Microscopic definition of entanglement M. PONMURUGAN, JING CAO, ALEXEI LIKHTMAN, University of Reading — We propose to define polymer entanglements as long-lived contacts between the mean paths. The mean path is defined as a path connecting average positions of every monomer over characteristic time of entanglement τ_e. We performed molecular dynamics simulations on variety of bead-spring models in equilibrium and under shear and investigated properties of entanglements defined in such way. A new algorithm for identification of entanglements allows tracing evolution of individual entanglements and quantifying such mechanisms as constraint release and convective constraint release.

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