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Mechanics of nanostructured polymers: Insights from molecular simulations

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Many polymers exhibit structural heterogeneity on the nanoscale, either by partially crystallizing or, in the case of copolymers, by phase separation. Their mechanical properties are controlled by molecular level mechanisms at interfaces between crystalline-amorphous or rubbery-glassy regions, respectively. In this talk, we employ multiscale molecular dynamics simulations to investigate deformation and plastic flow of such polymers. For the semicrystalline case, we consider an ensemble of randomly nucleated crystallites embedded in an amorphous matrix. When stretched at constant rate, crystallites first reorient and partially fragment in the strain-softening regime, while chain alignment and recrystallization is observed in the strain-hardening regime [1]. We show that a significant contribution to the fracture toughness originates in cross-ties between crystallites. We also present results for sphere-forming triblock elastomers, where chain ends embedded in glassy spheres effectively cross-link a rubbery matrix. The evolution of the spherical morphology and chain on formations are compared for different deformation protocols and polymer molecular weight, and the consequences for the macroscopic stress-strain response will be discussed [2]. By tracking polymer entanglements throughout the deformation process, we test and improve upon current network models for crosslinked entangled polymer networks.

[1] Sara Jabbari-Farouji, Joerg Rottler, Olivier Lame, Ali Makke, Michel Perez, and Jean-Louis Barrat, ACS Macro Lett. 4, 147 (2015)

[2] Amanda J. Parker and Joerg Rottler, Macromolecules 48, 8253 (2015)

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