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Macroscale modelling of Bridgman furnace solidification for the prediction of texture evolution and columnar to equiaxed transition

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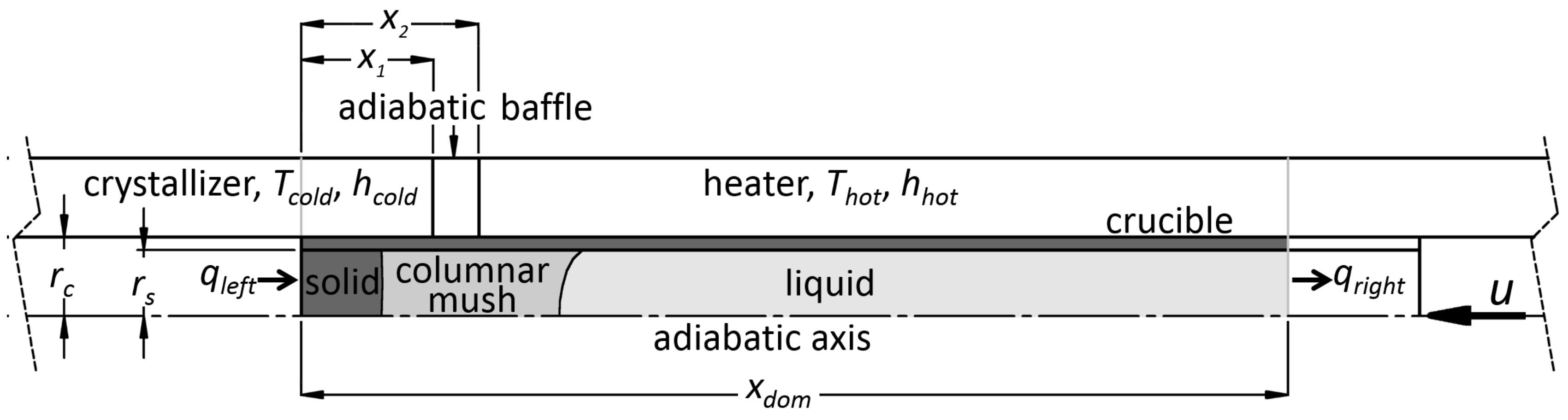
INTRODUCTION

The work outlined here describes the development of two macroscopic models for the prediction of texture evolution during Bridgman furnace experiments that use cylindrical shaped samples. The first model employs a 2D axisymmetric thermal model coupled to a front tracking algorithm for modelling the evolution of axial and radial columnar grains. The second model employs a 1D thermal model (suitable for small sample diameters) with axial columnar mush front tracking; equiaxed growth is analytically modelled using the Avrami's extended volume concept. Both models are demonstrated for typical experimental test case scenarios, specially, traditional Bridgman furnace solidification and power down solidification.

