CHiMaD Center for Hierarchical Materials Design

SPECIAL SEMINAR

Introduction of Thermodynamic-Fluctuation-Based Nucleation to Phase-Field Model

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Machiko Ode is a senior researcher in the Computational Materials Science Unit at National Institute for Materials Science (NIMS) in Japan. She graduated from the Department of Materials Engineering at the University of Tokyo and received her Ph.D. in 2002. She joined NIMS as a Post-Doctoral Fellow at first and then Tenure-Track Researcher in 2005. Dr. Ode published more than 20 papers on phase-field modelling and several papers on the experimental work related to the measurement of thermodynamic property such as diffusion constant.

ABSTRACT

Thermodynamic fluctuation-based nucleation model is introduced to phase-field simulations. The normally distributed random temperature fluctuation proposed by Landau and Lifshitz[1] is imposed on each calculation grid, and if the grid temperature is lower than the average temperature, the undercooling is converted to the increase of solid fraction, where the conversion factor is given as a function of the latent heat, heat capacity, and the phase-field threshold for nucleation. For the numerical simulation, small three-dimensional cubes surrounded by a heat bath are prepared. The random temperature fluctuation and solid fraction are set as the initial conditions. We repeated the calculation more than 50 times under

the same calculation conditions, starting with different random number seeds. The ratio of nucleation occurs to the total calculation trials is defined as the nucleation ratio. The nucleation ratio steeply increases at a certain range of undercooling and the transition temperature is regarded as the nucleation temperature. The obtained nucleation temperature is rather in good agreement with that by a classical nucleation theory. These nucleation criteria are successfully applied to the second-phase precipitation of peritectic solidification.

[1] L.D.Landau and M.J.Lifshitz, Statistical physics 3rd ed., Oxford, Butterworth-Heinemann (1975)