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Predicting the mechanical behavior of butadiene-rubber nanocomposites

Sepideh Zoghi, Ghasem Naderi, and Shirin Shokoohi

The physical and mechanical characteristics of butadiene-rubber-based nanocomposites can be reliably predicted using theoretical hyper-elastic models and finite-element simulations.

Butadiene rubber (BR), a kind of elastomer, is used in the production of a large number of products (e.g., shoe soles, conveyor belts, golf balls, and sealing dams) due to its high abrasion resistance, high resilience, and very low water absorption.[1] Several investigations have been conducted on elastomers with different additives, and significant improvements to the properties have been observed in the resulting composites.

To produce a new rubber product, however, many steps (that are not cost- or time-effective) must be repeated to achieve the best results. The use of models to simulate the final characteristics of rubber parts is therefore strongly encouraged.[2] Moreover, according to the literature, finite-element simulations based on theoretical models can provide details of the main qualitative features of materials, whereas experimental investigation of the elastomers requires costly tests.[3]

A variety of outstanding research has been carried out on the notable effect of nanofiller content on the degree of agreement between experimental data and theoretical values for elastomer nanocomposites. The composites thus studied include polyvinyl chloride/acrylonitrile butadiene rubber/organoclay (PVC/NBR/organoclay), natural rubber/ethylene propylene diene monomer (M-class) rubber (NR/EPDM), and BR/EPDM.[4–7] In the case of BR, it has been shown that micro- and nano-scaled additives can result in the improvement of a number of different characteristics in the resultant composites. A number of resins—including polyacrylate, polyurethane, epoxy, and polyester—have been used as modifiers for different polymers, but have not been fully explored for BR.[8,9]

To investigate the effect of a resin additive on the properties of BR nanocomposites, and to test the accuracy of the associated models, we introduced nanoclay and an epoxy-polyester hybrid (EPH) resin to BR. We then investigated the performance of the resultant nanocomposites against uniaxial load and compared results obtained from models to

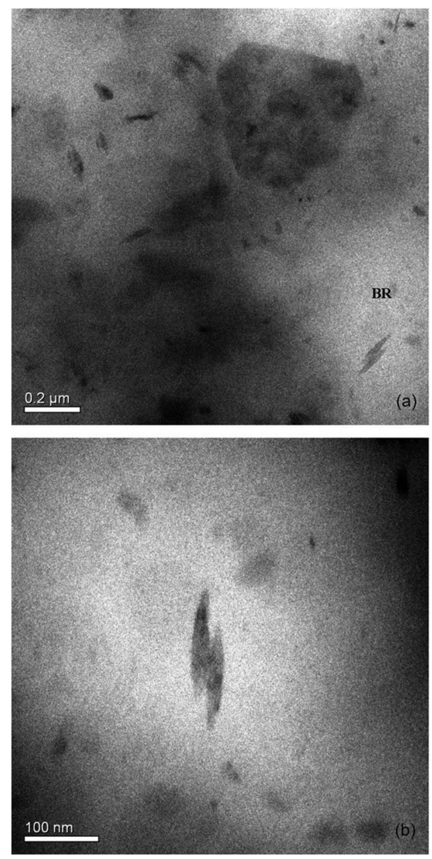

Figure 1. *Transmission electron microscopy images of the nanocomposite, BE20N5, comprising butadiene rubber (BR) with 20 parts per hundred rubber (phr) epoxy-polyester hybrid (EPH) and 5phr Cloisite 15A. (a) Intercalated/exfoliated nanoclay layers are visible in both BR and EPH phases. Black sections indicate either agglomerated nanoclay bundles or rigid calcium carbonate/titanium dioxide particles within the powder coating wastes (EPH). (b) A typical bundle of clay galleries after the nanocomposite has been subject to shear forces.*[10]

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our experimental results.[10] In addition to these routine approaches, we used transmission electron microscopy (TEM) to observe the dispersion state of nanoclay within the elastomer matrix. We then confirmed the results by calculating a number of parameters, including 'B' in Pukanszky's model, the aspect ratio in the Guth model, and the Young's modulus of the compounds using Halpin-Tsai theory. We analyzed all of the obtained data using ABAQUS software.[10]

We fabricated our BR/EPH composites with 20wt% EPH and added Cloisite 15A to the compound at contents of 3, 5, and 7 parts per hundred rubber (phr). We then investigated the characteristics of the different samples via non-isothermal differential scanning calorimetry analysis (DSC), thermogravimetric analysis (TGA), and TEM. Due to the interactions between epoxy groups in the EPH resin and the amine groups in the organoclay layers, we found that clay platelets were well intercalated and partially exfoliated within the BR/EPH matrix (shown in Figure 1). We confirmed this finding via calculations based on the Pukanszky model. Moreover, we evaluated the overall dispersibility of Cloisite 15A in the BR/EPH matrix according to the Halpin-Tsai and Guth models. According to our results, the BE20N5 (i.e., containing BR/20phr EPH/5phr Cloisite 15A) sample showed the highest dispersion, as we expected based on our calculations (see Figure 2).[10]