2D AXISYMMETRIC BRIDGMAN FURNACE FTM FOR COLUMNAR GROWTH

Thermal Model

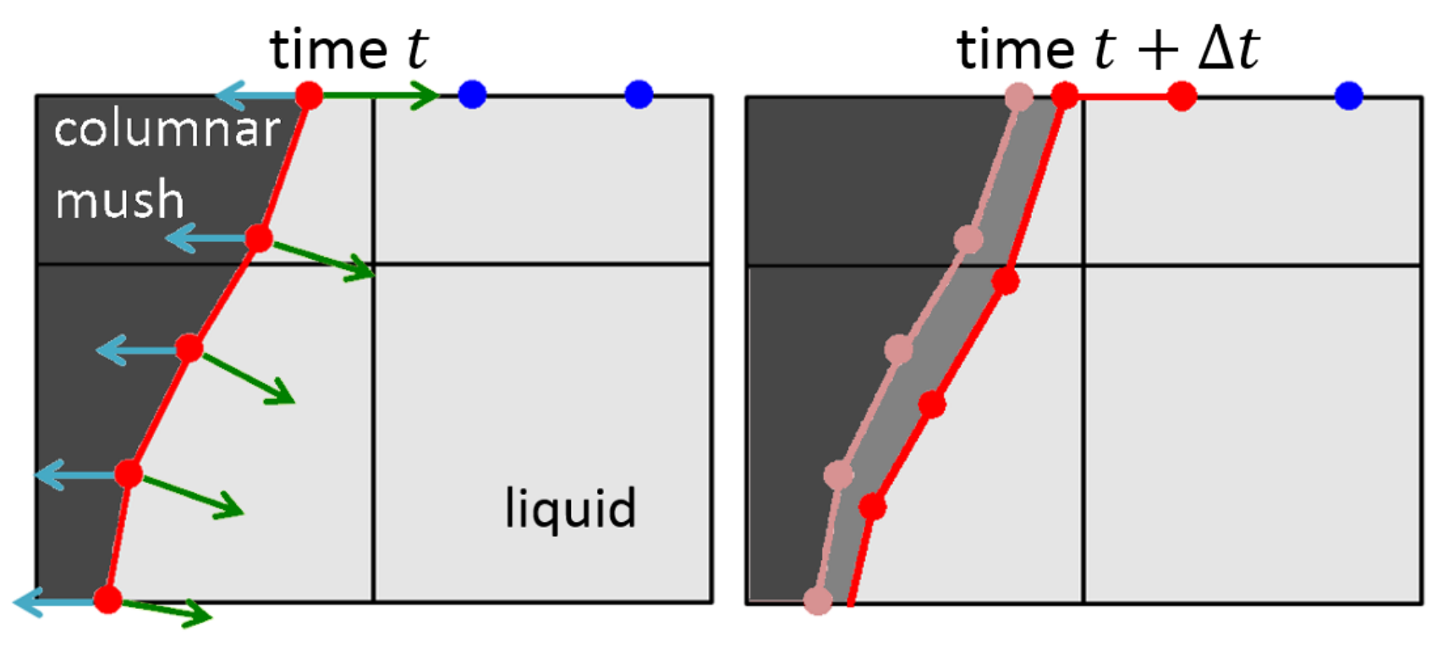


Temperature evolution in the domain is governed by the following heat transfer equation:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rk\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) - u\rho\frac{\partial\left(c_p T\right)}{\partial x} + \rho L\frac{\partial}{\partial t}\left(\frac{g_s V_m}{V_{CV}}\right) + u\rho L\frac{\partial}{\partial x}\left(\frac{g_s V_m}{V_{CV}}\right)$$

This equation was solved coupling a finite volume method [1] to a front tracking algorithm [2] for the evolution of the columnar dendrites region.

