Quantitative phase-field modelling for solidification with coupled heat and solute diffusion in multi-component alloys

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ABSTRACT

Understanding and controlling solidification microstructure of alloys are one of important subjects in the field of materials science and engineering, because features of the solidification microstructure such as the size and morphology of the solidified crystals and non-uniform distribution of alloying elements, viz., microsegregation determine the quality of as-cast materials. The alloy solidification, by its very nature, is a multi-physics problem involving heat transfer, solute diffusion and fluid flow and so on. Hence, analyses and prediction of the solidification microstructure require these physics and their coupling to be precisely described.

The phase-field model is a powerful tool to simulate the microstructural evolution processes during alloy solidification. This is a diffuse interface approach and one can avoid explicitly tracking the position of interface in complex microstructural patterns, which is the chief advantage of this model. It is common practice to assign an arbitrary value to the interface thickness in the simulation of alloy solidification because of the computational cost resulting from the description of a realistic thickness of the solid-liquid interface. It postulates that the computational result is independent of the interface thickness used in the simulation. However, it is known that the standard phase-field models suffer from anomalous interface effects which scale with the interface thickness and it accordingly yields the result dependent on the interface thickness. It precludes quantitatively correct simulations in the standard phase-field models. This problem was solved by development of quantitative phase-field model which is constructed based on the thin-interface limit analysis. This model is free from the drawback mentioned above and it enables highly-accurate and large-scale computation of the solidification microstructure. However, the quantitative model developed in early works can be applied to an alloy system with zero diffusivity in solid (one-sided model).

In this study, we developed the quantitative phase-field model which can be applied to non-isothermal solidification in multi-component alloys with finite diffusivities in the solid [1]. Hence, our model can handle the coupling between the heat and solute diffusion in the microstructural formation. In this presentation, we introduce our recent attempt for the quantitative phase-field modeling and its application to the analysis on the microsegregation in alloy systems.

REFERENCES

[1] M. Ohno, "Quantitative phase-field modeling of non-isothermal solidification in dilute multicomponent alloys with arbitrary diffusivities", *Phys. Rev. E*, Vol. 86, 051603 (2012).