MAR16-2015-020161

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

From chromosome crumpling to the interacting randomly branched polymers

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The conformational statistics of ring polymers in melts or dense solutions is strongly affected by their quenched microscopic topological state. The effect is particularly strong for non-concatenated unknotted rings, which are known to crumple and segregate and which have been implicated as models for the generic behavior of interphase chromosomes. In [1] we have used a computationally efficient multi-scale approach to identify the subtle physics underlying their behavior, where we combine massive Molecular Dynamics simulations on the fiber level with Monte Carlo simulations of a wide range of lattice models for the large scale structure. This allowed us to show that ring melts can be *quantitatively* mapped to coarse-grained melts of *interacting* randomly branched primitive paths. To elucidate the behavior of interacting branched polymers, we use a combination of scaling arguments and computer simulations[2]. The simulations are carried out for different statistical ensembles: ideal randomly branching polymers, melts of interacting randomly branching polymers, and self-avoiding trees with annealed and quenched connectivities. In all cases, we perform a detailed analysis of the tree connectivities and conformations. We find that the scaling behaviour of average properties is very well described by the Flory theory of Gutin et al. [Macromolecules 26, 1293 (1993)]. A detailed study of the corresponding distribution functions allows us to propose a coherent framework of the behavior of interacting trees, including generalised Fisher-Pincus relationships and the detailed analysis of contacts statistics. [1] Ring Polymers in the Melt State: The Physics of Crumpling, Angelo Rosa and Ralf Everaers, Phys. Rev. Lett. 112, 118302 (2014)
[2] Conformations of randomly branching polymers with volume interactions, Angelo Rosa, A.Y. Grosberg, M. Rubinstein and Ralf Everaers, in preparation.