Polymeric features in the glassy arrest of melts

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Melts of long flexible polymeric molecules are archetypal systems undergoing a glass transition, characterized by a sharp slowing down of the relaxational dynamics upon cooling, whereas no structural thermodynamic signature is observable. In a melt of flexible molecules, the huge intermingling of polymeric coils prevents the cristallization, and a microscopically homogeneous glassy state is very easily observed. A first theoretical approach to this kinetic transition has been done recently [1,2,3] via a generalization of the mode-coupling theory, (MCT) which had been successful in predicting the main features of the glass transition of simple fluids. However, these previous studies used approximations to get tractable expressions which altered the accuracy of the predictions, and got rid of important polymeric features of these liquids at large length scales. We propose to reinvestigate this approach, using an adaptation of the traditional mode-coupling theory which retains the polymeric scaling features from the microscopic to the mesoscopic length scales. The issue is particularly interesting in the present state of the glass theory, where the efforts focus now on the characterization of dynamical heterogeneities beyond the monomeric length scales : the extended and diffuse nature of the polymeric molecules, which pervade several length scales could provide an interesting dynamical probe of these intermediate and important new properties of the dynamics of supercooled liquids.

The project includes theoretical developments, as well as a comparison of the theory with numerical simulations. It assumes thus an interest for theoretical considerations and numerical computations of model liquids. A good knowledge of the liquid physics [4] is desirable.

[1] Chong, S.-H. and Fuchs, M., *Mode-Coupling Theory for Structural and Conformational Dynamics of Polymer Melts,* Phys.Rev.Lett*.* **88***, 185702 (2002).*

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[3] Aichele et al, *Static properties of a simulated supercooled polymer melt: Structure factors, monomer distributions relative to the center of mass, and triple correlation functions*, Phys. Rev. E, **69**, 061801 (2004).

[4] Hansen J-P. and MacDonalds, I.R., *Theory of Simple Liquids*, Academic Press (2006).