Multiphysics and Multiscale Modeling of Solidification Processes

Miha Založnik*, Hervé Combeau

Institut Jean Lamour, CNRS – Université de Lorraine
Parc de Saurupt, CS 50840, F-54011 Nancy CEDEX, France
e-mail: miha.zaloznik@univ-lorraine.fr, web page: http://www.ijl.univ-lorraine.fr

ABSTRACT

In the metallurgical production chain, the solidification of the molten metal during casting sets the basic crystalline microstructure of the material. The modification of this structure during subsequent processing steps is limited. During solidification several types of defects form, such as heterogeneities of chemical composition: microsegregation at the microstructure scale, macrosegregation at the scale of the product; heterogeneities of structures in terms of grain orientation, size and morphology [1]. The reduction of these defects is an important issue for the industry because they impair the final properties of products.

Process-scale models of solidification processes need to account for couplings of different physical phenomena across several length scales. This requires a multiscale description of crystal growth, of formation of dendritic growth morphologies, and of multiphase heat and mass transfer and fluid flow across several regimes of multiphase transport. Microscopic phenomena can be incorporated into macroscale models by various homogenization techniques; the volume averaging method is often used. This requires a careful simplification and averaging of the microscale phenomena and interactions [2]. Moreover, efficient and robust algorithms that can solve a large number of strongly coupled partial differential equations are needed for the solution of the models [3]. In our presentation we introduce the existing models and their fundamental principles. We present the most recent applications of these models to industrial solidification processes (casting of steel ingots, direct-chill casting of aluminium alloys). We demonstrate their ability to help in the understanding of complex phenomena, such as the competition between nucleation and growth of crystal grains in the presence of convection of the liquid and of grain motion, and we discuss their predictive capabilities. Finally, we address the key remaining questions for future research.

REFERENCES

[1] J.A. Dantzig and M. Rappaz, *Solidification*, EPFL Press, 2009.

[2] H. Combeau, M. Založnik, S. Hans, P.E. Richy, "Prediction of Macrosegregation in Steel Ingots: Influence of the Motion and the Morphology of Equiaxed Grains", *Metall. Mater. Trans B*, Vol. **40**, pp. 289–304, (2009).

[3] M. Založnik and H. Combeau, "An operator splitting scheme for coupling macroscopic transport and grain growth in a two-phase multiscale solidification model: Part I – model and solution scheme", *Comp. Mater. Sci.*, Vol. **48**, pp. 1–10, (2010).