Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2016-0020

Vol. **21**, No. 1, pp. 1-15
January 2017

Computing Optimal Interfacial Structure of Modulated Phases

Jie Xu[1], Chu Wang[2], An-Chang Shi[3] and Pingwen Zhang[1,*]

[1] *LMAM and School of Mathematical Sciences, Peking University, Beijing 100871, China.*
[2] *Program in Applied and Computational Mathematics, Princeton University, Princeton, New Jersey 08544, USA.*
[3] *Department of Physics and Astronomy, McMaster University, Hamilton, Ontario L8S4M1, Canada.*

Received 3 February 2016; Accepted (in revised version) 30 May 2016

Abstract. We propose a general framework of computing interfacial structures between two modulated phases. Specifically we propose to use a computational box consisting of two half spaces, each occupied by a modulated phase with given position and orientation. The boundary conditions and basis functions are chosen to be commensurate with the bulk phases. We observe that the ordered nature of modulated structures stabilizes the interface, which enables us to obtain optimal interfacial structures by searching local minima of the free energy landscape. The framework is applied to the Landau-Brazovskii model to investigate interfaces between modulated phases with different relative positions and orientations. Several types of novel complex interfacial structures emerge from the calculations.

AMS subject classifications: 82B24, 82-08

PACS: 05.70.Np, 82.35.Jk, 68.35.Ct

Key words: Interface, modulated phase, metastable state, compatibility, Landau-Brazovskii model.

1 Introduction

Interfaces are transition regions connecting two different materials, two different phases of the same material, or two grains of the same phase with different orientations (grain boundaries). Interfacial regions are where the symmetries and patterns of the ordered structures are interrupted. Frequently in these regions defects of various types emerge [1]. The structure of interfaces greatly affects the mechanical, thermal and electrical properties of a material. In particular, the strength and conductivity of a material depend

*Corresponding author. *Email addresses:* rxj_2004@126.com (J. Xu), chuw@math.princeton.edu (C. Wang), shi@mcmaster.ca (A.-C. Shi), pzhang@pku.edu.cn (P. Zhang)

critically on the distribution and morphology of grain boundaries. In first-order phase transitions, the interfacial properties play an important role in the nucleation-growth process.

Theoretical discussions of interfaces usually start from the coexistence of two homogeneous phases, for which the order parameters are spatially uniform. If the contribution of inhomogeneity is included in the free energy, the interfacial structure becomes an intrinsic property of the energy functional. A simple and widely-used energy functional describing coexisting homogeneous phase is proposed by Cahn and Hilliard [2]. Since interfaces are non-equilibrium structures with long relaxation time, two different points of view could be held. One regards the interface as a metastable state and its morphology is obtained as a local minimizer of the free energy under certain constraints. The minimization approach is able to reach full relaxation and resolves the interfacial structure. This approach has been applied to two-component fluid interfaces to study the thickness and shape in various circumstances [2–6], as well as isotropic-nematic interfaces in liquid crystals [4, 7, 8]. An alternative approach is to treat the interface as a transient state and focuses on its dynamics, which is governed by the free energy, in some complex processes (see [9,10] for two examples built on the Cahn-Hilliard energy). The dynamical approach enables the study of the dynamical evolution of interfaces.

Interfaces between modulated phases have unique features. Because of spatial modulation, the interfacial profile depends on the relative position and orientation of the bulk phases. Also interfaces may exist between two grains of the same phase, i.e. grain boundaries. These features make it extremely interesting to study the mechanism of how two modulated structures are connected, which is very helpful to understanding the origin of epitaxial relationship and the anistropic nucleation. Therefore, it is important to investigate the morphology of a single interface using the minimization approach. In previous studies, the minimization approach has been used successfully in the tilted grain boundaries of the lamellar phase [11–14] and the bcc phase [15], and twist grain boundaries of several cubic phases [16]. Some works use dynamical approach [17–19], but it usually generates several interfaces because there is limitation in choosing boundary conditions, which we will explain later in detail. From the computational perspective, dynamical approach is more time-consuming, while in the minimization approach fast optimization algorithms can be used. In what follows, our discussion is limited to the minimization approach.

To convert a non-equilibrium interface into a metastable state, we need some anchoring conditions. Let us explain the anchoring conditions using a planar liquid-vapor interface as an example, where the density ϕ can be viewed as varying only in the x-direction. Suppose that the density of the liquid is ϕ_1, and that of the vapor is ϕ_2. The density far away from the interface shall be identical to the bulk values,

$$\phi(-\infty)=\phi_1, \quad \phi(+\infty)=\phi_2. \tag{1.1}$$

Note that these conditions do not determine the location of the interface. If we want to fix it, say, at $x=0$, an extra constraint is needed. A possible constraint is to choose an