Supplementary Materials: A Rapid, Open-Source CCT Predictor for Low Alloy Steels, and its Application to Compositionally Heterogeneous Material

Joshua Collins, Martina Piemonte, Mark Taylor, Jonathan Fellowes and Ed Pickering

This document provides supplementary figures for the paper "A Rapid, Open-Source CCT Predictor for Low Alloy Steels, and its Application to Compositionally Heterogeneous Material". Alongside this document, all measured, modelled and analysed data associated with this work has been made available online (paper reference [70]).

The measured dilatometry cooling curves for EN3B, EN8, and SA-540 B24 steels are presented in Fig. S1, Fig. S2, and Fig. S3, respectively. Dilatometry curves have been superimposed above each other to help visualise the changes between cooling behaviour. Transformation start temperatures, T_s, were determined using a combination of an offset method and a second derivative method – as described in the “Experimental Measurements" section of the paper. An example of this analysis is displayed in Fig. S4, which shows the analysis used to measure the T_s values for the 20 °C s^{-1} cooled EN3B specimen. The Python code used to conduct this analysis has been published online and is free to use (paper reference [65]). Fig. S5 and Fig. S6 display the PAG size analysis conducted on EN3B, EN8, and SA-540 B24 steels. A linear intercept method was used to analyse the PAG boundaries of EN3B and EN8, as shown in Fig. S5. SA-540 PAG measurements were conducted using EBSD (electron backscatter diffraction) parent grain reconstruction, as shown in Fig. S6. Predicted CCT curves from Thermo-Calc and JMatPro are presented alongside experimental T_s measurements in Fig. S7. Optical micrographs showing the impact of chemical heterogeneity on the phase transformation behaviour of EN3B and EN8 when cooled at 0.1 °C s^{-1} are presented in Fig. S8. The measured EPMA (electron probe micro-analyser) maps of the bulk, as-received SA-540 B24 material are presented in Fig. S9 for elements Al, C, Cr, Mn, Mo, Ni, Si, and V. These EPMA maps were then used to model a more realistic continuous cooling behaviour of SA-540, that considered the chemical heterogeneity of the alloy. The predicted constituent maps over a 1 x 1 mm^2 area of these EPMA maps are presented in Fig. S10 for cooling rates 0.1, 0.2, 0.5, 1, 2, 5, 10, and 20 °C s^{-1}.

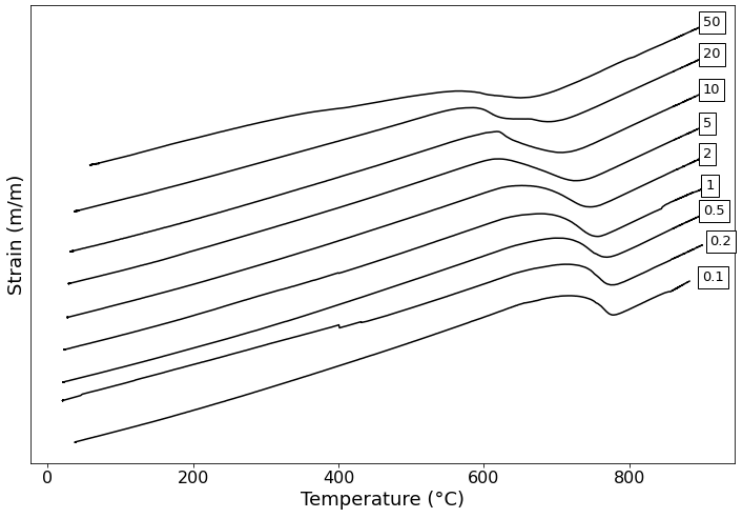


Figure S1. EN3B dilatometry cooling curves for cooling rates 0.1, 0.2, 0.5, 1, 2, 5, 10, 20, and 50 °C s^{-1}.

