A Rapid CCT Predictor for Low Alloys Steels, & its Application to Compositionally Heterogeneous Material

By J. Collins, M. Piemonte, M. Taylor, J. Fellowes and E. J. Pickering

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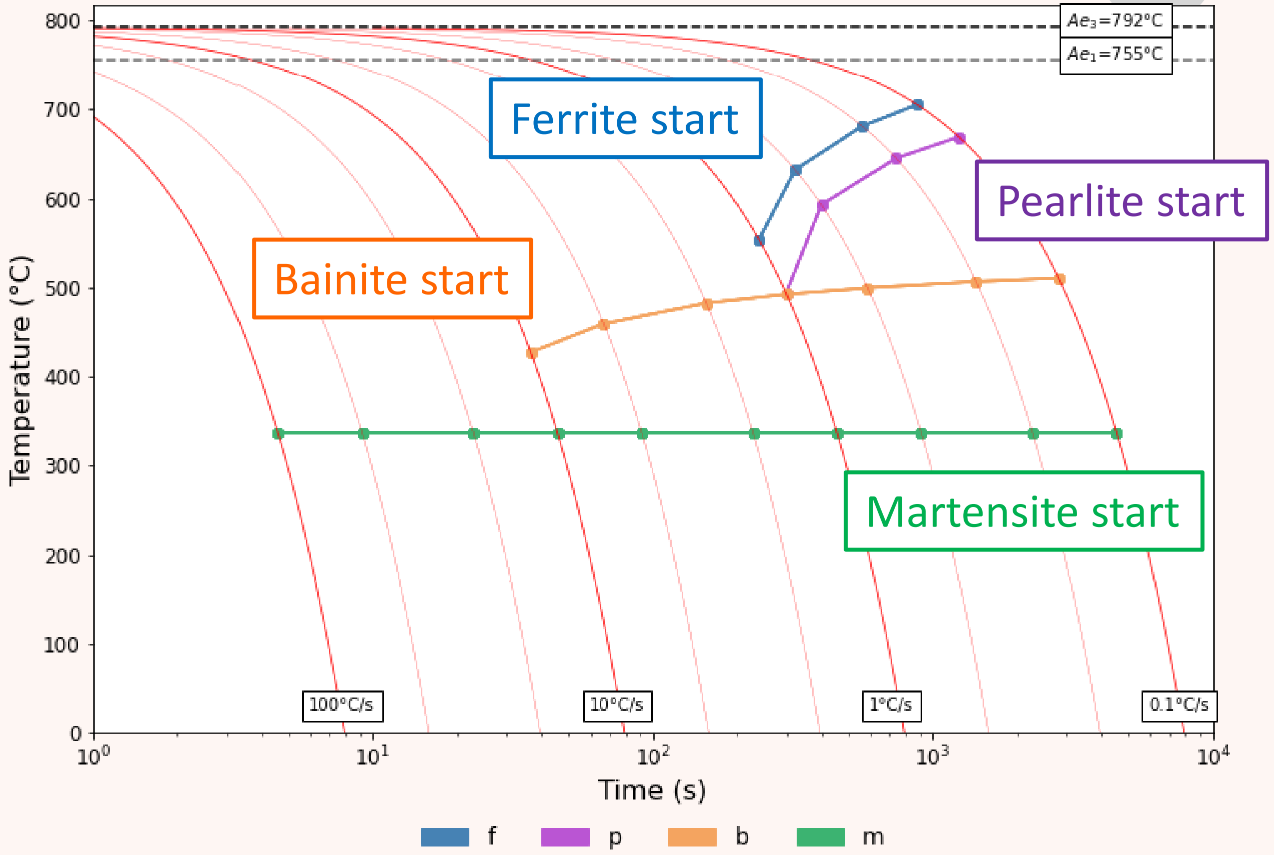
What is a CCT?

- Continuous Cooling Transformation (CCT) diagram
- Presents which constituents will transform on cooling
- Understand steel behaviour
- Optimise microstructure & properties



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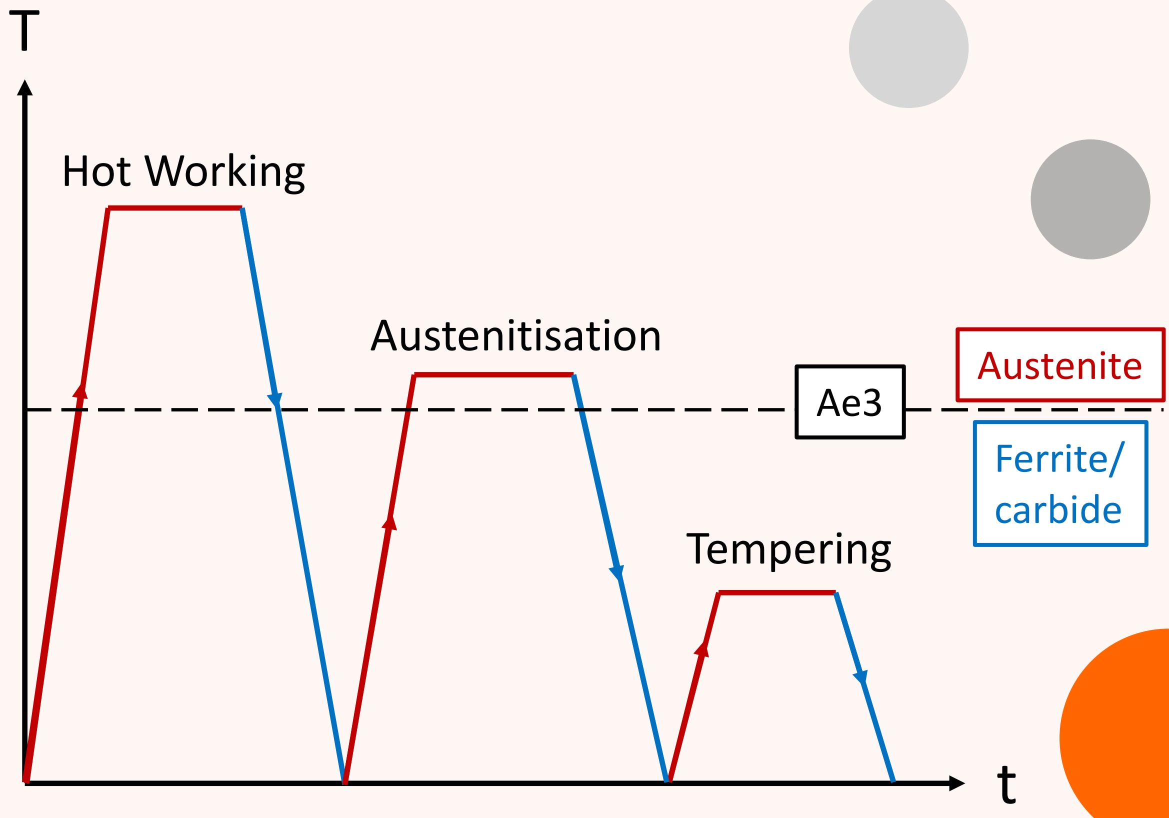
Why is this Important?

- Many commercial steel heat treatments involve a continuous cool
  - Forging/hot rolling
  - Austenitisation treatments
  - Homogenisation treatments

- Modelling CCT behaviour allows:
  - Better predict microstructure & properties
  - Save time (+ money)



Modelling CCTs – The Li Model

- Based off semi-empirical equations for isothermal transformation behaviour
  - Originally developed by Kirkaldy & Venugopalan [1], but modified by Li et al. [2]
- General form of equations:

$$\tau\left(X,T\right)=\frac{F(\mathrm{C},\mathrm{Mn},\mathrm{Si},\mathrm{Ni},\mathrm{Cr},\mathrm{Mo},G)}{\Delta T^{n}\exp(-Q/RT)}S(X)$$

Transformation time (s)

Function dependent on alloy composition and prior austenite grain size, G

Sigmoidal reaction rate function

Undercooling from equilibrium start temperature (i.e., Ae3 for ferrite)

Dependent on diffusion mechanism

Transformation activation energy

[1]: Kirkaldy and Venugopalan, Prediction of Microstructure and Hardenability in Low Alloy Steels, *Proceedings of an International Conference on Phase Transformations in Ferrous Alloys*, AIME (1984), 125.

[2]: Li et al., A Computational Model for the Prediction of Steel Hardenability, *Metallurgical and Materials Transactions B*, 29 (1998), 661.

Modelling CCTs – The Additivity Rule

- Converting between isothermal to non-isothermal behaviour

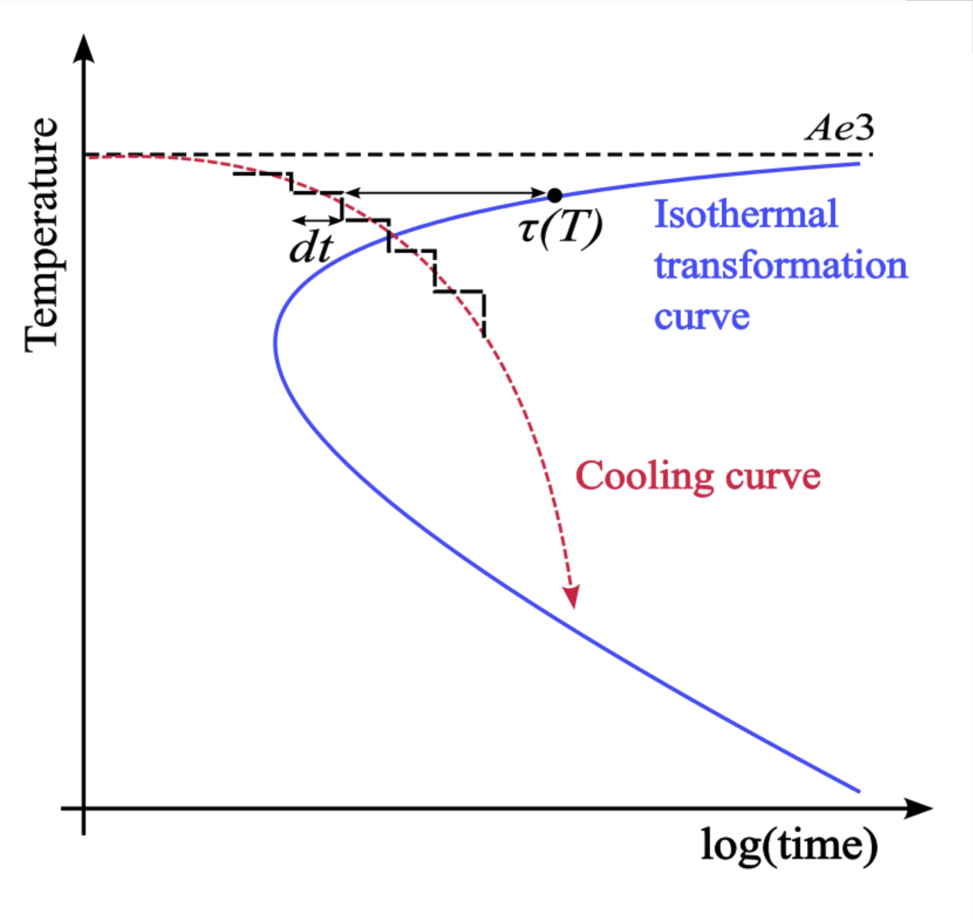
- The additivity rule [3]:

Time step

$$\sum \frac{\mathrm{d}t}{\tau(T)} = 1$$

Transformation time

$$\tau\left(X, T\right) = \frac{F(\mathrm{C}, \mathrm{Mn}, \mathrm{Si}, \mathrm{Ni}, \mathrm{Cr}, \mathrm{Mo}, G)}{\Delta T^n \exp(-Q/RT)} S(X)$$



[3]: E. Scheil. Anlaufzeit der Austenitumwandlung. Archiv für das Eisenhüttenwesen, 8:565–567, 1935.

Modelling CCTs – The Li Model

Li Model

$$\tau(X,T) = \frac{F(\mathrm{C}, \mathrm{Mn}, \mathrm{Si}, \mathrm{Ni}, \mathrm{Cr}, \mathrm{Mo}, G)}{\Delta T^{n} \exp(-Q/RT)} S(X)$$ [2]

+

$$\sum_i \frac{\Delta t_i}{t_i} = 1$$ [3]

Ferrite

Pearlite

Bainite

+

Martensite

$$\mathrm{M_S}(^{\circ}C) = 561 - 474\,\mathrm{C} - 33\,\mathrm{Mn} - 17\,\mathrm{Cr} - 17\,\mathrm{Ni} - 21\,\mathrm{Mo} + 10\,\mathrm{Co} - 7.5\,\mathrm{Si}$$ [4]

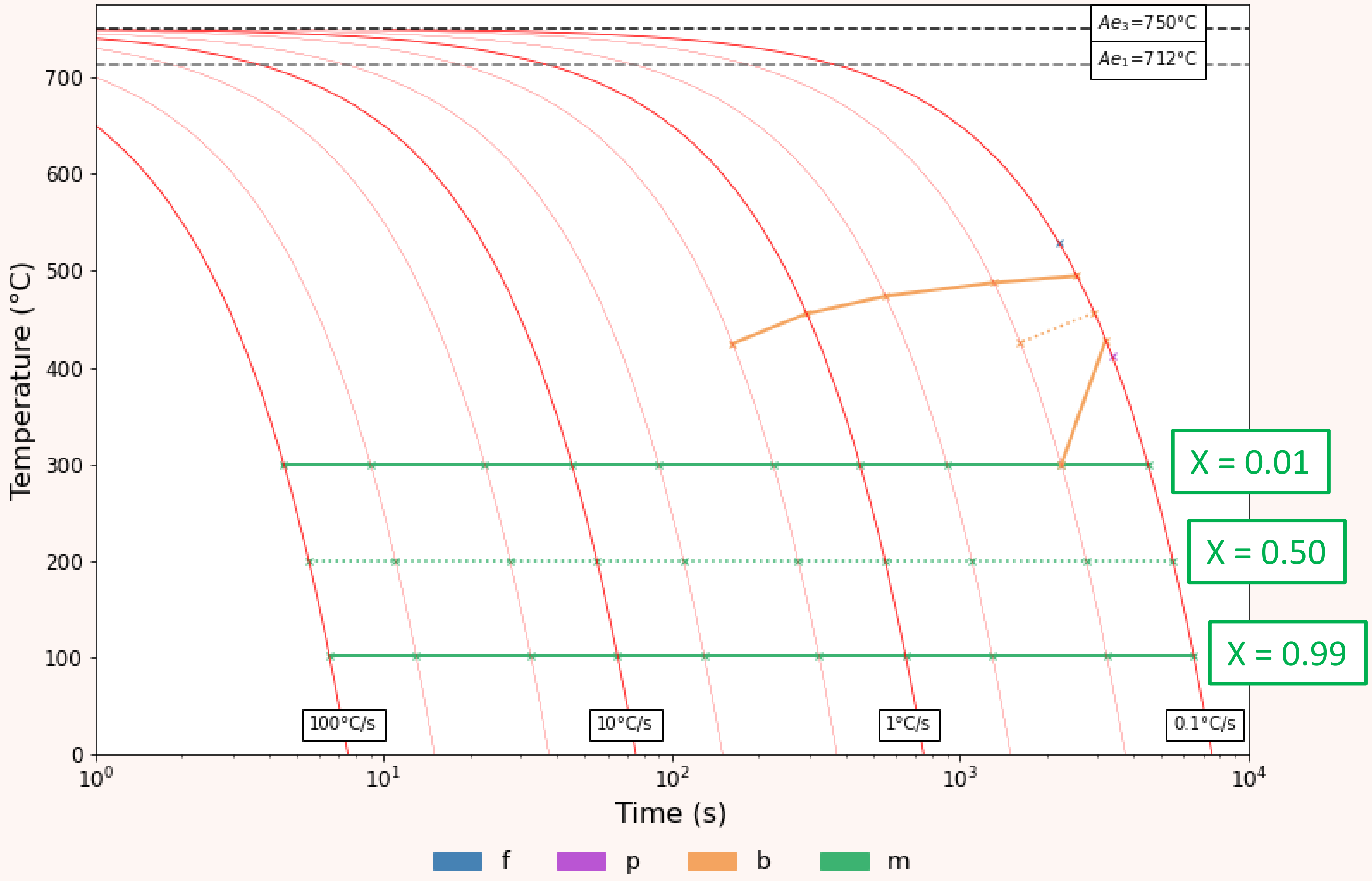
[2]: Li et al., A Computational Model for the Prediction of Steel Hardenability, *Metallurgical and Materials Transactions B*, 29 (1998), 661.

[3]: E. Scheil. Anlaufzeit der Austenitumwandlung. Archiv für das Eisenhüttenwesen, 8:565–567, 1935.

[4]: C. Y. Kung and J. J. Rayment. An Examination of the Validity of Existing Empirical Formulae for the Calculation of Ms Temperature. Metallurgical Transactions A, 13:328–331, 1982.

