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Microscopic Theory for Entangled Polymer Dynamics in Rod-Sphere Nanocomposites UMI YAMAMOTO, KENNETH SCHWEIZER, Univ of Illinois - Urbana — We have developed a self-consistent microscopic theory for the long-time dynamics of needles in an array of static spherical fillers. The approach exactly enforces the dynamical two-body rod topological uncrossability and sphere impenetrability constraints, leading to a generalized concept of entanglements that includes the filler excluded volume effect. How the diffusion anisotropy (transverse versus longitudinal motion) depends on the filler-needle aspect ratio, polymer concentration, and filler volume fraction is established. Due to the steric blocking of the longitudinal reptative motion by obstacles, a literal localization transition is predicted that is generically controlled by the ratio of filler diameter to the pure polymer tube diameter or needle length. For a window of filler sizes and loadings, the needle is predicted to diffuse via a "renormalized" reptation dynamics where the tube is compressed and the longitudinal motion is retarded in a manner that depends on all system variables. At high filler volume fractions the needle diffusivity is strongly suppressed, and localization ultimately occurs in the unentangled needle regime. Generalization of the approach to treat mobile fillers, flexible chains, and nonrandom microstructure is also possible.

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