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Molecular dynamics simulation of electromechanical breakdown of polyolefins under a high electric field[1] MAYANK MISRA, DANIEL SINKOVITS, SANAT KUMAR, Columbia University — Polymers are finding increasing use as dielectric materials. Due to their flexibility, polymer dielectrics in the presence of an electric field may undergo large deformations that result in mechanical instability, which leads to detrimental failures. We study this mechanical instability in polyolefins using all-atom molecular dynamics. We vary the simulated external electric field from 0 to 1200 V/μm to study the effect of high electric fields on polyolefins. At critical conditions, we observe a thinning effect leading to electromechanical breakdown. We also determine the critical voltage using theoretical models and relate it to the thinning effect detected in the molecular dynamics simulations.

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