Summary of thesis: The law of the phase growth accompanying latent heat

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Systems in which different phases coexist, such as growing crystal, exhibit a rich variety of dynamical behaviors. A typical situation is that an interface connects a stable phase and a metastable phase. Then, through the propagation of the interface, the stable phase grows and eventually the metastable phase vanishes. This phenomenon is ubiquitously observed in nature.

The propagation of the interface can be described by the time evolution of an order-parameter field that represents the extent of the order. When the order parameter is the only relevant dynamical variable of the system, the propagation velocity of the interface between the two phases is proportional to the difference in free energy densities, where the proportional constant is the mobility. However, as typically observed in crystallization, energy flow becomes a significant physical quantity, because latent heat is generated in the growth process. In this case, a temperature field also evolves under the influence of the generated latent heat, and this temperature field influences the time evolution of the order parameter. The set of coupled equations is called the phase-field model, which may be the most standard description of the phase growth that takes the effect of latent heat into account. It has been known that the interface position $R(t)$ at time t depends on the extent of the metastability Δ. Here, Δ is defined as

$$\Delta \equiv \frac{c_p}{T_c(\delta s)}|T_c - T_{\mathrm{ms}}|,$$

where T_c is the equilibrium transition temperature, T_{ms} is the temperature of the heat bath in contact with the metastable phase, δs is the entropy jump per unit volume, and c_p is the specific heat capacity per unit volume under constant pressure. When the extent of supercooling is less than unity, the interface displacement during some time interval is proportional to the square root of the time interval. This phenomena is observed by the numerical simulation using the phase-field model. Latent heat modifies the law of the propagation of interfaces. However, to our knowledge, there have been no theoretical studies of the $\sqrt{t}$-dependence in the phase-field model.

Furthermore, it is not obvious whether or not the phase-field model is appropriate for describing phase growth. Following the Onsager principle, we can derive an equation equivalent to the phase-field model. Because the noise intensity is determined by the fluctuation-dissipation relation of the second kind, the thermal noises are inevitable in the description. Thus, it is not evident whether noise effects are irrelevant to the phase growth, which is assumed in the phase-field model. Even worse, a typical interface width is the order of 10^{-7} cm. Thus, the interface may be out of the mesoscopic description. In the phase-field model, all such properties are universally represented by only the gradient term. These are issues on the validity of the phase-field model.

Based on the background, this thesis study the deterministic and stochastic phase growth with latent heat and examine the effect of the thermal fluctuation on the phase growth. In Chapter 2, we demonstrate the square root behavior by deriving a perturbative solution for a propagating interface in the phase-field model. The particular solution possesses the scaling form with two scaled coordinates and one dimensionless time-dependent small parameter. Expanding the solution in the small parameter, we calculate the leading-order contribution and the next-order contributions explicitly. we find that the solutions shows the square root behavior and the interface temperature deviates from the equilibrium transition temperature in proportion to the interface velocity.

In Chapter 3, we propose a stochastic growth model describing the phase growth accompanying latent heat. The model is based on an energy-conserving Potts model with a kinetic energy term defined on a sparsely random lattice only in one direction. For this model, we calculate the stable and metastable phases exactly using statistical mechanics. Furthermore, owing to the presence of the kinetic energy, the conversion from the potential energy to the kinetic energy of the Potts model can be described in the model, which corresponds to the generation of latent heat.

In Chapter 4, performing numerical simulations of the model, we measure the displacement of the interface. we find the scaling relation $R(t) = L_x\bar{\mathcal{R}}(Dt/L_x^2)$, where L_x is the system size between the two heat baths (See Fig. 1). The scaling function $\bar{\mathcal{R}}(z)$ shows $\bar{\mathcal{R}}(z) \simeq z^{0.5}$ for $z \ll z_c$ and $\bar{\mathcal{R}}(z) \simeq z^{\alpha}$ for $z \gg z_c$, where the crossover value z_c and the exponent α, $0.5 \leq \alpha < 1$, depend on the temperature of the heat bath in contact with the stable phase. The scaling relation in the late stage is not observed in the phase-field model. This means that the stochastic growth law is qualitatively different from that of the deterministic phase-field model.

The final chapter is devoted to the summary of the thesis.

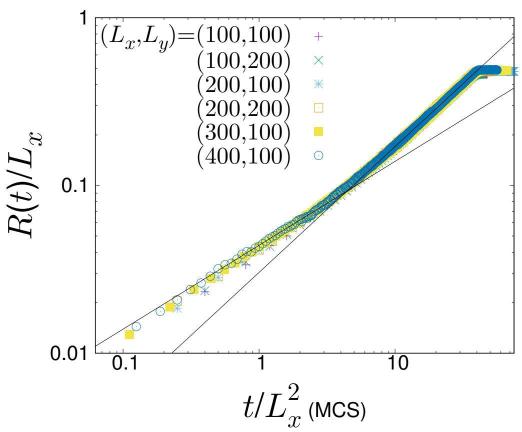

Fig. 1: One example of the numerical result. Log-log plot of $R(t)/L_x$ as a function of $z = t/L_x^2$. The two guidelines are $\bar{\mathcal{R}}(z) \sim z^{0.5}$ and $\bar{\mathcal{R}}(z) \sim z^{0.75}$, respectively.