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An efficient multiscale model of damping properties for filled elastomers with complex microstructures

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ABSTRACT

This work proposes an efficient framework for prediction of filled elastomer damping properties based on imaged microstructures. The efficiency of this method stems from a hierarchical multiscale modeling scheme, in which the constitutive response of subcell regions, smaller than a representative volume element (RVE), are determined using micromechanics; the resulting constitutive parameters then act as inputs to finite element simulations of the RVE, from which damping properties are extracted. It is shown that the micromechanics models of Halpin–Tsai and Mori–Tanaka are insufficient for modeling subcells with many filler clusters, and thus these models are augmented by an additional interaction term, based on stress concentration factors. The multiscale framework is compared to direct numerical simulations in two dimensions and extended to predictions for three dimensional systems, which include the response of matrix–filler interphase properties. The proposed multiscale framework shows a significant improvement in computational speed over direct numerical simulations using the finite element method, and thus allows for detailed parametric studies of microstructural properties to aid in the design of filled elastomeric systems.

1. Introduction

Filled elastomeric polymers have found many applications in a variety of fields spanning the automotive [1,2], civil engineering [3] and even food packing industries [4]. In many applications elastomers provide desirable damping or energy dissipation properties but can lack the strength needed to carry structural loads or resist wear. The addition of fillers adds strength to elastomer systems but can reduce damping properties as shown in [2,5]. Wang [2] gives a specific example where it is shown that the *wet grip* of tires is improved by increasing damping property values at room temperature. The addition of strengthening fillers, however, acts against these wet grip improvements by decreasing room temperature damping values. Thus, as damping decreases, performance decreases as well, which creates a design dilemma, trading performance with strength.

A powerful tool to aid in this design decision would be one that could accurately predict the damping properties of an existing material while simultaneously allowing for parameterized studies of new virtual materials. This model would allow a designer to determine if a material meets both the strength and damping goals before the material is produced and to gage what modifications are needed before production. Such a model is the goal of this work. This model will be based on the premise that knowledge of the three dimensional (3D) morphology of a filled system (for example from sectioned scanning electron microscopy) is key to accurate computational models. The major challenge to be addressed is that direct numerical simulations (DNS) using computational tools such as molecular dynamics or the finite element method (FEM) can be prohibitively slow if not intractable when modeling a 3D microstructure on the scale of a representative volume element (RVE). Thus, a multiscale approach is proposed here using micromechanics to homogenize the morphology of sub-RVE scale subcells. A coarse finite element model is then used to simulate the combined response of these subcells, resulting in a reduced computation size as compared to DNS of the entire microstructure. While a homogenized model cannot account for all of the information included in direct simulations, the advantage in computational speed will be substantial, making it a powerful tool for materials design of filled elastomer systems.

2. Background

Two micromechanics models are popular for representing the effective stiffness of a filled composite and will form the basis for

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the proposed work. These are the Mori–Tanaka [6] and Halpin–Tsai [7] models. Both predict the stiffness tensor, $\bar{\boldsymbol{L}}$, of a matrix/filler composite material. The Mori–Tanaka model and the self-consistent model (on which Halpin–Tsai model is based[2]) both account for the interaction of filler inclusions by allowing a single inclusion's stress to be altered by the presence of other inclusions. The author will define this as a *weak* interaction, in that, the explicit increase in stress due to a pair or group of inclusions in not modeled. The extensions proposed in Section 6 will attempt to capture a *strong* interaction between inclusions by modeling stress risers based on the influence of adjacent fillers.

The application of these models to viscoelasticity is achieved by using the elastic–viscoelastic correspondence principle. The details of which are given in the work of Brinson and Lin [10]. In short, an elastic modulus, such as Young's modulus, can be viewed as complex and a function of frequency, ω. The complex Young's modulus is given as

$$E^*(\omega) = E'(\omega) + iE''(\omega), \tag{1}$$

where E' and E'' are the storage and loss modulus respectively and $i = \sqrt{-1}$. Where E' represents the elastic response in-phase with the strain loading and E'' represents the response 90° out-of-phase with the loading due to time dependent viscoelastic effects. The ratio of the loss to storage modulus will be referred to here as $\tan\delta$ (where δ is the phase lag of the material) and is proportional to the energy dissipation or damping of the system [2]

$$\tan\delta = \frac{E''}{E'}. \tag{2}$$

This value can be directly related to properties of importance to many engineering applications (such as tire *wet grip*) and thus this work will focus on determining $\tan\delta$ for a filled elastomer.

