Polymers under Multiple Constraints

Polymer- & Soft-Matter-Seminar

Thursday, 19th December 2013

at: 5.15 pm

VSP1 1.26, Von-Seckendorff-Platz 1, 06120 Halle

Special Event

Prof. Dr. Jutta Luettmer-Strathmann and Kiran Khanal

Departments of Physics and Chemistry, The University of Akron, Akron, OH 44325, jutta@uakron.edu

“Liquid-crystalline ordering in semiflexible polymer blends"

Semiflexible polymers of sufficient stiffness exhibit liquid crystalline order at low temperature and high polymer concentration. Blends of stiff and flexible polymers have interesting physical properties and important applications in organic electronics. For example, in bulk heterojunction devices, amorphous and ordered regions with varying compositions coexist due to microphase separation of the blend components. Accounting for these effects in device simulations is difficult since the size of the active layer is too large to generate realistic morphologies from molecular simulations of the constituents. In this work we present Monte Carlo simulations of a coarse-grained lattice model for semiflexible polymers that allows us to study the formation of liquid crystalline regions in melts and blends. Structural properties show that the blends are well mixed at high temperature and phase separate on ordering. We investigate the effect of blending on the ordering transition and show how external fields affect the ordered domains. The long-term goal of this work is to generate relevant morphologies for device simulations and we discuss our steps in that direction.