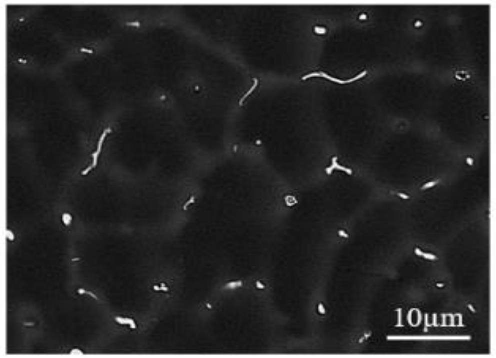
# Homogenization and dissolution model



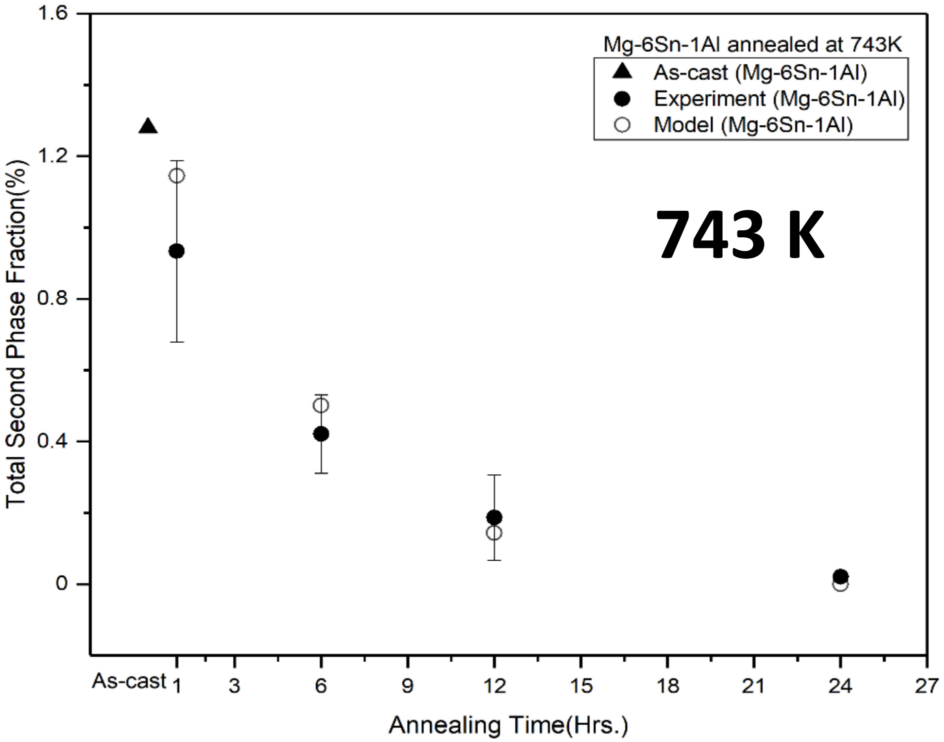



# Mg- 6 wt. % Sn – 1 