CALPHAD Based Cellular Model of Dendrite Growth in Welds

Abstract

A computational model of dendritic growth based on the CALPHAD thermodynamic model was developed in this study. The dendrite growth was simulated using cellular automata (CA) with the equilibrium conditions in interfacial cells. The developed novel model (CA-CALPHAD) overcomes the current limitation of the published CA models, in which linearized phase diagrams are used, and allows for the investigation of some practical alloys such as stainless steels. To reduce the computational time, the study proposes a specific data structure to store the thermodynamic information and an efficient interpolation scheme to retrieve the information during the simulation.

The model takes into account the curvature effect of the evolving solid/liquid (S/L) interface by incorporating the capillarity undercooling into the thermodynamic information during the simulation. The finite volume (FV) numerical scheme was used to solve the mass and heat diffusion equations.

The developed CA-CALPHAD model can be used to investigate the free growth, constrained growth, and competitive growth of dendrites in response to different solidification parameters. The results of modeling include the dendrite morphology, dendrite size, solute segregation in the dendrite, dendrite growth rate, dendrite tip radius, and the spacing between primary and secondary dendritic arms.

Finally, a procedure of linking the developed CA-CALPHAD model to a computational welding mechanics tool (CWM) was developed producing a holistic multiphysics model (CWM-CA-CALPHAD). Therefore, the model can be used to predict the microstructure of a weld in response to realistic welding parameters and weld joints design.