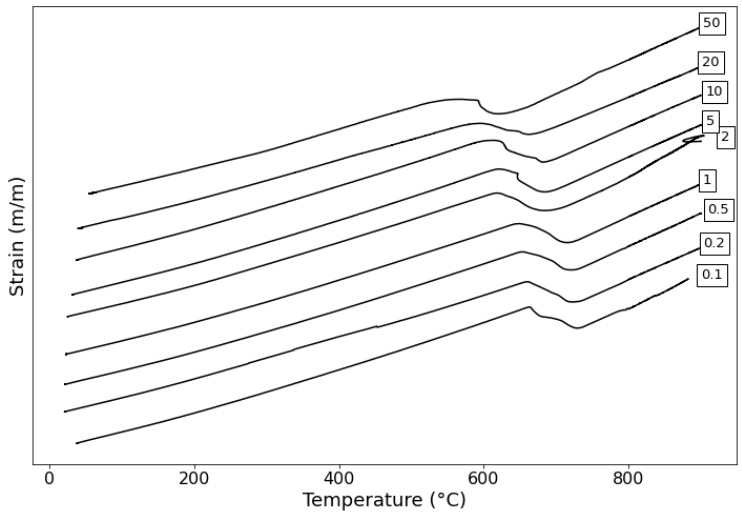


Figure S2. EN8 dilatometry cooling curves for cooling rates 0.1, 0.2, 0.5, 1, 2, 5, 10, 20, and 50 °C s^{-1}.

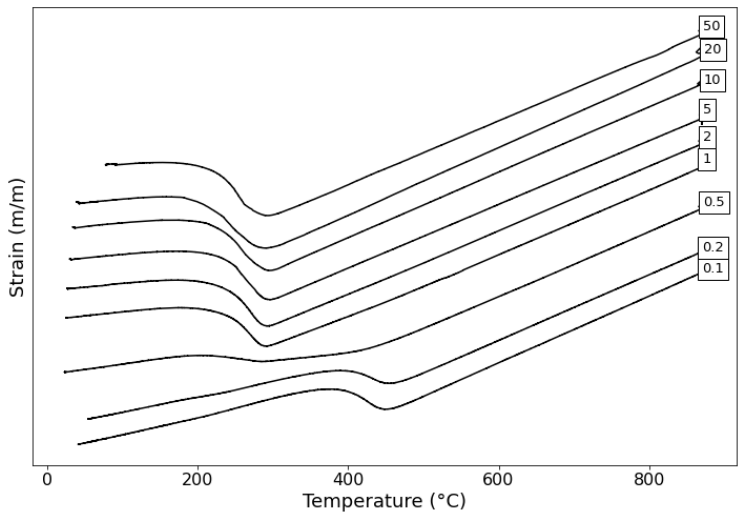
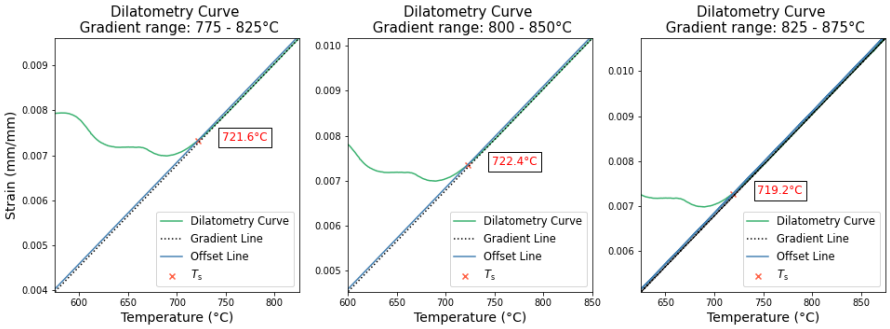
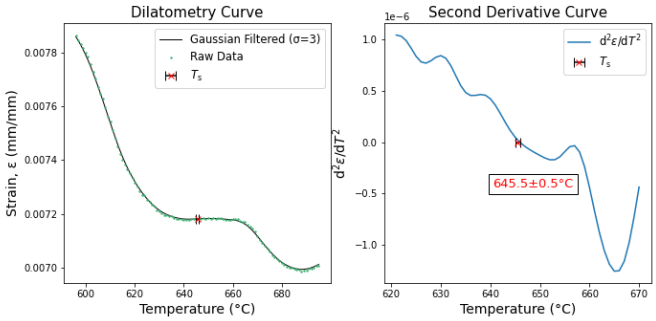


Figure S3. SA-540 dilatometry cooling curves for cooling rates 0.1, 0.2, 0.5, 1, 2, 5, 10, 20, and 50 °C s^{-1}.

