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Memory effect in simulations of asymmetric diblock copolymers under thermal processing

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Recent experiments [Kim et al. Science 356, 520 (2017); PNAS 115, 847 (2018)] observed that the temperature protocol used to heat and cool an asymmetric diblock copolymer from its disordered micelle liquid state to its ordered micelle crystal phase, and back, can influence which ordered phase is found. This suggests some memory of the initial ordered micelle phase is preserved in the disordered micelle state. To develop an understanding of this memory effect, we perform simulations of a time-dependent Landau-Brazovskii model, which has stability regions for disorder, disordered micelles, BCC, FCC, as well as Frank-Kasper phases. Our protocol is to equilibrate a low-temperature ordered micelle phase, rapidly heat to just above the order-disorder transition, anneal for a time tH, then quench back to the low temperature and observe the time, tL, it takes for the ordered phase to (re-)form. For small tH, we find that the ordered phase re-forms quickly (tL is small), regardless of whether the original ordered phase is stable or metastable. We measure tL as a function of tH and find a threshold tH above which the system remains in the disordered micelle liquid over our (long) simulation time. We examine trends of this memory effect as we move around the low temperature region of the phase diagram. These results shed light to the origin of the experimentally observed memory effect.

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