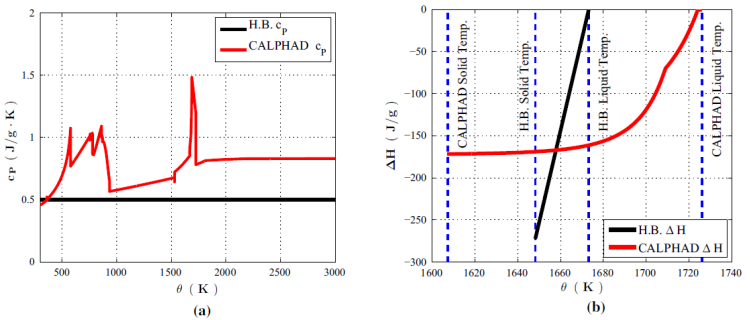
Thermo-Calc Software

Development of Non-Equilibrium Thermodynamic Tools for Additive Manufacturing

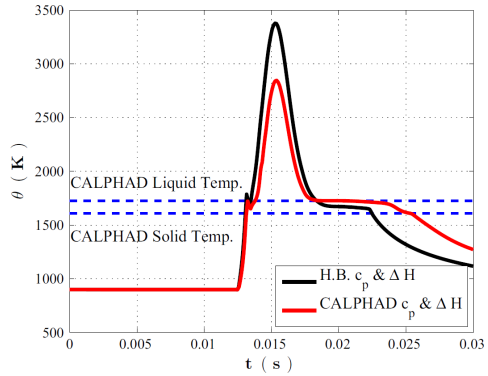
CALPHAD data: for mechanical/thermal FEA modeling

- Data is not always available for specific heats of material
- General ‘alloy’ data may be available from a handbook, but this is usually a constant value
- How do you tweak your model when the chemistry of your material is different heat to heat?
- Properties like specific heat, density, enthalpy, mobilities, latent heat can be calculated as a function of chemistry and temperature - and used as inputs into other codes to determine heat transfer, stress distributions etc.
- Comparison from Smith et al. of calculated specific heat and enthalpy change vs handbook value for a 316L stainless steel – note over 500K change in peak temperature prediction, as well as 2x change in solidification time – this also has an effect on weld pool geometry

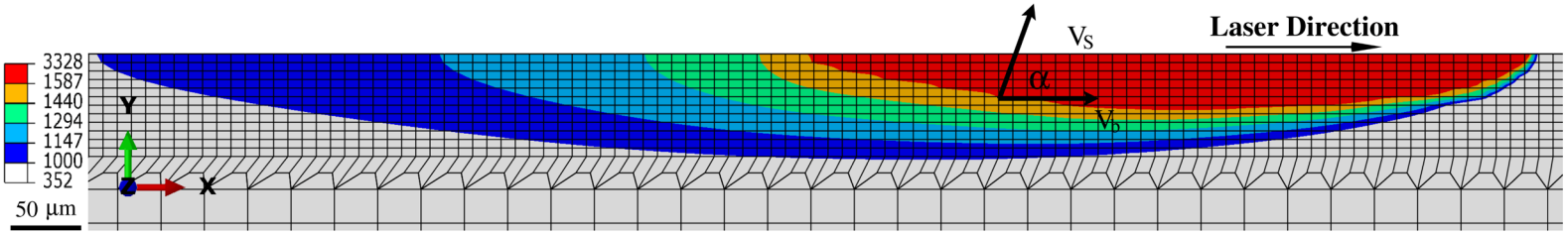


Comparison of handbook values and CALPHAD calculated values of Cp (left) and ΔH (right) – from Smith, et al. / *Computational Mechanics* 57.4 (2016): 583-610.

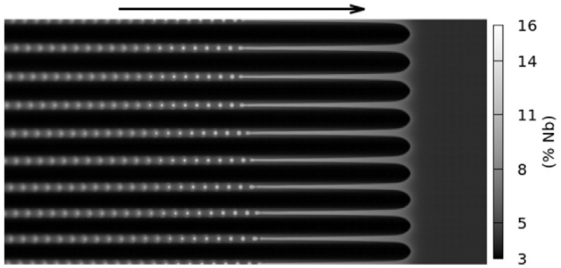
Resulting temperature vs time predictions for a selected node in an FEA simulation – also from Smith, et al.