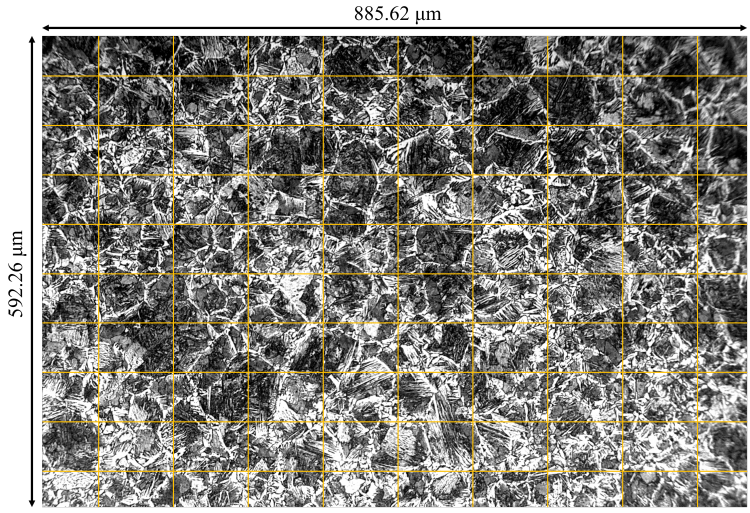


(a) Offset Method

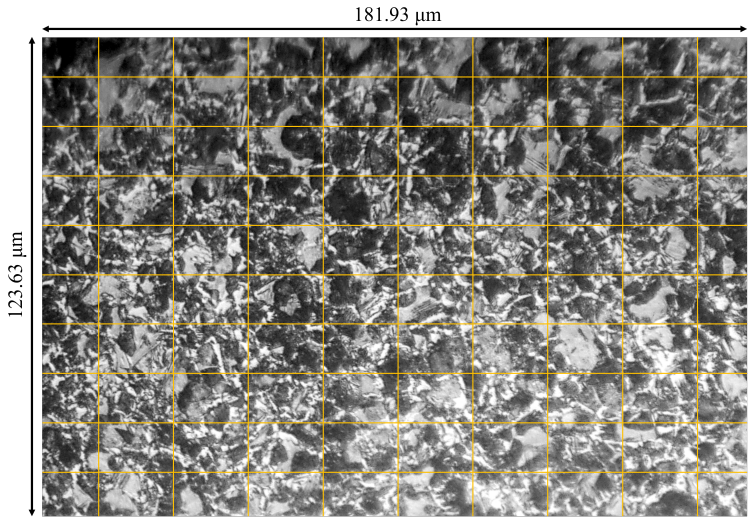


(b) Second Derivative Method

Figure S4. Analysis conducted on the EN3B dilatometry curve cooled at 20 °C s^{-1}. A combination of a) an offset method, and b) a second derivative method were used to measure the ferrite and pearlite start temperatures, respectively. The Python code used to conduct this analysis has been published online and is free to use (paper reference [65]).

