Micromechanically Motivated Modeling of Semicrystalline Polymers

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ABSTRACT

Semicrystalline polymers (SCPs) are of ever increasing technological importance due to their remarkable toughness, good impact strength, very low gas-permeability, superior wear resistance, and biocompatibility. 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 amorphous polymer chain networks and crystalline structures, they exhibit deformation mechanisms of both amorphous polymers and crystalline materials. One of the most fascinating 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, where the lamellae grow out from a common central nucleus. The spherulite diameters are normally in the range of 2 to 20 μm while the crystalline lamellae are 3 to 20 nm thick [1]. Due to this complicated and hierarchical microstructure of semicrystalline polymers, the deformation mechanisms are complex processes involving multiple stages.

In this work a micromechanically motivated constitutive model for the mechanical behavior of semicrystalline polymers that have spherulite microstructures is developed. The model consists of alternating amorphous regions and crystalline lamellae emanating from a common nucleus as in the case of a real spherulite microstructure. Individual constitutive models are used for the crystalline and the amorphous regions. In order to capture the high inhomogeneity observed in spherulite microstructures [2] the deformation field is assumed to vary in these regions. This is in contrast to the most inclusion models proposed for SCPs in the literature. The variation of the deformation field is parameterized in terms of some unknown constants which are determined by physically motivated equations such as traction equilibrium at the interfaces, compatibility equations and equilibrium equations. The performance and predictive capability of the proposed model are demonstrated through numerical tests and comparisons with real experiments.

REFERENCES

[1] Z. Bartczak and A. Galeski, "Plasticity of Semicrystalline Polymers", *Macromolecular Symposia*, **294**, 67-90 (2010).

[2] H. E. Oktay and E. Gürses, "Modeling of Spherulite Microstructures in Semicrystalline Polymers", *Mechanics of Materials*, **90**, 83-101 (2015).