

2-D 격자이론으로 해석한 네마틱-동방상 계면

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Nematic-Isotropic Interface by 2-D Lattice Analysis

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Introduction

Liquid crystalline (LC) polymer dispersed phase in isotropic polymer matrix is of great interests due to the ability of LC dispersion of making self-reinforced composites as well as of processing aids (Cogwell et al., 1983; Handlos and Baird, 1995). Also the LC-isotropic interface may be of interest for the applications such as multi-layered film where at least one component is LC polymer. One of striking properties in the interface is that dynamics of LC dispersions in an isotropic polymer matrix show strong size dependence (Riise et al., 1999; Lee and Denn, 1999, 2000; Lazkano et al., 2002). The dynamics of LC droplets is consistent with the Palierne model when we use the interfacial tension which is estimated by group contribution method where the orientation of LC polymer is not considered at all. However the dynamics of LC droplets is different from the above when the droplet size is smaller than a size of LC correlation length (Riise et al., 1999; Lee and Denn, 1999, 2000; Lazkano et al., 2002).

Li and Denn have studied the LC-isotropic interface by Monte Carlo simulations and found that the far-field orientation has a strong effect on the magnitude of the interfacial tension and the interfacial tension is an increasing function of the nematic order parameter S for parallel far field, while it is a decreasing function for a homeotropic far field, where S is defined as $S = \langle 3\cos^2\phi_i - 1 \rangle / 2$.

In this work, we present a simple lattice model for a reference plane in the LC-isotropic interfacial region, which is everywhere perpendicular to the local density gradient. This analysis shows clearly that the interfacial tension is exponentially depending on the orientation of LC polymer in the interfacial region.

Interfacial lattice model

Surface excess energy has been studied extensively by defining a reference surface. This surface is everywhere perpendicular to the local density gradient. In this work, we are to discuss surface excess energy of nematic-isotropic interface in a reference plane. A molar excess free energy in the interfacial region is obtained as follows,

$$\tilde{G} = \tilde{G}_{isotropic} + \tilde{G}_{orientation} \quad (1)$$

Results

In calculations, we use $x_{1m}=x_2=50$, which is close to a degree of polymerization of conventional engineering polymers. The interaction parameter χ_{12} is set to 0.08 which is large enough compared to the critical interaction parameter, $(\chi_{12})_c=0.04$, representing the binary mixture of two phases. From the calculations, we can see the excess free energy is increasing exponentially as follows,

$$\tilde{G} = 2\tilde{G}_{isotropic} \exp(2.3S) \quad (2)$$

It is worth to note that the excess free energy is increasing more rapidly than the values calculated from Eq. 2 in the highly ordered state (large S values) where minimum errors in the orientation factor is incorporated in the calculation model.

References

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