Gyroid Interface from Symmetric ABCD Tetrablock Quarterpolymers by Monte Carlo Simulation

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ABC triblock terpolymers consisted of three incompatible polymer chains naturally form three-phase structures in bulk state. Morphologies of the molecules whose volume fraction of A-chain is equal to that of C-chain, $\varphi_A=\varphi_C$, have been well studied, where they possess two interfaces, A/B and B/C, which do not intersect each other because the A- and C-phases are pulled apart by the B-chains. The symmetric terpolymers show the tricontinuous gyroid structure around $\varphi_B=0.5$ [1,2]. The two interfaces, A/B and B/C, are different from the Schoen's gyroid surface, because φ_A and φ_C are much smaller than 1/2, while the trajectory of the center of the B-chains can be statistically described as the gyroid surface. The visible A/B and B/C interfaces are a pair of level surfaces derived from the Schoen's gyroid. Triply periodic minimal (TPM) surfaces including gyroid have not been observed as interfaces of microphase-separated structures in block polymer systems so far, and interfaces with zero mean curvature formed by block copolymers have only been observed in lamellar phase, which can be simply recognized as a flat surface. In this study we try to obtain and visualize TPM "interface" in phase structures of symmetric ABCD tetrablock quarterpolymers where the two conditions with respect to volume fractions, $\varphi_A=\varphi_D$ and $\varphi_B=\varphi_C$, hold, while a volume fraction parameter, $\varphi=\varphi_C+\varphi_B$, as the sum of B- and C-phases, is defined.

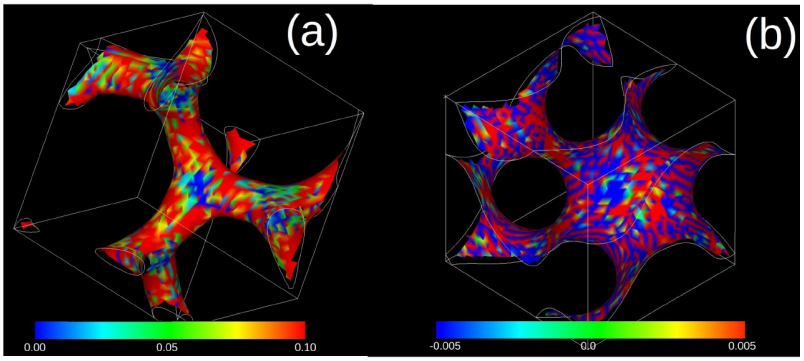

Figure 1 The shape and distributions of mean curvature *H* on the (a) A/B and (b) B/C interfaces using the color scale [3].

At first, we simulated the stable structure in the medium φ region, and obtained the lamellar structure whose repeating unit is ABCDCB in the range of $\varphi < 0.625$. A phase transition from the lamellar to tetracontinuous structures is observed at $\varphi=0.625$ with increasing φ. This newly found structure is stable for certain φ region, but finally another lamellar structure appears at $\varphi=0.8125$. The composition range of the tetacontinuous structure has been found to be $0.625 \leqq \varphi \leqq 0.75$, and the three-dimensional surfaces of A/B and B/C interfaces are shown in Figure 1. It is found that the A/B interface is equivalent to the C/D interface and the A/B and C/D interfaces can be regarded as the level surfaces to the gyroid surface. The B/C interface divide into two subspaces with equal volume. Figure 1 compares the distribution of mean curvature *H* on the interfaces using the color scale. The averaged *H* values with their standard deviations are $\langle H_{AB}\rangle=1.08\text{x}10^{-1}\pm0.110$ and $\langle H_{BC}\rangle=4.39\text{x}10^{-4}\pm0.0307$, indicating that the mean curvature of the B/C interface, where the centers of polymer chains stay on, is nearly zero, and hence we conclude the visible interface can be described as the Schoen's gyroid surface.

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