

Computational Method of Grain Boundary Energy Consistent for Different Orientations and Applications to Double Gyroid Beyond Twinning

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Abstract. We develop the method for computing grain boundary (GB) energy consistent for different grain orientations for phase-field type models. The computation is carried out in a parallelepiped domain such that periodicity is attained along two edges parallel to the dividing plane of two grains. The width of the normal direction is carefully chosen such that the part of each grain in the computational domain can be reassembled into several unit cells. In this way, the bulk energy per volume in the computational domain is identical to the energy density of a unit cell, so that GB energy of different orientations can be obtained in a unified standard. We apply this method to the study of four double-gyroid (DG) GBs with different orientations numerically using the Landau–Brazovskii free energy, including the (422) twin boundary studied recently, a network switching GB, and two tilt GBs. Topological variations and geometric deformations are investigated. It is found that deviations in strut lengths and dihedral angles from the bulk DG substantially exceed changes in strut angles and nodal coplanarity. We also examine the spectra along the contact plane of two grains and utilize them to evaluate the GB widths. Of the four GBs we study, the network switching GB changes to the least extent topologically and geometrically, meanwhile has the lowest energy and the smallest GB width.

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Key words: Grain boundary energy, orientation, phase-field model, double gyroid, network switching.

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1 Introduction

The double gyroid (DG) has been observed in various materials, including block copolymers [1–4], liquid crystal polymers [5, 6], lipid mesophases [7, 8], surfactants [9–11], and biological assemblies [12–14]. The ideal DG skeleton has two interpenetrating networks with opposite chirality [15, 16], typically given by the higher-concentration region of a component. Each network is featured by three coplanar struts of equal length from each node to three adjacent ones with the angle 120° . Such planes rotate $\pm \arccos(1/3)$ ($\approx \pm 70.5^\circ$) along the clockwise(+)/counterclockwise(–) network, generating the shortest ten-node circuits [17] and the unit cell of the $Ia\bar{3}d$ space group. The particular symmetries and skeletons lead to unique properties, including excellent mechanical [18–23], optical [14, 24, 25], mass transport properties [26, 27] and highly uniform porosity [28, 29]. These properties may be affected by defect structures [30] that are yet well-understood.

Defects in network structures involve changes of graph topology and geometry [17, 18, 31–36], thus are more complicated. For DG, a well-structured $(422)^\ddagger$ twin boundary (TB) with mirror symmetry, possibly first noticed in Ref. [37], has been analyzed in several recent works. This specific structure is examined by minimal surface [38, 39], followed by experiments [39, 40]. Specifically, the fusions of nodes on the TB plane and the resulting alterations of circuits are examined. To coordinate with the TB nodes, the network structure adjacent to these nodes, such as the changes of strut lengths and dihedral angles, undergoes complex deformation. TBs are generally regarded to have lower energy because of their better symmetries, which is suggested by the results of spherical structures [41–44]. However, for DG and other network structures, it requires further studies on GBs of other orientations to validate. Furthermore, it is intriguing to explore whether some mechanisms on the formation of the (422) TB also feature other GBs. To our knowledge, the above problem is yet to be covered experimentally, so we believe that it would be interesting if predictions can be made from the computational aspect.

To comprehend properties of GBs formed by DG or other network structures, it is crucial to examine their morphologies from the energy viewpoint. It thus calls for reliable and efficient computations of the GB energy. Conceptually, GB energy is the excess energy over the bulk energy in the GB system. Since the GB energy relies on the orientations of grains, the definition of the GB energy shall follow a consistent standard in order to be comparable for different orientations. A naive approach is to compute in a periodic domain that matches the period of each grain with the prescribed orientation [45], with each grain occupying half of the computational domain. In this case, the bulk energy per volume in this domain is identical to that of a unit cell. This setting actually studies the system with infinite many GBs in presence periodically, which may affect one another. Meanwhile, the requirement on the periodic domain could make it very large, leading to high computational costs. Another choice is to formulate the GB system in a bounded domain [42, 46]. This approach is more flexible on the computational domain since one

[‡]Miller indices