Abstract Submitted for the MAR10 Meeting of The American Physical Society

Ultrathin-films of diblock copolymers under shear ALEXAN-DROS CHREMOS, ATHANASSIOS PANAGIOTOPOULOS, Chemical Engineering, Princeton University — The behavior of diblock copolymers ultra thin-films under confined-shear conditions has been studied using coarse-grained Langevin dynamics simulations. The conformational properties of the diblock copolymers within the thin-film and the overall film's structural behavior are examined as functions of the composition (volume fraction) f, the segregation strength, Φ , and the strength of the shear-field, $\dot{\gamma}$. Below the order-disorder transition (ODT) the film generates a rich variety of structures composed by a monolayer of compressed micelles. Once a shear field is applied and above a critical shear rate, the system re-self-assembles into cylindrical micelles with orientation parallel to the shear flow. This study draws much of what is known from simulation and experiment on the formation of cylinders under shear and provides deeper insights into shear-induced sphere-to-cylinder order-order transition and realignment of cylinders. In addition to formation of cylinders formation parallel to the sheared direction, we have identified the conditions under which the formation of cylinders under the influence of shear flow have orientation *perpendicular* rather than parallel to the shear flow. This order-order steady-state orientation transition is temperature dependent.

> Athanassios Panagiotopoulos Chemical Engineering, Princeton University

Date submitted: 20 Nov 2009

Electronic form version 1.4