Front Tracking Model



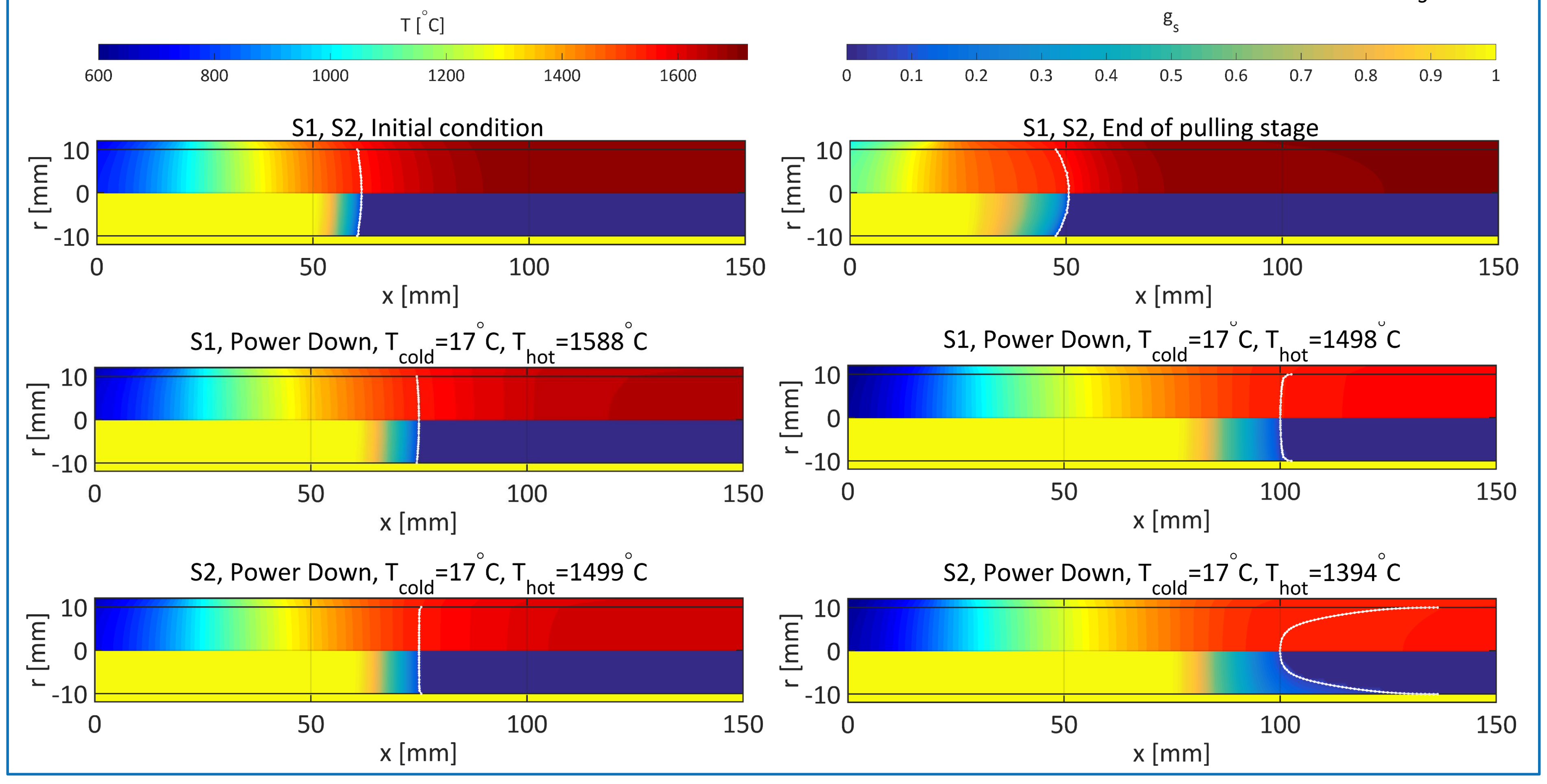
→ pulling velocity u
→ dendrite tip growth velocity $|v_t| = C(T_L - T)^n$
● active markers
● non active markers, nucleate if $T_L - T \geq \Delta T_{nucl}$
■ V_m at time t
■ $\Delta V_m/\Delta t$ at time $t + \Delta t$

Simulations set-up

SAMPLE	Ti-45.5Al-4.7Nb-0.2C-0.2B	r_s=10 mm	T_{liq}=1550 °C	T_{sol}=1434 °C	x_{dom}=150 mm
CRUCIBLE	Y_2O_3	r_c-r_s=2 mm			
THERMAL DATA	T_{cold}=17°C	T_{hot}=1720°C	h_{cold}=h_{hot}=100 W/(m² °C)	q_{left}=105.25 kW/m²	q_{right}=0.9 kW/m²
SIMULATIONS STAGES	Pulling stage		u=0.278 mm/s		t_{end}=72 s
	Power Down	S1	-dT_{hot}/dt=15 °C/min		t_{start}=72 s
		S2	-dT_{hot}/dt=30 °C/min		

Simulation Results

The following figures show the solution at different time steps. The upper half of each plot shows the distribution of T in the sample, while the lower half shows the distribution of g_s.



Discussion

Pulling Stage:

- The columnar front moved to the left maintaining a convex shape, due to positive radial thermal gradient. No radial columnar growth occurred.

Power Down:

- The columnar front started to advance, and its shape became gradually concave, due to the reversal of the radial thermal gradient in the heater zone.
- When the nucleation undercooling at the sample circumference was reached, nucleation and radial columnar growth occurred.
- For the same length of the axial columnar zone (given by the position of the axial marker), radial columnar growth was more significant when a higher cooling rate was applied (S2).

