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A simulation study on the effect of spring-shaped fillers on the viscoelasticity of rubber nanocomposite

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ABSTRACT

Background/Purpose: Rubber nanocomposites have been widely used in many engineering fields due to their unique properties such as high elasticity and viscoelasticity. Much attention has been paid to the viscoelasticity of rubbers because it directly relates to the performance of the rubber products.
Methods: Based on the micromechanical theory, the finite element method is used to analyze the effect of elastic modulus and volume content of spring-shape nanofillers on the dynamic viscosity of composites.
Results: The simulation results show that there is an optimal elastic modulus of spring-shape nanofillers to make the loss factor a minimum. There is a threshold value of spring-shape nanofiller content for the dissipation energy density of composite.
Conclusion: The elastic modulus of spring-shape nanofillers has a large effect on the loss factor of composites. The selection of elastic modulus of spring-shape nanofillers is critical for applications of composites. The efficiency of spring-shape nanofillers in reducing the dynamic viscosity of composites is so high that volume content of spring-shape nanofillers as low as 0.1% can greatly reduce the loss factor of composites with bonding interface.

1. Introduction

Rubber nanocomposites have been widely used in many engineering fields due to their unique properties such as high elasticity and viscoelasticity. It is important to control the viscoelasticity of rubber nanocomposites by mixing the rubber matrix with the appropriate nanofillers because under dynamic working conditions, the viscoelasticity dominates to a large extent the mechanical behavior and even the failure of the rubber components. Theoretically, the mechanical properties of nanofiller such as modules and flexibility, geometrical factors of nanofiller such as the shape, the size and the aspect ratio, the content of nanofiller, and the interface between the nanofiller and the matrix all have important effect on the viscoelasticity of rubber nanocomposite [1]. So far, extensive experimental studies have been performed on the viscoelasticity of rubber nanocomposites [2–10], including layered structured nanocomposites such as clay and grapheme nanocomposites, fibril structured nanocomposites such as carbon nanotube rubber nanocomposites, but never specifically on the effect of the spring-shape nanofillers on the viscoelasticity.

In our previous work based on molecular simulation we found that spring-shape nanofillers have more advantages than fillers of other shapes in reducing dissipation energy of rubber nanocomposites [11]. Despite all this, the effect of the content, the interface between nanofiller and matrix, and the mechanical properties of the spring-shape nanofillers on the viscoelasticity of rubber nanocomposites hasn't been analyzed in detail. However it is very important to guide the production of spring-shape nanofillers and their nanocomposites. In fact, it is difficult to perform such a study because it is difficult, if not impossible, to fix many of the experimental conditions, what's more, there aren't such appropriate spring-shape nanofillers for us to use in experiment. However, numerical simulation can get around such difficulties. Moreover numerical simulation has the advantage over experiment of fundamental understanding the deformation mechanisms and predicting the overall material behavior of nanocomposites.

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Numerical methods at both the molecular level and micro/macro scale have been developed to study the properties of composites. MD (molecular dynamics) is a method at the molecular level. Apart from microscopic properties such as molecular interactions, interlayer spacing, binding energy, macroscopic properties such as elastic properties can be computed by modeling the discrete atoms/molecules and its interactions [12–20]. At present MD can study only structures with a small number of particles and polymer chains because of limitations in computing capacity. At the micro/macro scale the mechanical behavior of nanocomposites is studied by creating representative volume element (RVE). One method to compute the RVE is to obtain closed-form analytical solutions by simplified models such as the Halpin–Tsai model and the Mori–Tanaka model, which are rough and originally developed to predict the material properties of short-fiber composites [21,22]. A more powerful method to compute the RVE is finite element method (FEM) without the need for a simplified model. FEM has been widely used in studying the properties of nanocomposites including stress transfer, fracture mechanics, crack propagation, residual thermal stress, thermal conductivity, elastic modulus, and viscoelasticity [23–35]. In addition, FEM is also used in analyzing the effect of the interface between the nanofillers and the matrix on the properties of nanocomposites [36].