Applications to mechanical/thermal FEA modeling



- Keller et al. used a transient thermal model in ABAQUS to model one layer of powder deposition of laser melted Alloy 625 powder.
- Specific heat capacity and density were taken as functions of temperature from a Thermo-Calc Scheil simulation and used as inputs in the ABAQUS model.
  - This allows for the full effect of segregation during solidification, and possible eutectic phase formation (NbC, Laves) to be taken into account in the Cp and density values.
- From this – the pool shape and resulting solidification speed Vs = V_{laser}*cos(α) can be determined along with thermal gradient G
- These two values are needed for a phase field simulation to predict the dendrite arm spacing
- Keller also simulated this, found reasonable agreement of dendrite arm spacing



Phase field simulation of cellular dendrite structure (brightness = wt% Nb)

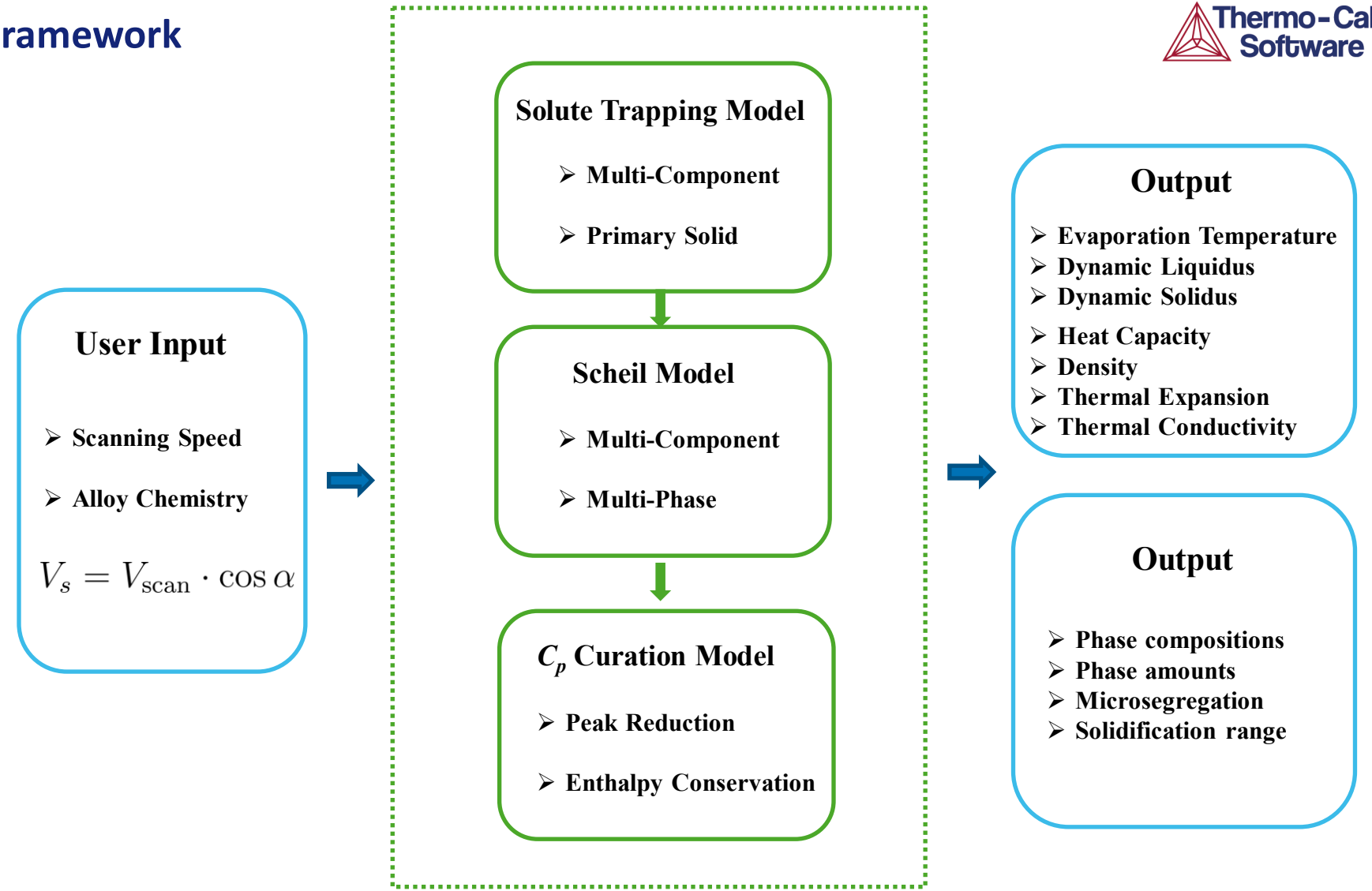
Keller, Trevor, et al. "Application of finite element, phase-field, and CALPHAD-based methods to additive manufacturing of Ni-based superalloys." *Acta materialia* 139 (2017): 244-253.