wt. % Al: Homogenization



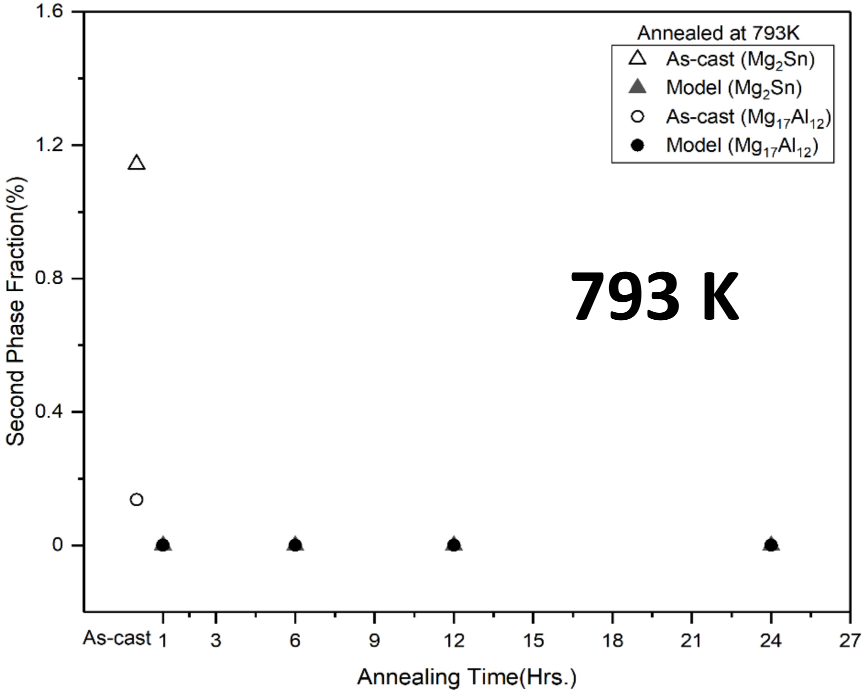



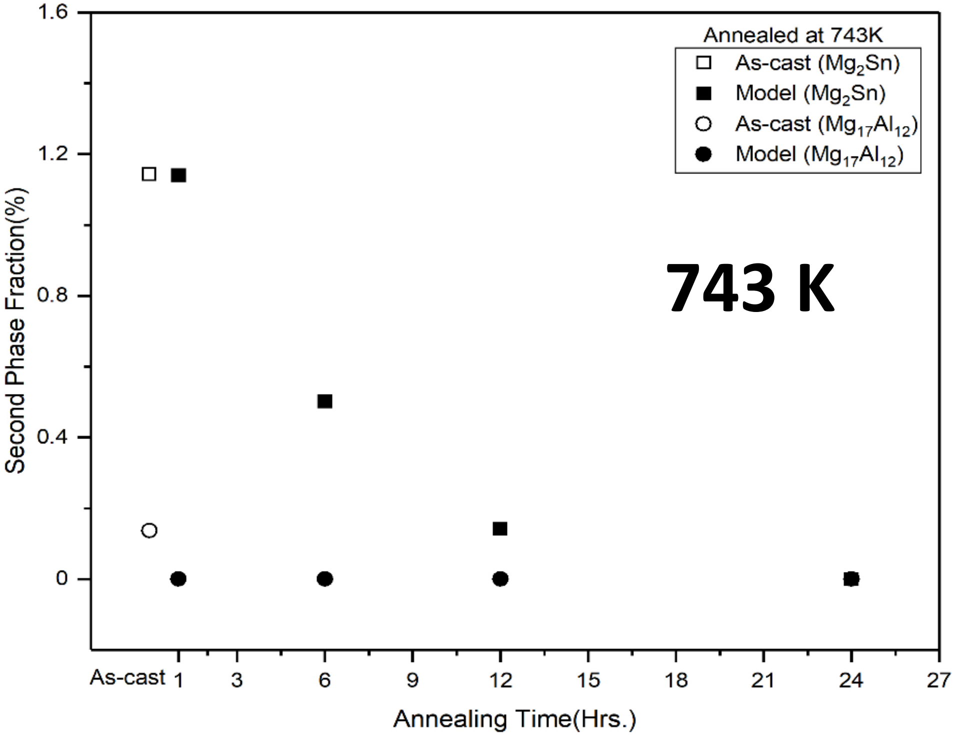

(cooling rate during casting 40K/sec)




