Simulating Mushy Zone Resolidification for Multiphase and Multicomponent Alloys Using ChemApp

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ABSTRACT

A sample that is exposed to a temperature gradient over a large temperature range will completely melt in the heating zone and remain completely solid in the cooling zone. In between the completely liquid and solid regions, respectively, there is a mushy zone with a gradient in solid fraction. Local, temperature dependent equilibration at the solid/liquid interfaces yields a concentration gradient that in turn causes mass transport out of the mushy zone towards the hot regions of the sample. The local concentration change in the mushy zone eventually leads to its complete resolidification.

A model for simulating mushy zone resolidification in a temperature gradient is presented. The diffusion equation is solved numerically using the Finite Difference Method. Temperature dependent local equilibria at each position in the mush are calculated using the thermodynamic software package ChemApp. Concentrations and phase fractions are calculated from thermodynamically consistent phase diagrams, avoiding typical simplifications for analytical models such as linear solidus and liquidus lines and, accordingly, constant distribution coefficients k_e and liquidus slopes m_L. The resolidification model treats multicomponent alloying systems and accounts for multiphase equilibria. The evolution of the concentration distribution on the macroscopic length scale and of the local phase fractions as a function of time are predicted. The final concentration and phase distributions along the former mushy zone and the total resolidification time are calculated. Simulation results for peritectic Cu-40wt%Al and eutectic Al-5wt%Si-1wt%Mg alloys are compared with microstructures from temperature gradient annealing experiments. It is shown that the model is well suited to predict mushy zone resolidification in multicomponent and multiphase alloys.