Purpose

- **Non-equilibrium conditions: property changes as function of solidification speed**
  - Solute trapping effect that changes the solute partition between liquid and solid phases
  - Microstructure changes due to varying solidification speed, e.g. microsegregation, solid phase amounts, etc.
  - Consequent changes of thermal and thermophysical properties

- **Data curation : suitable for FEM modeling**

Framework


User Input
Scanning Speed
Alloy Chemistry
$V_s = V_{\text{scan}} \cdot \cos\alpha$
Solute Trapping Model
Multi-Component
Primary Solid
Scheil Model
Multi-Component
Multi-Phase
C_p Curation Model
Peak Reduction
Enthalpy Conservation
Output
Evaporation Temperature
Dynamic Liquidus
Dynamic Solidus
Heat Capacity
Density
Thermal Expansion
Thermal Conductivity
Output
Phase compositions
Phase amounts
Microsegregation
Solidification range

Solute Trapping : Assumptions

Thermo-Calc Software

- Only one primary solid phase forms dendrite, NOT necessarily the first solid phase
- Solute trapping in primary solid phase only. Other solid phases have equilibrium compositions following Scheil model
- Amounts of solid phases are dependent on solute trapping and solidification speed
- Dynamic liquidus for primary solid phase is dependent on solute trapping and solidification speed
- Dynamic solidus is calculated as complete solidification

Dynamic Liquidus as Function of Solidification Speed

- Diffusion across the liquid/solid interface

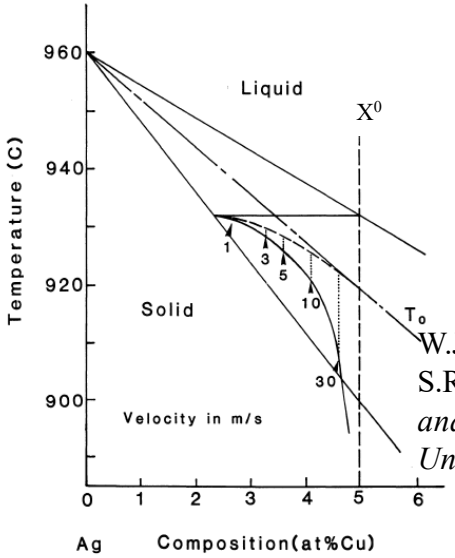
$$\left(X_i^0 - X_i^S\right)\frac{V}{V_i^D} = X_i^S X_n^0 \left(1 - \psi_i^e\right)$$

- Driving force for interface motion

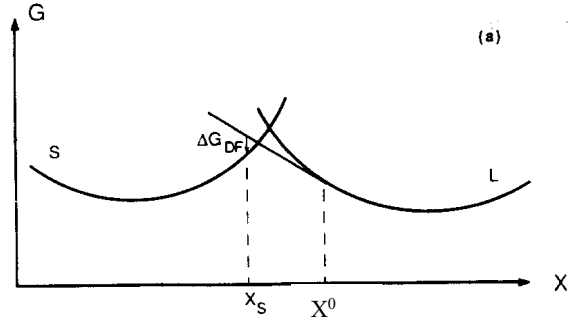
$$V = V_0\left[1 - \exp\left(\frac{\Delta G_{DF}}{RT}\right)\right]$$

- Obtain dynamic liquidus and initial primary solid composition

- If dynamic liquidus below T_0: amorphous



W.J.Boettinger, S.R.Cortell, in *Science and Technology of the Undercooled Melt*, 1986

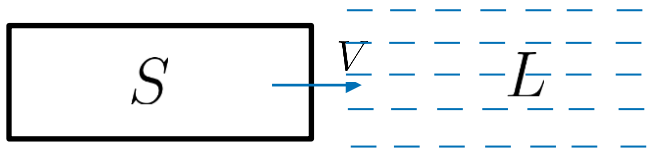


M.J.Aziz, *J. Appl. Phys*, 53(2)1158(1982)

Solute Trapping Model : Modified Aziz* Model

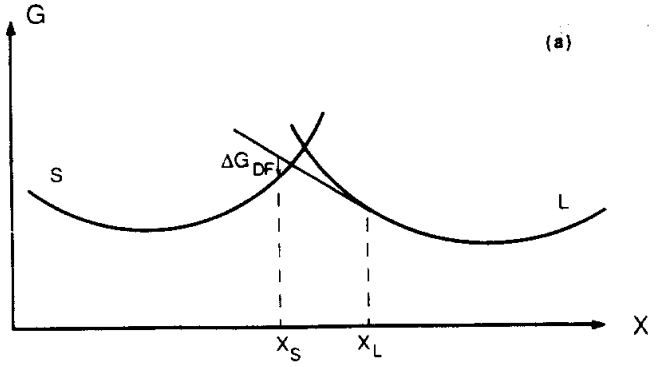
- Diffusion across the liquid/solid interface

$$\left(X_i^L - X_i^S\right)\frac{V}{V_i^D} = X_i^S X_n^L\left(1-\psi_i^e\right)$$



