Simulation Capability for Nanoscale Manufacturing Using Block Copolymers

David Clague
(925) 424-9770
clague1@llnl.gov

This project focused on simulation capability for nanoscale manufacturing using block copolymers. The capabilities published in the literature enable prediction of the polymer combination and the ratio of polymers involved to achieve desired nanoscale features during melt solidification. Additionally, the length of the polymer blocks qualitatively influences the temperature and time necessary for the annealing process.

Project Goals

The goal of this project was to reduce to practice published, predictive block copolymers simulation capabilities to augment and guide experimental efforts to controllably form nanoscale features.

Relevance to LLNL Mission

Repeatable control of nanoscale features such as lithographic masks and 3-D structures is a critical capability gap at LLNL. This project will provide custom nanofabrication technology that will enable the transition and deployment of many nanoscale devices and technologies into the programs. This enabling capability will impact nanoscience and technology at LLNL, and aligns with competency goals in predictive simulation and micro-, meso- and nanoscale engineering, computational engineering, and mesoscale fabrication.

FY2006 Accomplishments and Results

We reduced to practice 2-D and 3-D Cahn-Hilliard-Cook (CHC) type

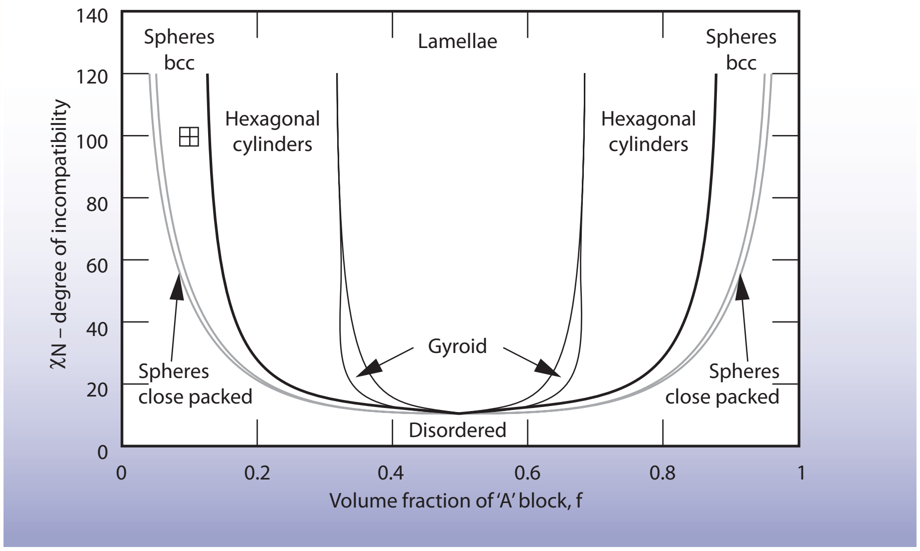

Figure 1. Phase diagram for polystyrene and PMMA, predicted using self-consistent mean field theory: χ is the Flory-Huggins parameter, which is a measure of block-block solubility; N is the degree of polymerization; and f is the number fraction of the reference polymer in the diblock.

models to predict nanophase formation in diblock copolymer systems. The models from the literature were reduced to both MatLab® scripts and Fortran90® simulation capabilities. The potential nanophases that can be predicted with the model include lamellae, cylinders, gyroids, and spheres (Fig. 1).

Two-dimensional results from this effort enabled elucidation of conditions that produced lamellae and cylindrical features. Additionally, through the literature, we were able to relate final features to real dimensions. When comparing predicted feature sizes with experiment, it was found that the simulation results were within 5% of the realized results. In Fig. 2, we show lamellae and cylindrical phase separations.

In addition to reduction to practice of the 2-D CHC model, a 3-D version of the capability was reduced to practice to enable prediction of 3-D effects and surface boundary conditions on nanoscale feature formation. Figure 3 shows the 3-D results for lamellae and spherical nanofeatures.

Using these newly available capabilities, simulation results have been collected to help guide block copolymer selection from commercial sources to achieve desired feature sizes.

