Technische Universiteit Eindhoven University of Technology

M. Sc. Project

Collective Dynamics in Deformed Polymer Glasses

Introduction – Everyday experience shows that polymers deform irreversibly under the application of high loads. While such behavior can not only be observed and quantified in experiments, and also described phenomenologically using macroscopic models, the relevant microscopic processes are still largely unknown. For example, it is still challenging to explain why polystyrene fails brittle while polycarbonate shows ductile deformation.

Goal – This M. Sc. project will help to unravel those microscopic structural changes in polymer glasses (e.g. polystyrene) that explain their large-deformation behavior.

Task – In the group of dr. Lyulin and prof. dr. Michels, Molecular Dynamics (MD) simulations have been performed on polystyrene samples in tensile deformation. While, the evolution of the structure in terms of all atom positions (trajectory files) is available, the main task now consists in analyzing the data. Particularly, few intuitive parameters should be found that play a key role in the deformation behavior of the entire sample. For example it is believed that chain segments can only rearrange collectively under deformation. Thus, natural questions are: how does the size and number of these cooperative regions depend on time and on the applied load, and which sections of the polymer chain primarily participating in the cooperative motions? These and similar questions shall be addressed in this project, since they are crucial for more coarse-grained modeling approaches.

Type of work – Develop a computer program for the detailed analysis of microstructure evolution; concepts proposed in the literature for the analysis of collective motion shall be tested specifically on the available trajectory files for polystyrene.

Requirements – Expertise in programming (f77,f90,C,C++, Matlab, Mathematica) and in numerical simulation; Interest in mechanical properties of materials.

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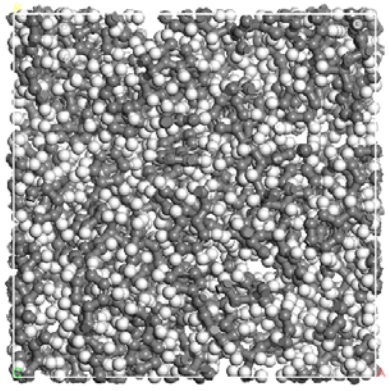

atomistically detailed simulation of polystyrene