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Structure and Dynamics of Polymer nanocomposite hydrogels DI XU, MIRIAM RAFAILOVICH, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University. NY-11794 — Polymer hydrogels are widely used in fields like food science, tissue engineering and drug delivery. A lot of research has focused on developing hydrogels with novel properties. However, a lack of understanding of the dynamics and structure of the hydrogel has become a big obstacle. We use molecular dynamic simulations, which provide a direct observation of gel formation and gel structures, to study the local structural and dynamic properties of hydrogels. Our work focuses on using coarse-graining molecule dynamic simulations to study physically linked polymer nano-composite hydrogels. Our goal is to study how the aspect ratio and shape of the nanofiller introduced to the hydrogel can lead to different mechanical behavior. Our simulation looks at the effects of polymer species, chain length, and water content and the effect on the mechanical properties of the hydrogel.

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