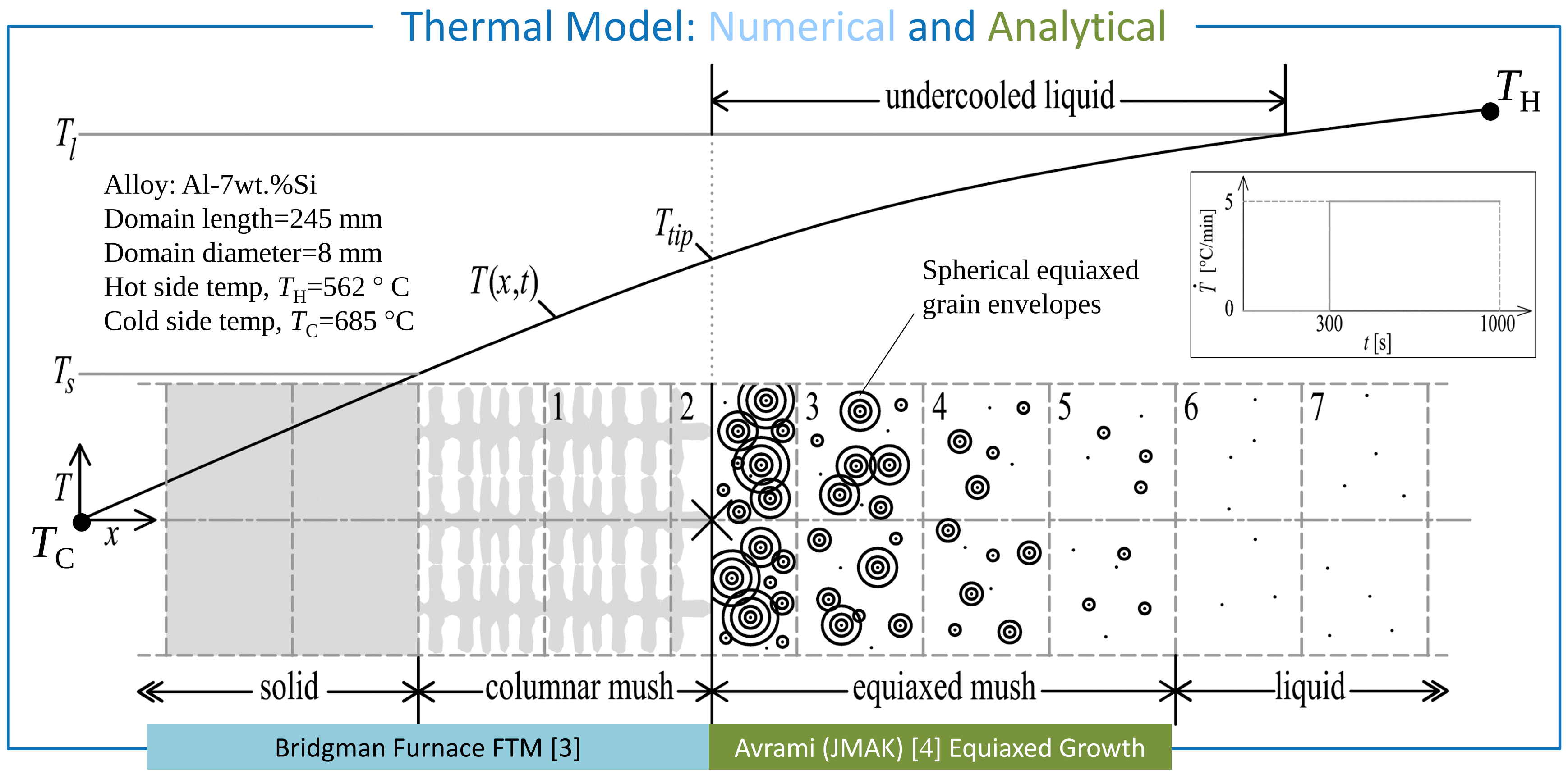
Bibliography

[1] S. Battaglioli, S. McFadden, A. J. Robinson, "*Numerical simulation of Bridgman solidification of binary alloys*," Int. J. Heat Mass Transf. 104 (2017) 199–211.

