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S E M I N A R

aus

Halbleiterphysik und Nanotechnologie

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Hörsaal für Physik

"The role of reversible cross-links on the mechanical properties of polymeric systems- A Monte Carlo study"

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Natural materials are a constant source of inspiration for material scientists in manufacturing materials with new and desired mechanical properties. However, this requires a thorough understanding of the structure and the mechanisms that make biological materials achieve their outstanding mechanical properties. One strategy to improve the mechanical performance of natural materials is using reversible cross-links in their structures. These so called sacrificial bonds can be found in bone, wood, and in some softer biological materials like silk, mussel byssus threads. Sacrificial bonds (SBs) are weaker than the covalent bonds that hold the structure together. Thus, upon loading SBs break before the covalent bonds rupture. The rupture of these cross-links reveals hidden length providing a very efficient energy dissipation significantly toughening the structure.

The first part of the results focuses on the influence of SBs on the mechanical properties of single polymer chain using Monte Carlo method. In our model, the chain consists of several beads linked together via covalent bond. In addition some of the beads so called "sticky sites" are allowed to form SBs. SBs in this model always formed from only two sticky sites and are allowed to open and close reversibly. At the beginning the influence of entropy on the efficacy of SBs is investigated. Then, the influence of SB density and arrangement is discussed on the mechanical properties of the chain by determining the load-displacement curves.

In the second part, emphasis is placed on the influence of grafting density and cross-link density on the mechanical properties of the chain bundle. Most surprisingly the results show that only two cross-links are sufficient to break the backbone of the system although the cross-links are weaker than the covalent bond by factor of four. This failure is caused by the topology of the interchain cross-links in the chain bundle where sacrificial bonds are distributed in an ordered arrangement. This backbone failure weakens the strength of the material, but increases the amount of work to elongate the system as well as the apparent stiffness of the bundles.