**As-cast: $Mg_2Sn$ + $Mg_{17}Al_{12}$**

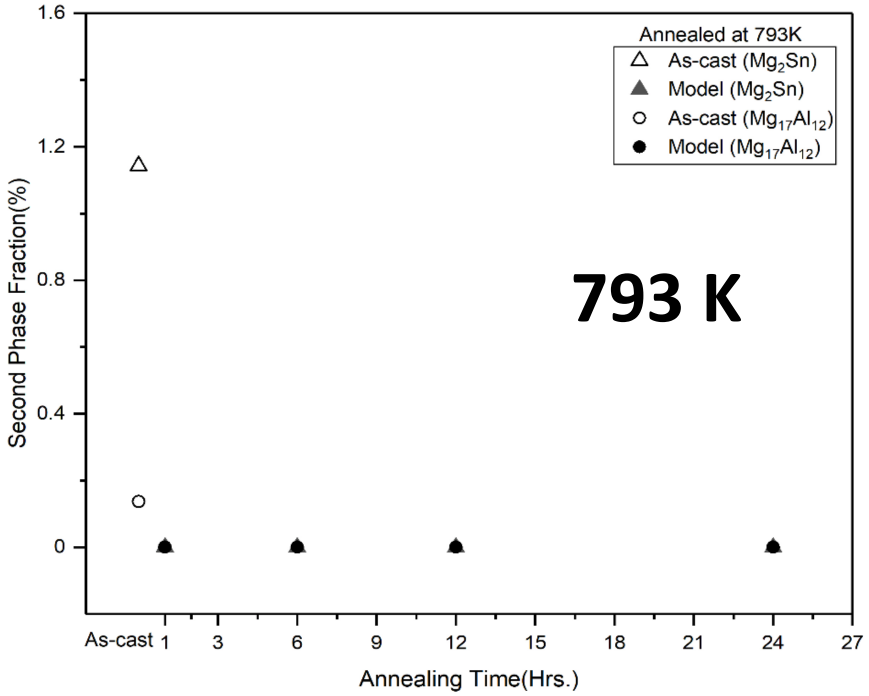
# Mg- 6 wt. % Sn – 1 wt. % Al

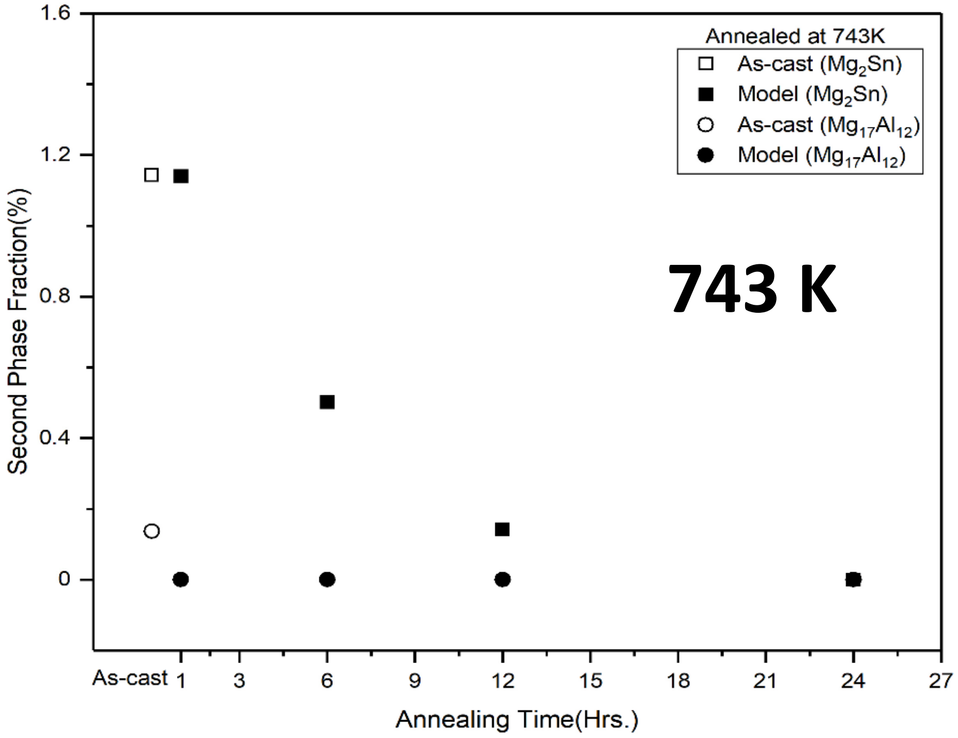



**Dissolution kinetics of $Mg_2Sn$ and $Mg_{17}Al_{12}$ phases are different**

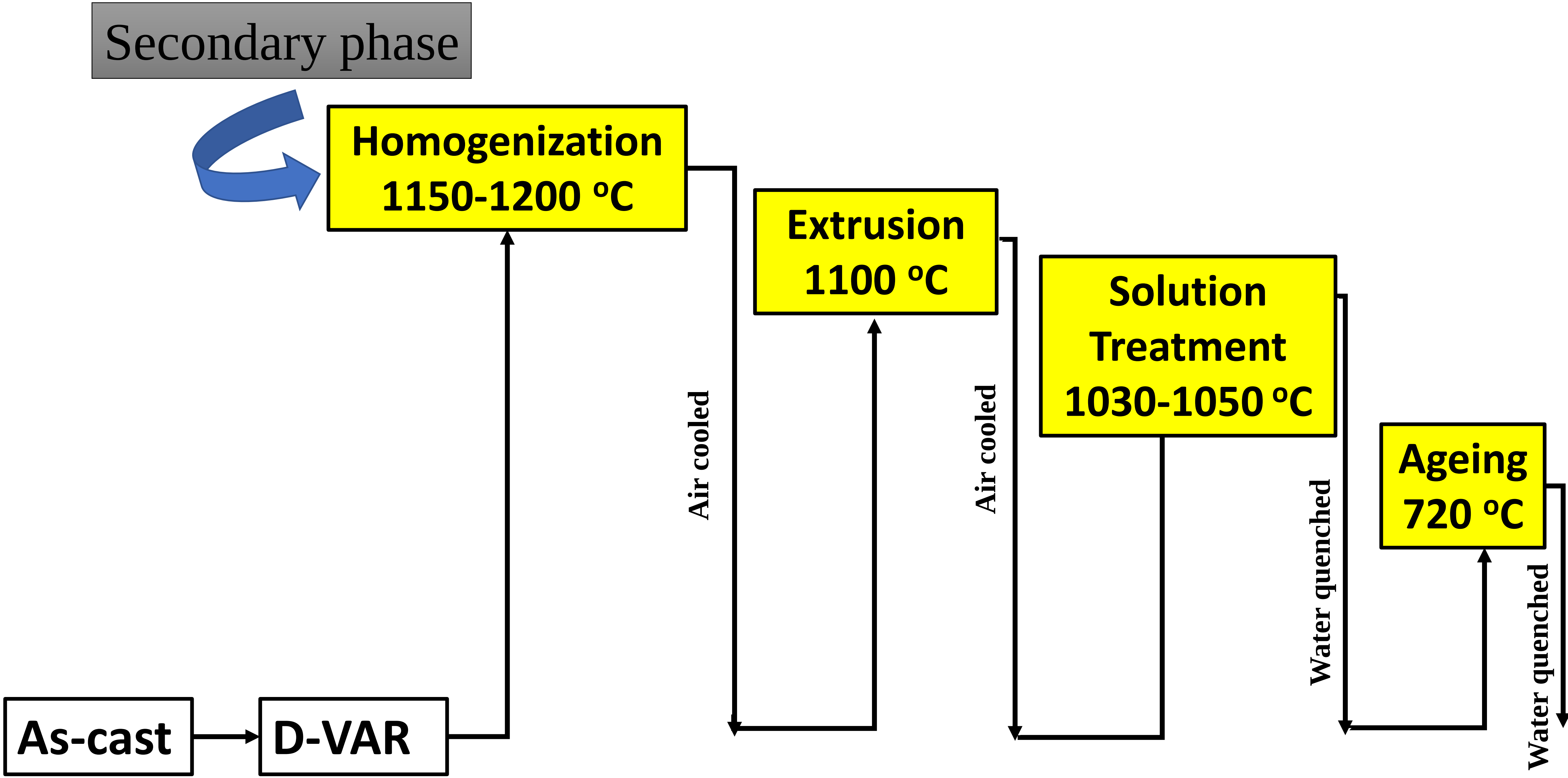