Throughout this document $(\cdot)^*$ will represent complex values and $(\cdot)_m$ and $(\cdot)_f$ will represent matrix and filler properties respectively. Using this notation, consider a composite with a complex Young's modulus in the loading direction, $\bar{E}^*_{yy}$. If this composite consists of a matrix material with a complex Young's modulus of E^*_m and a filler material with an aspect ratio, $\mathcal{R}$, a volume fraction, c_f, and a Young's modulus, E_f, then the Halpin–Tsai model can be expressed in a complex form as,

$$\frac{\bar{E}^*_{yy}}{E^*_m} = \frac{1 + 2\mathcal{R} c_f \eta^*}{1 - c_f \eta^*}, \tag{3}$$

$$\eta^* = \frac{(E_f/E^*_m) - 1}{(E_f/E^*_m) + 2\mathcal{R}}, \tag{4}$$

from which $\tan\delta$ can be determined. Likewise, if only two phases are considered, then $\bar{E}^*$ of the composite can be determined from the complex Mori–Tanaka stiffness tensor [10], given as

$$\bar{\boldsymbol{L}}^* = \boldsymbol{L}^*_m \left\{ \boldsymbol{I} - c_f [\boldsymbol{S}^*_f c_m + c_f \boldsymbol{I} + (\boldsymbol{L}^*_f - \boldsymbol{L}^*_m)^{-1} \boldsymbol{L}^*_m]^{-1} \right\}^{-1}, \tag{5}$$

where $\boldsymbol{I}$ is a fourth-order identity tensor, $\boldsymbol{L}^*_m$ is the complex matrix stiffness, $\boldsymbol{L}_f$ the filler stiffness and $\boldsymbol{S}^*_f$ the complex Eshelby tensor as defined in [11].

Brinson and Lin [10] have studied $\bar{\boldsymbol{L}}^*$ using Mori–Tanaka and have shown good agreement with finite element simulations of a periodic computational unit cells with a single inclusion. Brinson's work, however, was not intended to model larger cells with many interacting inclusions.

A number of works have included a region of modified properties between the filler and matrix, known as the interphase region (or IP region), into micromechanical models. Gusev and Lurie [12] used a four phase model of spherical filler particles to predict $\tan\delta$ for ordered and random microstructures, but used viscoelastic models only in the interphase regions at a single frequency (1 radian/s). Liu and Brinson [13] have also carried out detailed finite element analysis to inform models of IP effects by numerically computing a strain concentration tensor for various inclusion geometries, such as nanotubes and nanoplates. This analysis requires a specific finite element analysis for all filler geometries and thus may become computationally expensive for arbitrarily complex microstructures. A similar approach was employed by Song and Zheng [14]. This model introduced a scalar strain amplification factor pre-multiplying the complex matrix modulus of a filled system. The amplification factor was expressed in an semi-empirical form accounting for a number of microstructural parameters but also used empirical factors to match experimental data.

The model presented here will be capable of including IP effects but will first focus on computing mechanics of a sub-RVE cell containing many interacting filler particles. Then the IP properties will be added for a 3D demonstration. The model will rely on extracting data from a microstructural image. This image is broken down into binary voxels which represent either matrix or filler and are illustrated in Fig. 2. A recent work by Mishnaevsky [15] used 2D voxel based images such as in Fig. 2 combined with micromechanics, to predict the stiffness of complex microstructures. However, only isostress (Reuss) and isostrain (Voigt) models were used.

The work of Deng et al. [5] used this voxel representation to determine the interphase properties of a filled polymer system by comparing finite element analysis of a 2D, 300 × 300 voxel, reconstructed image to experimental results. This work was extended to 3D in the study by Breneman et al. [16]. For both of these works, interphase thickness was limited to integer multiples of the mesh size. The proposed model will speed up the voxel based calculations of Deng et al. and Breneman et al. and also allow for more flexibility in interphase thickness modeling.

The work shown here uses both Halpin–Tsai and Mori–Tanaka models extended to capture *strong* interactions between particles (and IP in 3D) and will also capture arbitrarily complex structures through the voxel representations.

3. Material properties

In this work, elastomeric polymers with stiff fillers will be addressed. A viscoelastic polymer with frequency dependent properties will be used for the matrix. Values of matrix properties E'_m and E''_m used in this work are based on the *soft material* studied by Brinson and Lin [10].

The polymer matrix is considered nearly incompressible with a Poisson's ratio of $\nu_m = 0.48$. The density of both phases is considered small ($\rho_m = \rho_f = 1 \times 10^{-9}$ kg/m^3) to avoid any inertial effects in finite element analysis which are absent in micromechanical modeling and negligible in dynamic mechanical analysis (DMA) testing used to characterize viscoelastic properties. The filler is considered to be stiff as compared to the matrix and of a brittle nature. Thus, the filler is considered to have $E_f = 1 \times 10^9$ Pa. A filler Poisson's ratio of $\nu_f = 0.4$ is used in this work based on the value used in [5]. The values of E_f and ν_f are considered frequency independent.

4. Finite element model

Finite element modeling will be used for two purposes in this work: first, as a verification tool for both subcell and cell models, and second, as an RVE level simulation tool of the cell (see Fig. 1). The properties of an RVE are defined in the micromechanics text [11]. For this work, an RVE cell (Fig. 1a) is broken down into

[2] The Halpin–Tsai equations simplify the self-consistent approaches of Hermans [24] and Hill [9] as summarized in [8].