COMPUTER SIMULATION OF PHASE SEPARATION IN DIBLOCK COPOLYMERS ON CURVED SURFACES

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ABSTRACT

In this talk, we consider phase separation on curved surfaces in 3D by numerically solving a nonlocal Cahn-Hilliard equation for diblock copolymers. In the proposed model, a curved surface is implicitly defined as a level set of a phase-field function. We use a discrete narrow band grid that neighbors the curved surface. We use the closest point method and apply a pseudo-Neumann boundary. Due to boundary condition we can replace the Laplace-Beltrami operator by the standard Laplacian operator. We use an unconditionally gradient stable scheme, which was introduced by Eyre. We also use the minimum number of grid points for the discrete narrow band domain. The proposed scheme is efficient. Computational tests are provided to study phase separation patterns for diblock copolymers on curved surfaces in 3D.

REFERENCES

1. I.P. Campbell, G.J. Lau, J.L. Feaver, M.P. Stoykovich, Macromolecules **45**, 1587 (2012).
2. C. Singh, M. Goulian, A.J. Liu, G.H. Fredrickson, Macromolecules **27**, 2974 (1994).
3. F. Liu, N. Goldenfeld, Phys. Rev. A **39**, 4805 (1989).
4. R. Choksi, M.A. Peletier, J.F. Williams, SIAM J. Appl. Math. **69**, 1712 (2009).
5. P. Tang, F. Qiu, H. Zhang, Y. Yang, Phys. Rev. E **72**, 016710 (2005).
6. T. Baumgart, S.T. Hess, W.W. Webb, Nature **425**, 821 (2003).
7. A.R. Bausch, M.J. Bowick, A. Cacciuto, A.D. Dinsmore, M.F. Hsu, D.R. Nelson, M.G. Nikolaides, A. Travesset, D.A. Weitz, Science **299**, 1716 (2003).
8. P. Sens, S.A. Safran, Eur. Phys. J. E **1**, 237 (2000).
9. K. Binder, S. Puri, S.K. Das, J. Horbach, J. Stat. Phys. **138**, 51 (2010).
10. G. Brown, A. Chakrabarti, J. Chem. Phys. **102**, 1440 (1995).
11. K. Binder, J. Non-Equil. Thermodyn. **23**, 1 (1998).
12. H. Xiang, K. Shin, T. Kim, S.I. Moon, T.J. McCarthy, T.P. Russell, Macromolecules **37**, 5660 (2004).
13. R. Choksi, M. Maras, J.F. Williams, SIAM J. Appl. Dyn. Syst. **10**, 1344 (2011).
14. M. Pinna, A.V. Zvelindovsky, Eur. Phys. J. B **85**, 1 (2012).
15. D. Jeong, J. Shin, Y. Li, Y. Choi, J.-H. Jung, S. Lee, J. Kim, Curr. Appl. Phys. **14**, 1263 (2014).