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Multiscale Modeling of Polymer Systems comprising Nanotube-like Inclusions by Considering Interfacial Debonding under Plastic Deformations

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Abstract

The mechanical properties of polymer nanocomposites are severely governed by the situation of the interphase region. Yet, a few was known about interfacial adhesion/debonding in the vicinity of polymer-nanofiller interface. The inadequateness of our information on such region takes its origin in the assumptions involved in theoretical models describing interfacial debonding. Particularly, zero interphase region, constant modulus, and elastic deformation assumptions make predictions unreliable when experimental mechanical characteristics are meticulously analyzed. In this work, multiscale modeling approach was implemented in prediction of plastic deformation of stress-strain of a typical thermoplastic polymer filled with nanotube-like inclusions. In contrast to the above-mentioned assumptions that take a naïve look at the interphase region, a finite element code was developed here to assist in interfacial debonding evaluation by considering a variable modulus for non-zero layer between polymer and nanotube-like filler phases under plastic deformation. Experimental plots of stress-strain on typical nanocomposites prepared varying the amount and surface chemistry of the nanofiller were used for approval of the model outcome. The use of finite element method in such a complex systems improved significantly the predictability of theories by making possible monitoring the effect of thickness of interphase on debonding behavior.

Keywords: Multiscale modeling, Interfacial debonding, Nanocomposites, Interphase, Mechanical properties