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Mechanisms of Stress-Transfer in Polyethylene-Hexagonal Boron Nitride Composite Fibers toward Platelet Exfoliation

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By coupling experimental and computational approaches this work explores the exfoliation mechanism for hexagonal boron nitride (h-BN) in polyethylene (PE) matrices during processing of composite fibers. A shear-flow gel-spinning apparatus was utilized to fabricate PE/h-BN composite fibers with 11 wt% h-BN loading. The fiber processing method enables direct crystallization of the PE onto h-BN to promote interfacial interactions. Spectral analysis of the major h-BN peaks related to inter-layer interaction and stacking shows significant changes, suggesting exfoliation of the h-BN in the fibers as a function of processing. Wide-angle X-ray diffraction (WAXD) patterns showed the disappearance of the major h-BN (002) peak in the composite fibers after hot-drawing processes. This peak is present due to the stacked h-BN layers within the platelets. The diminishment of this WAXD peak suggests exfoliation of the h-BN due to shearing (i.e., fiber drawing). This phenomenon was further confirmed experimentally by Raman spectroscopy, where there is an intensity decrease of the major (1366.2 cm^{-1}) peak indicating the weakening of the h-BN inter-layer interactions caused by the additional vibration of boron and nitrogen atoms. The deformation of the polymer matrix during fiber formation is considered to play a direct role on the exfoliation processes for the h-BN platelets due to interfacial interactions. A full atomistic steered molecular dynamics (SMD) approach was used to obtain baseline force and work requirements for h-BN layer separation, as well as to simulate the h-BN exfoliation behavior as a result of the PE matrix deformation during processing. Computational results indicated that a large interactive area between the polymer and the fillers is required to induce enough stress-transfer in order to exceed the h-BN exfoliation force/energy threshold. By exceeding this threshold, exfoliation of the platelets to monolayer h-BN is validated. This work provides new insight toward understanding the relationship between interfacial area and interaction strength for the polymer matrix and filler, as well as their interplay for affecting ultimate structural changes in the composite material as a function of processing.

Keywords: composite; boron-nitride; polyethylene; interfacial; stress-transfer