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Understanding the interfacial chain dynamics of fiber-reinforced polymer composite[1] MONOJOY GOSWAMI, JAN-MICHAEL CARRILLO, AMIT NASKAR, BOBBY SUMPTER, Oak Ridge National Lab — The polymer-fiber interface plays a major role in determining the structural and dynamical properties of fiber reinforced composite materials. We utilized LAMMPS MD package to understand the interfacial properties at the nanoscale. Coarse-grained flexible polymer chains are introduced to compare the various structures and dynamics of the polymer chains. Our preliminary simulation study shows that the rigidity of the polymer chain affects the interfacial morphology and dynamics of the chain on a flat surface. In this work, we identified the 'immobile inter-phase' morphology and relate it to rheological properties. We calculated the viscoelastic properties, e.g., shear modulus and storage modulus, which are compared with experiments. MD simulations are used to show the variation of viscoelastic properties with polymer volume fraction. The nanoscale segmental and chain relaxation are calculated from the MD simulations and compared to the experimental data. These observations will be able to identify the fundamental physics behind the effect of the polymer-fiber interactions and orientation of the fiber to the overall rheological properties of the fiber reinforced polymer matrix.

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