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An atomistic-to-continuum coupling method for fracture simulations of amorphous polymers

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In this contribution, we present a concurrent atomistic-to-continuum coupling method for fracture simulations of amorphous polymers. This method is based on the Capriccio method [1], which couples a particle domain resolved by molecular dynamics (MD) simulations and a continuum domain descritized by Finite Element (FE) method. Recently, it was extended to inelasticity [2] by employing an inelastic constitutive model [3] in the FE domain.

Since fracture of materials is usually a problem that has to consider fine-scale processes at molecular or atomistic resolution in the vicinity of the crack tip, but is subject to macroscopic boundary conditions, an atomistic-to-continuum coupling method is appropriate for adequate simulations of fracture. To this end, we further develop the inelastic Capriccio method for multi-scale simulations of polymer fracture by embedding an MD domain with a pre-crack into a continuum domain with a notch. The MD domain can then be deformed in a non-affine way by prescribing the boundary conditions of the FE domain. Using this method, we conducted Mode-I deformation of amorphous glassy polystyrene under isothermal condition to study the crack behavior of the MD domain.

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