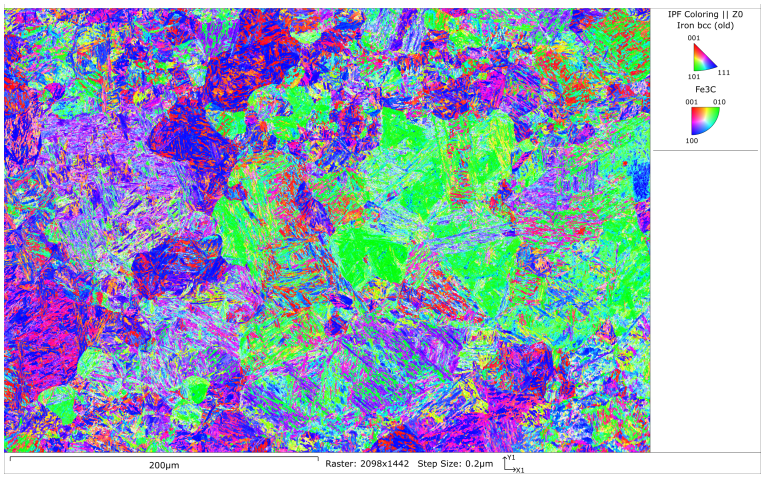


(a) EN3B

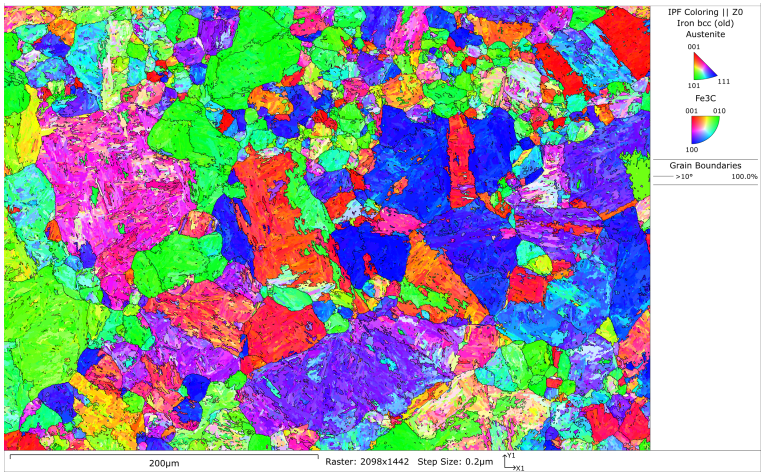


(b) EN8

Figure S5. The linear intercept method used to measure a) EN3B, and b) EN8 PAG sizes. Both images were taken from samples cooled at $50\,^{\circ}\mathrm{C\,s^{-1}}$. The small fractions of allotriomorphic ferrite that nucleated during these cools were used to highlight the position of PAG boundaries. A total of 18 intercept lines were used (9 horizontal and 9 vertical). Each line length was divided by the number of PAG boundary intercepts and an average was calculated. The PAG size for EN3B and EN8 were measured to be 46 and 7 μm respectively.

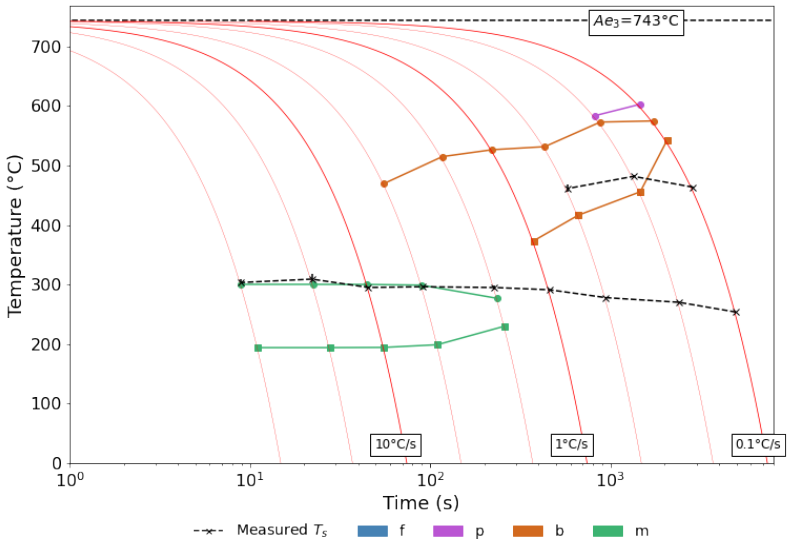


(a) EBSD Map

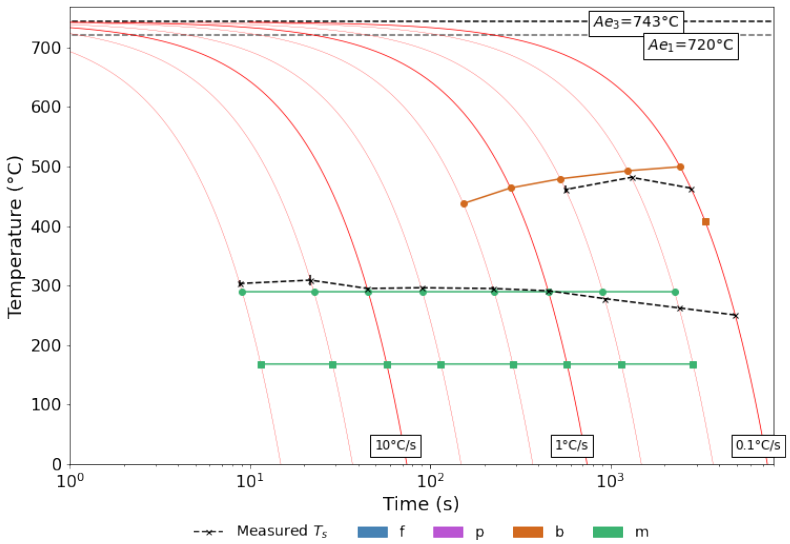


(b) Parent Grain Reconstructed Map

Figure S6. EBSD data for SA-540 showing a) the “cleaned" EBSD map taken from the bulk material of a vacuum cooled sample, and b) the parent grains (PAGs) reconstructed from the original EBSD map using Aztec Crystal software. An area-weighted equivalent circular diameter of all the PAGs measured was calculated as 36 μm and taken to be the average PAG size. A Thermo Scientific Apreo 2 scanning electron microscope (SEM) fit with an Oxford Instruments Symmetry EBSD detector was used to map the sample. A single EBSD map was collected over a 420 μm x 290 μm area using a 0.2 μm step size. An accelerating voltage of 20 kV and a 26 nA beam current was used.

