Determining mechanical properties of complex materials using the computer

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In this talk I will discuss how Monte Carlo simulations can be used to determine the mechanical properties of complex materials. In particular I will discuss two special systems: carbon nanostructures and a polymeric system that is inspired by the fascinating material of the mussel byssus-a material that considerably improves its mechanical performance by using sacrificial bonds. Carbon nanostructures combine high stiffness with low weight and exceptional toughness that makes carbon a promising candidate for applications in structural mechanics. Understanding the mechanical behavior of these structures on an atomistic length scale is inevitable in describing the mechanical performance and stability of large, hierarchical structures like carbon onions and fibers. In the presented work *ab initio* calculations were used to extract classical potentials describing deformations of C-C bonds that were used in subsequent Monte Carlo simulations to perform computational mechanical tests on larger structures[1]. These tests included stretching, bending and buckling simulations on graphene, allowing to determine the value of the Poisson ratio, as well as the membrane and bending stiffness of graphene, from which the effective elastic modulus and the effective thickness can be consistently derived[2].

The second system discussed is inspired by sacrificial bonding that is one strategy to improve the mechanical properties of natural materials. Sacrificial bonding can be found in a large variety of biological materials like bone, wood and in some softer biological materials like silk, mussel byssus threads and whelk egg capsules. Sacrificial bonds (SBs) are reversible bonds which are weaker than the covalent bonds that hold the structure together. Thus, upon loading SBs break before the covalent bonds rupture. The rupture of SBs reveals hidden length providing a very efficient energy dissipation mechanism. Furthermore, SBs can reform after their rupture providing molecular repair and self-healing. We use Monte Caro simulations to examine the influence of the topology and SBs density on the mechanical properties of single polymeric chains[3]. The polymers in the model investigated are modeled as a string of hard spheres that are covalently connected to their two neighboring beads. Additionally some of the beads are defined as "sticky" and are allowed to form a SB. The SBs were assumed to be a factor of 4 weaker than the covalent bonds. The influence of SB density, topology and thermal backbone fluctuations on the mechanical behavior of the chains are investigated by computationally mimicking tensile and cyclic loading tests[4,5].

[1]D. Holec, M. A. Hartmann *et al.*, Phys. Rev. B **81**, 235403 (2010)
[2]M. A. Hartmann *et al.*, Europhys. Lett. **103**, 68004 (2013)
[3]S. S. Nabavi, M. J. Harrington, O. Paris, P. Fratzl, M. A. Hartmann, New J. Phys. **16**, 013003 (2014)
[4]S. S. Nabavi, M. J. Harrington, P. Fratzl, M. A. Hartmann, Bioinsp., Biomim., Nanobiomater. **3**, 139 (2014)
[5]S. S. Nabavi, P. Fratzl, M. A. Hartmann, Phys. Rev. E **91**, 032603 (2015)