Modelling CCTs – The Li Model (SA-540 B24)

SA-540	
	Wt.%
C	0.40
Si	0.26
Mn	0.75
Ni	1.81
Cr	0.86
Mo	0.32



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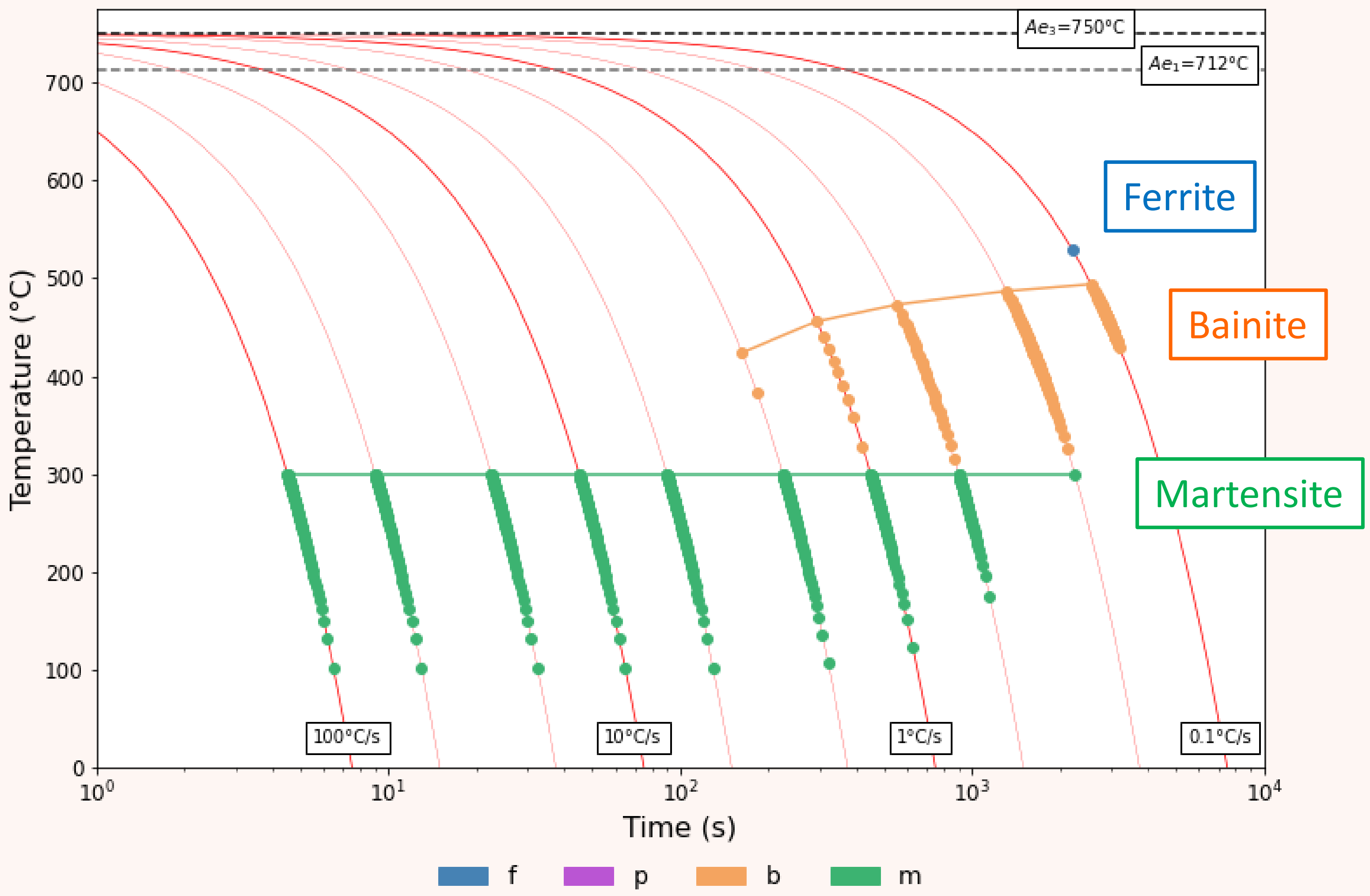

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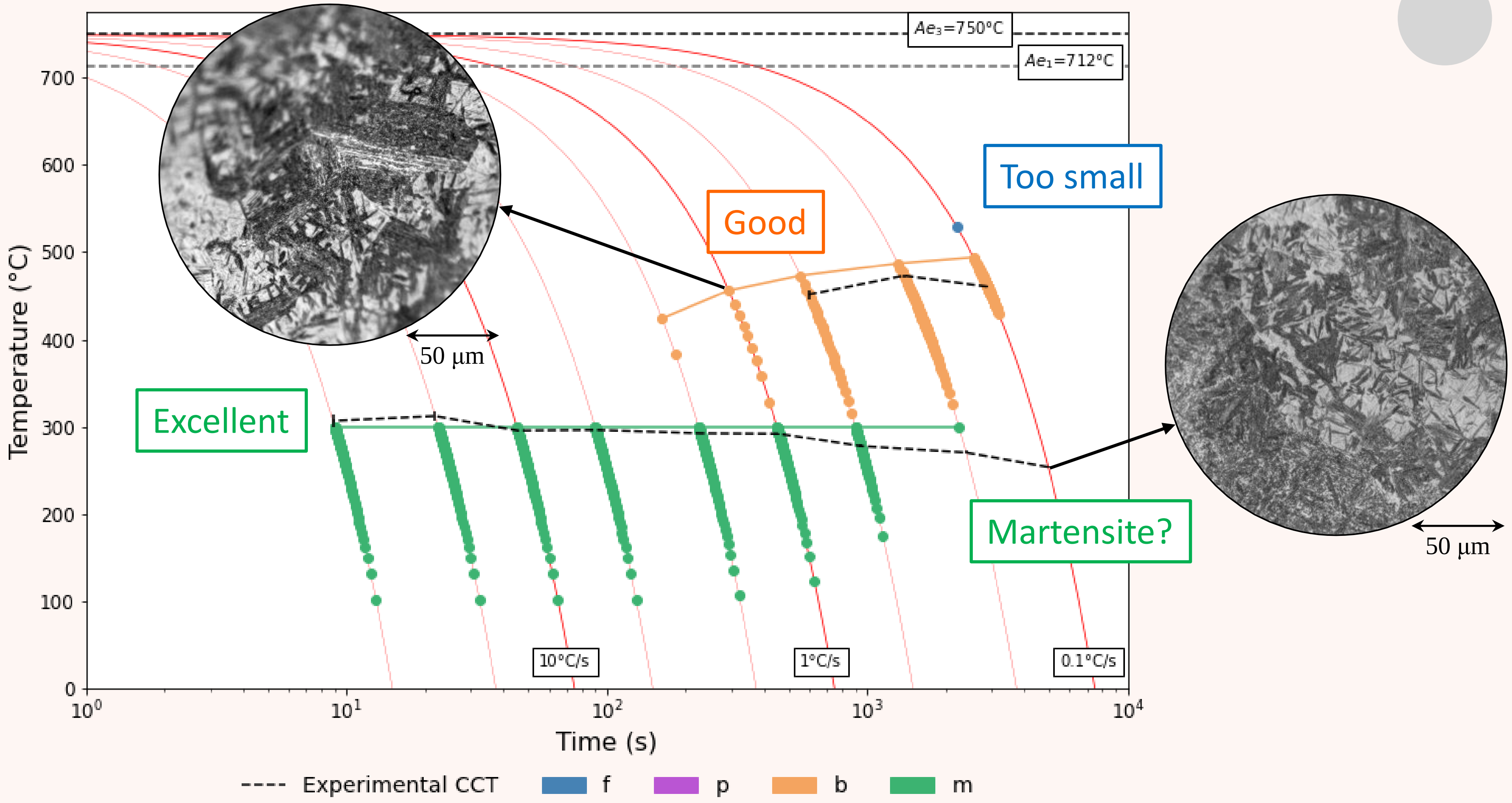
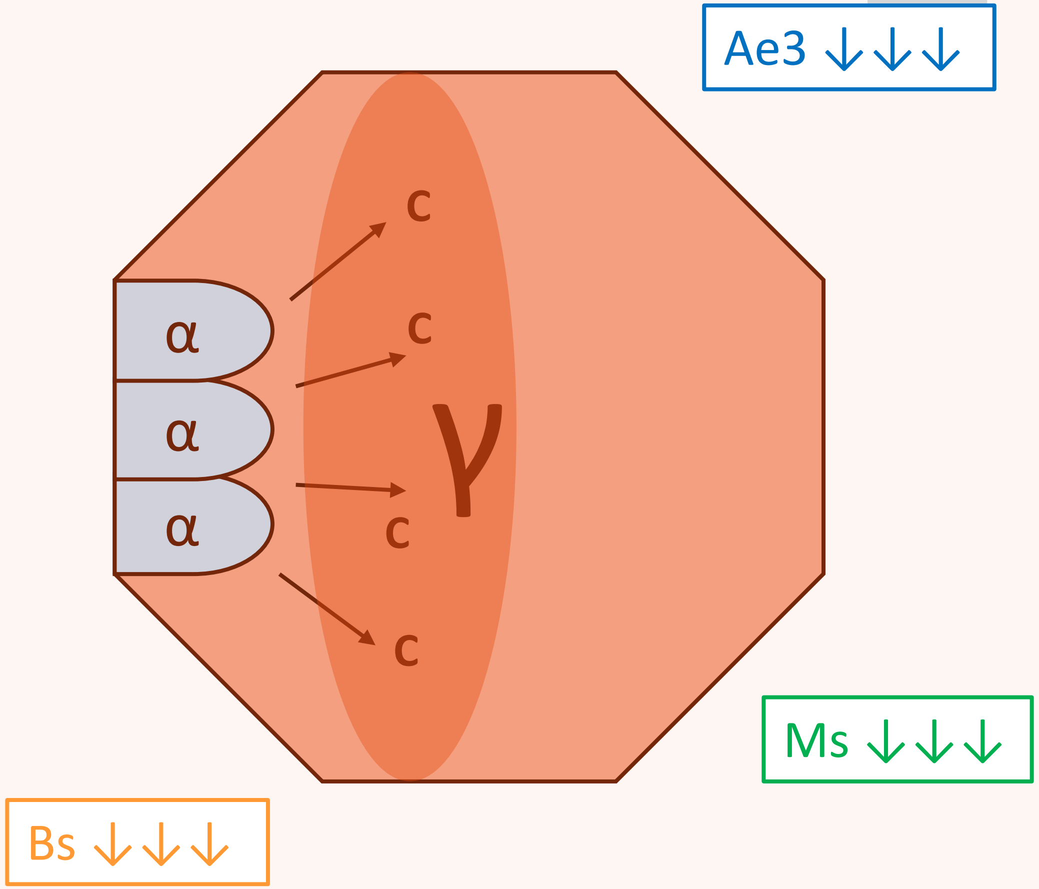


Modifying the Li Model – Carbon Partitioning

- The Li Model doesn't consider

  Carbon Partitioning

- As austenite transforms into ferrite:
  - Ferrite kicks out excess carbon
  - Enriching the austenite with carbon
  - Altering the stability of austenite



Modifying the Li Model – Carbon Partitioning

- Concentration of carbon in untransformed austenite [5]:

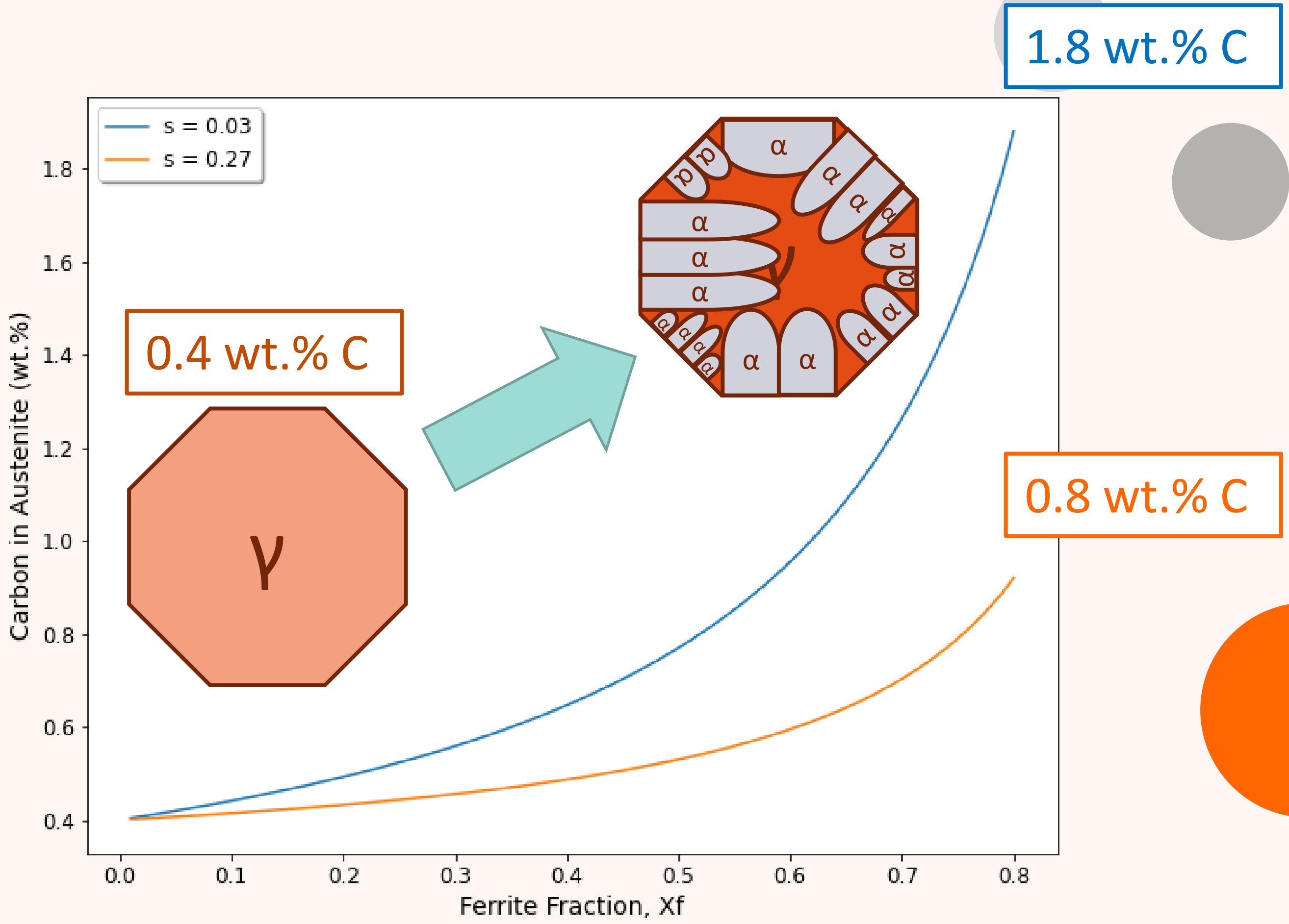
Average C composition

$$x_\lambda = \bar{x} + \frac{X\left(\bar{x} - s\right)}{(1 - X)}$$

Retained C composition

Phase fraction

- Upper bainite/ferrite:
  - s = 0.03 wt.% C
- Lower bainite:
  - s = 0.27 wt.% C



[5]: H. K. D. H. Bhadeshia and D. V. Edmonds. The Mechanism of Bainite Formation in Steels. Acta Metallurgica, 28:1265–1273, 1980.

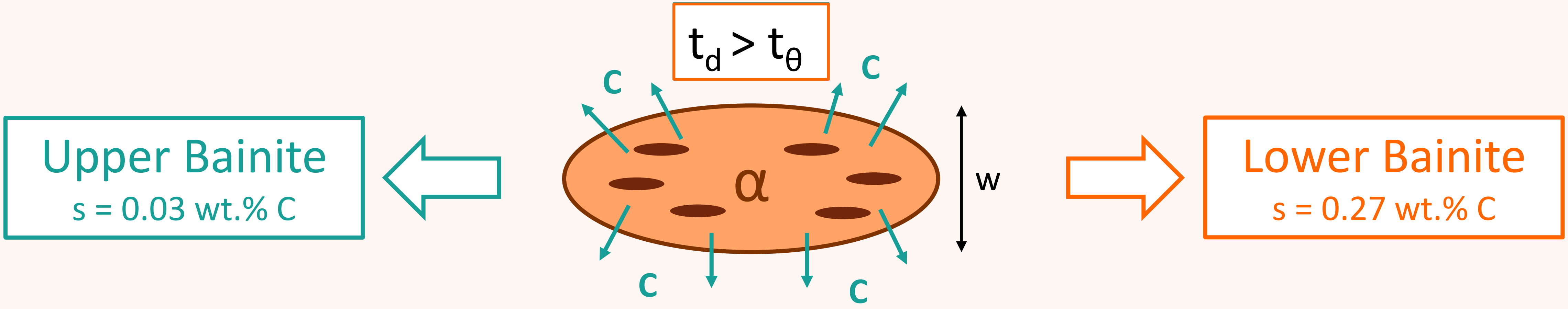
Upper-to-Lower Bainite Transition, L_s

- Model developed by Takahashi and Bhadeshia [6]:
  - Ferrite decarburisation, t_d:

$$t_{\mathrm{d}} = \frac{w^2 \pi (\bar{x} - x^{\alpha\gamma})^2}{16 \underline{D} (x^{\gamma\alpha} - \bar{x})^2}$$

- Cementite precipitation, t_θ:

$$\xi(t) = 1 - \exp\left(k\, t^{0.62}\right)$$



[6]: M. Takahashi and H. K. D. H. Bhadeshia. Model for transition from upper to lower bainite. Materials Science and Technology, 6:592–603, 1990.

Modifying the Li Model

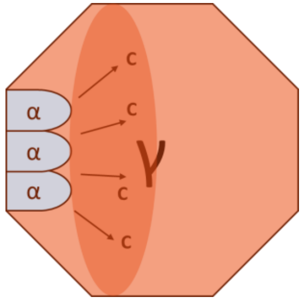
Li Model

$$\tau(X,T) = \frac{F(\mathrm{C, Mn, Si, Ni, Cr, Mo}, G)}{\Delta T^n \exp(-Q/RT)} S(X)$$ [2]

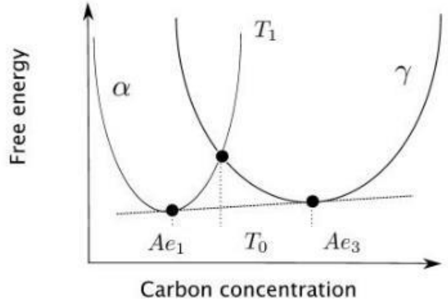
$$+ \sum_i \frac{\Delta t_i}{t_i} = 1$$ [3]

Modifications

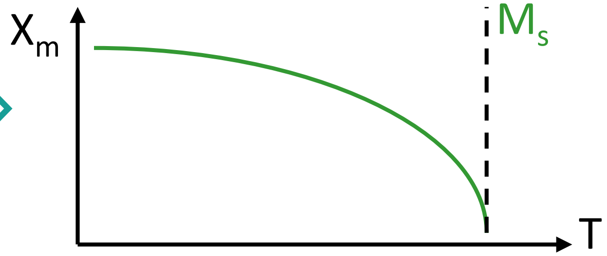
Carbon Partitioning



Adjusted Boundary Conditions



K-M Martensite Model [7]



[2]: Li et al., A Computational Model for the Prediction of Steel Hardenability, *Metallurgical and Materials Transactions B*, 29 (1998), 661.

