Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Discovering Ordered Phases of Block Copolymers: A New Fourier-space Approach FENG QIU, Dept. of Macromolecular Science, Fudan University, Shanghai, 200433, China, AN-CHANG SHI, Dept. of Physics and Astronomy, McMaster University, Hamilton, Ontario L8S 4M1, Canada, ZUOJUN GUO, HONGDONG ZHANG, YULIANG YANG — A new method to solve the self-consistent field theory of block copolymers is developed. This method is based on the fact that, for any computational boxes with periodic boundary conditions, all spatially varying functions are spanned by the Fourier series determined by the size and shape of the box. This method is well suited for the discovery of ordered structures of block copolymer systems. The symmetry of the ordered structures emerges from the minimization of the free energy density. Application of the technique to diblock copolymers recovers all the previously known ordered structures plus a few new metastable ones. As an example of application, the method is used to construct a phase diagram for a model of frustrated triblock copolymers. A variety of stable or metastable three-dimensional ordered structures are discovered. Furthermore, the capability of the method to reproduce experimentally observed structures is demonstrated by the knitting pattern in triblock copolymers.

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Date submitted: 25 Nov 2007 Electronic form version 1.4