An anti-trapping current for use in phase-field simulation with arbitrary (CALPHAD) thermodynamics

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Work on the development of a general anti-trapping current for use in phase-field models with arbitrary CALPHAD type thermodynamics, including the sub-lattice models used for non-stoichiometric intermetallics, is now complete and the model published [1, 2].

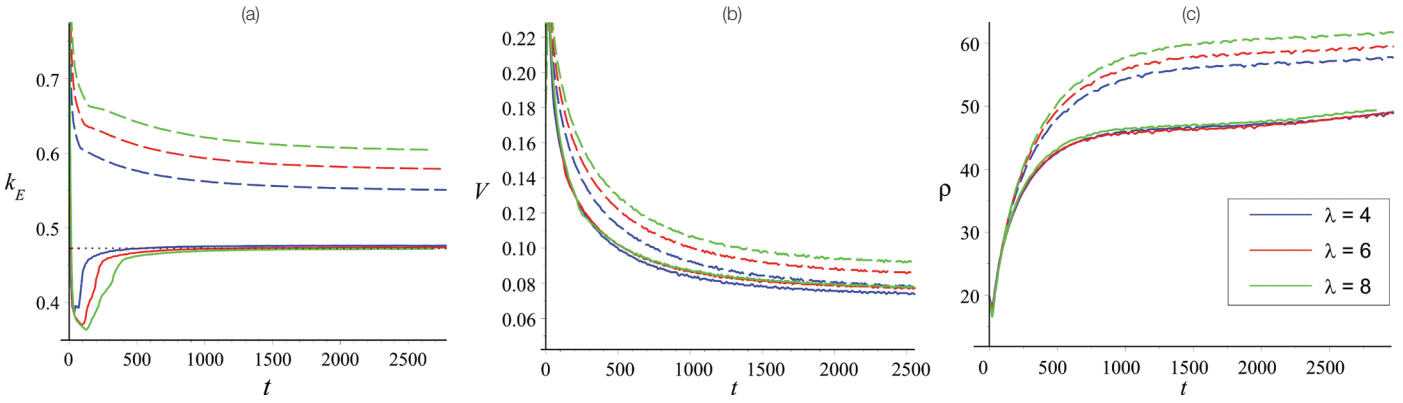

FIGURE 1. Values for (a) the partition coefficient, (b) the crystal growth rate and (c) the dendrite tip radius obtained from phase field simulations with interface widths of 4 (blue), 6 (red) and 8 (green) both with (solid lines) and without (dashed lines) the use of an anti-trapping current.

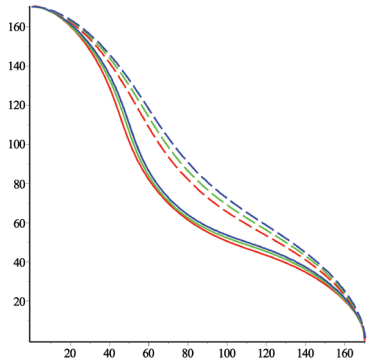

FIGURE 2. Morphology of a dendritic crystal with (solid) and without (dashed) anti-trapping.

Such anti-trapping currents are required to compensate for artificial solute trapping introduced by the diffuse interface used in phase-field simulations but are generally limited to simple thermodynamics in the dilute solution limit. As such, this development is applicable to all fields in which phase-field simulation is used with complex engineering alloys.

The new anti-trapping current is remarkably successful, not only in mitigating the effects of model induced solute trapping, but also in rendering the solution fully independent of interface width effects. This is illustrated in Figure 1 in which we compare the measured partition coefficient, kE, the crystal growth velocity, V, and the dendrite tip radius, ρ, in phase-field simulations for three values of the interface width, λ, with (solid lines) and without (dashed line) the anti-trapping current. It is clear from Figure 1a that with the new anti-trapping current the equilibrium partitioning coefficient (dotted) is recovered exactly in all simulations, whereas without the current strong interface width dependence is observed. However, as can be seen from Figures 1b-1c, the new current also renders the velocity and dendrite tip radius independent of the interface width, allowing fully quantitative simulation. Due to the success of the new current, it is now routinely used in all of our phase-field simulations.

However, the inclusion of anti-trapping currents also qualitatively changes the simulation, in that the morphology of the predicted crystals is changed. This point has previously received little attention with it generally being claimed that even non-quantitative phase-field simulations have some qualitative value. The effect can be seen in Figure 2, in which we plot out the outer envelope of a dendritic crystal, again for three values of the interface width, λ, with (solid lines) and without (dashed line) the anti-trapping current. The effect can be understood by realising that different parts of the dendrite are growing at different rates and that therefore, in the absence of an anti-trapping current, will be subject to differing levels of solute trapping. The effect is to make the simulation without the anti-trapping current closer to the equilibrium Wulff shape. Consequently, the model incorporating the new anti trapping current is better suited to non-equilibrium simulation.

REFERENCES:

[1] P.C. Bollada, P.K. Jimack and A.M. Mullis. Numerical approach to compensate for phase-field interface effects in alloy solidification. *Computational Materials Science*, In Press, (2018).

[2] A.M. Mullis, P.C. Bollada and P.K. Jimack. Development of an anti-trapping current for phase-field models using arbitrary CALPHAD thermodynamics.THERMEC' 2018, International Conference on Processing and Manufacture of Advanced Materials, Paris, France, 2018, *Materials Science Forum*, In Press, (2018).

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