Supplementary

Appendix A

PFM solution with double-well potential

To explore the influence of the double-well potential equation (Eq. 11) on the PFM simulation results, the following explanations and the findings were presented. First, we substitute Eq. 2 with Eq. 10:

$$F^{CH} = F_d^{CH} = \int \left[\frac{\delta f_d(c)}{\delta c} + \frac{\kappa_d}{2} |\nabla c|^2 \right] dv \quad (10)$$

where $f_d(c)$ is the double-well potential, and κ is the gradient energy coefficient. Initially, for the completion of modeling the pearlitic transformation in API X60 steel, the double-well potential was expressed as Eq. 11, where A is a positive constant determining the magnitude of the energy barrier between ferrite and cementite in equilibrium.

$$f(c) = Ac^2(1-c)^2 \quad (11)$$

The double-well potentials intrinsically produce two phases, reflected in the data. With a specific interest in the pearlitic transformation, the austenite phase was omitted from analysis, and only ferrite and cementite were considered. **Error! Reference source not found.** demonstrates the application of Eq. 11 at various levels of the constant A, showcasing the equation's resolution under different conditions. Figure A 2 illustrates the microstructural evolution during the pearlitic transformation in API X60 steel. The initial phases are observed to segregate without significant resistance. The fundamental goal of phase field modeling is the minimization of the total free energy. In this scenario, as time progresses, the model predicts that the layers are inclined to evolve into spherical shape.

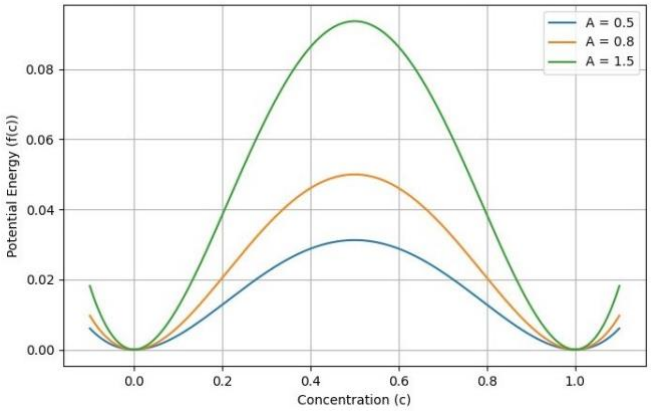

Figure A 1 Change in potential relative to chemical composition at different values of A.

However, as shown in Figure A 2, the higher value of a constant A suggests that the pearlite layers display a reduced inclination towards spherical structuring. This analysis is

corroborated by the observations in Figure A 2 (b), where the layers demonstrate a persistent form without transitioning to a spherical structure.