# Mg- 6 wt. % Sn – 1 wt. % Al



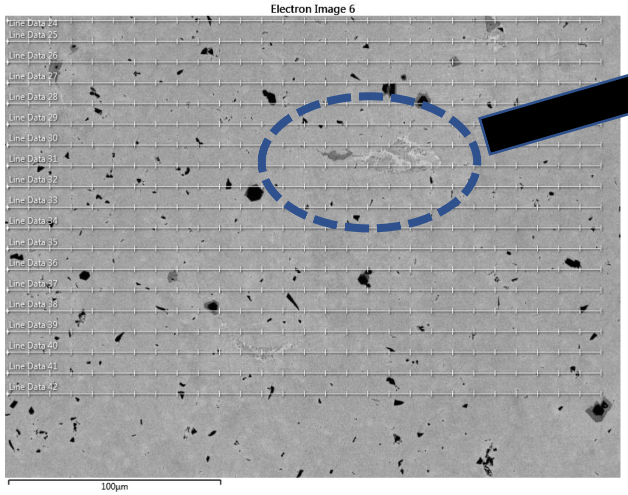




**Dissolution kinetics of $Mg_2Sn$ and $Mg_{17}Al_{12}$ phases are different**

# Ni alloy making route: Downstream process for 925 alloy

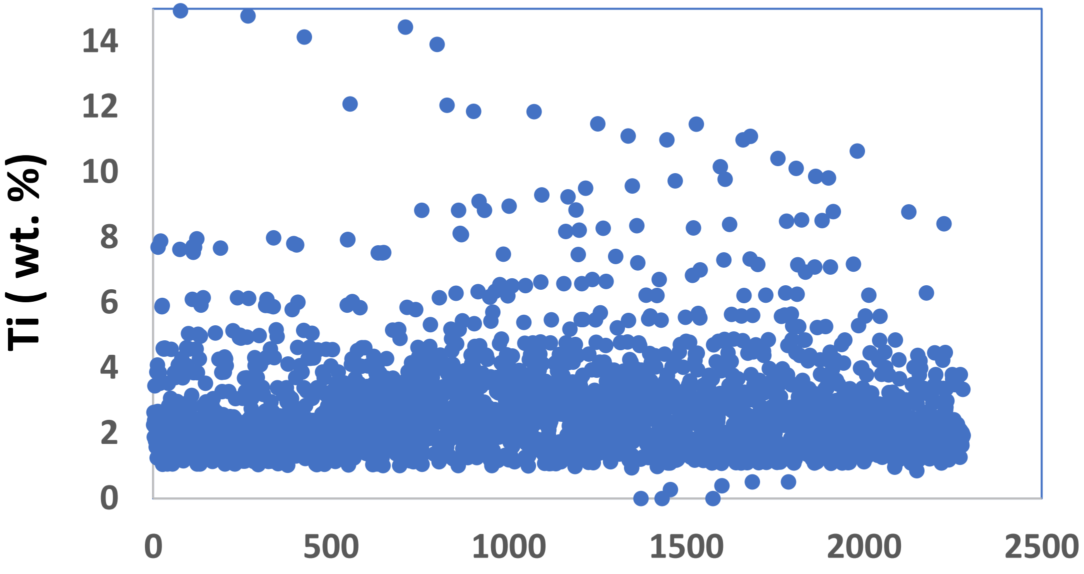


# 925 Alloy: As-cast microstructure characterization



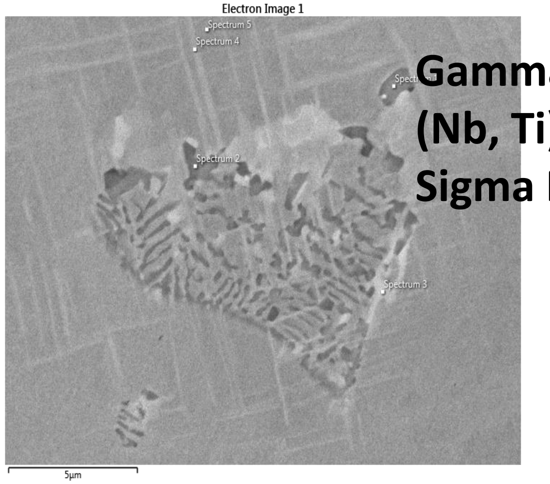


Complex microstructure



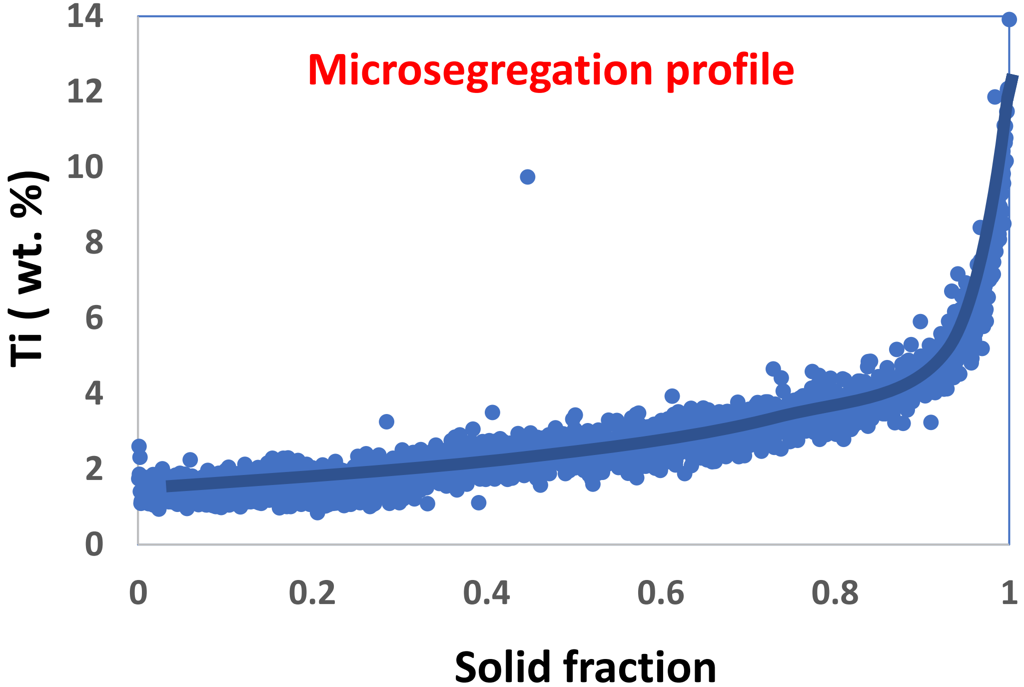

Sorting Algorithm: Microsegregation