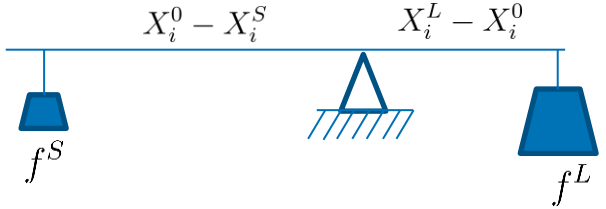
- Driving force for interface motion

$$V = V_0\left[1-\exp\left(\frac{\Delta G_{DF}}{RT}\right)\right]$$



- Mass conservation (lever rule)**

$$\frac{X_i^0 - X_i^L}{X_i^S - X_i^L} = \frac{X_j^0 - X_j^L}{X_j^S - X_j^L}$$



*M.J.Aziz, *J. Appl. Phys*, 53(2)1158(1982); M.J.Aziz and T.Kaplan, *Acta Metall.*, 36(8)2335(1988)

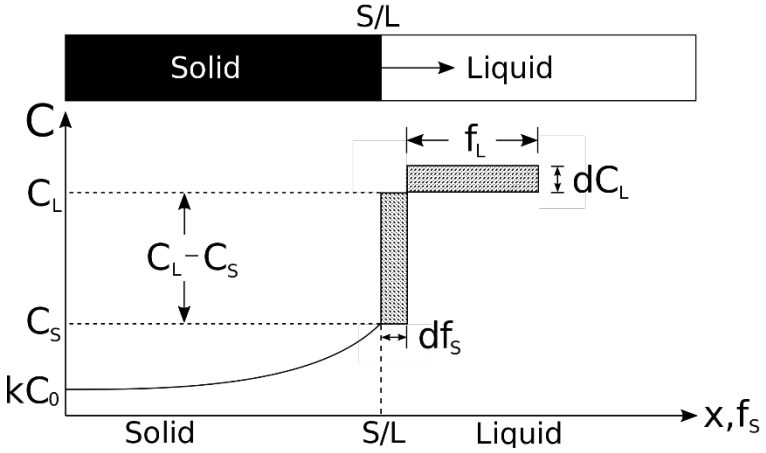
** M. Hillert, in *Phase Equlibria, Phase Diagrams and Phase Transformations*

Scheil Model* : Modified with Solute Trapping

- No back diffusion in primary solid, complete mixing in liquid

$$C_L(1-k)df_S = (1-f_S)dC_L$$

- Solute partitioning coefficient k comes from solute trapping calculation



Wikipedia

- Amount of other solid phases calculated based on

  ✓ Equilibrium calculation for solute compositions

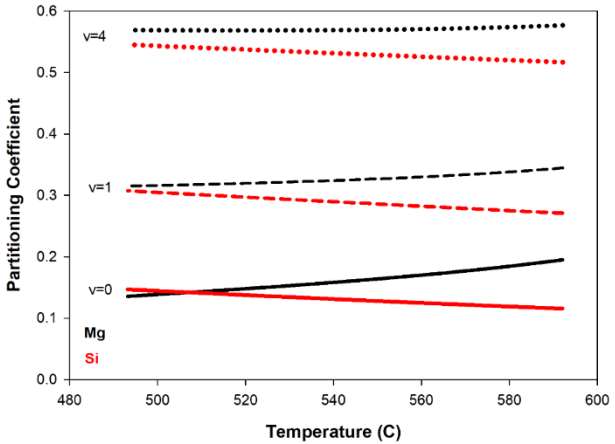
  ✓ Reduction of energy dissipation due to withholding by solute trapping