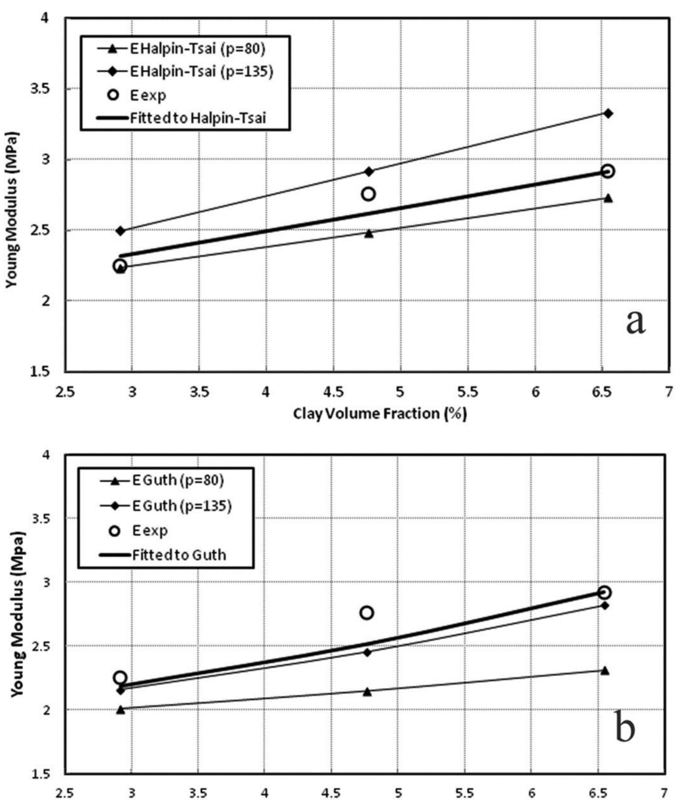

Figure 2. Comparing experimental Young's modulus values for BE20N5 with the values estimated through (a) the Halpin-Tsai relation and (b) the Guth model.[10] p: Aspect ratio.

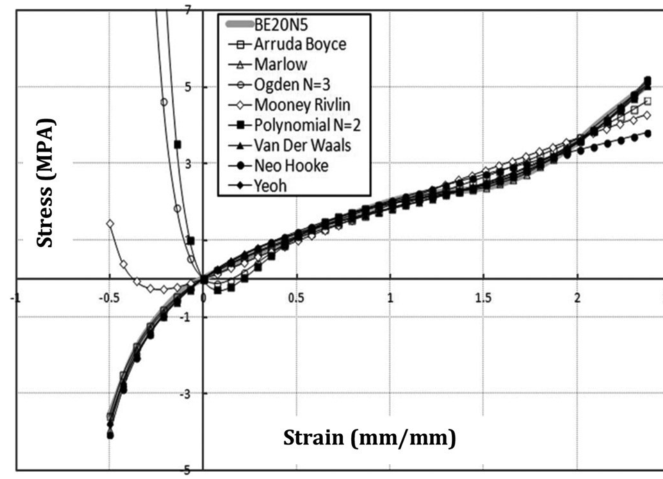

Figure 3. *Experimental stress-strain data fitted to hyper-elastic models for the BE20N5 nanocomposite.[10]*

In the final part of our study, we considered a wide range of hyper-elastic models—including Arruda-Boyce, Marlow, third-order Ogden, Mooney-Rivlin, second-order polynomial, van der Waals, Neo-Hooke, and Yeoh models—to fit the values that we obtained through uniaxial tensile tests. We carried out these experiments on molded dumb-bell samples in both tension and compression modes. By comparing the experimental and theoretical results we found that, of these models, Marlow, van der Waals, and Yeoh achieved the closest results to the experimental values in the range of strains studied (see Figure 3).[10]

In summary, we fabricated BR nanocomposites reinforced with an EPH resin and Cloisite 15A to determine the effect of this resin on the properties of BR nanocomposites. Additionally, we compared experimental and theoretical data of the nanocomposite characteristics to determine the accuracy of numerical models. The most significant outcome was the prediction—by the Halpin-Tsai, Guth, and Pukanszky models—of the level of integration achieved by the nanoclay (i.e., the clay layers were intercalated and partially exfoliated), as well as its dispersion. Additionally, we found that hyper-elastic models achieved good consistency with the experimental stress-strain data that we obtained for the nanocomposites. The best results were obtained with Marlow, van der Waals, and Yeoh hyper-elastic models, which were able to correctly anticipate the nanocomposites' reaction to load. In the next stage of our work, we will investigate the hyper-elastic behavior of nanocomposites in all deformation modes by carrying out equibiaxial

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and volumetric experimental tests to achieve more precise results.[10]

Author Information

Sepideh Zoghi
Department of Polymer Engineering
Islamic Azad University, South-Tehran Branch
Tehran, Iran

Sepideh Zoghi received her BSc in food science and technology engineering. She subsequently changed her field of study to polymer engineering, in which she received her MSc, and has registered two invention patents based on her work. Her research is focused on polymer nanocomposites.

Ghasem Naderi
Department of Rubber
Iran Polymer and Petrochemical Institute
Tehran, Iran

Shirin Shokoohi
Chemical, Polymeric and Petrochemical Technology
Development Research Division
Research Institute of Petroleum Industry
Tehran, Iran

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