Secondary Phases




Gamma Phase,
(Nb, Ti) (C,N)
Sigma Phase

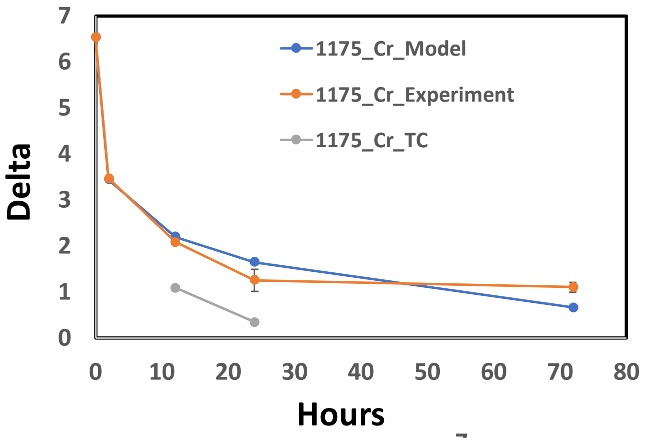
Homogenization calculations

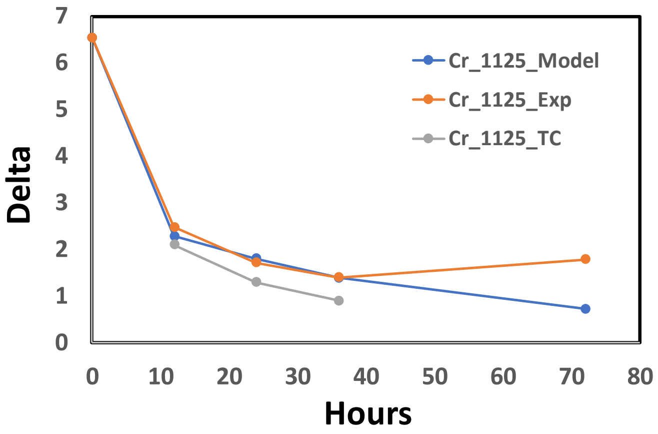


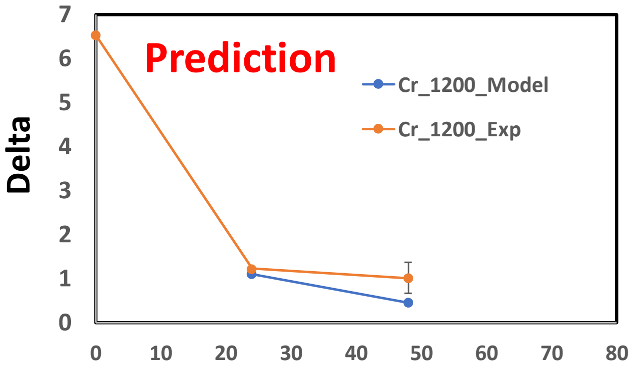
# Ni 925 alloy: Homogenization

| C | Si | Mn | Cr | Ni | Mo | W | Co | V | Ti | Cu | Al | Nb | B | N | Mg |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.01 | 0.2 | 0.39 | 20.25 | 42.75 | 3.03 | <0.01 | 0.033 | 0.054 | 2.38 | 1.92 | 0.26 | 0.31 | 0.0029 | 0.007 | 0.032 |