FEM has been demonstrated as a powerful and effective tool in discussing the viscoelasticity of rubber nanocomposites. Qiao [36] developed a 2-D finite element model to study the impact of interface zones on the overall properties of the composite. The simulation results showed that the loss modules of the composite is either broadened or shifted corresponding to the absence or presence of a geometrically percolating interface network. From micromechanics modeling of the linear viscoelasticity of carbon-black filled styrene butadiene rubbers (SBR), Diani [37] et al. concluded that a 4-phase micromechanical model, which accounts for a bounded rubber layer coating the fillers, provides satisfactory estimates of the linear viscoelasticity of filled rubbers from the rubbery state to the glassy state. N. Gil-Negrete [38] discussed the amplitude-dependent dynamic stiffness of filled rubber isolators using FEM and predicted the dynamic stiffness of a real bushing in working conditions with very satisfactory results. Ghoreishy [39] predicted the hyper-viscoelastic behavior of rubber compounds using Bergström–Boyce hysteresis model by FEM software ABAQUS.

In this paper, FEM approach is applied to analyze the effect of the properties of spring-shape nanofillers on the viscoelasticity of rubber nanocomposites. Two types of interface between the nanofillers and the matrix – the "bonding interface" and the "frictional interface" – are assumed to discuss the effect of the interface on the viscoelasticity of rubber nanocomposites. Interesting and important results are presented by our research.

2. Finite element model

FEM software ABAQUS is used in this paper and the VISCO procedure is adopted to perform a quasi-static analysis.

2.1. Representative volume element(RVE)

The effect of the distribution and orientation of spring-shape nanofillers on the viscoelasticity of rubber nanocomposites will be analyzed in our future work. In the current work, we focus on the effect of volume content and elastic modulus of spring-shape nanofillers on the viscoelasticity of rubber nanocomposites. A RVE composed of a rubber matrix with only one filler at the center of it is created for the simulation (Fig. 1).

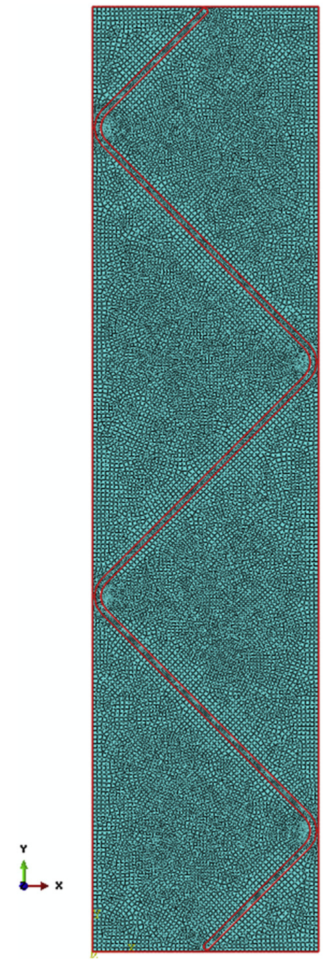

Fig. 1. RVE of composites with spring-shape filler.

The spring-shape nanofiller is firstly created, and then the overall dimensions of RVE is computed from the area and volume content of the spring-shape nanofiller. The length and width of RVE is 8.7 um and 2.1 um, respectively. The rubber matrix and the nanofiller are meshed with CPS4R in FEM software ABAQUS. After mesh sensitivity analysis, the element size is determined and the number of node and element is 19016 and 18585, respectively.

2.2. The interface region

Experimental results of some previous investigations suggest that there exists an interface region between fillers and the matrix in rubber composites and the interface plays a crucial role in determining the overall mechanical response of the composites [40–42]. But other investigators reported that no discernible interface could be detected when the matrix was able to diffuse into the filler sizing [24]. To account for the effect of the interface, some researchers introduced a third phase with mechanical properties on the order of magnitude of the matrix to optimize composite performance. In fact, it is impossible to model a composite with an interface whose size and mechanical properties can be accurately specified because at present there are no such experimental data.

To analyze the influence of interface on the viscoelasticity of rubber nanocomposite, two types of interface are taken into account. One is called the "bonding interface," in which the nanofiller and the matrix are bonded tightly and no relative displacement