Micromechanical and Multiscale Modeling of Strain-Induced Crystallization in Polymers

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ABSTRACT

The present talk treats a polymer affected by the strain induced crystallization (SIC) as a heterogeneous medium consisting of regions with the different degree of network regularity and thus significantly differs from the common approaches based on the use of the Langevin expression for the free energy [1]. Our concept allows depicting the nucleation and the growth of crystalline regions as well as the change of effective material parameters depending on the level of the strain applied. The model proposed is thermodynamically consistent. It is based on the assumptions for the free Helmholtz energy and dissipation. Both of them primarily include bulk- and surface terms due to the deformation and crystallization. The external variables are deformations and temperature, whereas the inelastic deformations and degree of the network regularity are internal variables. Their evolution equations are derived according to the principle of maximum of dissipation [2]. The explained framework is advantageous for several reasons. First, it is suitable to answer the crucial question of which process predominantly influences SIC: the nucleation of new crystalline regions or the growth of already existing ones. Secondly, the proposed model is ideal for a direct implementation within the standard multiscale finite element concept [3]. This numerical homogenization procedure is compatible with the theory of finite strains and is applicable for modeling the cases where the ratio of characteristic lengths of scales tends to zero. Both of these features are necessary for the effective modeling of SIC. The solution of the tasks itemized will make it possible to achieve the final goal: the advanced simulations of SIC which can significantly contribute to the more efficient designing and usage of polymers. This is especially motivated by the fact that SIC has to be understood as a kind of reinforcement already successfully applied for some rubber materials. The proposed concepts are of general nature and can be taken as a basis for the modeling of similar processes involving crystallization processes.

REFERENCES

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