[3]: E. Scheil. Anlaufzeit der Austenitumwandlung. Archiv für das Eisenhüttenwesen, 8:565–567, 1935.

[7]: D. P. Koistinen and R. E. Marburger. A general equation prescribing the extent of the austenite-martensite transformation in pure iron-carbon alloys and plain carbon steels. *Acta Matllurgica*, 7:59-60, 1959.

Modelling CCTs – The Final Product (SA-540 B24)

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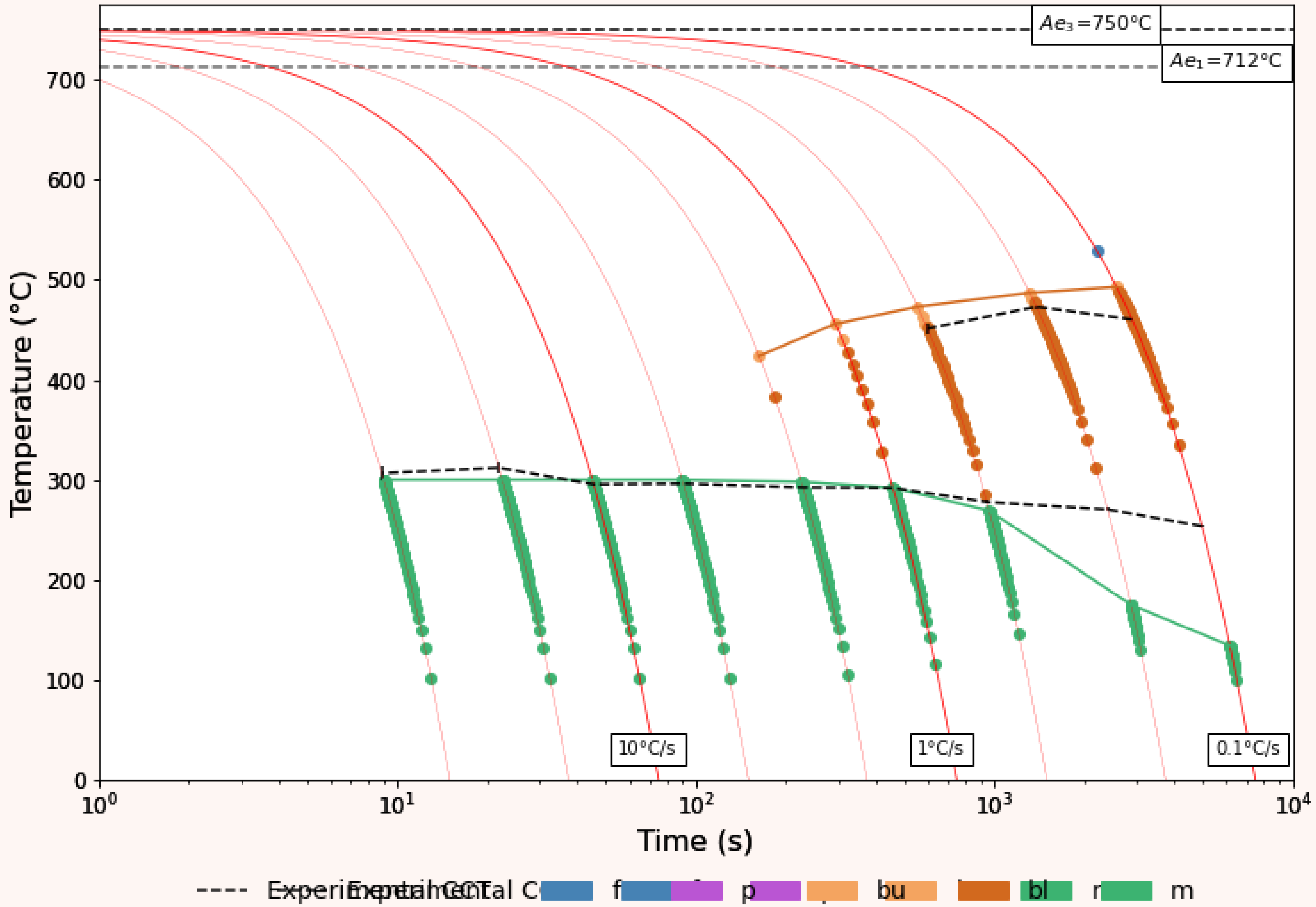

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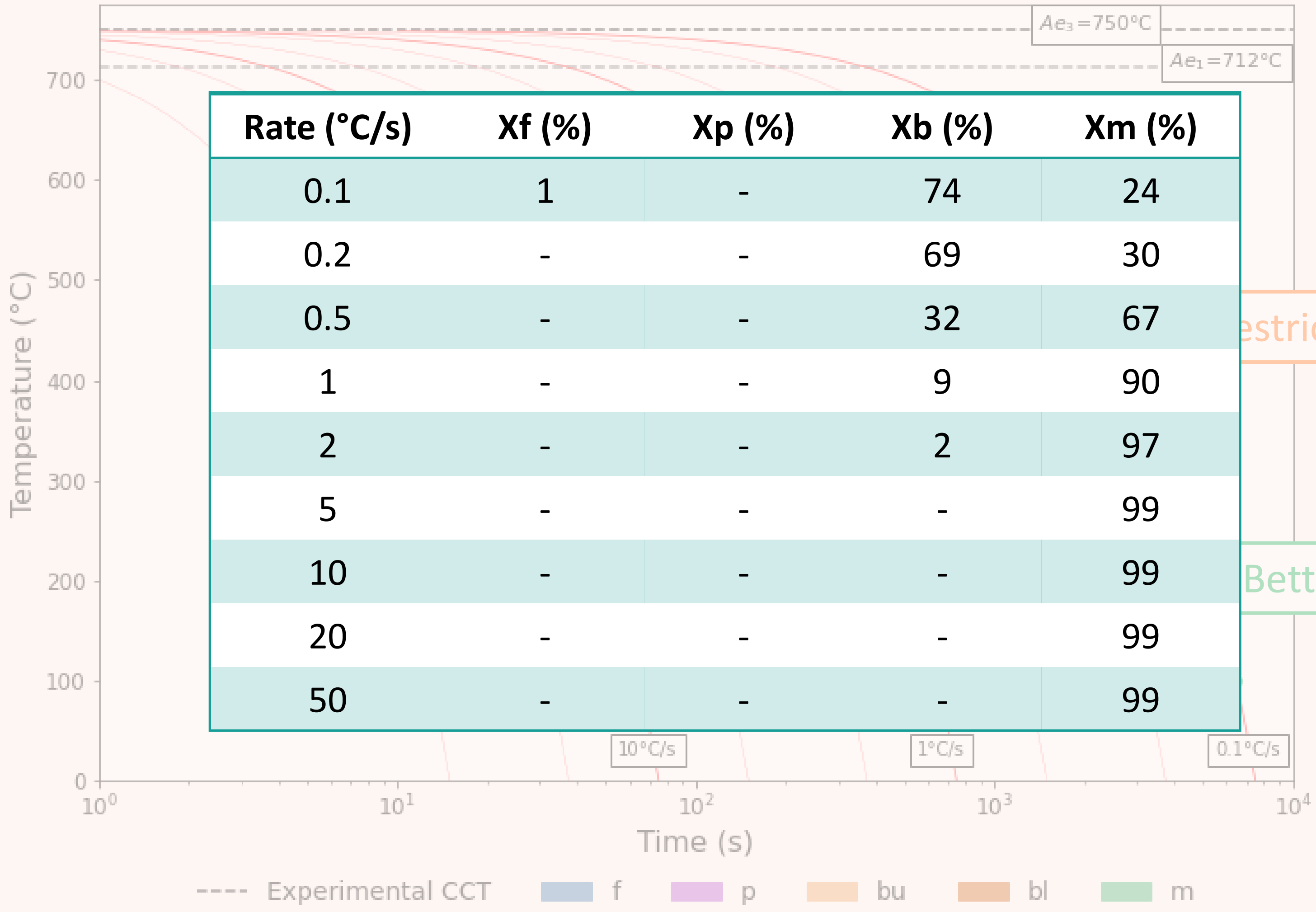
Modelling CCTs – The Final Product (SA-540 B24)

SA-540	
	Wt.%
C	0.40
Si	0.26
Mn	0.75
Ni	1.81
Cr	0.86
Mo	0.32

Rate (°C/s)	Xf (%)	Xp (%)	Xb (%)	Xm (%)
0.1	1	-	74	24
0.2	-	-	69	30
0.5	-	-	32	67
1	-	-	9	90
2	-	-	2	97
5	-	-	-	99
10	-	-	-	99
20	-	-	-	99
50	-	-	-	99



estrict bainite

Better martensite (suppressed)

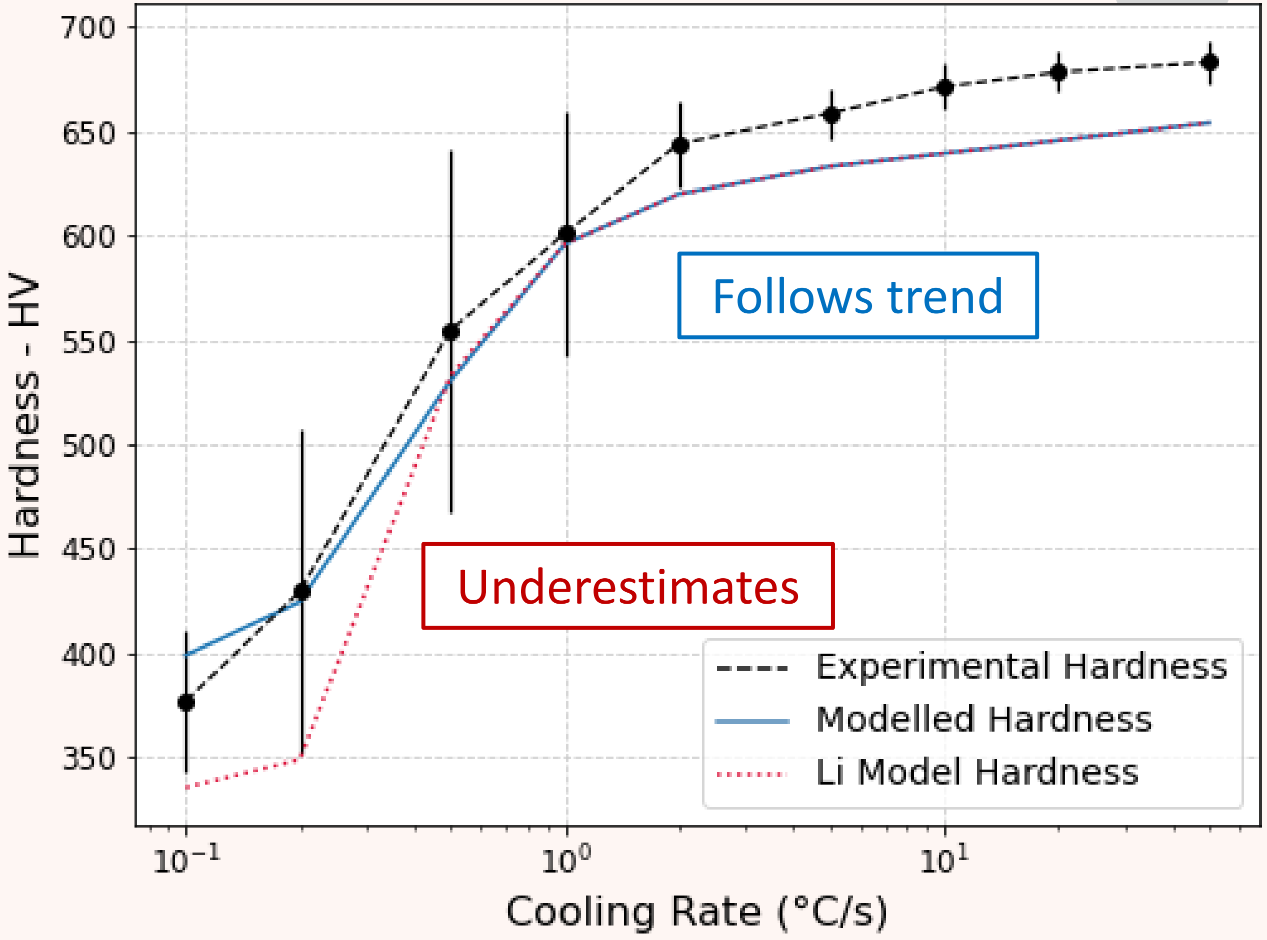
Modelling CCTs – Hardness Predictions (SA-540 B24)

$$Hv_{F+P} = 42 + 223C + 53Si + 30Mn + 12.6Ni + 7Cr + 19Mo + (10 - 19Si + 4Ni + 8Cr + 130V) \log Vr$$ [8]

$$Hv_B = -323 + 185C + 330Si + 153Mn + 65Ni + 144Cr + 191Mo + (89 + 53C - 55Si - 22Mn - 10Ni - 20Cr - 33Mo) \log Vr$$ [8]

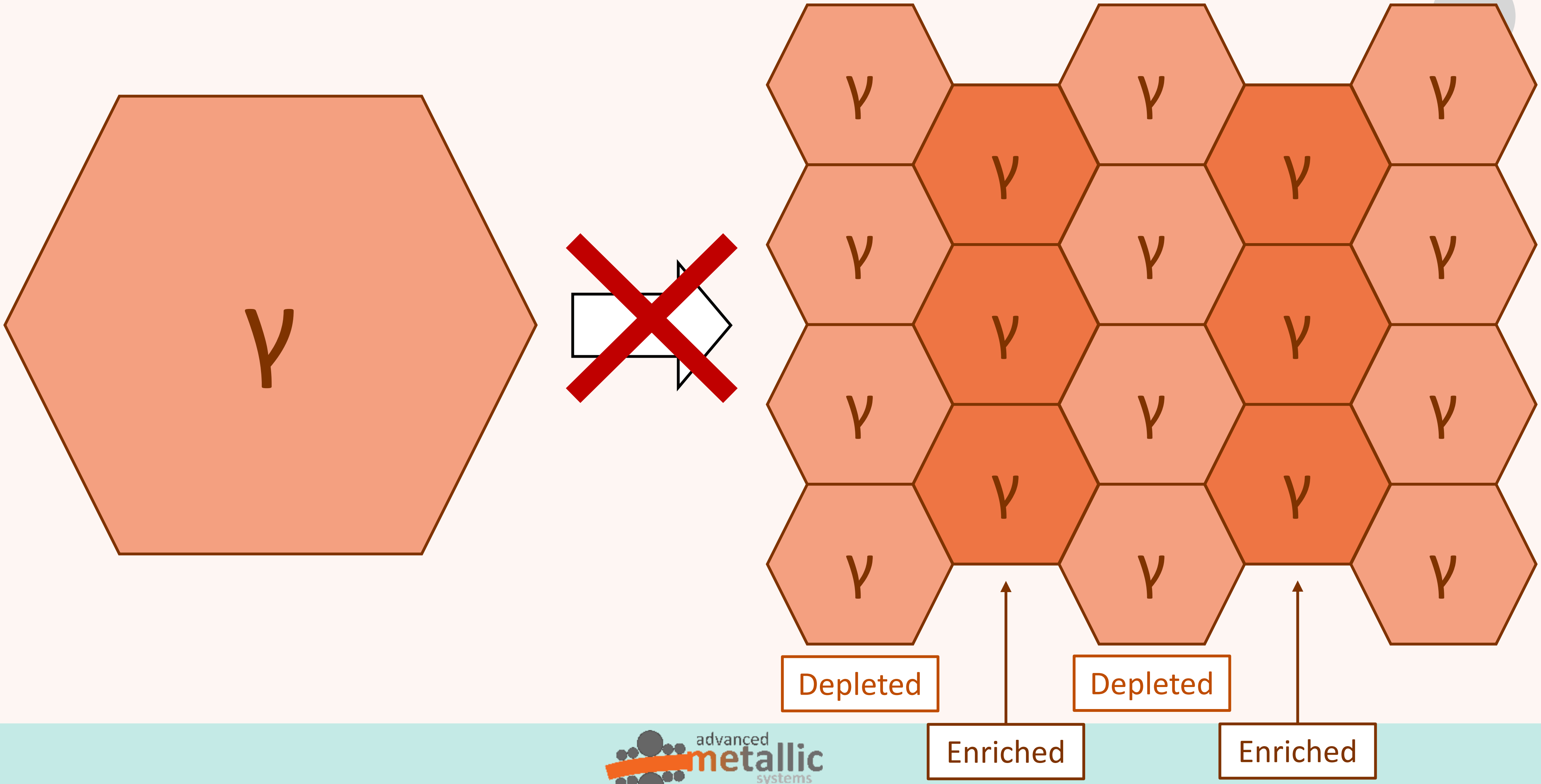
$$Hv_M = 127 + 949C + 27Si + 11Mn + 8Ni + 16Cr + 21 \log Vr$$ [8]

$$Hv = X_M Hv_M + X_B Hv_B + (X_F + X_P) Hv_{F+P}$$



[8]: R. Blondeau, Ph. Maynier, J. Dollet, and B. Vieillard-Baron. mathematical model for the calculation of mechanical properties of low-alloy steel metallurgical products: a few examples of its applications. In Heat Treatment '76, page 189,