*E.Scheil, *Z. Metallk.*, 34(1942)70

Solute Trapping : Al-10Si-0.6Mg

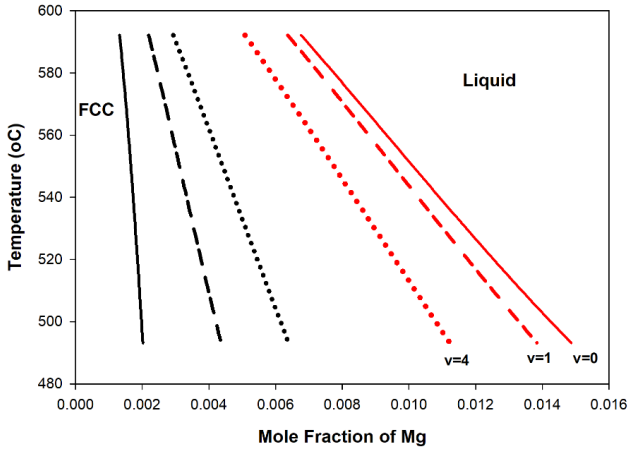
Al	Si	Mg
Bal	10.0	0.6

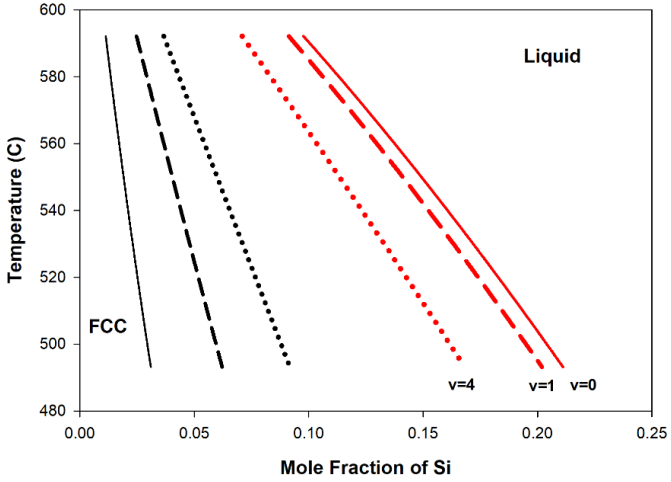
Solute Partitioning



- Multi-component
- Deviation from ideal solution
- Temperature dependence of solute partitioning

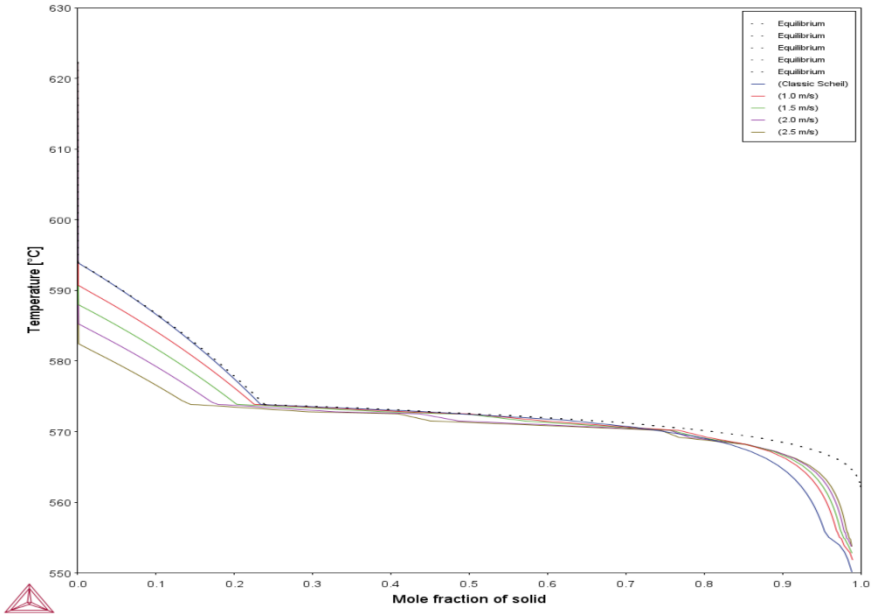
Phase Boundaries

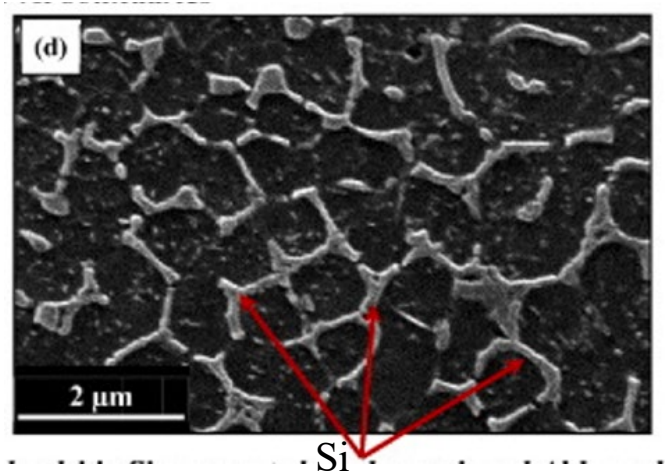




Solidification : Al10SiMg Alloy

Al	Si	Mg	Fe	Ti	Mn	Cu	Zn	Ni	Pb	Sn
Bal	10.0	0.325	0.275	0.075	0.225	0.025	0.05	0.025	0.025	0.025





