

Multiscale computational modeling of alloy solidification

L. Tan and Nicholas Zabarar
Materials Process Design and Control Laboratory
Sibley School of Mechanical and Aerospace Engineering
188 Frank H. T. Rhodes Hall
Cornell University
Ithaca, NY 14853-3801

E-mail: tanlijian@gmail.com, zabarar@cornell.edu
URL: <http://mpdc.mae.cornell.edu/>

In this work, alloy solidification is modeled in three scales: atomic scale, meso scale and macro scale. At the atomic scale, phase diagrams are computed using molecular dynamics approach [1]. NPT ensemble with variable cell size is used in the molecular dynamics simulation, since volume of the system is not fixed due to phase change. Empirical potential functions are utilized to compute phase structure corresponding to minimum energy. At the meso scale, a level set method combining features of front tracking methods and fixed domain methods is presented to model meso scale structure evolution in the solidification of multi-component alloys using inputs from atomic scale computations, e.g. phase diagrams [2]. Adaptive meshing is used to bridge meso scale and macro scale [3]. Parallel computation using domain decomposition based on the adaptively refined mesh allows us to analyze the effects of nucleation and fluid flow on segregation.

References

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