Séminaire

mardi 17 décembre 2024 à 10h30

Amphithéâtre Henri Benoît

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Controlling semicrystalline polymer properties by modulating the topology of amorphous chains

The thermophysical properties of semicrystalline polymers are believed to be strongly dependent on the topological features of the chain segments found in the amorphous domains. Theoretical modelling and computer simulation are essential tools for investigating this hypothesis due to the experimental challenges associated with resolving the contour of individual polymer chains. I will discuss how the number density and mean length of bridges and trapped entanglements – the inter-crystalline “stress transmitters” – affect small-molecule permeability, postyield response, welding quality, and degradation rate in semi-crystalline polymers. I will also demonstrate how self-consistent field theory can be leveraged to estimate the topological features of the amorphous chains as a function of the polymer’s molecular weight, crystallinity and lamellar thickness. In line with previous work, the theory predicts an increase in length and decrease in the number of stress transmitters with increasing inter-lamellar spacing. Furthermore, chain ends are found to preferentially segregate at the crystal/amorphous interphase to relieve the excess of injected chains in the amorphous domains, thereby providing theoretical support to recent experimental observations.

Les personnes souhaitant rencontrer M. Valsecchi sont priées de prendre contact avec H. Meyer.