Abstract

The demand for constitutive models is expanding to improve filled-rubber compounds towards sustainability. Fillers provide strength to the compounds, and the introduction of fillers causes a restructuring of the internal cross-linked rubber network. The restructuring results in a fusion of three networks, e.g., polymer-polymer, polymer-filler, and filler-filler interactions. We used two commonly used fillers in the rubber industry: carbon black and silica, for studying the formation of the network in CB-filled compound using the constitutive model (Mooney-Rivlin) and atomic force microscopy. Using the model, the study establishes the quantification of cross-link density (physical and chemical) and changes in physical entanglement in restructured networks. Also, the study proposes a parabolic equation for physical entanglement with increasing filler loading. Moreover, the onset of non-linearity in the filler-polymer network for larger deformation is crucial for exploring the viscous response. The optimization uses three hyperelastic models for large deformation, e.g., Ogden, Yeoh, and Arruda Boyce. The Prony series was adopted and quantified to have a grasp on the viscoelastic behavior, and the combination of the Ogden and Prony series provides an excellent match to the experimental features. The study verifies by applying the constitutive model and material parameters to probe into the geometrical defects on the specimen, achieving good agreement between simulation and experimental results. Moreover, the study is expanded to construct a finite-deformation yield-surface-free elastoplastic constitutive model using the Ogden model to decouple and quantify the effect of different deformation and damage mechanisms. For the study, we have used compounds filled with three different ingredients as fillers (carbon-black, silica-silane-DPG, and silica-silane-hexylamine). The effect of different deformation and damage mechanisms are decoupled and quantified (providing significance to the networks) using the advanced constitutive model, which yielded excellent agreement between experimental data. The study also proposes an eco-friendly and sustainable rubber nanocomposite as an alternative to traditional silane systems. The proposed nanocomposite exhibits excellent physicomechanical properties with homogeneously dispersed fillers in the matrix with an average particle size of 9 nm. The eco-friendly nanocomposite resulted in good cure characteristics, low flocculation rate, and low Mullin's softening. Overall, the study provides an understanding and quantification of the network mechanism using constitutive law and finding a sustainable alternative for the toxicological effects of silanes in polymer product formulation, making it a promising candidate for large-scale industrial applications of elastomer nanocomposites.

Keywords: Constitutive model, Filler network, Mechanical properties, Entanglement, Cross-link density, Sustainable