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Prediction of Mechanical and Fracture Properties of Rubber Composites by Microstructural Modeling of Polymer-Filler Interfacial Effects

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Abstract

In nano-dispersed filler containing rubbers, mechanical properties of composites are dictated by the characteristics of surface layers in the interphase as well as the manner in which rubber interacts with filler at the interface. In the present contribution, surface-related and volume-related effects of filler on the reinforcement were distinctively considered in the finite element prediction of mechanical and fracture properties. A unit-cell containing three phases of a single particle, an interphase perfectly bonded to the particle, and the rubber matrix was built. The particle represents the total volume fraction of the filler, and the interphase symbolizes all surface related phenomena of the filler including filler surface area, filler structure, filler-filler interaction and filler-polymer interaction. The J- integral was evaluated to approximate the energy release rate of a crack interacting with the interphase layers having hyper-elastic or hyper-viscoelastic properties. It was shown that the interphase layers are capable of lowering the crack driving force by reducing the level of local strain fields or inducing viscoelastic dissipations. Substitution of the “perfect bonding” interface with a “freely moving” one greatly affected the energy release rate, confirming the experimental evidence that a perfect bonding is not desirable for crack growth resistance.

Keywords: Finite Element Method (FEM), Microstructural Model, Energy Release Rate, Interfacial Effects, J-integral, Rubber Composites

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