Accounting for Compositional Heterogeneity



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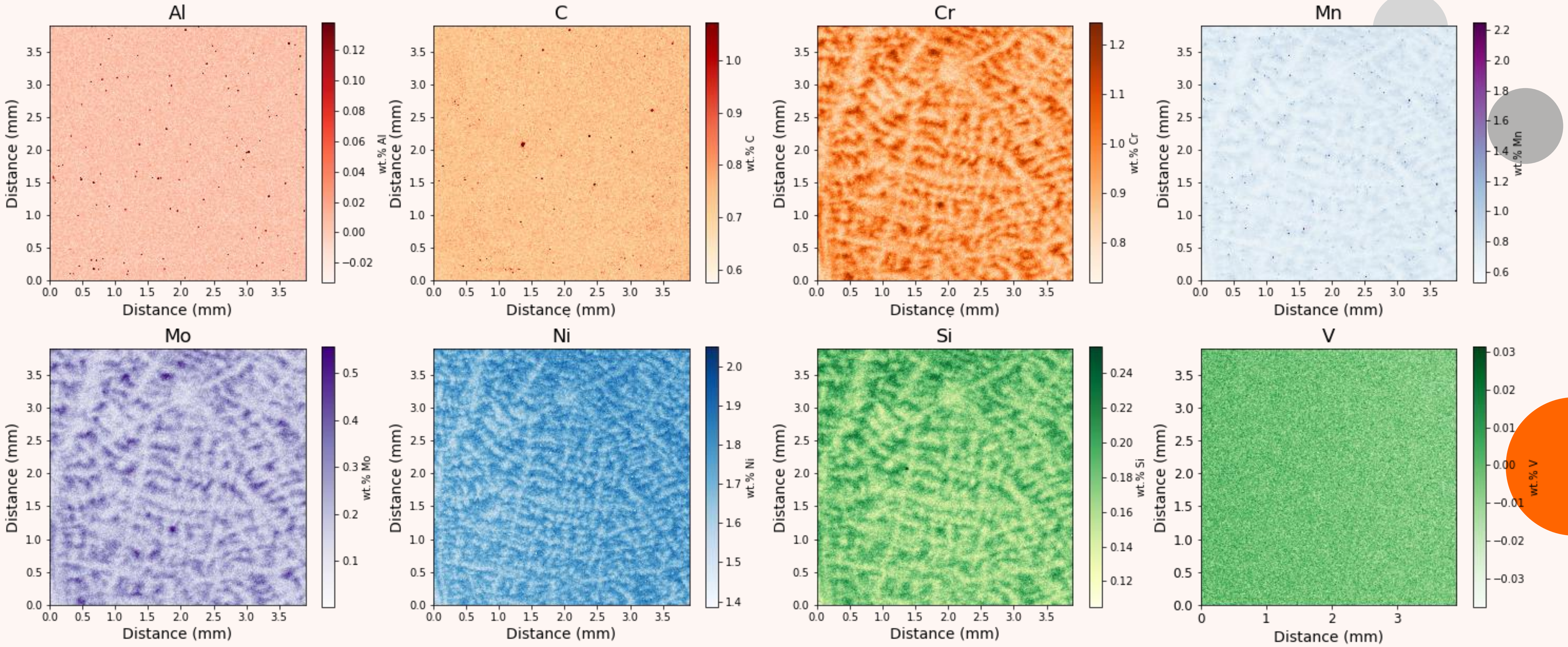
Compositional Heterogeneity – EPMA (SA-540 B24)



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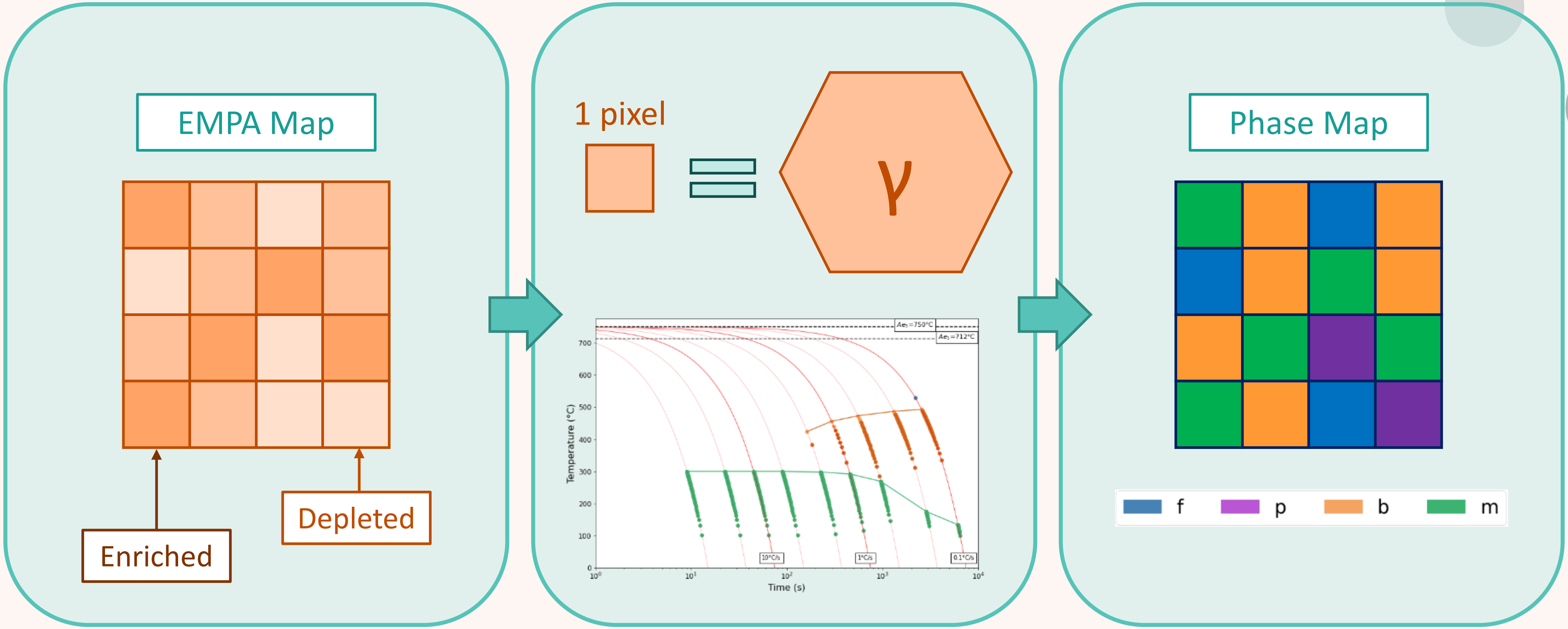
Compositional Heterogeneity – Applying the Model



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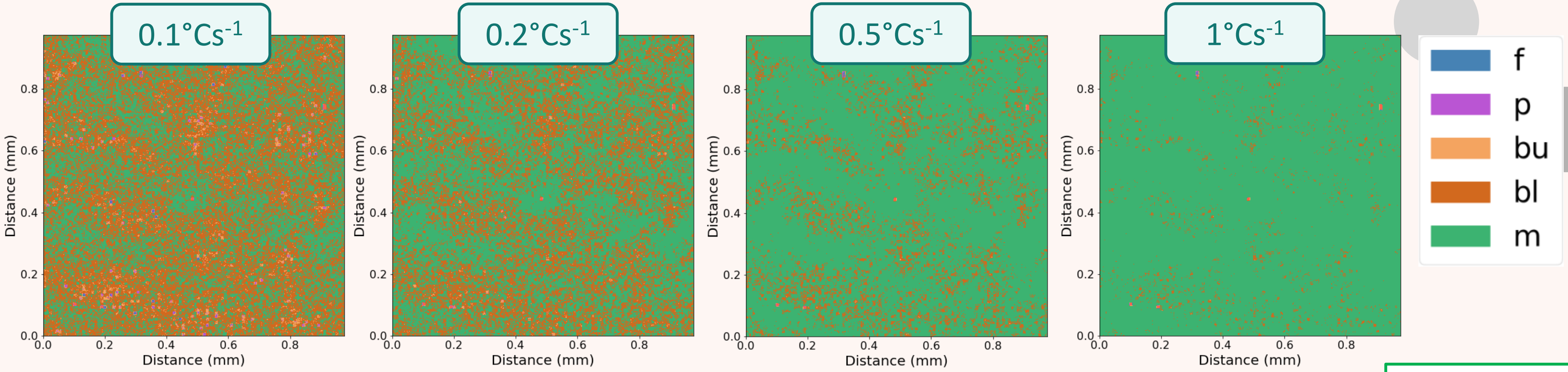
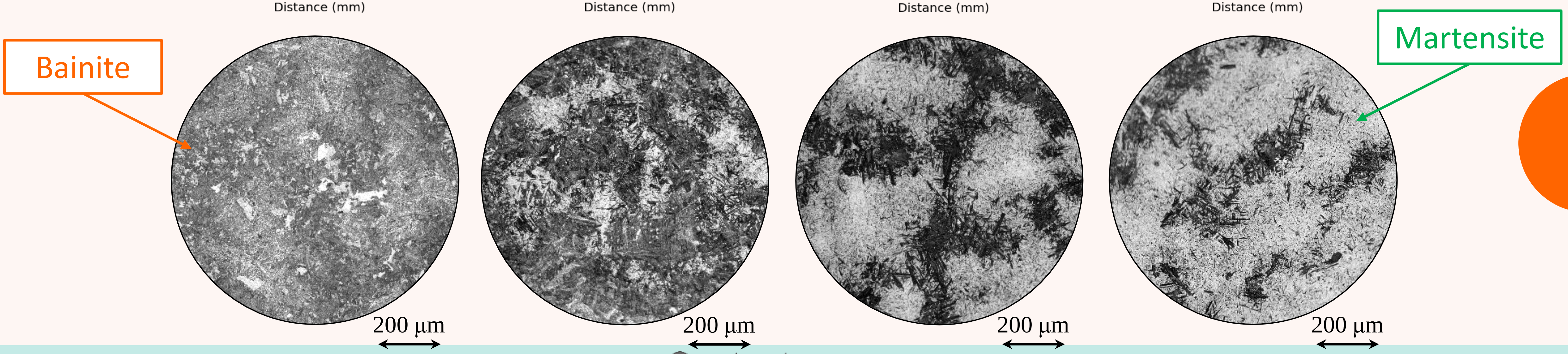
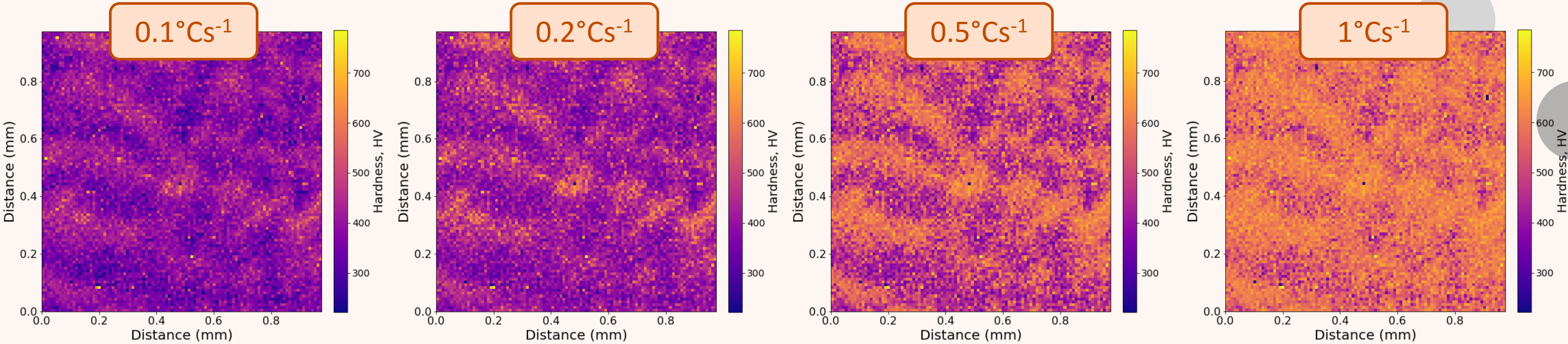
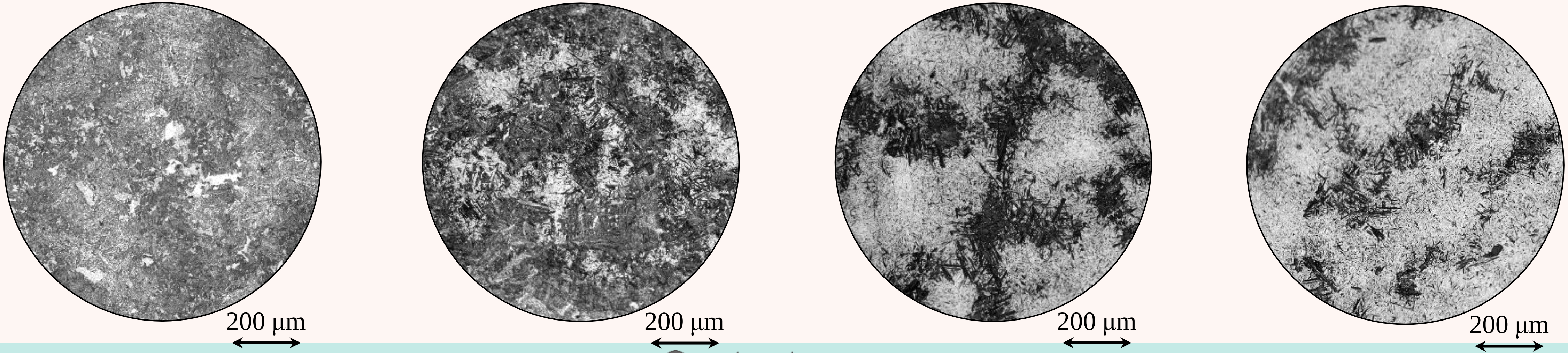
Applying the Model – Phase Maps (SA-540 B24)





Applying the Model – Hardness Maps (SA-540 B24)





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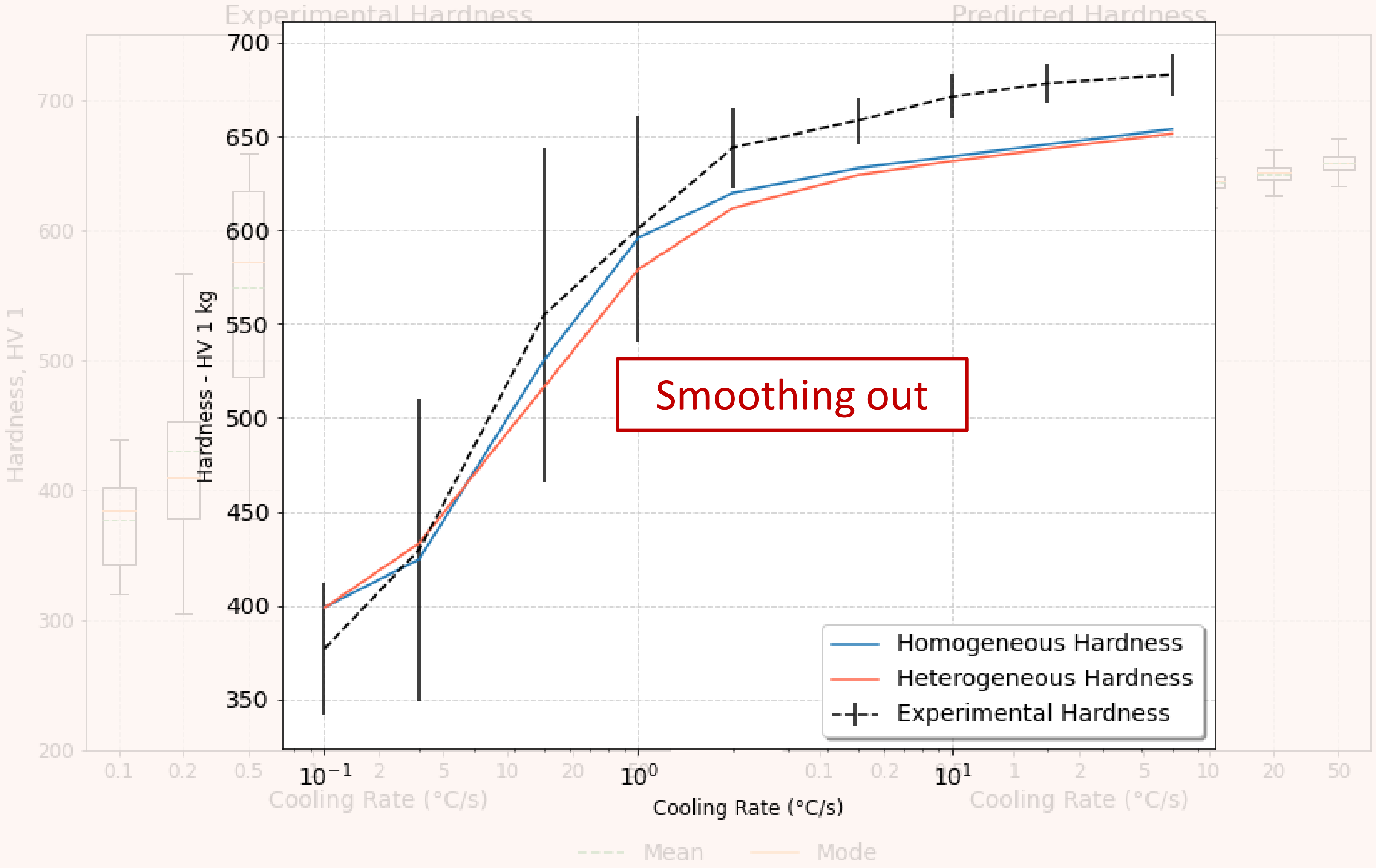
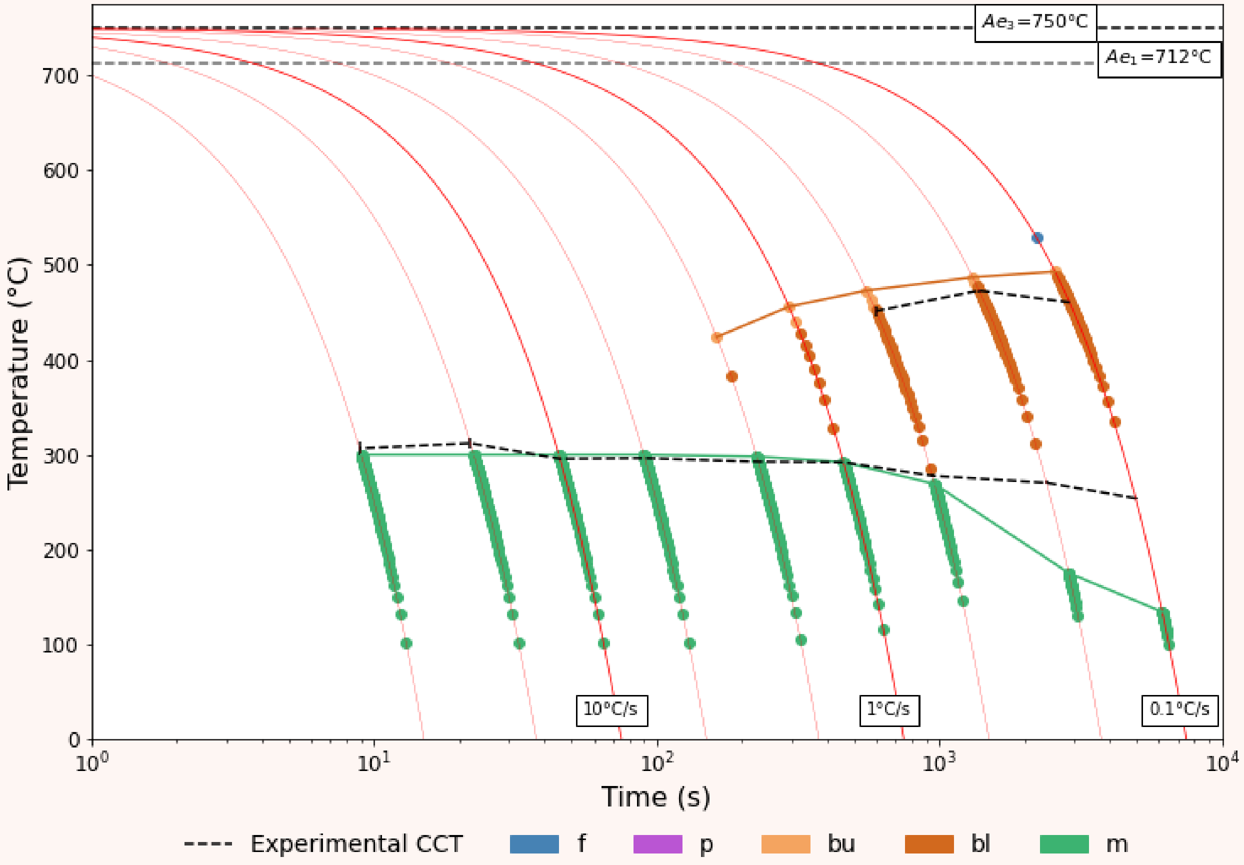
Applying the Model – Hardness (SA-540 B24)

