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Homogenized Molecular Chain Plasticity Simulation for Crystalline Polymer Using Craze Evolution Model Based on Chemical Kinetics

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Fracture of ductile polymers occurs on the boundary between molecular chain-oriented region and non-oriented region after neck propagation due to concentration of craze that is particular microscopic damage of polymers. In this study, craze evolution behavior is decomposed into nucleation and growth of craze. Craze evolution equation is newly developed on the basis of chemical kinetics introducing strain rate and strain dependencies as an activation energy model. Furthermore, a multiscale FE analysis based on homogenized molecular chain plasticity model coupling the craze evolution equation is carried out for crystalline polymer. It is attempted to reproduce computationally characteristic behaviors of craze evolution, i.e., propagation of craze concentration region with neck propagation and cessation of craze evolution in oriented molecular chain region. In addition, applying failure criteria obtained from experiment on fibril strength to the above numerical results, fracture predictions based on craze concentration are demonstrated.

Keywords: Crystalline polymer, Molecular chain plasticity, Homogenization, Craze, FEM