

DESCRIPTION FOR THE GENERAL PUBLIC

Polymers are omnipresent in our everyday life. Their applications extend to nearly every branch of technology; they have also increasing role in contemporary medicine, where they are used as components of drug delivery systems and biomaterials (including implants, tissue engineering products, carriers for gene therapy etc.). In many applications, from car tires to hydrogel wound dressings, polymers are used in a crosslinked form. That means that their long, linear chains are linked together to form insoluble and usually elastic 3D networks. While industry can nowadays manufacture a large variety of polymers in diverse forms, still many questions remain unanswered as to the detailed mechanism of chemical reactions and physical processes underlying polymer synthesis and modification (e.g. by crosslinking). It is believed that by expanding our understanding of these processes we would be able to more precisely control the synthesis and in this way design products of even better (or totally new) properties compared to those available today. In this project we will study some of the important processes involved in polymer formation and modification, in order to deepen our understanding of the dynamics and mechanism of these reactions.

Our approach is novel and innovative for at least two reasons. First of all, we will employ in parallel experimental work and computer simulations. Secondly, both the selected simulation and experimental approach are based on original concepts that have been so far rarely used to explain general phenomena in polymer physics and chemistry. Computer simulations, based on the novel DLL (Dynamic Lattice Liquid) approach, can not only reduce the cost and duration of testing some hypothesis when compared to experiments, but allow us to go beyond of what is possible to measure experimentally - we can isolate single processes, we can test them in precisely controlled conditions, we can also eliminate unwanted side factors and experimental errors, as well as technical limitations. However, as with any new tool, our approach must be careful - we will first test if our simulation approach and model reproduce well these situations that can be studied experimentally. Only if this is the case, we can use simulations to answer questions that cannot be assessed by experiments. In our experimental approach we will initiate the studied reactions by ionizing radiation. In this way we can deliver to the system precisely known amount of energy in precisely defined time, while at the same time eliminating the need of using any chemicals which could complicate our studies. Ionizing radiation generates reactive chemical species - free radicals, that can initiate polymerization and cross-linking. By using fast spectroscopy (following in very short times as micro- and milliseconds the way our samples absorb light) we can directly observe how a polymer chain is growing or how crosslinks between the chains are formed.

Using simulations and experiments in parallel, we will study various cases of polymerization (simple or proceeding side-by-side with cross-linking), and later various pathways of cross-linking itself, either between the chains - leading to large 3D crosslinked polymer structures, or between the segments of the same chain. The latter process is of considerable interest, since it leads to the formation of nanogels - molecular cages of nano dimensions, that are being tested e.g. as drug, gene or radioisotope carriers in medicine. In all cases we will aim at understanding the dynamics and mechanisms of the studied processes. We shall learn how the experimental parameters and properties of the starting materials influence not only the reactions themselves, but also the structure of final products. In this way, besides providing basic qualitative and quantitative description of the studied reactions and processes, important for polymer chemistry and physics, we will contribute to practical knowledge on how to synthesize a complex, sophisticated, functional polymer-based material of precisely defined properties.