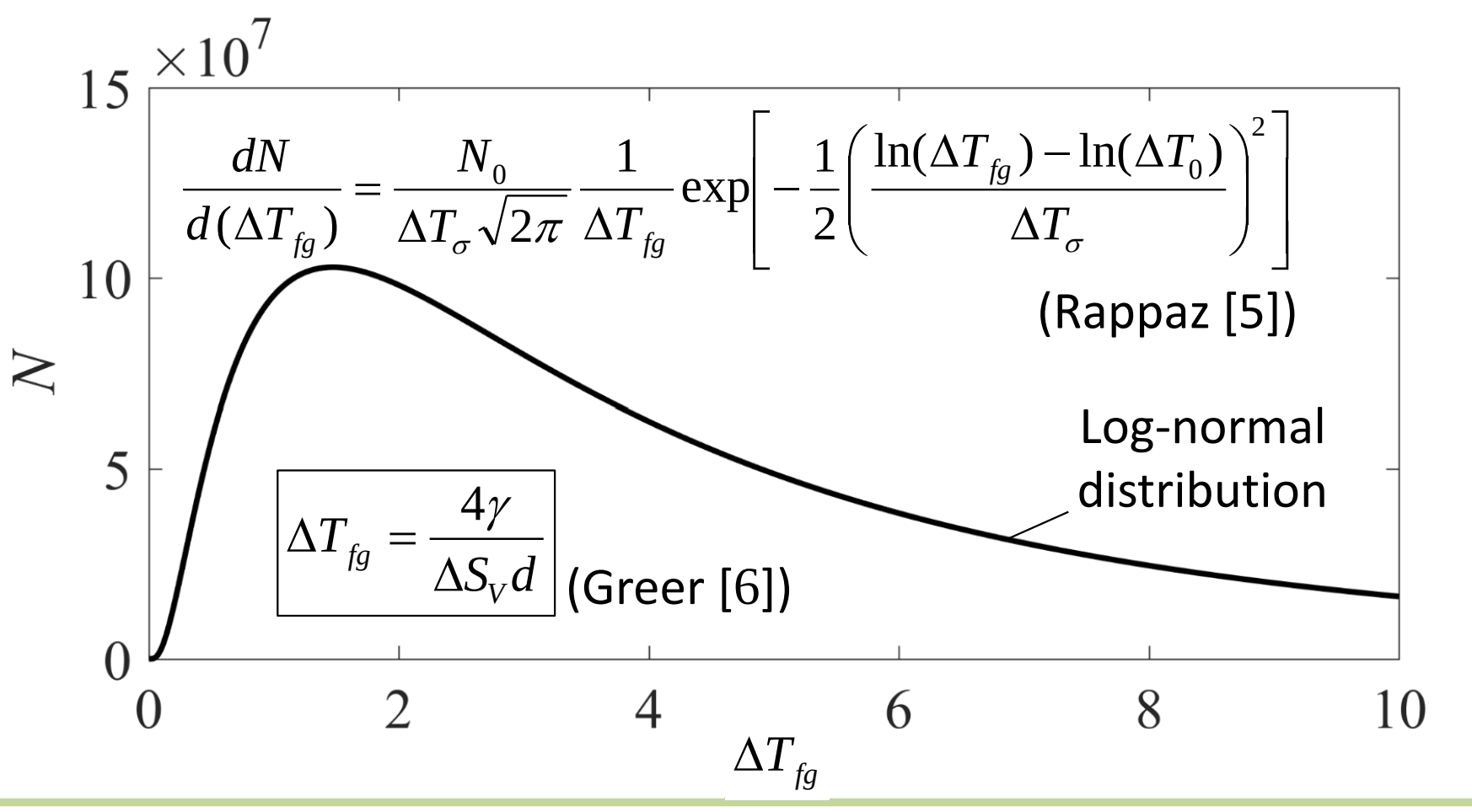
[2] D. J. Browne, J. D. Hunt, *"A fixed grid front-tracking model of the growth of a columnar front and an equiaxed grain during solidification of an alloy*, "Numer. Heat Trans. B 45 (2004) 395–419.

