CHARACTERIZATION OF LOCAL STATIC AND DYNAMIC PROPERTIES OF POLYMER SYSTEM IN BOND-FLUCTUATION MODEL

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Abstract:

Polymers are nowadays present in many areas of science, e.g. physics, chemistry, biology, nonlinear optics and material engineering. Despite the interest in polymer systems their theoretical description still constitutes a challenge. Wide range of time and space scales characteristic for polymers make their analysis much more difficult. Depending on the temperature the system can be treated as a liquid (above glass transition temperature T_g) or as a solid (below T_g). Therefore for their analysis methods of computer science are usually used.

Commonly used in polymer science is Monte Carlo bond-fluctuation (lattice) model introduced by Carmesin and Kremer [1]. It uses some simplifications and allows the effective modelling of behaviour of polymer system, its dynamics and related effects. Many issues connected with polymer systems were modelled and explained with bond-fluctuation model [2]. Still one can find areas of polymer science where the knowledge about the behaviour of polymers is insufficient. One of such topics is microscopic structure of polymer systems.

The main goal of my thesis is the characterization of structural microscopic static and dynamic properties of model polymer system. We believe that the description of its microscopic structure is crucial for modelling of physical phenomena, understanding of polymers internal processes and for interpretation of experimental results. For the analysis of local structure we use *local void parameter*. It describes local neighbourhood of chosen lattice site in the system.

The thesis is divided into three main chapters in which the following topics are discussed: static properties, dynamic properties and model of chosen nonlinear optics phenomenon (*all-optical poling*) based on parameters describing local structure.

The distribution of local void parameter is inhomogeneous. In the system we distinguish two types of correlations of lattice sites with the same values of local void parameter: *liquid-like* and exponential. We affirm clusterization of lattice sites with high values of *local void parameter*. The distribution of sizes of clusters can be fitted by power law. Clusters show some 2-dimensional and some fractal features.

Analysis of Monte Carlo kinetics (dynamics) of the system is in its preliminary stage. We found that it depends on the temperature: for low temperatures kinetics is *frozen-like* and for high temperatures it is *mobile-like*. Analysis of dynamic parameters suggests the presence of heterogeneous kinetics.

In the third part we propose the model of *all-optical poling* effect [3] where the influence of polymers onto guest molecules is based on local parameters of polymer system. We reproduce the

build-up of noncentrosymmetric (polar) order and *angular hole burning* effect, due to the intercation of guest molecules with linearly polarized light. Obtained results show the transfer of complex kinetics from the polymer system onto guest molecules, manifested via time dependence of *stretched exponential* type and power laws. Those effects are the strongest close to the glass transition temperature. We affirm monotonic dependence of some investigated physical quantities on the experimentally tunable parameter.

Bibliography:

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[3] Radosz, W.; Pawlik, G.; Mitus, A.C. Complex Dynamics of Photo-Switchable Guest Molecules in All-Optical Poling Close to the Glass Transition: Kinetic Monte Carlo Modeling. J. Phys. Chem. B 2018, 122, 1756-1765.