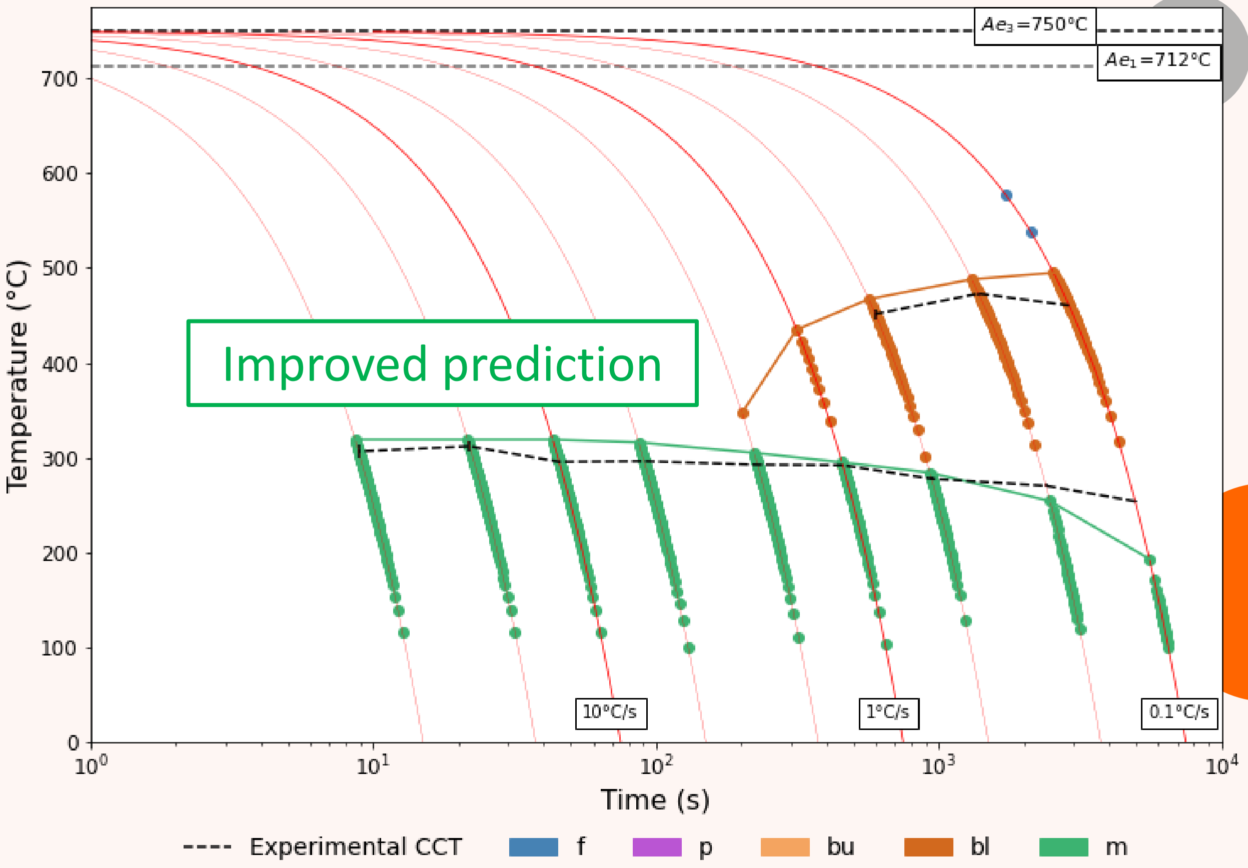


Applying the Model – CCT (SA-540 B24)

Homogeneous

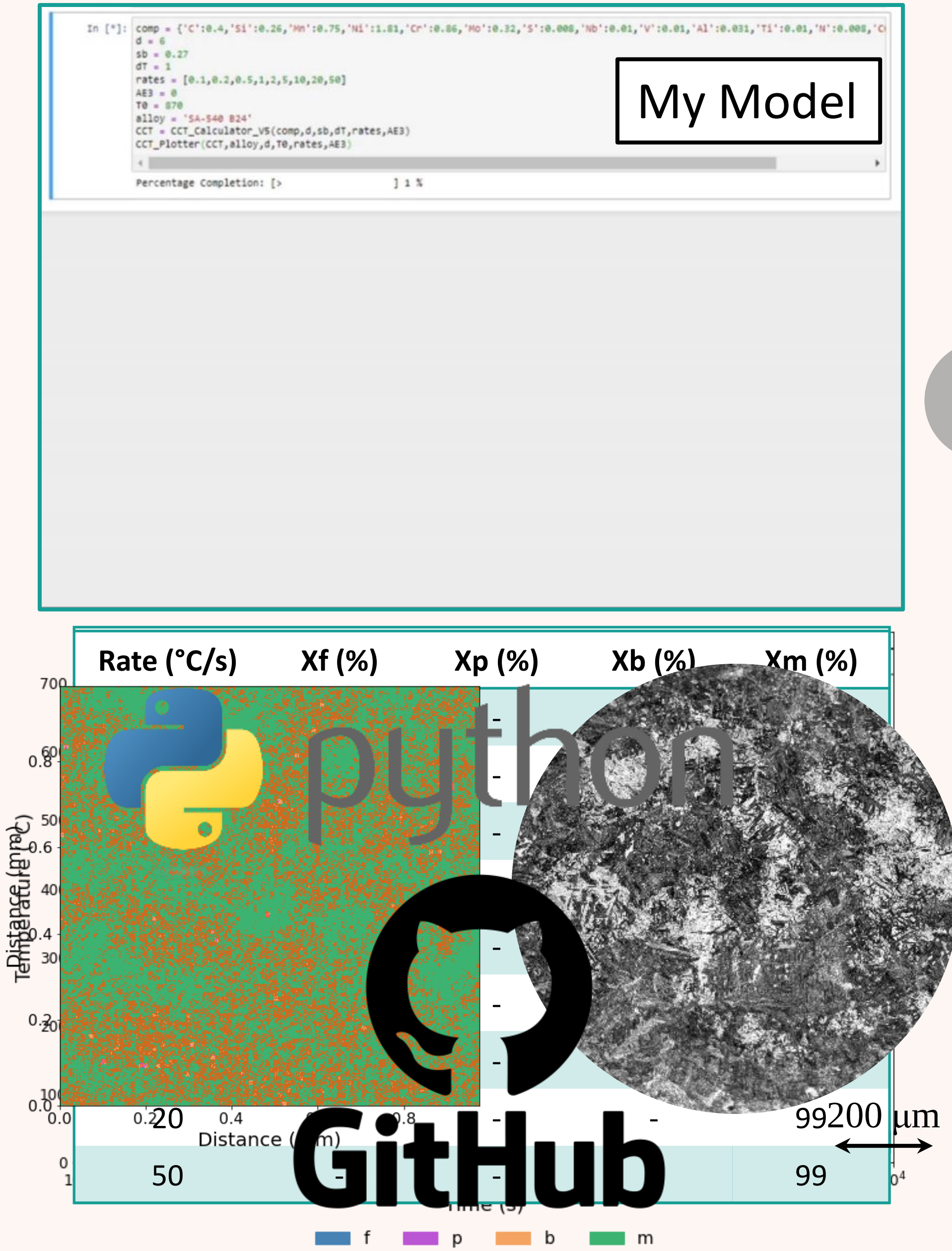


Heterogeneous



Advantages of My Model

1. Rapid simulation times
   - ~ 10s per CCT
2. Improved CCT predictions
   - Novel modifications
3. Expanded predictive capabilities
   - Outputs final constituent fractions
4. Improved versatility
   - Adapted well into more complex model
5. Free, open source & accessible



Thank you for Listening

The authors gratefully acknowledge the EPSRC (Engineering and Physical Sciences Research Council, UK), SFI (Science Foundation Ireland) and Rolls-Royce for their financial support.

Add me on LinkedIn!

Check out my CCT predictor!

Modelling CCTs – Li Equations

Ferrite

$$\tau_{\mathrm{F}} = \frac{\mathrm{FC}}{2^{0.41\,G}\,(\mathrm{Ae}_3 - T)^3 \exp(-27500/RT)} S(X)$$

$$\mathrm{FC} = \exp(1.00 + 6.31(\%\,\mathrm{C}) + 1.78(\%\,\mathrm{Mn}) + 0.31(\%\,\mathrm{Si}) + 1.12(\%\,\mathrm{Ni}) + 2.70(\%\,\mathrm{Cr}) + 4.06(\%\,\mathrm{Mo}))$$

[2]

Pearlite

$$\tau_{\mathrm{P}} = \frac{\mathrm{PC}}{2^{0.32\,G}\,(\mathrm{Ae}_1 - T)^3 \exp(-27500/RT)} S(X)$$

$$\mathrm{PC} = \exp(-4.25 + 4.12\,(\%\,\mathrm{C}) + 4.36\,(\%\,\mathrm{Mn}) + 0.44\,(\%\,\mathrm{Si}) + 1.71\,(\%\,\mathrm{Ni}) + 3.33\,(\%\,\mathrm{Cr}) + 5.19\sqrt{(\%\,\mathrm{Mo})})$$

[2]

Bainite

$$\tau_{\mathrm{B}} = \frac{\mathrm{BC}}{2^{0.29\,G}\,(\mathrm{B}_s - T)^2 \exp(-27500/RT)} S(X)$$

$$\mathrm{BC} = \exp(-10.23 + 10.18\,(\%\,\mathrm{C}) + 0.85\,(\%\,\mathrm{Mn}) + 0.55\,(\%\,\mathrm{Ni}) + 0.90\,(\%\,\mathrm{Cr}) + 0.36\,(\%\,\mathrm{Mo}))$$

[2]

[2]: Li et al., A Computational Model for the Prediction of Steel Hardenability, *Metallurgical and Materials Transactions B*, 29 (1998), 661.

Modelling CCTs – Transformation Start Equations

Ferrite + Pearlite

$$Ae_3(^\circ F) = 1570 - 323\,\mathrm{C} - 25\,\mathrm{Mn} + 80\,\mathrm{Si} - 32\,\mathrm{Ni} - 3\,\mathrm{Cr}$$

[9]

Pearlite

$$\begin{aligned} A_{\mathrm{cm}}(^\circ C) = 224.4 + 992.4\,\mathrm{C} - 465.1\,\mathrm{C}^2 + 46.7\,\mathrm{Cr} + 19.0\,\mathrm{C}\,\mathrm{Cr} \\ -6.1\,\mathrm{Cr}^2 + 7.6\,\mathrm{Mn} + 10.0\,\mathrm{Mo} - 6.8\,\mathrm{Cr}\,\mathrm{Mo} - 6.9\,\mathrm{Ni} \\ +3.7\,\mathrm{C}\,\mathrm{Ni} - 2.7\,\mathrm{Cr}\,\mathrm{Ni} + 0.8\,\mathrm{Ni}^2 + 16.7\,\mathrm{Si} \end{aligned}$$

[10]

Bainite

$$\mathrm{B}_s(^\circ C) = 637 - 58\,\mathrm{C} - 35\,\mathrm{Mn} - 15\,\mathrm{Ni} - 34\,\mathrm{Cr} - 41\,\mathrm{Mo}$$

[2]

Martensite

$$\mathrm{M_S}(^\circ C) = 561 - 474\,\mathrm{C} - 33\,\mathrm{Mn} - 17\,\mathrm{Cr} - 17\,\mathrm{Ni} - 21\,\mathrm{Mo} + 10\,\mathrm{Co} - 7.5\,\mathrm{Si}$$

[4]

[9]: R. A. Grange. Estimating Critical Ranges in Heat Treatment of Steels. *Metal Progress*, 79:73–75, 1961.

[10]: S-J. Lee and Y-K. Lee. Thermodynamic Formula for the Acm Temperature of Low Alloy Steels. ISIJ International, 47:769–771, 2007.

[2]: Li et al., A Computational Model for the Prediction of Steel Hardenability, *Metallurgical and Materials Transactions B*, 29 (1998), 661.

[4]: C. Y. Kung and J. J. Rayment. Metallurgical Transactions A, 13:328–331, 1982.

Modelling CCTs – K-M Equations

$$X_{\mathrm{M}} = X_{\mathrm{A}}^{0}(1 - \exp(-k(\mathrm{M}_s - T)))$$ [7]

$$k = \frac{-\ln(0.01)}{M_{\mathrm{s}} - M_{\mathrm{f}}}$$

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[7]: D. P. Koistinen and R. E. Marburger. A general equation prescribing the extent of the austenite-martensite transformation in pure iron-carbon alloys and plain carbon steels. *Acta Matllurgica*, 7:59-60, 1959.

Upper-to-Lower Bainite Transition, L_s

- Model developed by Takahashi and Bhadeshia [6]:
  - Ferrite decarburisation, t_d:

$$t_{\mathrm{d}} = \frac{w^2 \pi (\bar{x} - x^{\alpha\gamma})^2}{16 \underline{D} (x^{\gamma\alpha} - \bar{x})^2}$$

Lath width

Local para-equilibrium compositions

Carbon diffusivity

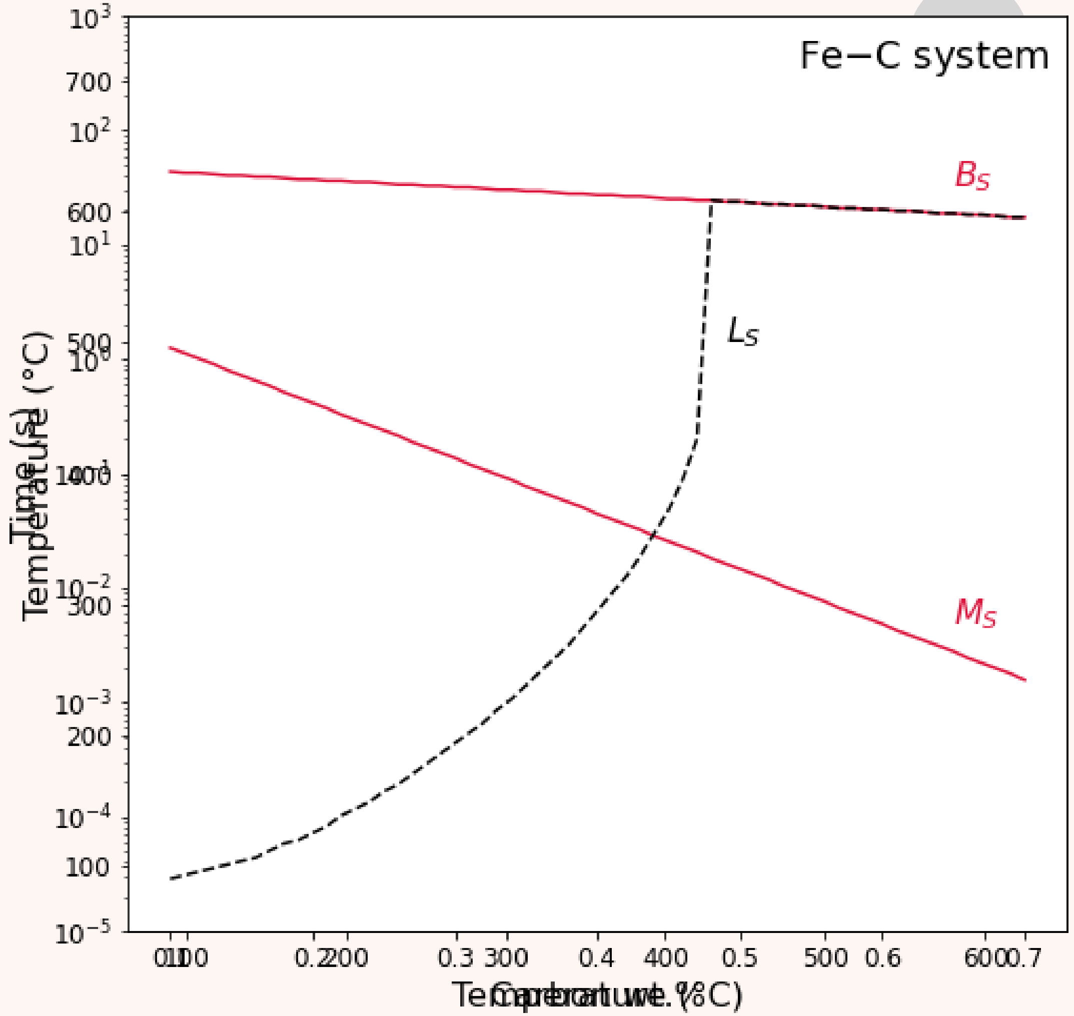
  - Cementite precipitation, t_θ:

$$\xi(t) = 1 - \exp\left(k\, t^{0.62}\right)$$

t_θ

Cementite volume fraction

Temperature dependent term



[6]: M. Takahashi and H. K. D. H. Bhadeshia. Model for transition from upper to lower bainite. Materials Science and Technology, 6:592–603, 1990.