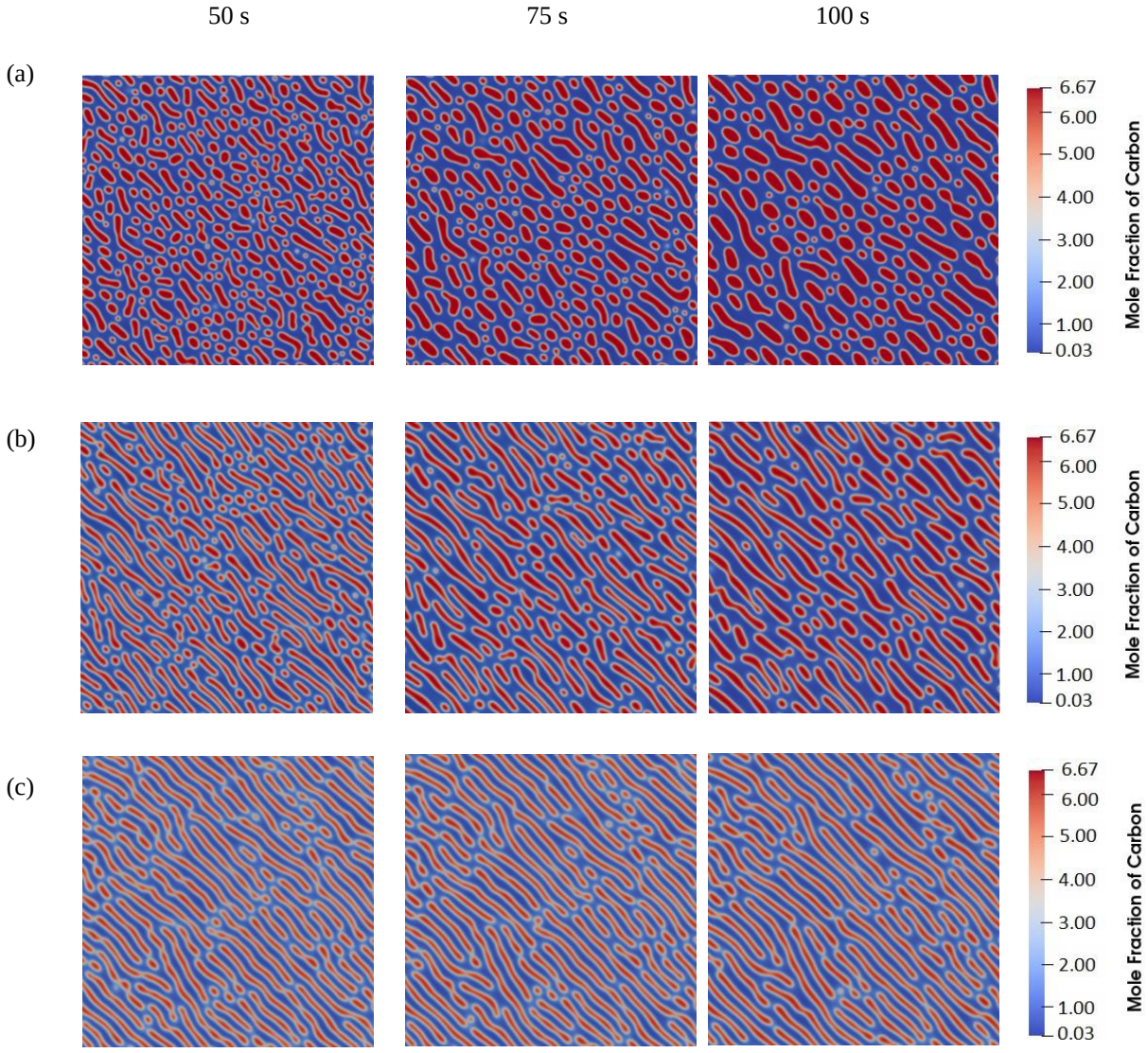

Figure A 2 Phase evolution using a double-well potential with (a) $A = 0.5$, (b) $A = 0.8$, and (c) $A = 1.8$ for 50 s, 75 s, and 100 s. The figure is colored by the concentration of red layers are cementite and blue matrix is ferrite.

Employing the Digimizer software, the thickness and interlamellar spacing of the layers were quantitatively determined, with the findings presented in Figure A 3.For this analysis, 10 layers were randomly chosen, and the software facilitated the calculation of an average for both thickness and interlamellar spacing. An increase in the constant A correlates with a microstructure characterized by thinner layers and interlamellar spacings. However, Figure A 2 indicates that varying the constant A does not markedly influence the thickness and interlamellar spacing. Consequently, the application of a double-well potential does not constitute a particularly precise method for examining the pearlitic phase transformation. Due to limitation of the double-well

potential to model exclusively binary phase systems, coupled with the observed differences when compared with experimental results, the application of a double-well potential framework appears to be inappropriate for the investigation of pearlitic phase transformations.

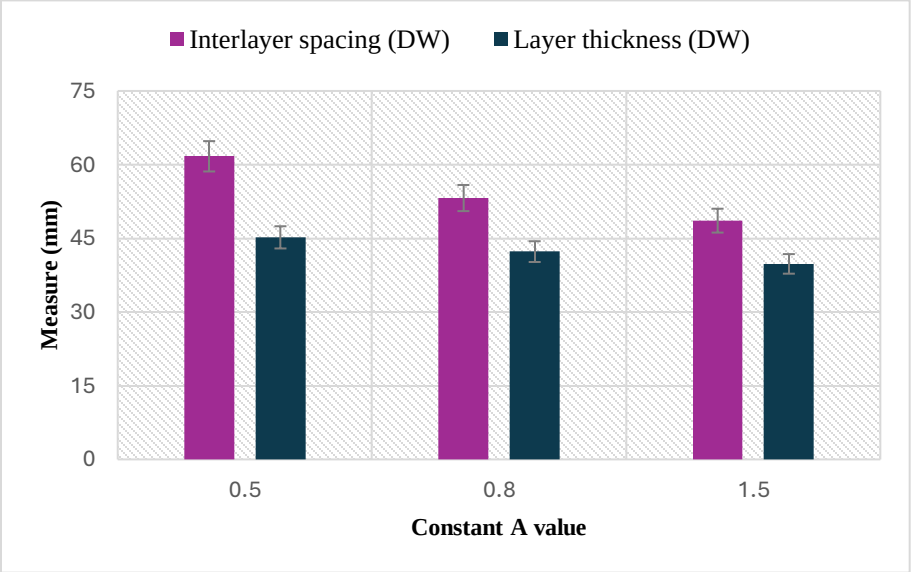

Figure A 3 Interlamellar spacing, and layer thickness obtained from computation using double-well potential.