1D AXISYMMETRIC BRIDGMAN FURNACE FTM FOR COLUMNAR GROWTH WITH AVRAMI-BASED EQUAIXED GROWTH MODEL

Thermal Model: Numerical and Analytical



Nucleation



$$\frac{dN}{d(\Delta T_{fg})} = \frac{N_0}{\Delta T_\sigma \sqrt{2\pi}}\frac{1}{\Delta T_{fg}}\exp\left[-\frac{1}{2}\left(\frac{\ln(\Delta T_{fg}) - \ln(\Delta T_0)}{\Delta T_\sigma}\right)^2\right]$$

$$\boxed{\Delta T_{fg} = \frac{4\gamma}{\Delta S_V d}}$$

Growth

The '**Extended Volume**' (below) is the sum of all equiaxed sphere envelopes, regardless of any geometric overlapping.

$$V_{eq.mush}^{extended} = \frac{4\pi}{3}\int_0^t I\left(\int_{t'}^t v_{equiaxed}\,dt''\right)^3 dt'$$

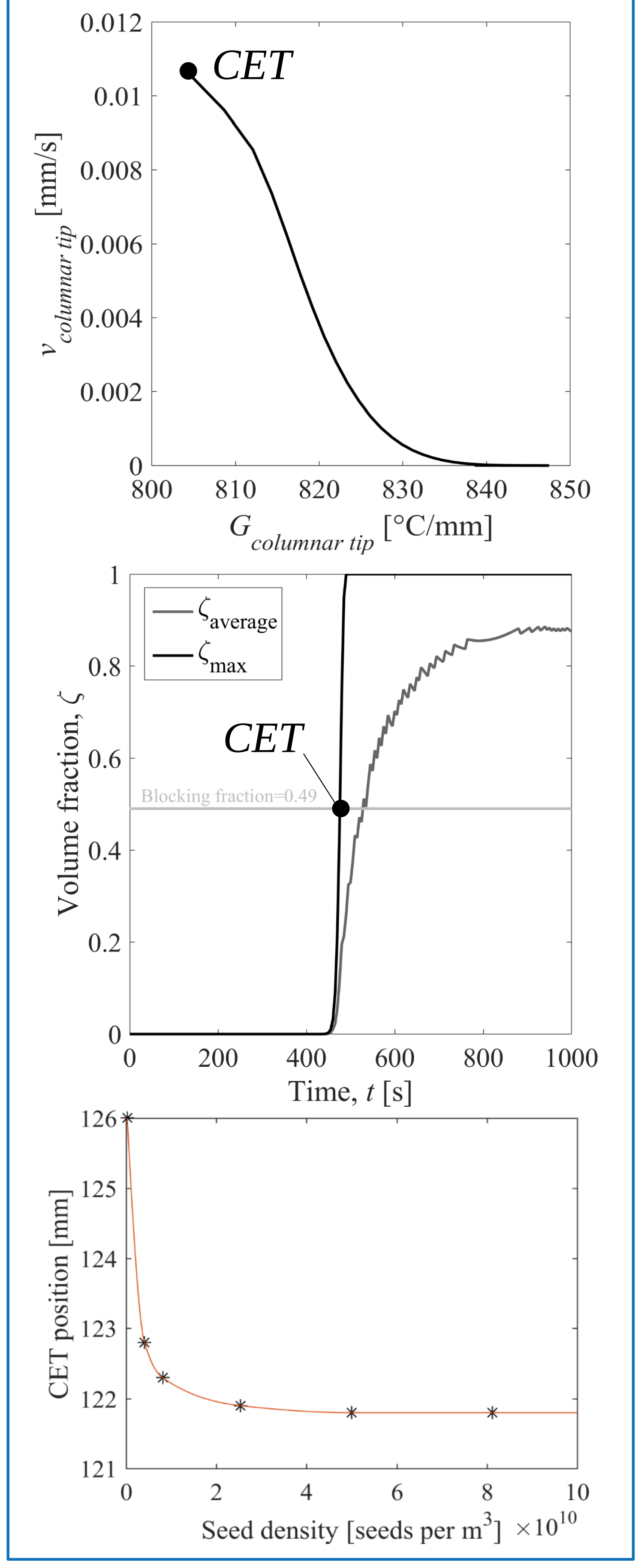
However, the **Avrami equation** (below) accounts for impingement based on the assumption of homogenous probability of nucleation events in all untransformed areas.