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Incomplete Reaction Phenomenon

- The sudden halt in bainite transformation
  - Austenite carbon concentration increases
  - The free energy change for transformation tends to 0
    - $\Delta G_{(\gamma \rightarrow \alpha)} = 0$
  - Described by the T0' equation:

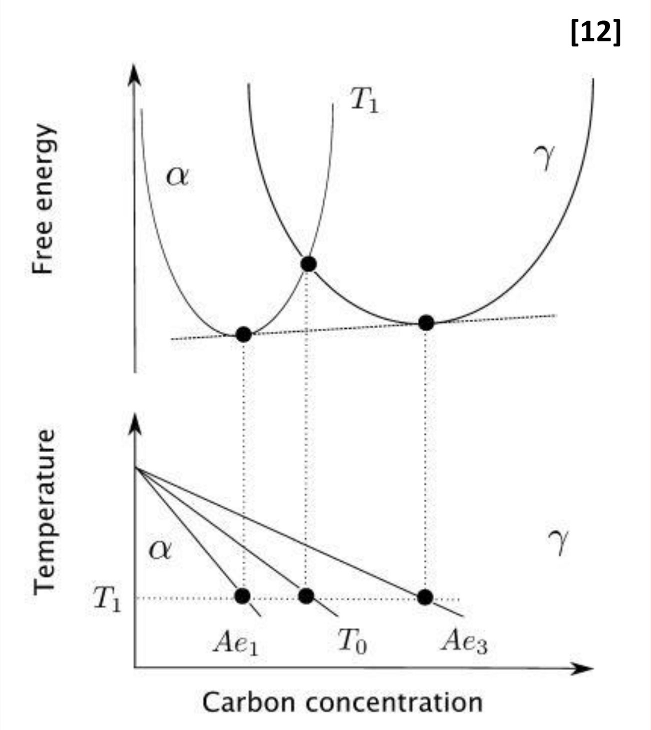
$$T_0'(K) \simeq 970 - 80\,x_C - \Delta T_0$$

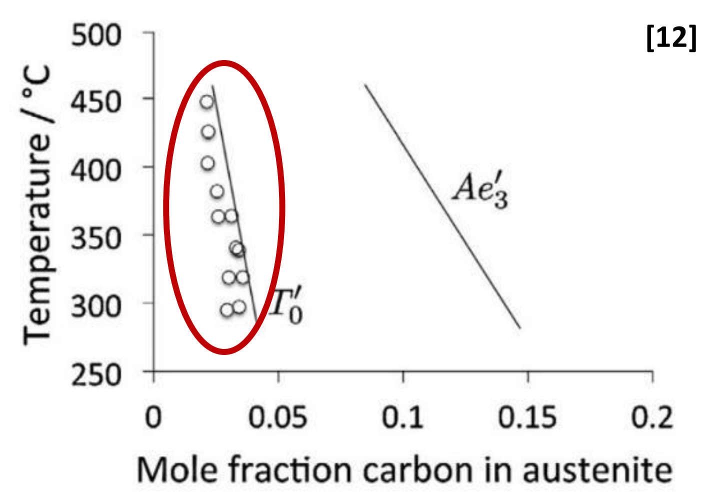
$$\Delta \mathrm{T}_0 = \frac{\Sigma_i\, x_i(b_{NM}\Delta T_{NM_i} + b_M \Delta T_{M_i})}{b_{NM} + b_M}$$

xc = at.% of carbon

xi = at.% of substitutional alloying element, i.

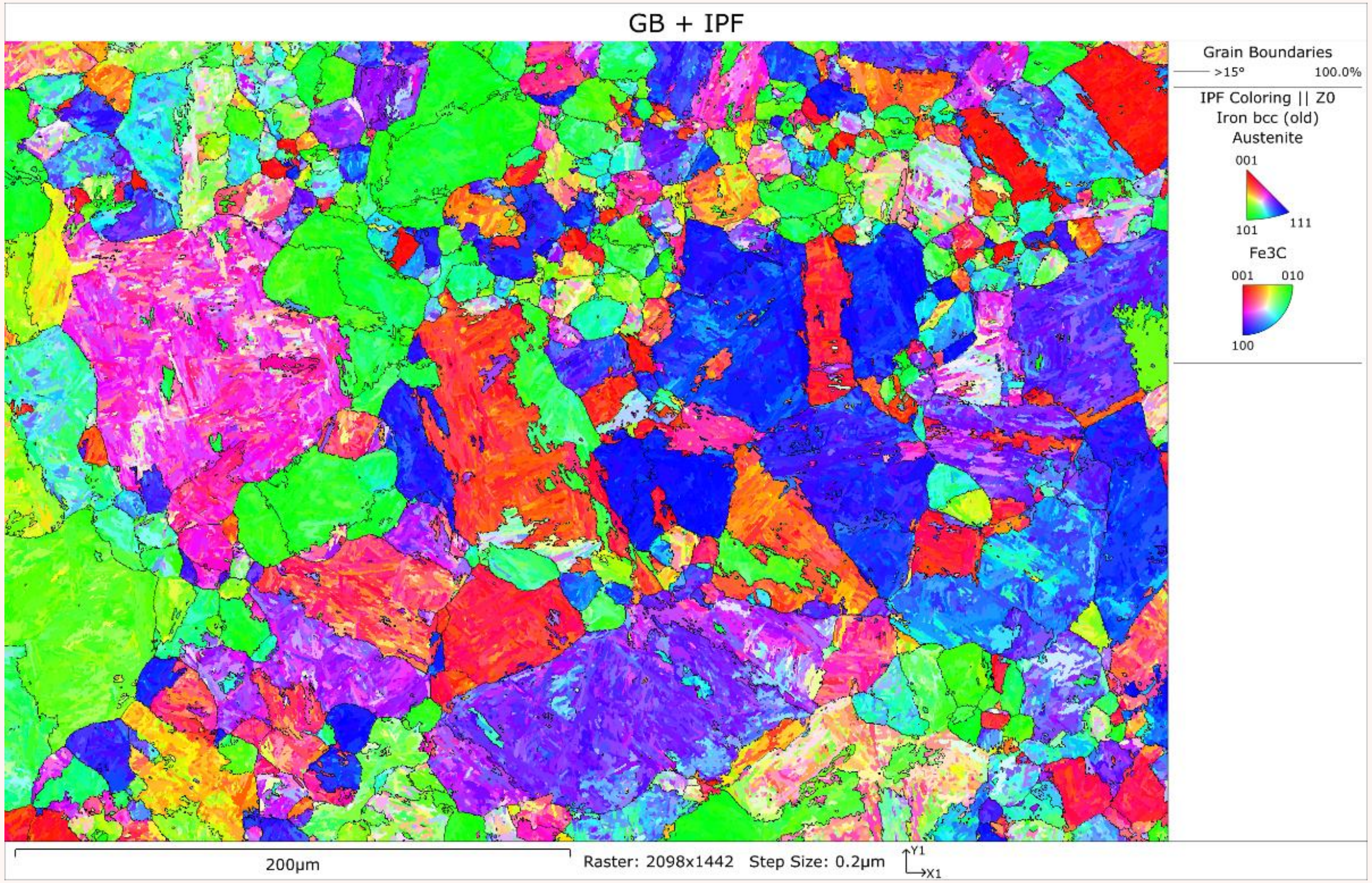
Predefined constants





[11]: H. Bhadeshia and R. Honeycombe. Steels: Microstructure and Properties, chapter 15, pages 421–455. Butterworth-Heinemann, 4th edition, 2017.

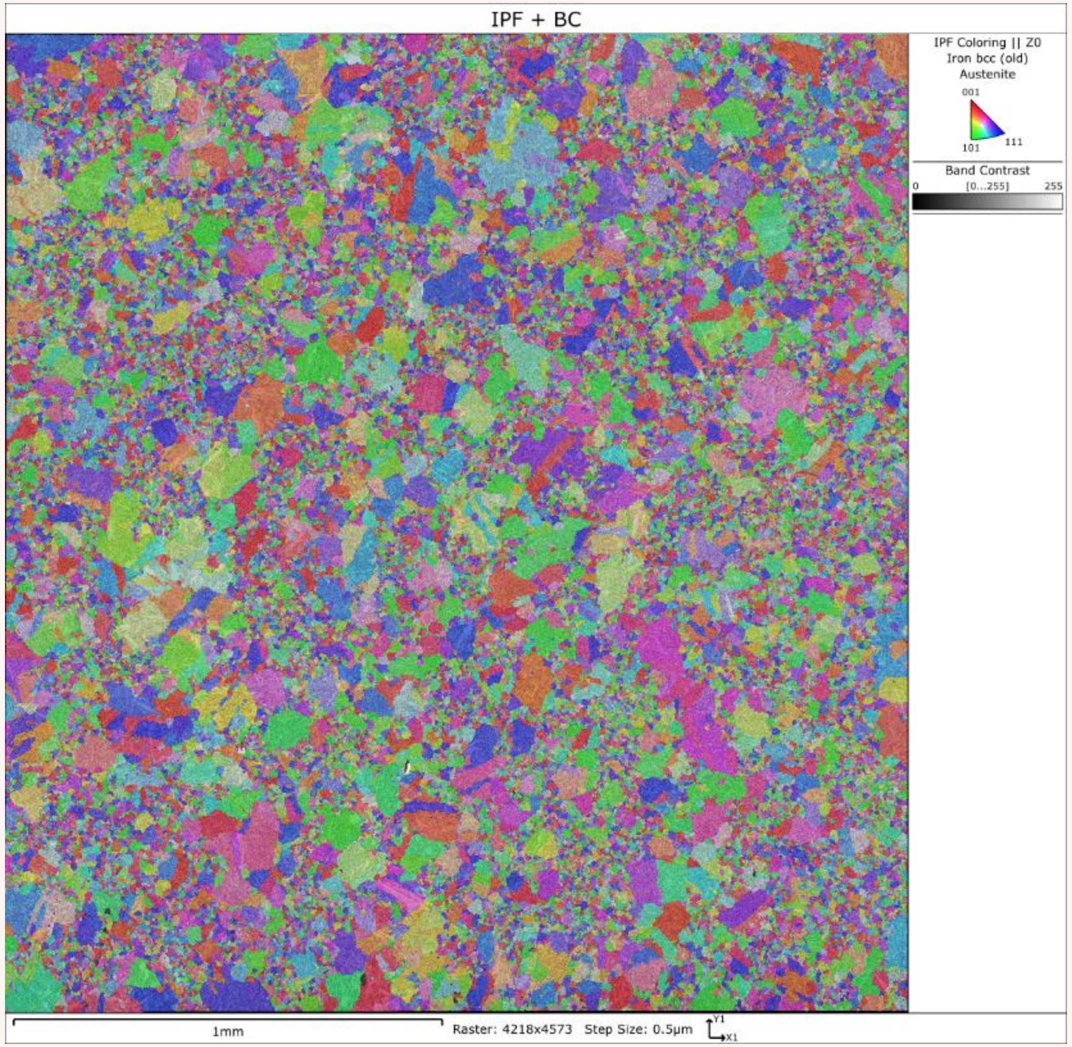
SA-540 B24 – Prior Austenite Grain (PAG) Size

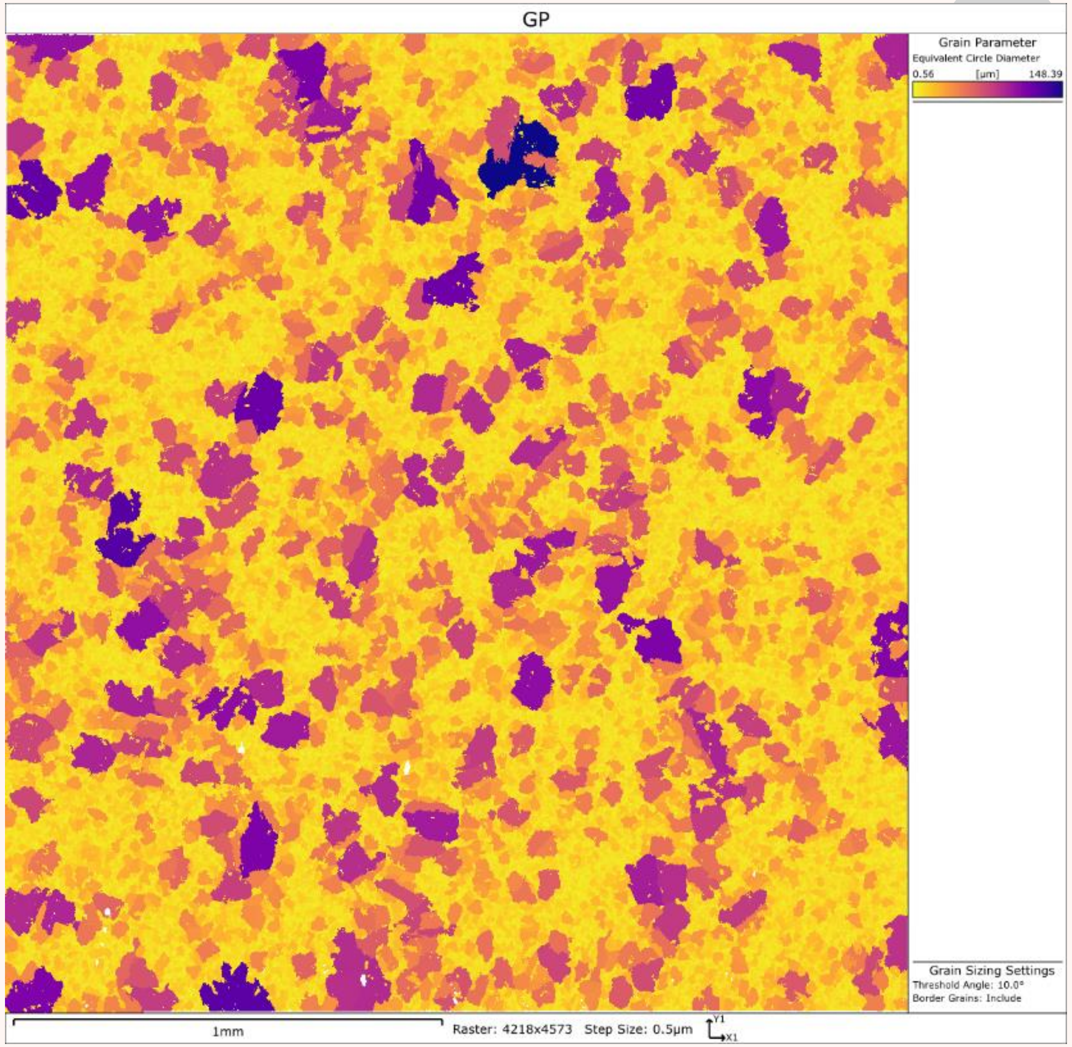


PAG Analysis

Grain Count: 2830
Mean: 3.5 µm
A-weighted Mean: 36.2 µm
Min: 0.7 µm
Max: 97.5µm
St.-Dev.: 6.5 µm
ASTM Grain Size: 11.5

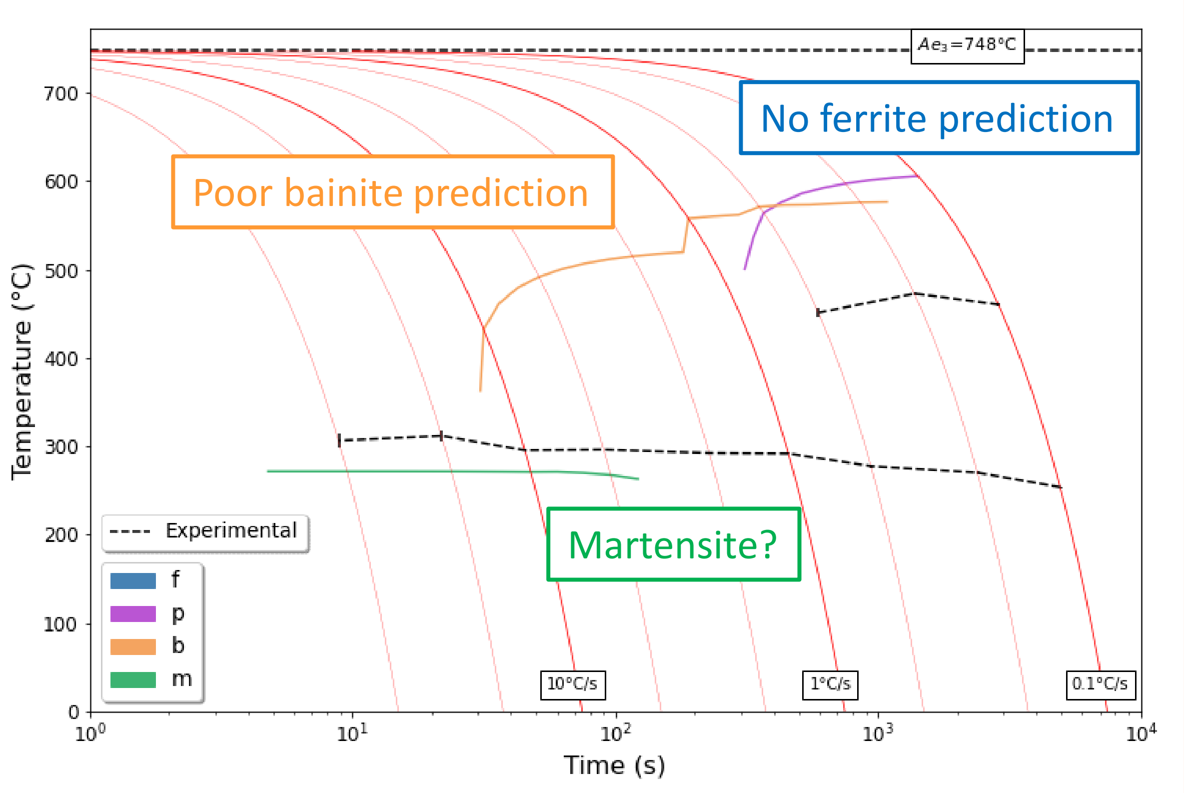
SA-540 B24 – Prior Austenite Grain (PAG) Size