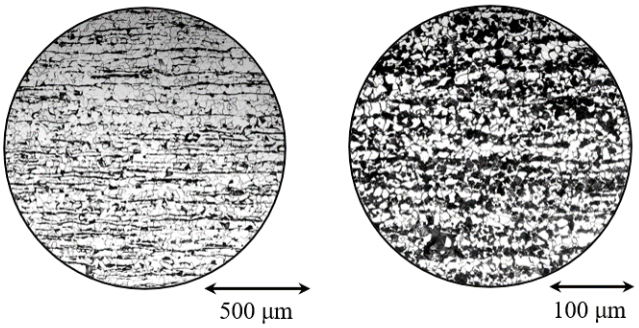


(a) Thermo-Calc Prediction



(b) JMatPro Prediction

Figure S7. Modelled SA-540 B24 CCT curves by (a) Thermo-Calc and (b) JMatPro for cooling rates 0.1, 0.2, 0.5, 1, 2, 5, 10, 20 and 50 °C s^{-1}. CCT curves are plotted as predicted start temperatures, T_s (circle markers) and finish temperatures, T_f (square markers). Constituent nomenclature includes: f - ferrite, p - pearlite, b - bainite and m - martensite. Experimental T_s measurements are plotted alongside the predicted results as a dashed black line. Predictions were made using Thermo-Calc Version 2022.1.93985-389 and JMatPro-v13.1.



(a) EN3B **(b)** EN8

Figure S8. Optical micrographs of the 0.1 °C s^{-1} cooled (a) EN3B and (b) EN8 microstructures, imaged looking down their transverse direction (TD) perpendicular to their rolling direction (RD). The impact of microsegregational banding on the phase transformation behaviour of both alloys is revealed when observing the microstructures from their TD. At a 0.1 °C s^{-1} cool, both alloys display characteristic ferrite-pearlite banding (i.e., light-dark etched microstructures respectively).

