Abstract Submitted for the MAR06 Meeting of The American Physical Society

Self-consistent field theoretic calculations of stress in diblock PANAGIOTIS MANIADIS, KIM O. RASMUSSEN, TURAB LOOKMAN, ED-WARD M. KOBER, Theoretical Division, Los Alamos National Laboratory — The elastic properties of diblock copolymers are studied using self-consistent field theoretical calculations. Our starting point is the approach of Fredrickson (J. Chem. Phys. 117, 6810, 2002) in which microscopic expressions of the elastic energy and stress of polymer chains are self-consistently incorporated into the free energy expression for a homopolymer. We extend this theory to phase separating diblock copolymers and calculate numerically the complete stress tensor in the presence of external strain. Our numerical method can be easily generalized to multi-block copolymers, and our method can be used to study the elastic properties of phase separating polymer materials in general.

> Kim O. Rasmussen Los Alamos National Laboratory

Date submitted: 11 Jan 2006

Electronic form version 1.4