ESPCI
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Séminaire PMMH

Bureau d'Études, Bâtiment L, 2 ème étage

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Plastic deformation mechanisms in amorphous and semicrystalline polymers

Solid-like polymers are found in amorphous or semicrystalline state which consist of crystalline and amorphous regions. These polymeric materials have a diverse range of applications from packaging to more high-performance products such as bullet resistant vests and helmets. The wide-spread application of polymers is owing to their large region of plastic flow and their ability to dissipate energy before failure. The deformation mechanisms of the plastic flow in amorphous polymers is rather well understood. However, 70% of synthetic polymers are semicrystalline and their underlying mechanism of deformation is still a matter of debate.
Employing large scale molecular dynamics simulations, we obtain the uniaxial tensile response of amorphous and semicrystalline states of a crystallizable bead-spring model [1]. 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 their amorphous counterparts ?
Our obtained stress-strain curves encompass strain softening and strain hardening regimes similar to the experimental data. Simulations allow us to observe detailed structural changes during deformation which are normally difficult to investigate in real experiments [2,3]. We find that the strain-softening regime is dominated by deformation of crystallites via reorientation of chain-folded lamellae towards the tensile axis and fragmentation of largest crystalline domains. The strain hardening regime coincides with unfolding of chains and recrystallization as a result of strain-induced chains alignment.

[1] H. Meyer and F. Muller-Plathe, J. Chem. Phys. 115, 7807 (2001).
[2] S. Jabbari-Farouji, J. Rottler, M. Perez, O. Lame, A. Makke and J.-L. Barrat under consideration of Macro Letters.
[3] S. Jabbari-Farouji, J. Rottler, M. Perez, O. Lame, A. Makke and J.-L. Barrat submitted to Journal of Physics : Condensed Matter