Microstructure of SLM Al10SiMg

N.T.Aboulkhair et al, *Progress in Materials Science*, 106(2019)100578

- Increasing solidification speed decreases liquidus temperature
- Increasing solidification speed generally decreases solidification range comparing with classic Scheil, though anomaly cases are possible due to formation of low temperature solid phases

Solidification : IN718

Fe	Cr	Nb	Mo	Al	Ti	Ni
18.14	17.9	5.3	2.99	0.5	0.97	bal

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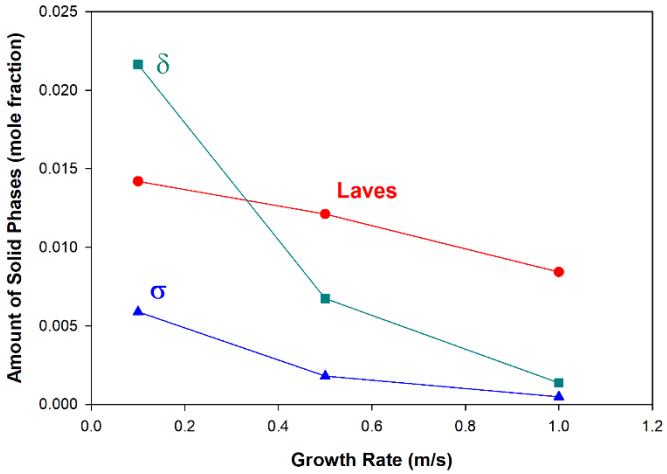
Solid Phase Amounts



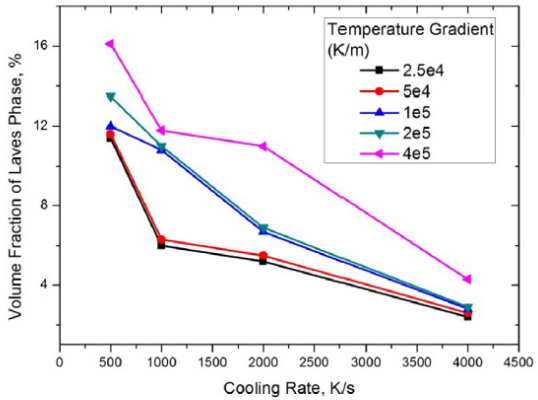
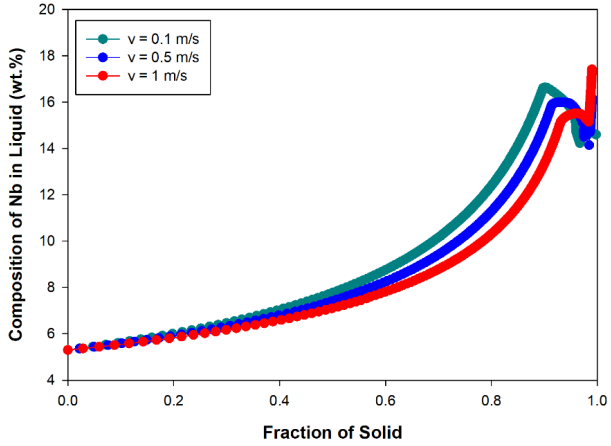
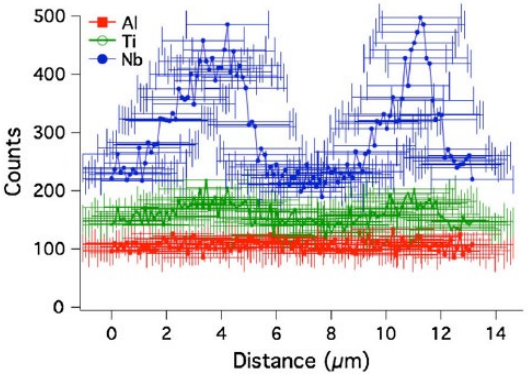


Fig. 5. Predicted volume fraction of Laves phase.

P.Nie et al. *Acta Mater.* 77(2014)85

Microsegregation





Y.Tian et al., *Met. Mater. Trans.* 45A(2014)4470

New Database: Thermal Conductivity*

Electrical Resistivity (ELRS)

- Prefitting with semi-empirical model
- Refitting with polynomial

Matthiessen's rule

$$\rho = \rho_0 + \rho_{e-p} + \rho_m$$

$$\rho_{e-p} = A \cdot \left(\frac{T}{\theta_R}\right)^5 \cdot J_5\left(\frac{\theta_R}{T}\right) \qquad A = \frac{3\pi\hbar {q_D}^6 (G')^2}{4e^2 (m^*)^2 n_c k_B \theta_D {k_F}^2 {v_F}^2}$$

