Polymers under Multiple Constraints

Kolloquium

Thursday,

13th June 2013

at: **5.15 pm**

Gustav-Mie-Hörsaal, Theodor-Lieser-Str. 9, 06120 Halle

Coffee will be served from 4.45 pm!

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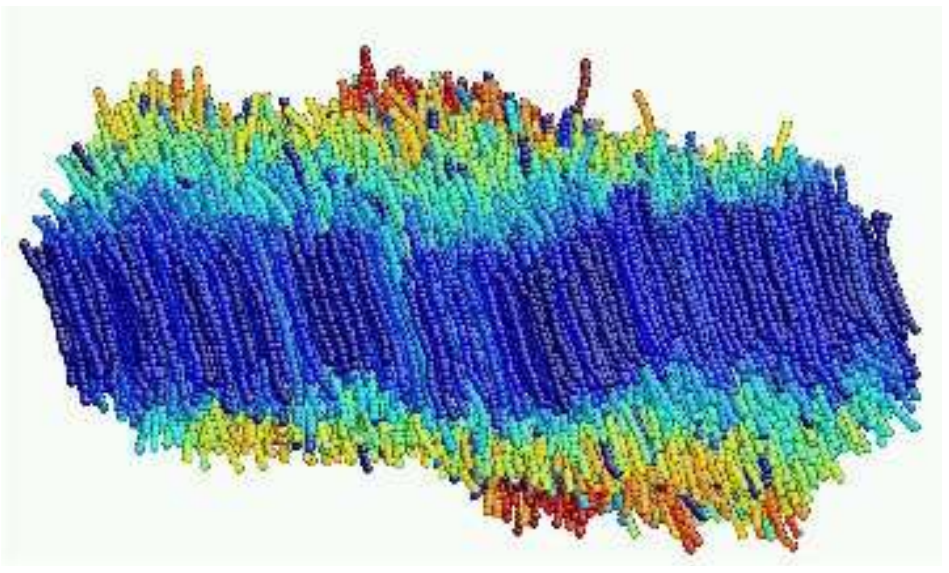
Polymer Crystallization: Ordered Structures in Complex Systems

Jens-Uwe Sommer and Chuanfu Luo

The crystallization of long chain molecules requires two ordering processes which take place simultaneously: Transition of each chain from the randomly coiled state into the partially folded and extended state, and the growth of many chains forming a regular crystalline structure. This leads to complex crystallization and nucleation pathways which usually result in non-equilibrium meta-stable states. I will first discuss some issues of possible equilibrium states of chain crystals [1]. Large scale molecular dynamics simulations are presented which allow to investigate molecular details of single lamellar growth out of an entangled polymer melt. The figure shows a snapshot of single lamellar as obtained in the simulations. Spatial-temporal measures of the state of order are introduced to detect precursor states of crystallizing chains during the crystallization pathway [2]. The local entanglement density during crystal growth is analyzed by primitive path analysis [3]. This leads us to establish a relation between entanglement and lamellar thickness.

[1] J.-U. Sommer, *Eur. Phys. J. E* **19**, 413 (2006)[2] C.-F. Luo and J.-U. Sommer *Macromolecules* **44**, 1523 (2011)[3] C.-F. Luo and J.-U. Sommer, *ACS Macro Lett.* **2**, 31 (2013)



Snapshot of a crystalline lamellar obtained in simulations using a coarse grained model of PVA. Shown are only the chain parts which are in a extended state(stems).

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