11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

MODELING OF SPHERULITE MICROSTRUCTURES IN SEMICRYSTALLINE POLYMERS

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Key words: *Semicrystalline polymers, Crystal Plasticity, Crystalline Materials, Amorphous Materials, Finite Element Method.*

Polymers constitute an important class of materials with a wide range of application areas in modern life. Among these, semicrystalline polymers (SCP), such as high-density polyethylene (HDPE), Nylon-6, poly(ethylene terephthalate) (PET), isotactic polypropylene (iPP) and ultra high molecular weight polyethylene (UHMWPE), form a sub-set with a significant technological interest. Owing to remarkable deformability and toughness, good impact strength, very low gas-permeability, superior wear resistance and biocompatibility, semicrystalline polymers are of ever increasing technological importance [1]. They have been used in applications such as ballistic plates, model aircraft, liquid and gas containers, plastic bags, piping systems, electrical insulation systems, substrates for flexible electronic devices and joint implants. Owing to crystalline structures and amorphous polymer chain networks, they exhibit both deformation mechanisms of crystalline materials and amorphous polymers. To this end, semicrystlline polymers can be considered as two-phase materials consisting of a soft amorph phase and a hard crystalline phase. One of the most common microstructures that are observed in melt crystallized semicrystalline polymers is the spherulite microstructure. In a spherulite microstructure ribbon-like crystalline lamellae are embedded in a matrix of amorphous material, that the lamellae grow out from a common central nucleus. The crystalline lamellae are 3 to 20 nm thick, whereas spherulite diameters are normally in the range of 2 to 20 microns [2]. Due to this complicated and hierarchical microstructure of semicrystalline polymers, the deformation mechanisms are complex and multistage processes. Therefore, a complete quantitative description of semicrystalline polymers requires different approaches at different scales of their microstructure [2].

In this work the large deformation mechanical behavior of semicrystalline polymers is studied by direct finite element modeling of the spherulite microstructure. Finite element meshes of spherulite microstructures are generated where different constitutive models are assigned to radially grown crystalline phase and amorphous polymer phase. A crystal plasticity model, which takes into account geometric constraints induced by inextensible polymer chains, is used for the crystalline phase, while an elastic microsphere model [3] is employed for the amorphous phase. The effects of several parameters, such as spherulite size and crystallinity, on the mechanical behavior are studied under different loading scenarios. Furthermore, it is shown that the model captured the evolution of inhomogeneous plastic deformation activity in spherulite microstructure reported in the literature.

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