$$\zeta = \frac{V_{eq.mush}}{V_{CV}} = 1 - \exp\left[-\frac{V_{eq.mush}^{extended}}{V_{CV}}\right]$$

Other simulation inputs

Simulation end time	t_{end}	[s]	1000	**Dendrite growth coefficient**	C	[m/°C^n]	2.9×10^{-6}
Numerical time step	Δt	[s]	1×10^{-3}	**Undercooling exponent**	b	[-]	2.7
Seed particle density	N_0	[seeds/m³]	5×10^{10}	**Latent heat of fusion per unit volume**	L_V	[J/m³]	1064×10^6
Seed diameter geometric mean	d_0	[mm]	0.67	**Equilibrium liquidus temperature**	T_l	[°C]	618
Seed diameter standard deviation	ΔT_σ	[mm]	0.867	**Equilibrium eutectic temperature**	T_s	[°C]	577
Blocking fraction	$\zeta_{blocking}$	[-]	0.49				

Simulation Results



Discussion

- The proposed model builds on an existing FTM [*] for columnar growth in a Bridgman furnace by introducing an equiaxed growth model.
- Nucleation of equiaxed grains is based on the 'free growth' model of Greer [†] where a lognormal distribution of inoculant particle diameter is assumed and related directly to get the nucleation undercooling, ΔT_{fg}.
- Growth of the equiaxed mush envelope is modelled using the Avrami extended volume concept. The transformed volume fraction of equiaxed mush, ζ, is calculated ahead of the columnar front.
- A simulation of a power down scenario is carried out where a cooling rate of 5 K/min is applied. The model can be used to estimate columnar to equiaxed transition (CET) by defining a blocking fraction, $\zeta_{blocking}$.
- It was found that at high seed density, N_0, the position the CET position reaches a lower limit of approx. 122 mm, in the given test scenario.

Bibliography

[3] R. P. Mooney, S. McFadden, M. Rebow, and D. J. Browne, "*A Front Tracking Model for Transient Solidification of Al–7wt%Si in a Bridgman Furnace*," Trans. Indian Inst. Met., vol. 65, no. 6, pp. 527–530, 2012.

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[6] A. Greer, A. . Bunn, A. Tronche, P. . Evans, and D. . Bristow, "*Modelling of inoculation of metallic melts: application to grain refinement of aluminium by Al–Ti–B*," Acta Mater., vol. 48, no. 11, pp. 2823–2835, Jun. 2000.

CONCLUSION

Firstly, the work outlines the development of a 2D axisymmetric model for heat flow in cylindrical samples directionally solidified in a Bridgman furnace; columnar dendritic growth is simulated using a front tracking method. The model is not restricted to low Biot number (<0.1) cases and, therefore, is useful where radial temperature gradients play an important role in microstructure development. The model is demonstrated by simulating traditional Bridgman solidification of a multicomponent Ti-Al alloy followed in series by power down solidification. Secondly, the work outlines how an analytical equiaxed growth model, based on the Avrami extended volume concept, can be implemented in a similar 1D axisymmetric front tracking Bridgman furnace model. A lognormal distribution of nucleation undercooling is assumed. The model is used to simulate CET in a notional power down scenario. It is demonstrated that the CET position reaches a lower limit when seed particle density is increased. It is intended, in the future, to implement the analytical equiaxed growth model into the 2D axisymmetric model.

Acknowledgements

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