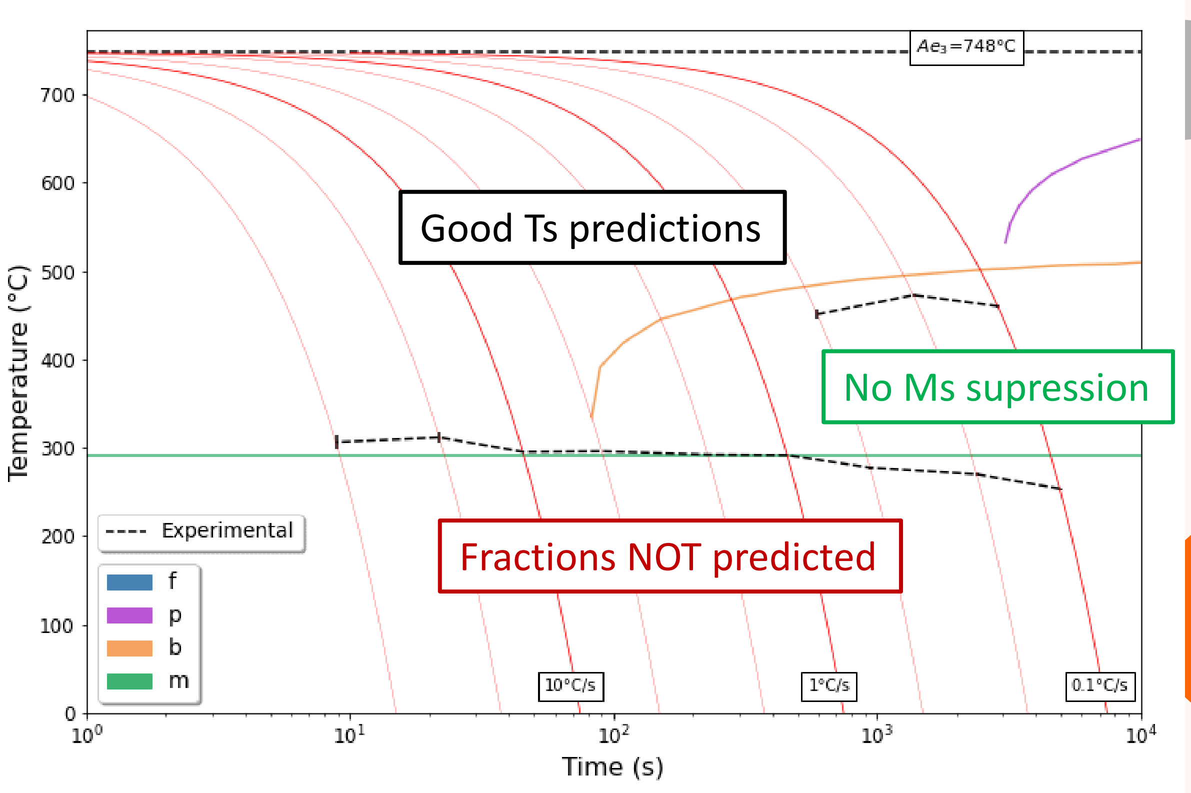


Comparing Other Models (SA-540 B24)

Thermo-Calc

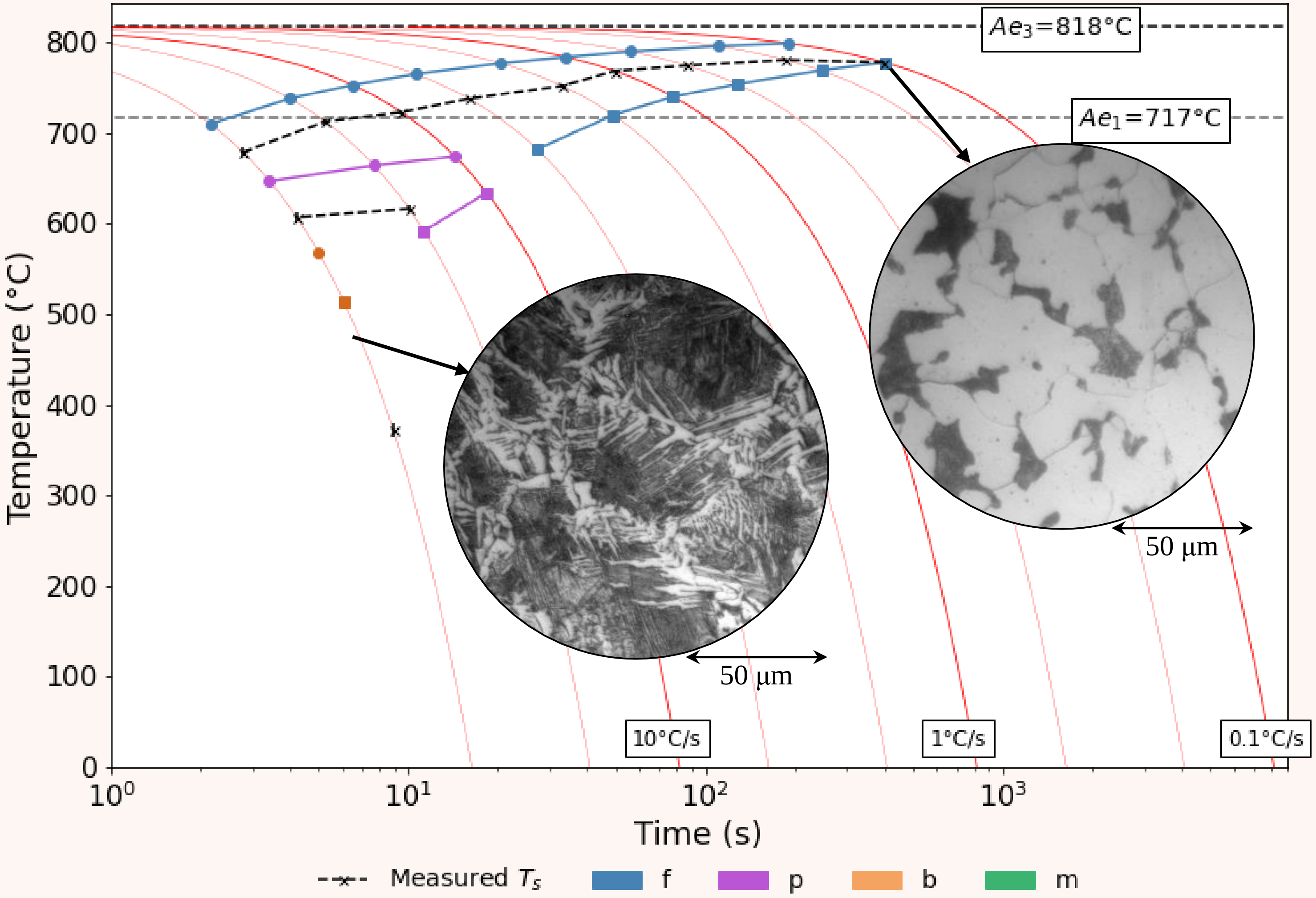


JMatPro



Modelling CCTs – The Li Model (En3B)

En3B	
	Wt.%
C	0.18
Si	0.16
Mn	0.73
Ni	-
Cr	-
Mo	-



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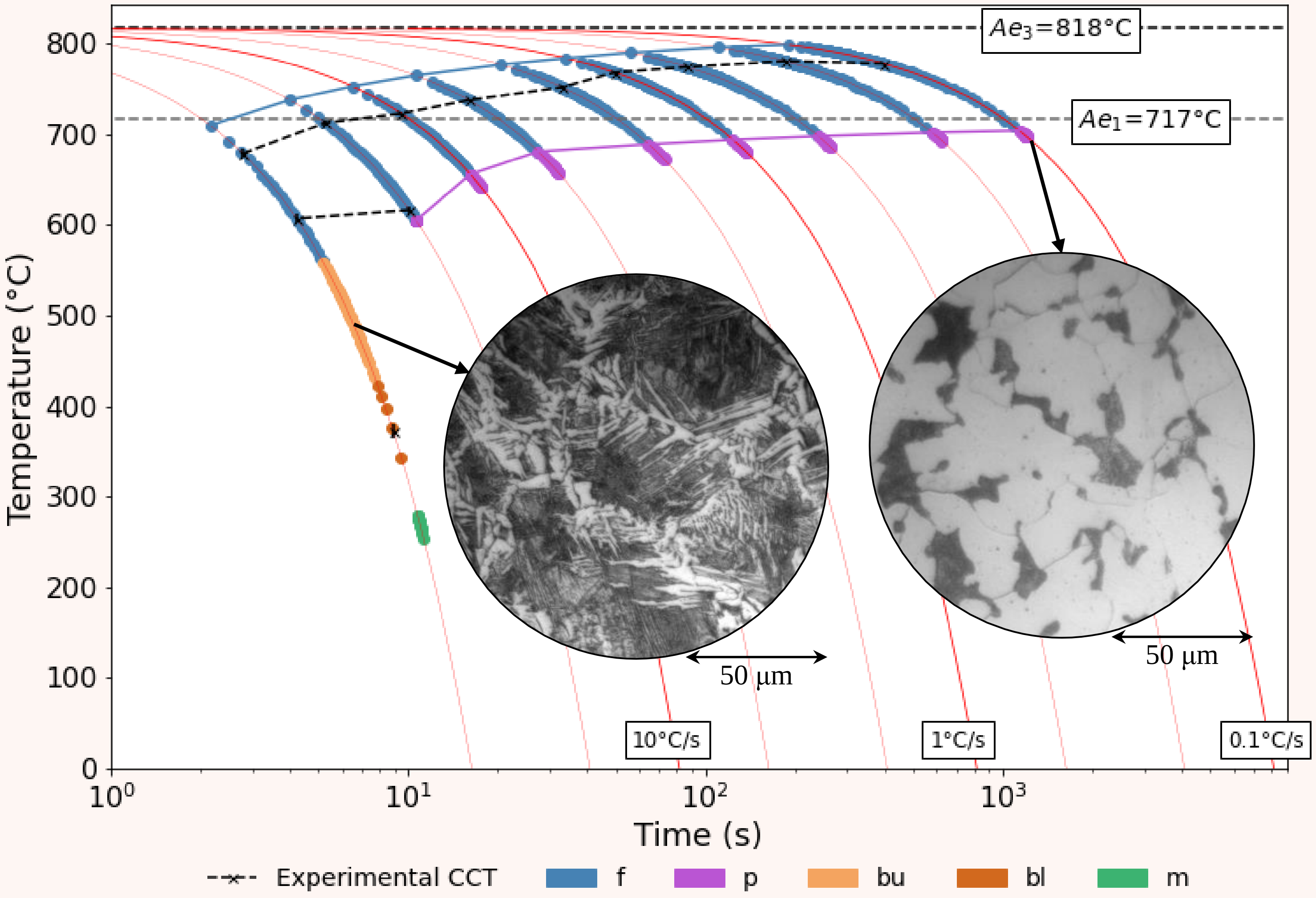
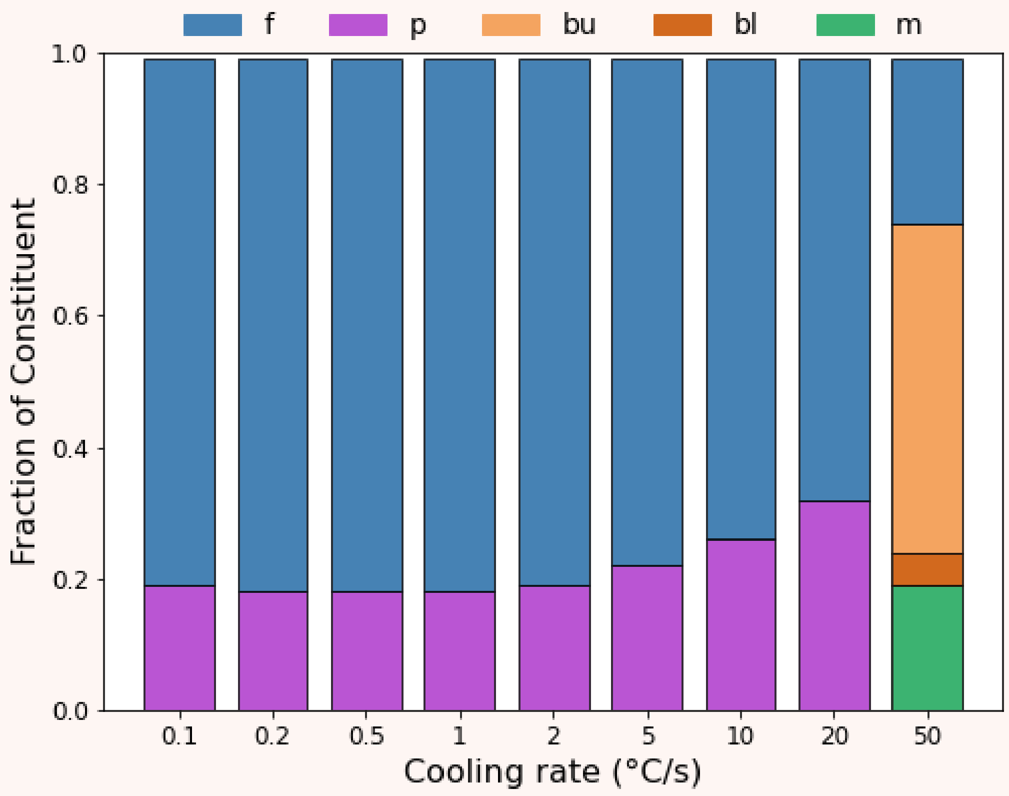
Modelling CCTs – My Model (En3B)

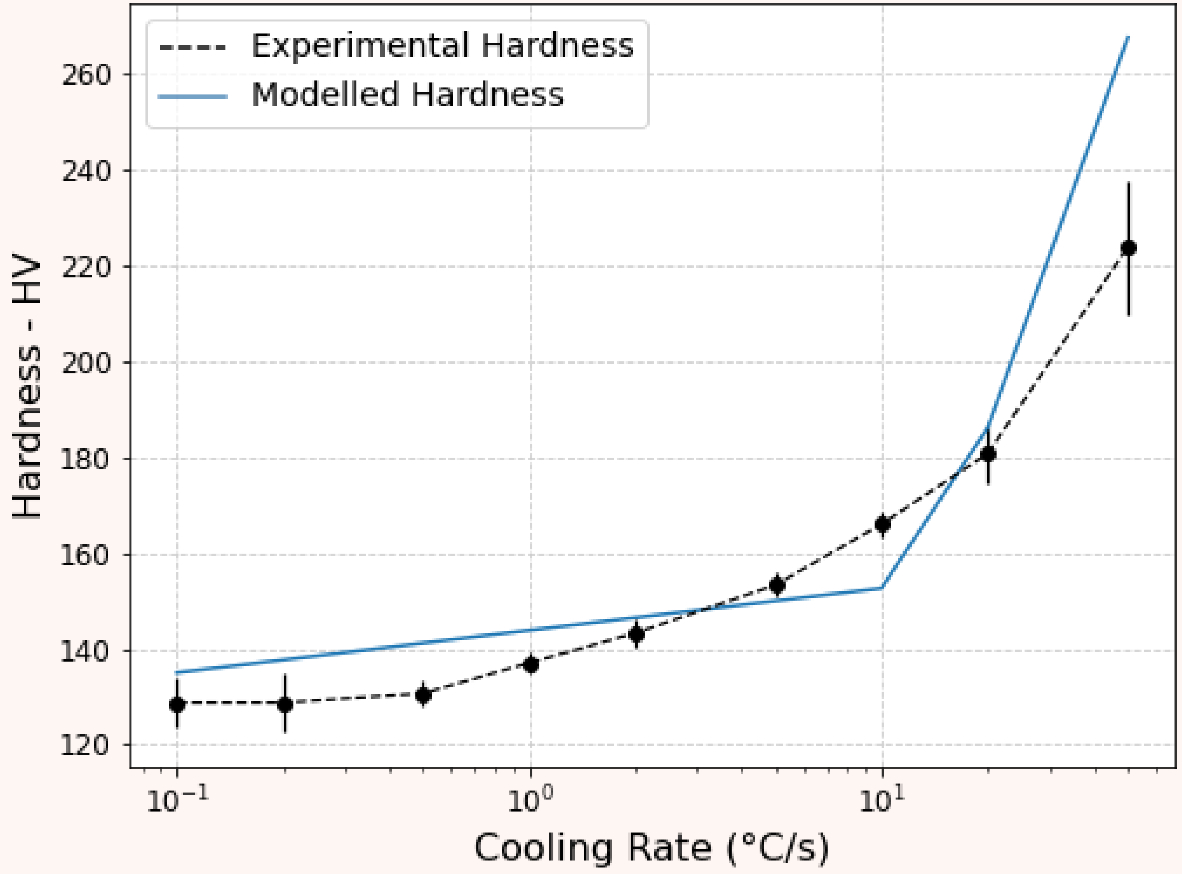
En3B	
	Wt.%
C	0.18
Si	0.16
Mn	0.73
Ni	-
Cr	-
Mo	-



