Transition pathways in Cylinder-Gyroid interface

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Abstract. When two distinct ordered phases contact, the interface may exhibit rich and fascinating structures. Focusing on the Cylinder-Gyroid interface system, transition pathways connecting various interface morphologies are studied armed with the Landau–Brazovskii model. Specifically, minimum energy paths are obtained by computing transition states with the saddle dynamics. We present four primary transition pathways connecting different local minima, representing four different mechanisms of the formation of the Cylinder-Gyroid interface. The connection of Cylinder and Gyroid can be either direct or indirect via Fddd with three different orientations. Under different displacements, each of the four pathways may have the lowest energy.

1 Introduction

Modulated phases of similar patterns can be formed by block copolymer melts [1, 2] and many totally distinct materials, such as biological cells [3] and metal nanoparticles [4, 5]. Of these modulated phases, the most commonly observed patterns include Lamellae (L), Cylinder (C), Sphere (BCC, FCC), Gyroid (G) and Fddd, for which extensive studies have been carried out both experimentally [6–8] and theoretically [9–13]. These phases, while possessing distinct symmetries, can coexist in many cases. The interface between two phases would exhibit fascinating structures, which also characterize first-order phase transitions [14–16].

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Because of the intrinsic ordered structures, their relative positions and orientations are essential to the interface, which is evidenced by several epitaxial relations [17–20]. In particular, multiple interface morphologies and epitaxies are found for the C-G coexistence systems [18], which result in distinct processes of phase transitions. These experimental findings bring us a number of glamorous phenomena, meanwhile raise theoretical problems on the formation mechanisms that require enlightening perspectives.

Some theoretical attempts have been made to understand the underlying mechanism of interfaces. One convenient approach is to follow relaxation dynamics, typically carried out in a large cell, to let interface emerge and evolve [21–23]. Usually, the results from the dynamic approach contain multiple interfaces that might interact one another. Furthermore, it is not easy to fix the relative orientation and displacement in large cell simulations. To arrive at closer examinations of the interfacial structures, some posed two phases delicately in a small computational box with special orientations and displacements. Using this approach, grain boundaries of L [24–26], BCC [27] and cubic phases [28] were examined.

Interfaces of general relative positions and orientations are also studied. For example, to provide insights on epitaxy, an artificial mixing ansatz is adopted followed by searching the minimum exceeding energy [29–31]. However, the interfacial morphology obtained from this approach may be far from optimal in many cases. A framework dealing with general relative positions and orientations was proposed later [32], where the boundary conditions and basis functions are carefully chosen to fix the bulk phases at certain positions and orientations consistently. This framework is further equipped with delicate numerical methods that can successfully deal with quasiperiodic interface [33]. The interfacial structures obtained from this framework prove to be much more complicated than simple mixing. Even in the simplest cases, a series of energy minima can occur depicting the process of phase transition. Moreover, when we alter the relative positions and orientations, a few fascinating results are then obtained, implying that the underlying mechanism can be quite complex in the formation of interfaces, such as deformation, wetting by a third phase, zigzagging, etc.

The above results indicate that the interface system could possess multiple energy minima. The relationships between minima can be characterized by the minimum energy paths (MEPs) on the free-energy landscape, which represent the most probable transition pathways [34–36]. The crest of a MEP connecting two minima is regarded as the transition state that is an (Morse) index-1 saddle point. Thus, if multiple minima exist, one could imagine that the interface shall be moving along the transition pathways through a series of transition states and minima. Nevertheless, the existing results are far from well-understood on the transition pathways in the interface systems.

In this work, we examine the transition pathways connecting different interface morphologies using the Landau–Brazovskii (LB) model which is a generic model for modulated phases. Specifically, we apply an efficient numerical method based on the index-1 saddle dynamics to the LB model in order to obtain MEPs connecting various local minima. Our focus is the C-G interface system. We present four primary transition path-