Bloch-Grüneisen

$$J_n\left(\frac{\theta_D}{T}\right) = \int_0^{\frac{\theta_D}{T}} \frac{x^n e^x}{(e^x - 1)^2} dx$$

$$\rho_m = \rho_{spd} \cdot \left(1 - e^{\left(-\frac{3}{2}\left(\frac{T}{T_c}\right)^3\right)}\right)$$

Our model in Thermo-Calc

Thermal Conductivity (THCD)

- Fitted with polynomials
- Predictions for κe and κg

Wiedemann-Franz Law

$$\frac{1}{\kappa_e} = W_e = \frac{\rho_0 + \rho_m + \rho_i}{L_0 T}$$

$$\rho_i = \frac{A}{L_0 T} \cdot \left(\frac{T}{\theta_R}\right)^5 \cdot J_5\left(\frac{\theta_R}{T}\right) \cdot f$$

$$f = 1 + \frac{3}{\pi^2} \cdot \left(\frac{k_F}{q_D}\right)^2 \cdot \left(\frac{\theta_R}{T}\right)^2 - \frac{1}{2\pi^2} \cdot \frac{J_7\left(\frac{\theta_R}{T}\right)}{J_5\left(\frac{\theta_R}{T}\right)}$$

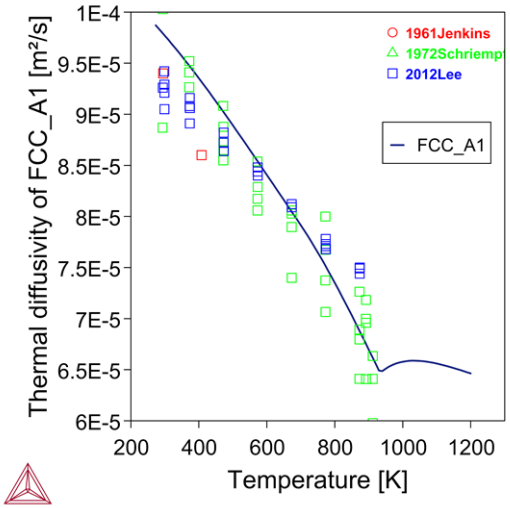
$$\kappa_p^U = A' \cdot \frac{M_a \cdot {\theta_D}^3 \cdot \delta}{\gamma^2 \cdot n_c^{\frac{2}{3}}} \cdot \frac{1}{T} \qquad A' = \frac{2.43 \cdot 10^{-5}}{1 - \frac{0.514}{\gamma} + \frac{0.228}{\gamma^2}}$$

Slack Model

*courtesy of Hai-Lin Chen, Thermo-Calc Software AB

Implementation in Thermo-Calc*

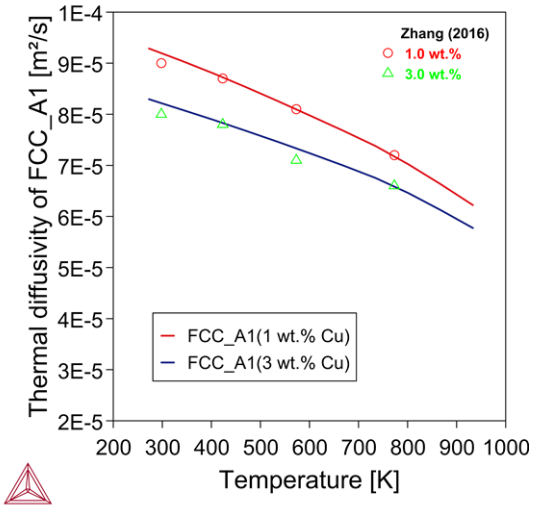
Unary, Al, THDF



- ➔ Jenkins, (1961), as in WADD-TR-61-95
- ➔ Schriempf, High T High P, (1972) 411
- ➔ Lee et al, Intl. J. Thermophys., (2012) 540

Available in TCAL7 !

Binary, Al-Cu FCC_A1, THDF



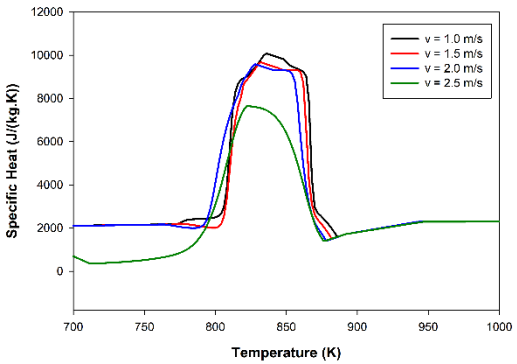
- ➔ Zhang, et al. Thermochim. Acta 635 (2016) 8

