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Cross-linked fiberglass packs: Microstructure reconstruction and finite element analysis of the micromechanical behavior

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ABSTRACT

An automated computational framework is introduced for simulating the micromechanical behavior of a fiberglass insulation pack with cross-linked fibers under compression. A new microstructure reconstruction algorithm is proposed that utilizes the NURBS representation of fiber geometries, together with statistical descriptors extracted from imaging data, to synthesize realistic microstructures by virtually packing fibers with the desired volume fraction, diameter distribution, and spatial orientations. Given the highly nonlinear micromechanical behavior of this nonwoven entangled material due to large deformations and contact-friction between fibers, a reduced-order finite element model is utilized to simulate its deformation response. In this approach, beam elements are used for modeling fibers, while a truss-shaped set of bushing-like connector elements are utilized to model binder particles that provide cross-linking between fibers. The accuracy of this model is verified through comparison with high-fidelity 3D simulations. Appropriate boundary conditions for simulating the mechanical behavior of microstructural models are then studied and the size of representative volume element (RVE) of the fiberglass pack is identified. The model is then employed to analyze the impacts of cross-linking and presence of fiber bundles in the microstructure on the deformation response of this materials system subject to a compressive load.

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1. Introduction

Fiberglass packs used for thermal insulation are nonwoven entangled networks of glass fibers that are cross-linked via a polymer binder phase. The low volume fraction of glass fibers (often < 2%) in such materials entraps a high volume of air across their thicknesses, which is crucial to their thermal insulation performance [1]. The binder phase, which is sprayed on glass fibers during the manufacturing process in the form of micro-droplets, provides cross-linking between fibers to improve structural stability and avoid the separation of fibers. In this article, rather than studying thermal properties, we aim to virtually reconstruct realistic 3D microstructural models of a fiberglass pack to simulate its micromechanical behavior subject to a compressive load. This type of loading is applied to fiberglass packs to reduce their thicknesses to a small fraction of the original value (here, 15%), which is essential for the economic storage and shipping of this material.

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The mechanical behavior of fiberglass insulation packs is highly dependent on their internal architecture [2,3], *i.e.*, the volume fraction and spatial orientation of fibers, as well as the number and strength of cross-links. Upon applying a compressive load, contact and friction forces are developed between fibers that also affect the deformation response of this nonwoven entangled material. While several studies have been conducted on the mechanical behavior of fiberglass packs, majority of prior research efforts rely on experimental techniques [4]. For example, impacts of contacts between fibers and the binder phase on the nonlinear elastic response of light fibrous materials is experimentally investigated in [5]. Evolution of the microstructure of a bundle of fibers during a compression test and the corresponding mechanical behavior at the macroscale are investigated in [6]. Mechanical behavior of various fibrous materials without cross-linking under compression tests are studied in [7], where the deformation response is linked to the number of contact points between fibers. Various nonwoven entangled materials with and without cross-linking are studied in [2,8] via quasi-static compression tests, showing that crosslinking could significantly increase their stiffness. These studies also show that the macroscopic stress response of such materials

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with a low fiber volume fraction follows a power law with respect to their decreasing density under compression.

Among existing analytical models developed for analyzing the mechanical behavior of fibrous materials, we can mention [9-12]. These models provide a closed-form solution for homogenized mechanical properties of nonwoven entangled materials as a function of different microstructural parameters [13]. A number of numerical studies relying on the finite element method (FEM) has also been carried out to predict the deformation response of such materials. Contact-friction interactions between fibers [14], as well as the impact of the number of contact points on the macroscopic mechanical behavior are analyzed in [15]. A numerical model for non-bonded fiber networks is developed in [16], which considers fibers as straight line segments with a random spatial arrangement. A beam-to-beam, frictionless contact model between fibers is introduced in [17] for simulating the mechanical response of fibrous materials. A continuum-based 3D periodic model of entangled nonwoven materials is presented in [18], in which fiber cross-linkers are modeled as beam elements. The failure response of notched and unnotched models of a multilayered cross-linked fiberglass pack subject to a tensile load is analyzed in [19] using FEM.

One of the limitations of most of the numerical studies outlined above is the use of simplified geometrical models (some in 2D) to represent the intricate microstructure of entangled nonwoven materials. Note that analyzing the impact of different microstructural features on the mechanical behavior of a nonwoven entangled material requires reconstructing multiple realistic repeating unit cells (RUCs) of that materials system. Creating such intricate microstructural models is one of the key challenges of the modeling process due to small diameters of fibers that are in contact at multiple points. To address this issue, one could directly convert digital data such as scanning electron microscopy (SEM) or micro-computed tomography (micro-CT) images of the material into a virtual microstructure [20,21]. For example, the characterization and direct reconstruction of 3D microstructures of a fiberreinforced polymer from micro-CT data are presented in [22]. One of the main difficulties during this process is to properly identify material interfaces within the microstructure, which is highly magnified when there is a low contrast between different phases or due to the close proximity of interfaces [23]. Both these challenges are encountered during the direct image-based modeling of fiberglass packs, where identifying interfaces between fibers that are in contact and might even be cross-linked using a polymer binder would be practically impossible in 3D.