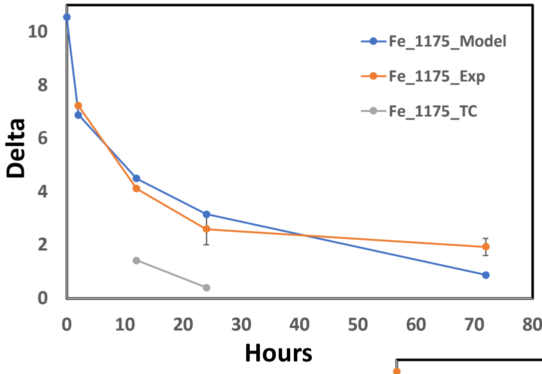
## Cr

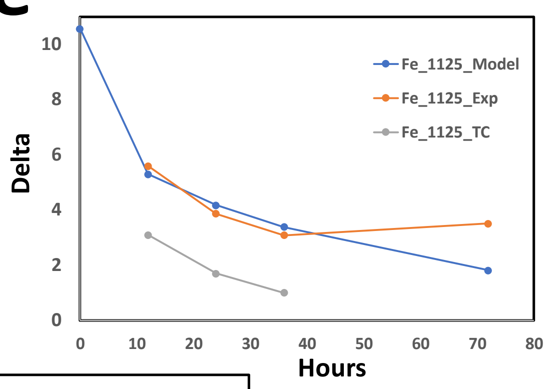


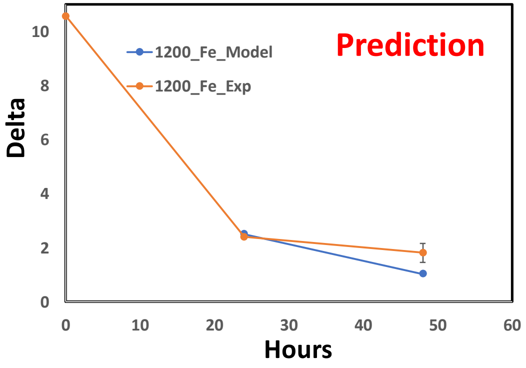




## Fe

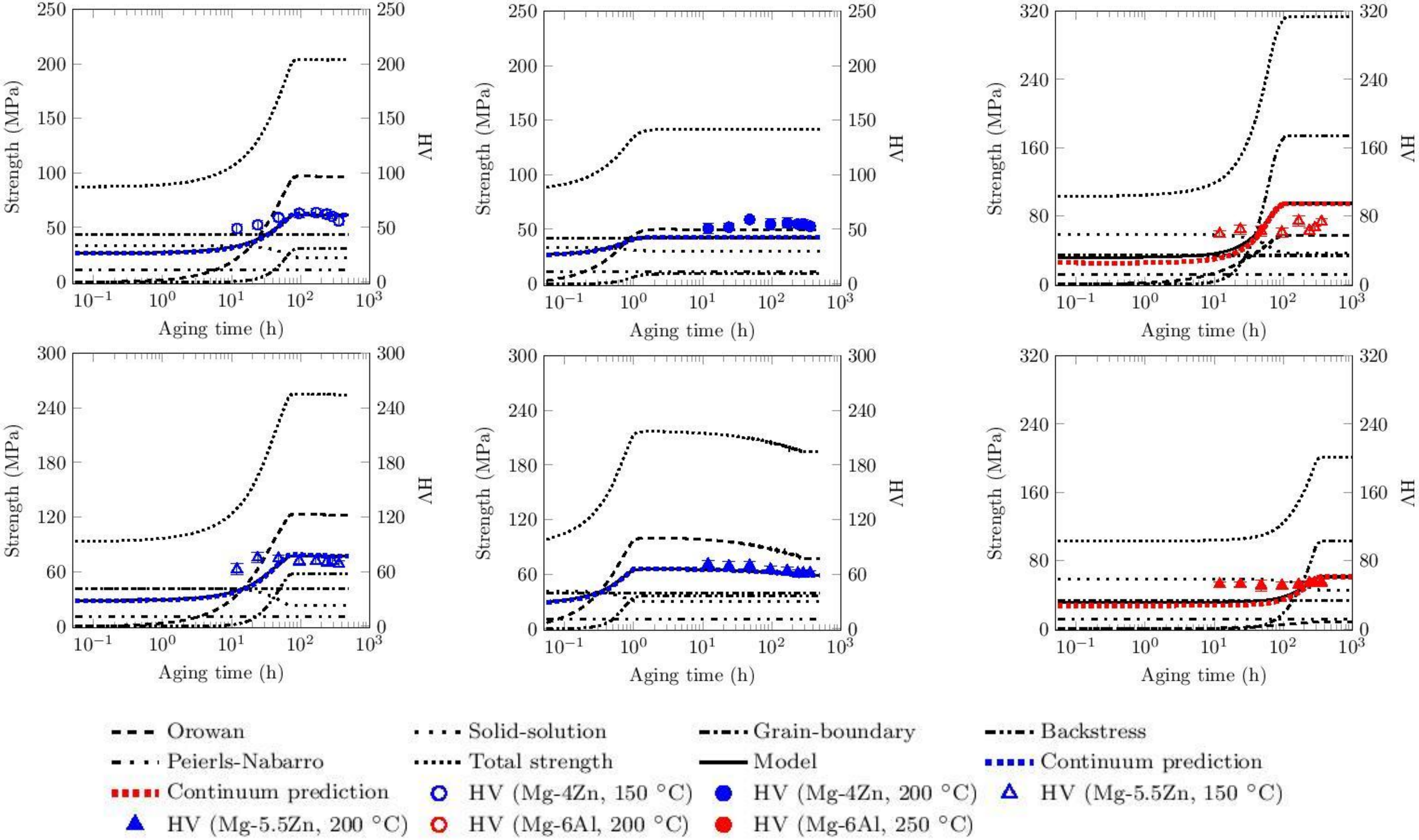


# Summary and future/current work

## Strength Prediction




* Samrah et al. Mechanics of Materials 2022

**Thank you**

**manas.paliwal@metal.iitkgp.ac.in**