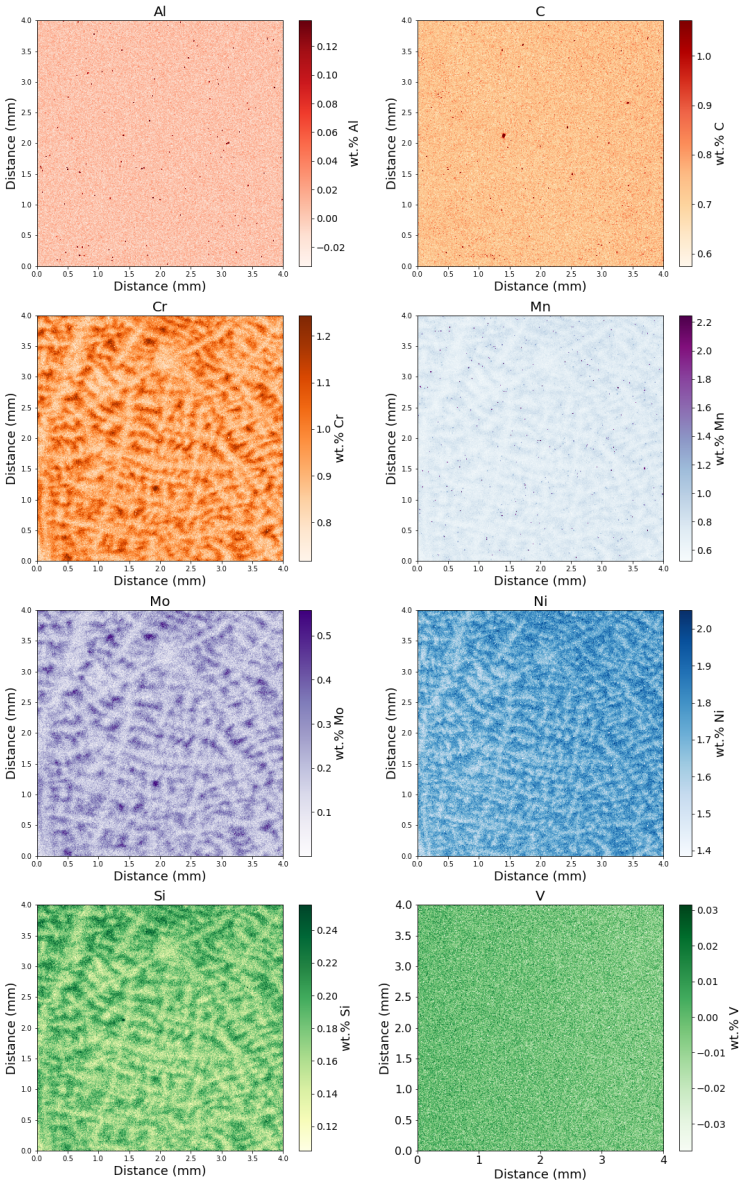


Figure S9. Quantitative EPMA maps of the as-received, SA-540 material for elements Al, C, Cr, Mn, Mo, Ni, Si, and V in wt.%. Map scale-bars have been restricted between the 0.1% and 9.99% percentiles of data in order to better view solute variation within the compositional ranges of interest.

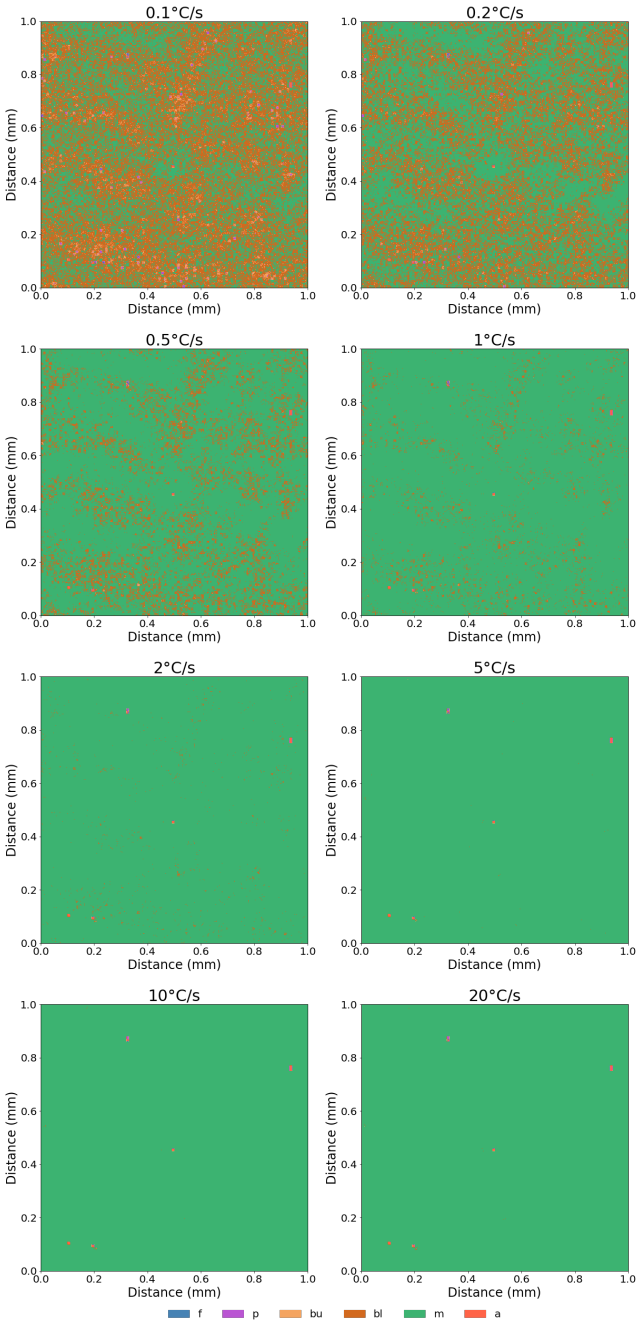


Figure S10. The predicted SA-540 constituent maps at cooling rates 0.1, 0.2, 0.5, 1, 2, 5, 10 and 20 °C s^{-1}. The maps were predicted by modelling the continuous cooling behaviour, using the proposed CCT model, at each pixel (i.e., each spatial composition) across a 1 x 1 mm^2 area of the measured EPMA maps (shown in supplementary Fig. S8). The constituent nomenclature is as follows: f - ferrite, p - pearlite, bu/bl - upper/lower bainite, m - martensite, and a - austenite. The data gathered from each map was used to predict a more realistic CCT behaviour of SA-540, that considered the chemical heterogeneity of the alloy, and was presented in CCT form in paper Fig. 12c. The prediction for the 50 °C s^{-1} cool has been omitted here, however it can be viewed online (paper reference [70]).