Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Influence of Angular Potentials on the Crystallization of Model Polymer Chains HENDRIK MEYER, CNRS, Institut Charles Sadron, 67083 Strasbourg, France, THOMAS VETTOREL, JÖRG BASCHNAGEL — A simplified polymer model appeared to be extremely efficient for the study of polymer crystallization in molecular dynamics simulations [1]. This model goes one step further than usual united-atom models and resumes all atoms of a monomer into one sphere. It still retains information of the possible conformations in an angular potential with 3 local minima. We systematically varied this angular potential which allows to tune crystallization and melting temperatures. The chain rigidity characterized by the fraction of stretched conformations in the melt is an important driving force for crystallization in these models: the higher this fraction, the easier is the crystallization and thus the higher the temperature where ordering starts. But interestingly, no trivial correlation with other examined quantities, and in particular with the persistence length, could be found.

[1] H. Meyer and F. Müller-Plathe, J. Chem. Phys. 115 (2001) 7807; Macromolecules 35 (2002) 1241. H. Meyer in Lecture Notes in Physics 606, J.U. Sommer, G. Reiter (eds.) Springer 2003.

Hendrik Meyer
CNRS, Institut Charles Sadron, 67083 Strasbourg, France

Date submitted: 04 Dec 2004 Electronic form version 1.4