

Knots are a fascinating subject not only for mathematicians. In fact, it turns out that knots and links, which are forming from the reciprocal entanglement of two or more knots, appear also in nature, for instance in the atmosphere of our sun, where the closed lines of the solar magnetic field create complicated topological structures. These structures are very relevant for the inhabitants of the Earth because, depending on the degree of their complexity, the lines of the magnetic field can undergo the so-called magnetic reconnection. This is a process in which the magnetic lines disconnect and reconnect changing their topological structure. The enormous amounts of energy released cause the phenomenon of solar flares, in which large fluxes of particles and electromagnetic waves are emitted. If they hit the Earth, they can disturb the telecommunications or destroy distribution transformers. In space, they could endanger the life of the astronauts. Similar topological structures characterize also the behavior of polymer systems, which are the main subject of this proposal. Polymers are consisting of long chains which are often closed forming in this way knotted rings. Like magnetic lines, these rings are additionally entangled together giving rise to links of complex topology. In biopolymers, like for example the DNA, this kind of topological entanglement is dictated by the necessity of shrinking the DNA, whose length is of the order of meters, into the tiny space of a cell nucleus, whose radius is of the order of a few micrometers. In the case of artificial polymer materials the presence of topological structures is also important. For example, without taking into account the existence of knots and links it is not possible to describe in a satisfactory way the behavior of elastic polymer materials and the agreement between theory and experiments is only within a twenty percent of error. Another characteristics of knots is that they diminish the resistance of materials under mechanical stress, a fact that can be important for recycling. The effects connected with the topological properties of polymer systems are measurable by experiments thanks to the recent technological progresses, which allow the manipulation of knots and links formed by a small number of polymers. Much more difficult is to isolate possible topological effects in the case of real materials, which contain billions of polymers. The aim of the present project is exactly a better understanding of the topological effects on the mechanical and thermal properties of polymer materials with the help of numerical methods. Such methods are already widely used in polymer physics. The results coming from numerical simulations can be easily compared with the experiments. Their predictions can also shed light on important aspects that cannot be clarified by experiments because they are out of the reach of present technologies. At present, thanks to computational techniques developed by our Szczecin group, it is possible to consider single polymers that contain four thousands segments or a link, in which ten polymer rings, each one of a length of four hundred segments, are entangled together. For polymers of such lengths the approximated models used in this research become realistic. We can for instance observe the formation of crystallized structures in polymers similar to those appearing in snowflakes. An important characteristics of the project is that for the first time polymer links will be studied containing up to ten knots entangled together. Up to now, mainly the physical properties of single knots have been studied. The questions that will be answered by this project are relevant both for the biophysics research and material engineering. Using polymer links it is possible to realize small nets or capsules in which it is possible to put drugs. What will be the thermal properties of such nets and capsules? Moreover, what will be the resistance under mechanical stress of a polymer link when it is stretched by external mechanical forces? In which parts of this system the stress will be higher? The latter is an important problem which should be solved in order to be able to predict where ruptures could occur inside the material. Finally, do conformations exist that are particularly stable, in the sense that they correspond to energy minima of the system? Preliminary numerical calculations suggest, that the energy landscape of polymer knots is very complicated, similarly to that of proteins. Finally, can we fine tune the properties of polymer materials with the help of the topological effects. The purpose of this project is to answer all these questions and to develop innovative numerical techniques that will be relevant not only in polymer physics, but also in all other disciplines, in which topological effects are important.