

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. Large scale molecular dynamics simulations are presented which allow to investigate molecular details of single lamellar growth out of an entangled polymer melt. Using a variant of a self-seeding techniques we are able to simulated single lamellar growth from entangled polymers melts containing chains of 1000 repeat units. Spatial-temporal measures of the state of order are introduced to detect precursor states of crystallizing chains during the crystallization pathway [1]. We have applied primitive path analysis to calculate the local entanglement properties during crystal growth. In general two competitive processes, a slow decrease of average entanglement length during cooling caused by stiffening of chains and a strong increase during crystallization, can be observed. In both homogeneous and heterogeneous nucleation, disentanglement occurs via forming folds from locally unentangled segments and continues in post-crystallization processes (slow reorganization), in particular during annealing [2].

[1] C.-F. Luo and J.-U. Sommer, *Macromolecules* **44**, 1523 (2011)

[2] C.-F. Luo and J.-U. Sommer, *ACS Macro Lett.* **2**, 31 (2013)