Besides the time-consuming and expensive process of preparing micro-CT images, even if the aforementioned challenges associated with the image processing phase are resolved, each set of digital data only yields a single microstructural model of an existing fiberglass pack. Clearly, this would not be sufficient for the virtual design of such materials, which requires reconstructing and simulating the micromechanical behavior of multiple models with distinct microstructural features. An alternative approach to overcome these challenges is to implement an appropriate virtual microstructure reconstruction algorithm [24]. Several descriptorbased [25-27] and correlation function-based [28-31] algorithms have introduced for reconstructing 2D/3D heterogenous microstructures based on geometrical features and the statistical data extracted from imaging data. The former class of algorithms attempt to replicate microstructural descriptors such the shapes of inclusions (fibers or particles), their volume fraction, and the spatial arrangement (*e.g.*, two-point correlation function). In such methods, it is necessary to implement an optimization phase relying, for example, on the Genetic Algorithm (GA) [32,33] or Simulated Annealing (SA) [34,35] to simulate the desired spatial arrangement of inclusions.

In correlation function-based techniques, which have been employed for modeling a wide array of materials [36,37], different algorithms can be implemented for reconstructing the microstructure. Among these algorithms, we can mention the nearest neighbor algorithm (NNA) [38,39], random sequential adsorption (RSA) [40,41], Voronoi tessellation (VT) [42-44], and random fieldbased method [45,31,46]. While some of these algorithms (e.g., RSA and NNA) are limited to microstructures with specific inclusion shapes (spheres/ellipsoid), there are algorithms that are more general and capable of reconstructing heterogenous microstructures with arbitrary-shaped embedded particles. However, in order to accurately replicate the target spatial arrangement of inclusions, one must combine these techniques with algorithms such as the Monte-Carlo method [47], pixel switching [48,49], and massspring mutation [28,50], which could impose a significant computational cost. Despite such advances in the development of descriptor-based and correlation function-based techniques, to the best of our knowledge, no algorithm is available for reconstructing realistic microstructural models of nonwoven entangled materials with fiber cross-linking.

Main objectives of this manuscript are threefold: (i) Introducing a new microstructure reconstruction algorithm to automatically synthesize 3D microstructural models of nonwoven entangled fibrous materials with cross-linking; (ii) developing a reducedorder FE model to simulate the mechanical response of such materials; and (iii) analyzing effects of different microstructural features on the mechanical behavior of a fiberglass pack subject to a compressive load. In Section 2, we present a NURBS-based algorithm to reconstruct fibrous microstructures according to a set of statistical microstructural descriptors, including the volume fraction, diameter, length and spatial orientation of fibers. We then introduce a reduced-order FE model relying on beam and bushing-like connector elements for discretizing the fiber and binder phases, respectively (cf. Section 3). Under compression, an explicit dynamic solver is employed to simulate the geometrically nonlinear behavior of fibers, as well and contact and friction forces between them. The proposed modeling framework is implemented to reconstruct the microstructure and analyze the micromechanical behavior of a fiberglass pack subject to a compressive load shrinking its thickness to 15% of the original value. In Section 5, we study the impact of boundary conditions on the fidelity of FE simulations and determine appropriate RVE size for the fiberglass pack. A comprehensive study on effects of cross-linking and presence of fiber bundles on the behavior of this material is presented in Section 6.

2. Reconstruction of the fiberglass microstructure

2.1. Imaging, image processing, and statistical descriptors

The fiberglass pack studied in this work has a nonwoven entangled microstructure with a low fiber volume fraction of $V_f \approx 1.2\%$. Two scanning electron microscope (SEM) images of this materials system (with no polymer binder) are depicted in Fig. 1. Given the high length-to-diameter ratio of fibers, with diameters ranging between 10 and 20 µm, the preparation of high-resolution 3D imaging data such as micro-computed tomography (micro-CT) images for this material is extremely challenging. The main reason is the small volume of the material that can be captured in such images, as increasing the resolution decreases the voxel size. Consequently, the visualized volume (often < 10 mm³) would include only a handful of fibers that cannot be a representative volume element (RVE) of the fiberglass pack. Further, even at very high resolutions with voxel sizes approaching sub-microns, it would be nearly impossible to distinguish between individual glass fibers

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