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Computational treatment of polymer fracture across the scales

Scientific area: Computational Solids And Structural Mechanics

Polymers have become indispensable in the past decades regarding resource efficiency and the associated lightweight constructions. Since material failure is crucial in this context, there is a large amount of ongoing research activities concerning crack phenomena. When it comes to computational approaches, a large variety of methods is applied to understand the distinctly multiscale nature of polymer fracture. As far as continuum mechanical techniques are concerned, local approaches such as the Finite Element Method (FEM) are well established. Prominent use cases well-suited to investigate crack propagation are the extended finite element method (XFEM) and FE formulations for phase field or cohesive zone models. Nevertheless, also promising nonlocal strategies such as peridynamics have emerged as an alternative way of modeling deformations with discontinuities. By means of particle-based techniques such as (coarse-grained) Molecular Dynamics (MD), molecular mechanisms related to material failure can be examined with quantum mechanics (QM) providing important insights into bond scission. Furthermore, various multiscale strategies have been proposed, which bridge the different time and length scales involved. For instance, efforts to couple MD with FE have been pursued, whereby special attention must be paid to the interface or interphase between the combined techniques.

In this minisymposium, we aim to provide a platform for intensive discussions of recent advances in the computational treatment of fracture and fracture-related behavior of polymers. We welcome all approaches concerning thermoplastics, thermosets, and rubber-like materials as well as polymer-based (nano-)composites. Ideally, links to experiments and current as well as future applications should be addressed.

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