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A Flux-Corrected Phase-Field Method for Surface Diffusion

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Abstract. Phase-field methods with a degenerate mobility have been widely used to simulate surface diffusion motion. However, apart from the motion induced by surface diffusion, adverse effects such as shrinkage, coarsening and false merging have been observed in the results obtained from the current phase-field methods, which largely affect the accuracy and numerical stability of these methods. In this paper, a flux-corrected phase-field method is proposed to improve the performance of phase-field methods for simulating surface diffusion. The three effects were numerically studied for the proposed method and compared with those observed in the two existing methods, the original phase-field method and the profile-corrected phase-field method. Results show that compared to the original phase-field method, the shrinkage effect in the profile-corrected phase-field method has been significantly reduced. However, coarsening and false merging effects still present and can be significant in some cases. The flux-corrected phase field performs the best in terms of eliminating the shrinkage and coarsening effects. The false merging effect still exists when the diffuse regions of different interfaces overlap with each other. But it has been much reduced as compared to that in the other two methods.

AMS subject classifications: 82C24

Key words: Phase-field method, surface diffusion, bulk diffusion, profile correction, flux correction.

1 Introduction

Phase-field method is a very useful tool for simulating interfacial phenomena and has been widely used in the modeling of binary alloys [1–3], solidification [4–6], microstruc-

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ture evolutions [7,8] and two-phase flows [9–11]. The major advantages of the phase-field method are its conservation nature and its ability of capturing topological changes naturally. A relatively recent application of the phase-field method is in the simulation of surface diffusion [12–18]. Although it has been proven in [19] that the sharp-interface limit of the Cahn-Hilliard equation with degenerate mobility $M(\phi)=1-\phi^2$ describes the interface motion induced by pure surface diffusion only if the potential is chosen to be logarithmic or double-obstacle form, in practice, a smooth polynomial double-well potential is often used [12–18] in order to avoid singularity. Unfortunately, as remarked by Cahn and Taylor [20], using a biquadratic potential might not drive the phase-field variable ϕ close enough towards ± 1 to sufficiently suppress bulk diffusion, a phenomenon which is caused by the normal gradient of the chemical potential and governed by a equation similar to that of quasi-stationary porous medium diffusion [21–23]. As a consequence, some adverse effects have been observed.

Yue et al. [24] pointed out that if a double-well potential was used, the phase-field variable inside/outside of a circular drop would be deviated away from its original value, ± 1, and in the meantime the radius of the circular drop would reduce in order to minimize the total energy. This shrinkage effect leads to a volume loss even though mass conservation is satisfied. Another effect caused by using double-well potentials in the phase-field method is the coarsening effect [21–23]. In the presence of the coarsening effect, larger solid domains will grow at the expense of nearby smaller ones. Such a phenomenon should not occur in a motion purely induced by surface diffusion. Different from the shrinkage effect, coarsening effect exists even in the sharp interface limit. In the sharp-interface limit, the interface velocity consists of two terms as shown in (1.1) [21–23]. One comes from the tangential flux, which contributes to the evolution of the interface driven by surface diffusion. The other one comes from a normal flux, which helps to maintain a diffuse interface with a finite thickness, but at the same time, brings the shrinkage and coarsening effects.

$$v_n=\frac{2}{3}\Delta_s\kappa+\frac{1}{4}\mu\nabla_n\mu. \tag{1.1}$$

In order to minimize the shrinkage effect, a profile-corrected phase-field method was proposed in [25] by adding a penalty flux. The function of this additional flux is to enforce a hyperbolic tangent profile of the phase-field variable in order to reduce the volume loss. The overall effect, however, depends on the competition between the original normal flux and the additional penalty flux in shaping the interface profile. In the initial stage of the simulation, the penalty flux is very small and the evolution is dominated by the original normal flux, which deviates the profile from its initial hyperbolic tangent form, resulting in a volume loss in most cases. Only when the deviation is sufficiently large, the effect of the penalty flux becomes stronger and it competes with the original normal flux to restore the profile back to the hyperbolic tangent form. The final profile, and thus the volume loss, is determined by the net effect of the two fluxes. In addition, as in the original phase-field method, the cause of the coarsening effect, that is, the bulk diffusion motion brought by the normal flux, still presents in the profile-corrected phase-