*courtesy of Hai-Lin Chen, Thermo-Calc Software AB

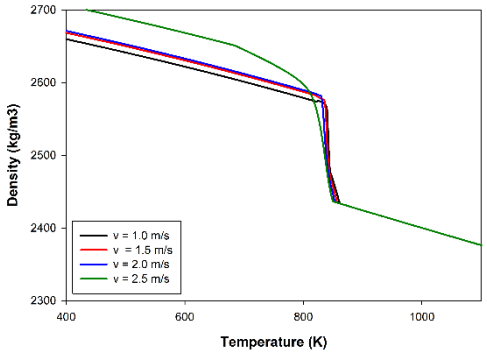
Thermophysical Data

Thermo-Calc Software

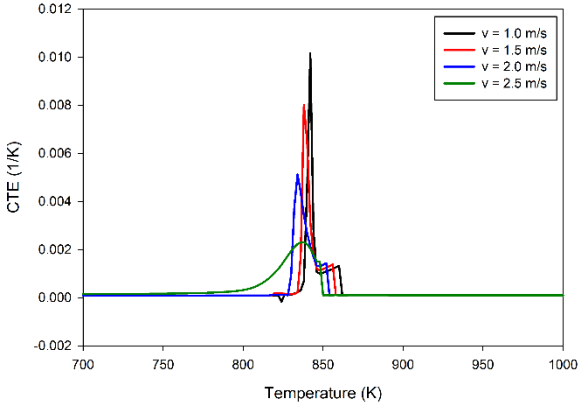
Heat Capacity



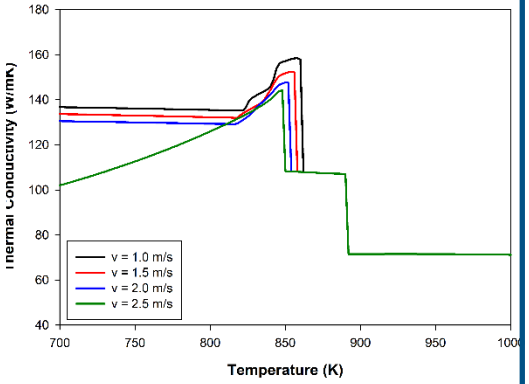
Density

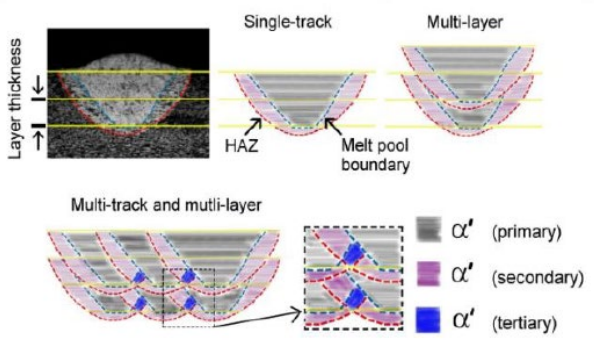


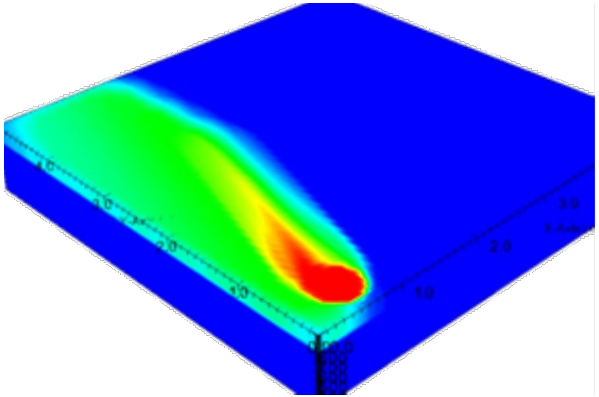
Thermal Expansion



Thermal Conductivity (on-going)







Summary

- **Non-equilibrium thermodynamic tools**
  - Solute trapping at the interface between liquid and dendric primary solid
  - Multi-component, multiphase with CALPHAD databases
  - Alloy chemistry- and solidification speed- dependent

- **Curation of thermodynamic and thermophysical data**
  - Peak reduction and smoothing of heat capacity data
  - Database for thermal conductivity
  - Output format compatible with FEM simulations

Future Work

- **Validation & feasibility test**
- **More thermophysical data (in more databases)**
  - Viscosity
  - Surface tension
  - Thermal conductivity
- **Evaporation**
  - Pressure dependence of evaporation temperature
  - Density and heat capacity data for FEM modeling
- **Solid state precipitation**
  - Improvement of PRISMA models to deal with cyclic thermal conditions in AM

Thermo-Calc Software

Thank You!

www.thermocalc.se

Save Time ♦ Reduce Costs ♦ Increase Innovation