P.36 Plastic deformation mechanisms in glassy and semi-crystalline polymers

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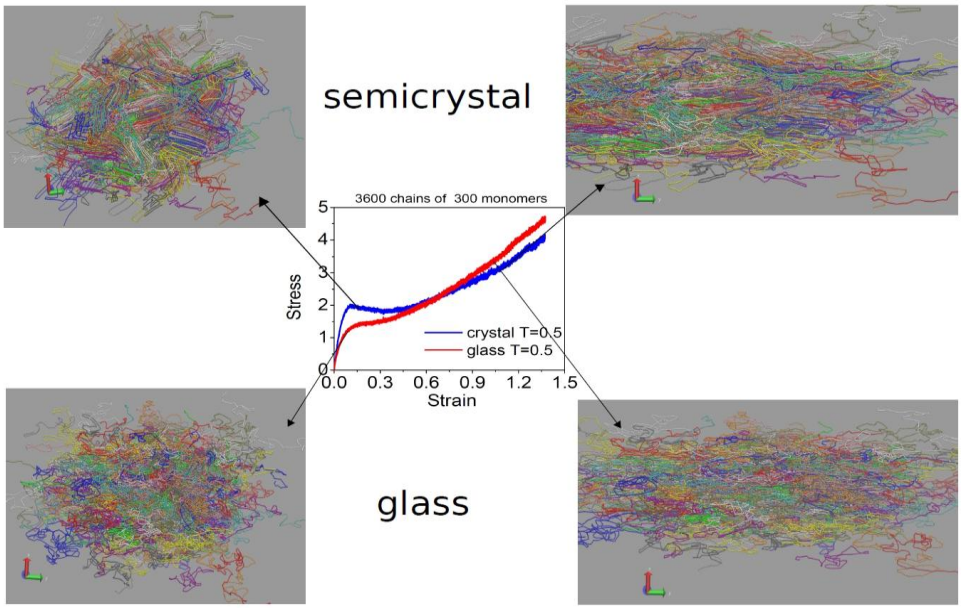
In polymeric materials, the connectivity of the long chain molecules usually hinders the formation of perfect crystals. However, upon slow enough cooling, polymers with regular side chains form partially crystalline structures that consist of stacking chain folded lamella and amorphous regions. The interplay of crystalline and amorphous regions leads to non-brittle solid materials with increased toughness that makes them favorable for various industrial applications. Although there is a wide agreement on the structure of this semicrystalline phase [1] mechanisms of deformation under stress, particularly at single chain level, are poorly understood and a subject of debate.

In order to gain an insight into the mechanical response of semi-crystalline and glassy polymers, we use molecular dynamics simulations. We employ a coarse-grained model for semiflexible polymers (CG-PVA) [2] which displays both crystallization and glassy behaviour via changing the cooling rate. We investigate the mechanical response of polymers by means of uniaxial tensile tests [3]. We address two key questions: i) How do ordered and amorphous regions transform under uniaxial tension? ii) How do mechanical properties of semicrystalline polymers differ from glassy ones?



We obtain the stress-strain curves in both elastic and plastic regimes of deformation and analyze the configurations of deformed samples (see figure). For semi-crystalline samples, in the elastic (linear) regime, deformation leads to a slight stretching of amorphous chains. Upon further increase of strain and yielding of samples, we observe a partial loss of crystallinity accompanied by partial alignment of crystallites with the tensile direction. Very large deformations cause unfolding of lamella and further stretching and alignment of chains along the tensile direction. In glassy samples, small deformations leads to stretching of chains and further increase of tension leads to a greater extent stretching and alignment of chains with tensile direction.

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