Related References

1. Kielhorn, L., and M. Muthukumar, "Spinodal Decomposition of Symmetric Diblock Copolymer/Homopolymer Blends at the Lifshitz Point," *J. Chem. Phys.*, **110,** 8, 1999.
2. Chakrabarti, A., and R. Toral, "Late Stages of Spinodal Decomposition in Three-Dimensional Model System," *Phys. Rev. B,* **39,** 7, 1989.
3. Matsen, M. W., and F. S. Bates, "Unifying Weak- and Strong-Segregation Block Copolymer Theories," *Macromolecules,* **29,** 4, 1996.

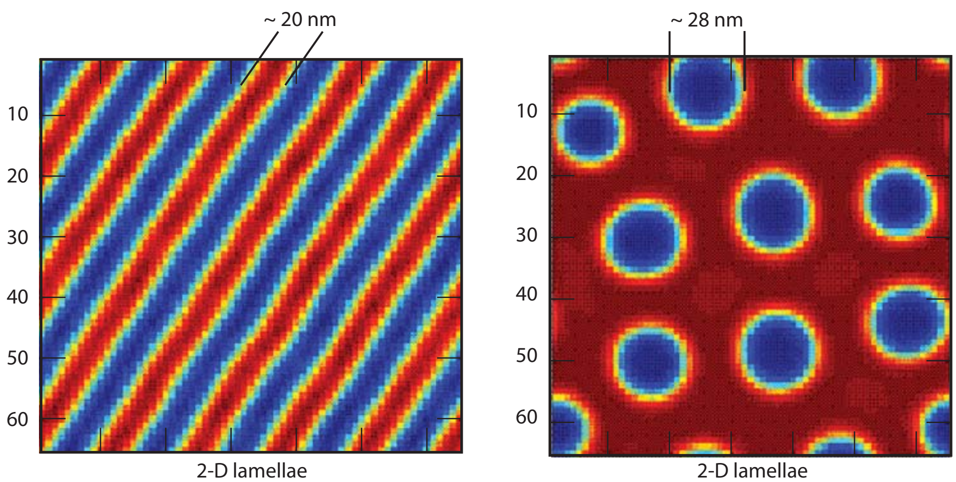

Figure 2. Predicted lamellae and cylindrical nanofeatures using 2-D CHC-like model for a polystyrene/PMMA diblock copolymer system. The volume fractions of the reference block were consistent with the phase diagram shown in Fig. 1. Results were in very good agreement with experiments.

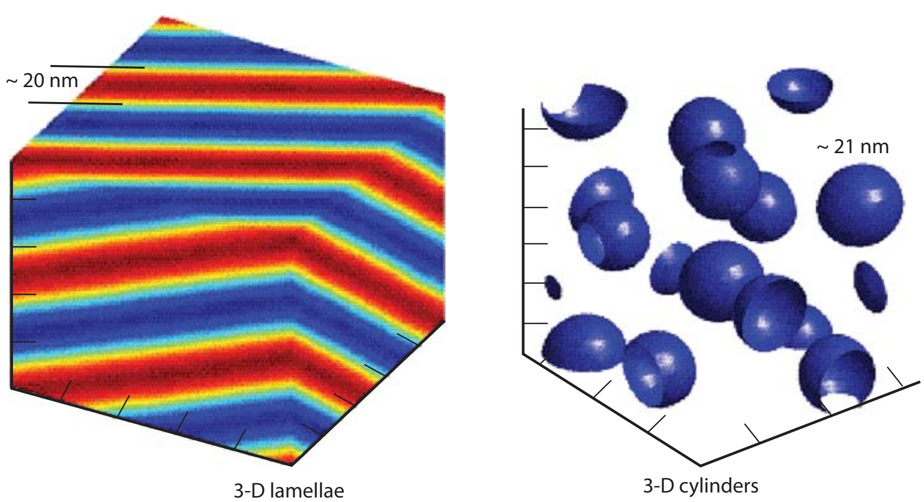

Figure 3. Predicted 3-D lamellae and spherical nanofeatures for a polystyrene/PMMA system. The average feature size is given on the images.