advanced metallic systems

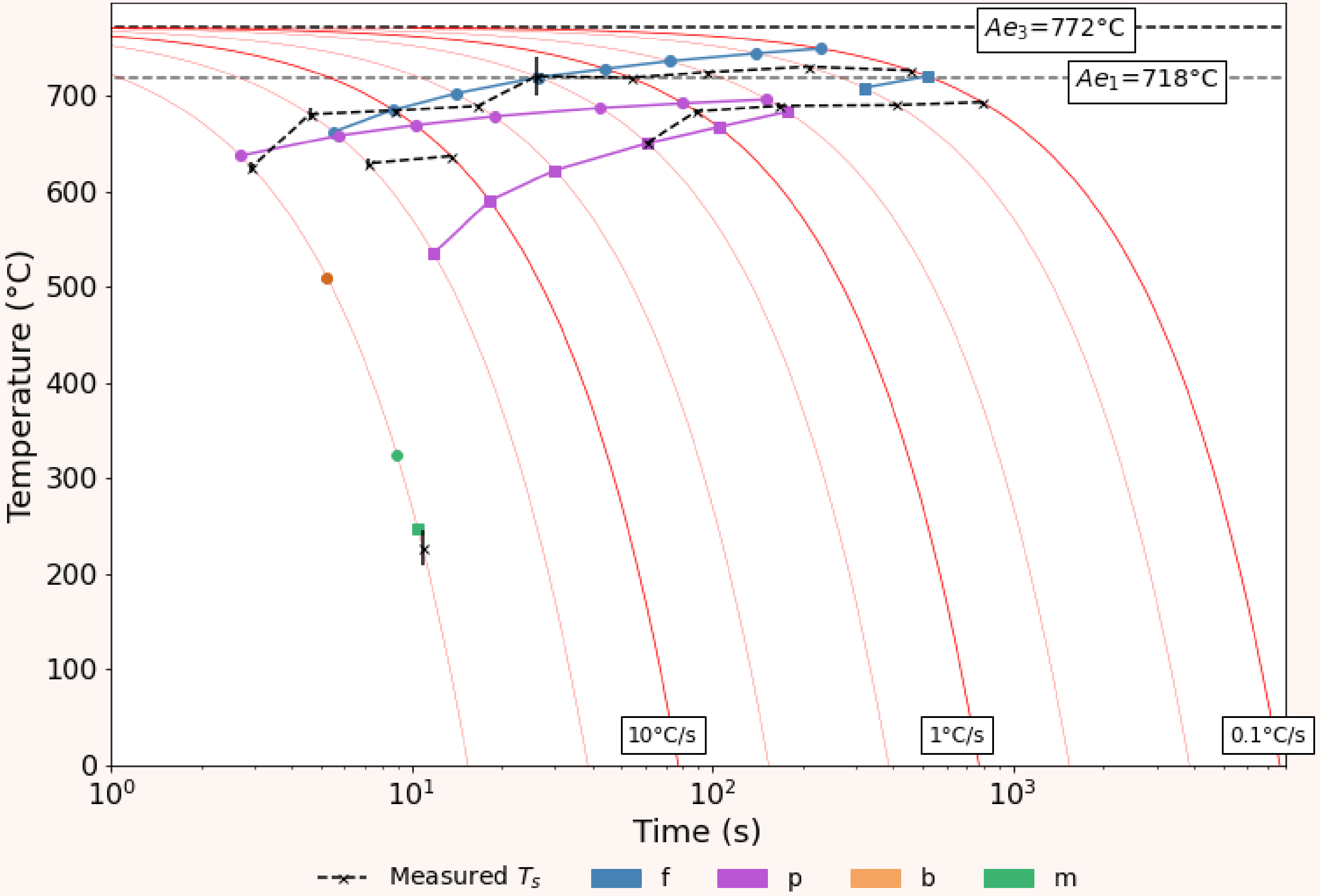
Modelling CCTs – Hardness (En3B)





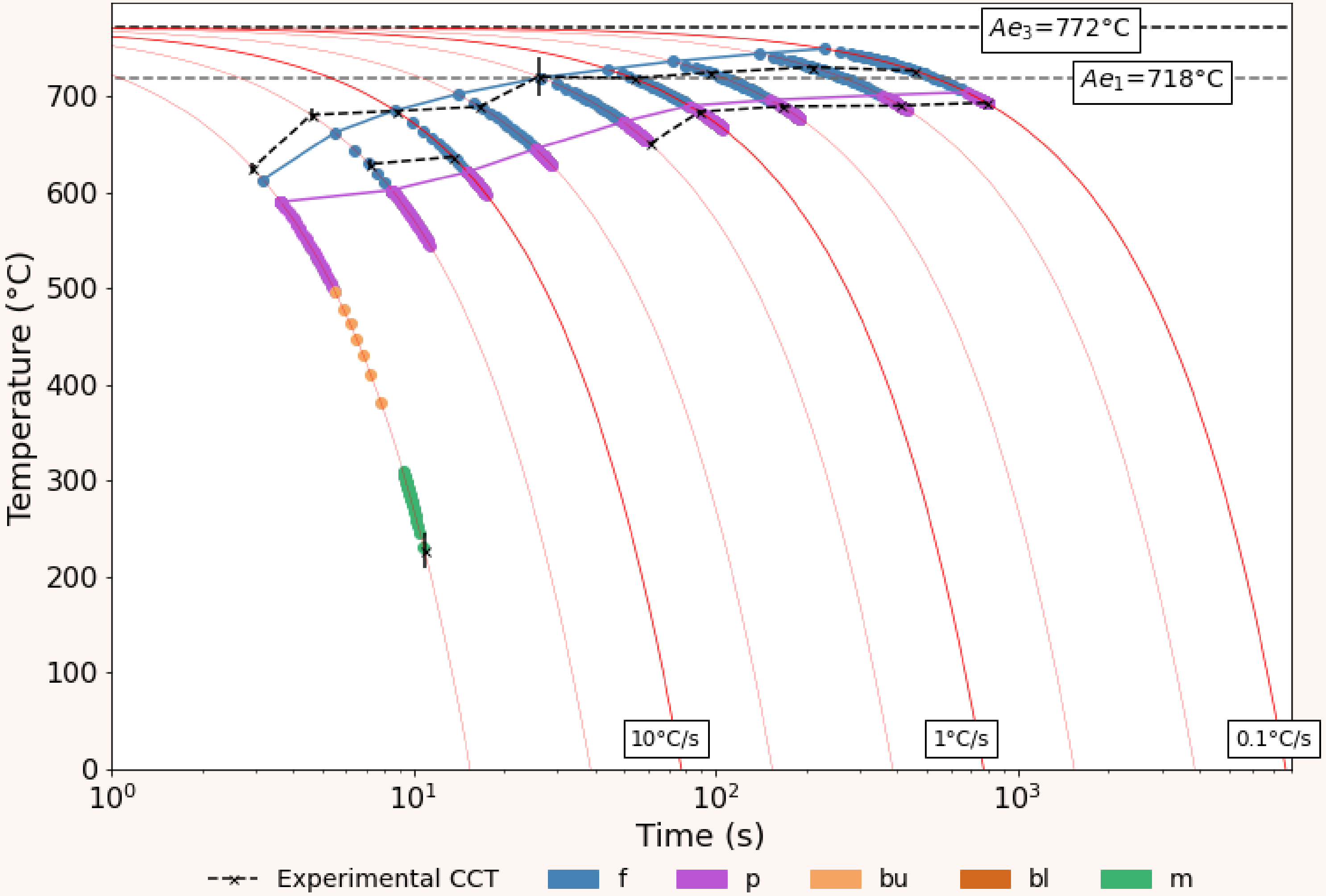
Modelling CCTs – The Li Model (En8)

En8	
	Wt.%
C	0.44
Si	0.20
Mn	0.77
Ni	-
Cr	0.14
Mo	-

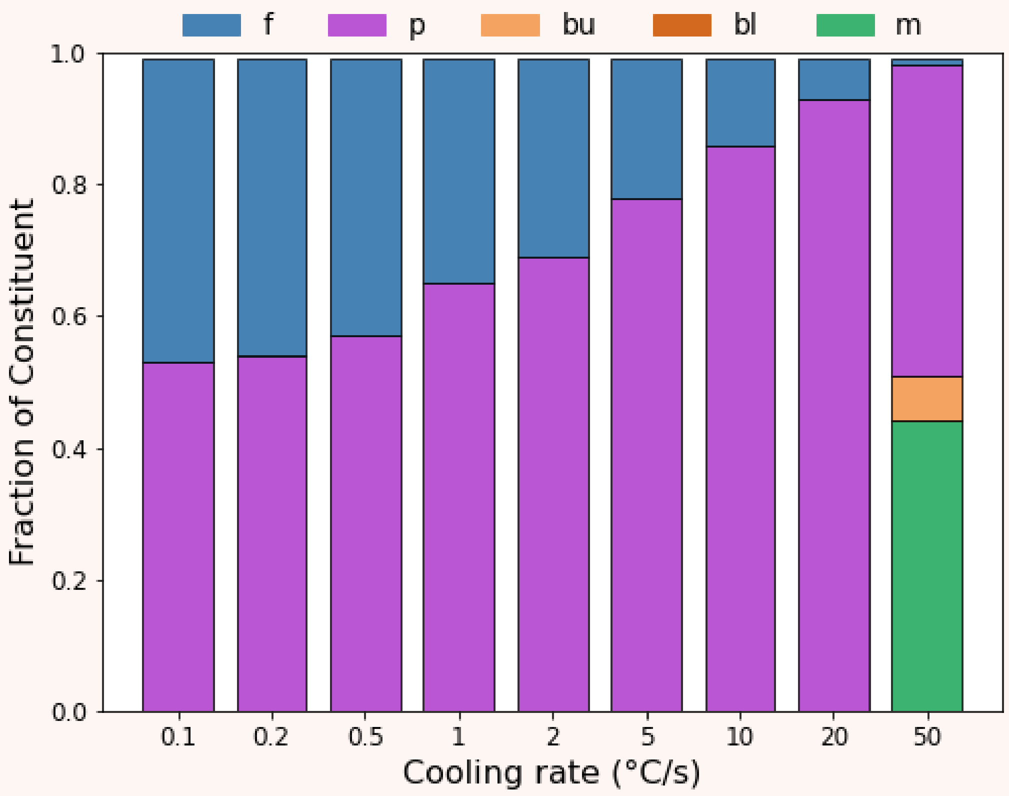


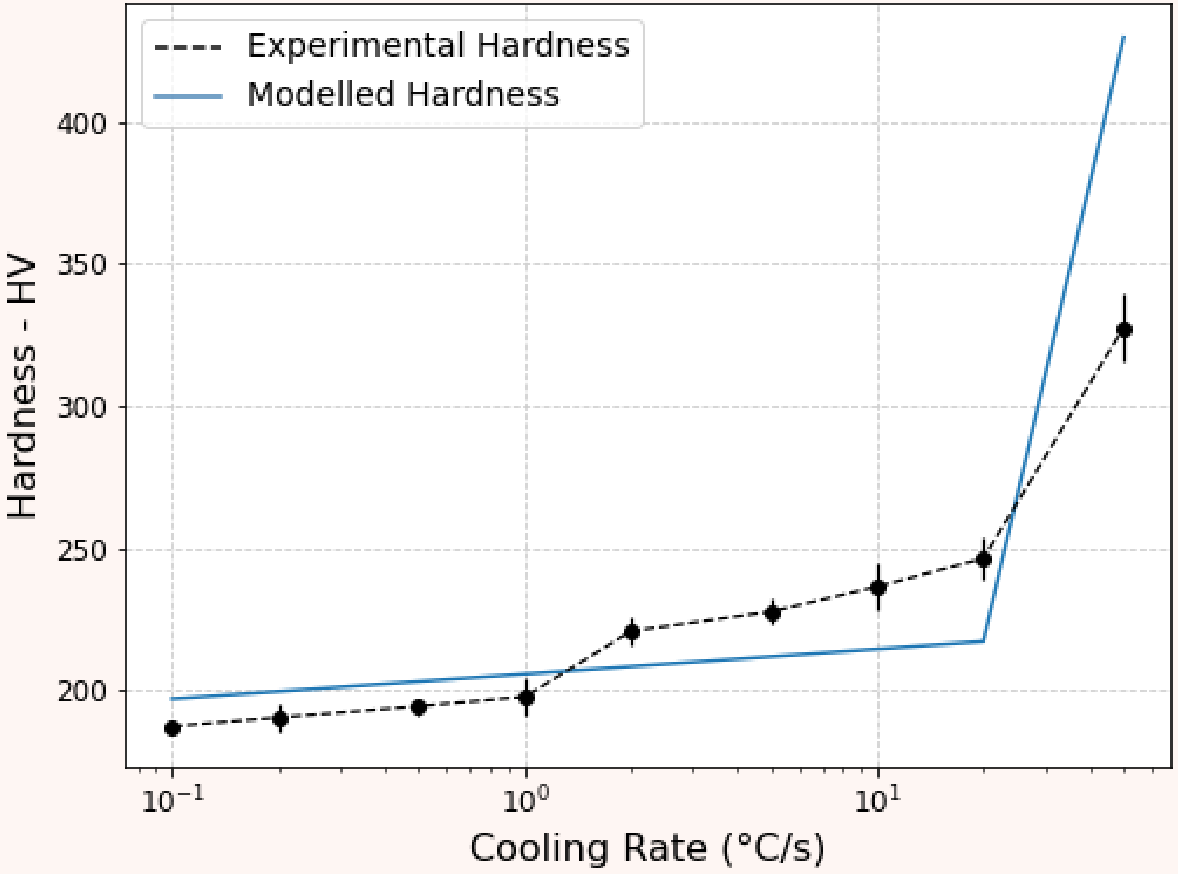
Modelling CCTs – The My Model (En8)

En8	
	Wt.%
C	0.44
Si	0.20
Mn	0.77
Ni	-
Cr	0.14
Mo	-



Modelling CCTs – Hardness (En3B)

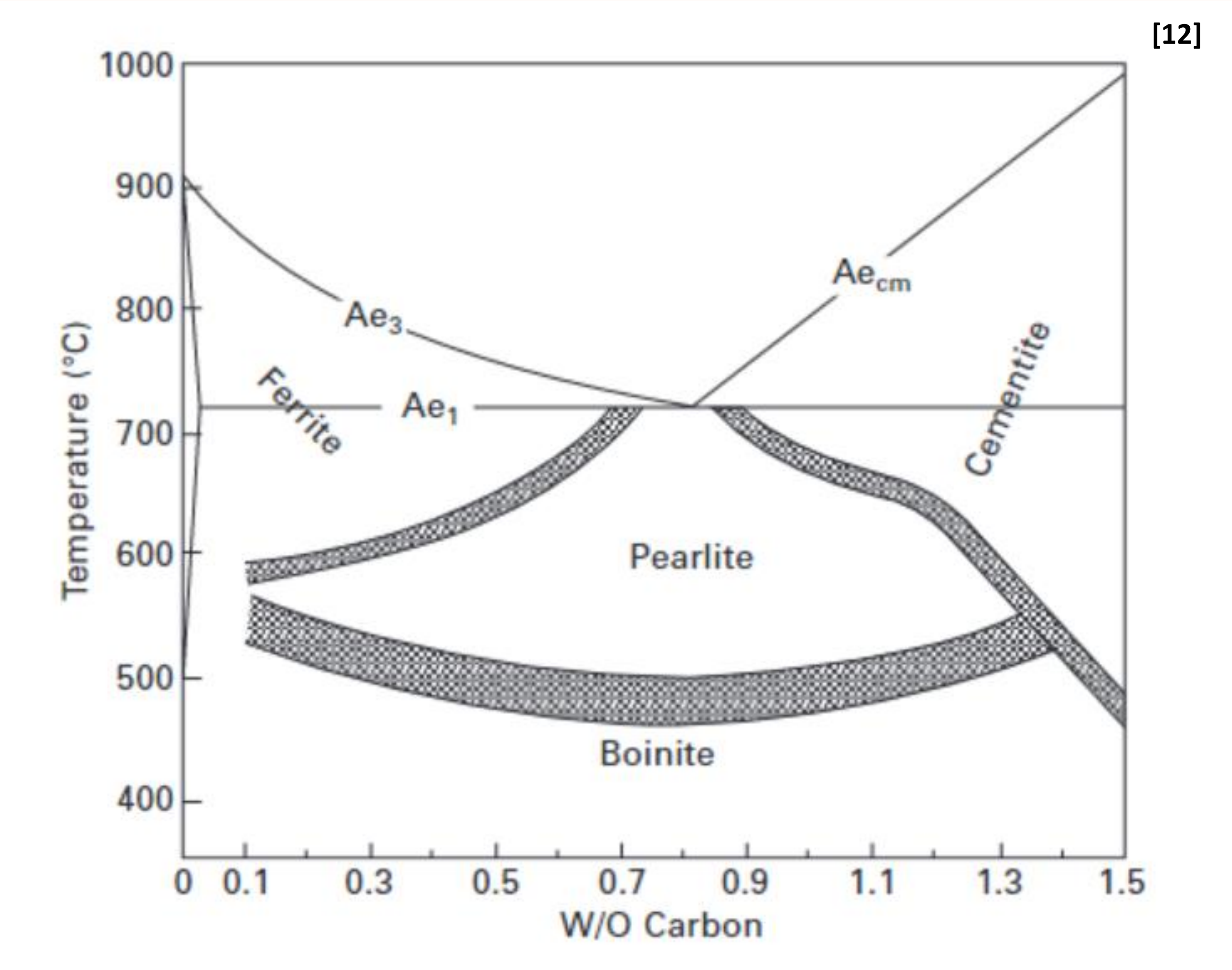




Model Boundary Conditions

Phase/Constituent	Transition Temperature	Additional Limitations
Ferrite	Ae3	Maximum ferrite limited by the ferrite/austenite equilibrium (lever rule)
Pearlite	Ae3 + Acm = Ae1	Pearlite start dependent on austenite/ferrite/carbide equilibrium
Bainite	Bs	Bainite transformation limited by the incomplete reaction phenomenon, T'0
Martensite	Ms	Martensite transformation rate follows Koistinen-Marburger behaviour (K-M)

Transformation Limits - Pearlite



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