International Journal of Solids and Structures 75–76 (2015) 247–259

Contents lists available at ScienceDirect

International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

A micromechanical model with strong discontinuities for failure in nonwovens at finite deformations

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ARTICLE INFO

Article history:
Received 14 April 2015
Received in revised form 25 July 2015
Available online 31 August 2015

Keywords:
Fracture
Nonwovens
Micromechanics
Network models
Reorientation
Homogenization of soft matter materials
Strong discontinuities
Finite deformations

ABSTRACT

This paper presents a new methodology to model failure phenomena in nonwoven materials with a random network microstructure at finite deformations. The recently developed homogenization technique for nonwoven materials (Raina and Linder, 2014) is combined with an enhanced deformation gradient arising due to strong discontinuities within the bulk. This allows to capture the anisotropic and nonlinear material bulk response with propagating cracks in the failing nonwoven at finite strains. The homogenization technique averages the microscale one-dimensional linear response over an orientation space to yield an accurate macroscale nonlinear behavior. Fiber reorientation and straightening phenomena are incorporated in an orientation space to account for non-affine deformation in a phenomenological manner. The failure in the form of cracks is incorporated locally as displacement jumps, so-called strong discontinuities. The local nature of displacement jumps allows their static condensation from the global governing equations, resulting in a compact and computationally efficient formulation. The computation of an objective enhanced deformation gradient, at a material point where failure is detected, follows the well-known incorporation of constant and linear separation modes directly into the finite element. The orientation space is subjected to this enhanced deformation gradient to yield the corresponding Kirchhoff stress tensor and elasticity modulus. Based on a micromechanically computed fracture strength, the proposed methodology is verified in terms of quantitative comparisons of the simulation results with experimental data from the literature.

1. Introduction

Nonwoven materials made from advanced synthetic fibers are known for their high specific strength making them attractive for demanding industrial applications. These materials possess a random fiber network microstructure constituting of one-dimensional elements, which is similar to materials such as biological tissues with randomly connected filamentous-actin or rubbery polymers with randomly connected polymer chains. Recently, a model was introduced in Raina and Linder (2014) with a predictive capability to simulate the anisotropic elastic behavior of nonwovens at finite deformations. The scope of industrial applications of such materials is vast which ranges from military and space equipments to nanofilters and reinforced concretes. For safer design of equipments, a complete predictive knowledge of such materials up to failure is required. The computational modeling of fracture, being in itself a numerically difficult proposition, becomes drastically complex when applied to soft matter materials such as nonwovens undergoing finite deformations, which presents the main goal of this paper.

The study of the mechanical behavior of nonwovens goes back to Backer and Petterson (1960), where the first continuum material model for nonwovens is proposed based on orthotropic theory of elasticity. Recent experiments (Zhang et al., 1998; Kim et al., 2000; Chocron et al., 2002; Hou, 2010; Ridruejo et al., 2010; Ridruejo et al., 2015; Martínez-Hergueta et al., 2015) provide a more complete understanding of their deformation mechanism under different loading conditions. Cox (1952) presented the first micromechanical modeling approach based on a fiber orientation distribution. In the following decades, various improvements to the material modeling capability were suggested (Bais-Singh and Goswami, 1995; Narter et al., 1999; Kothari and Patel, 2001; Liao and Adanur, 1997; Rawal, 2006). The experiments by Jearanaisilawong (2008) and Chocron et al. (2008) on needle-punched nonwovens made from *Dyneema* fibers and Ridruejo

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http://dx.doi.org/10.1016/j.ijsolstr.2015.08.018
0020-7683/

et al. (2010) on chemically bonded nonwoven felts made from *E-glass* fibers provide extensive data about deformation and failure behavior. The complex deformation mechanism, in the aforementioned experiments, is observed to be governed by fiber unfolding and stretching, inter-fiber friction, volume compaction due to change of volume fraction of fibers, reorientation of fibers, disentanglements due to fiber slipping from junctions, or fiber breakage. The main contribution of our approach presented in Raina and Linder (2014) was to identify the microstructural changes responsible for the non-linear stiffening in terms of the fiber undulations and the reorientation phenomena within a continuum rather than a lattice model setting (Onck et al., 2005; van Dillen et al., 2008). Specifically, a two-dimensional *network model* was developed by forgoing the standard volumetric-isochoric split of the deformation gradient and statistically distributing the constituent fibers in a non-uniform manner in the referential orientation space described by a unit circle. As a result, fibers are asymptotically aligned with the maximum loading direction in the reference geometry with each monotonic loading step. The evolved referential unit vectors are then mapped to the spatial geometry by the macro deformation gradient to compute the macroscopic Kirchhoff stress and the associated spatial elasticity modulus.

To model failure phenomena in nonwoven felts, the computationally efficient *strong discontinuity approach* (Simo et al., 1993; Armero and Garikipati, 1996; Oliver, 1996; Armero, 1999; Oliver et al., 2003; Linder and Armero, 2007; Armero and Linder, 2008) extended to finite deformations is combined with the aforementioned advanced network model based homogenization procedure in this work. A key characteristic of this approach is the enhancement of the deformation within a finite element through local degrees of freedom, which characterize the displacement jumps of a strong discontinuity. This construction allows the static condensation of the local degrees of freedom from the global equilibrium equations, which makes the framework easy to implement and apply for a large variety of fracture problems (Steinmann, 1999; Callari and Armero, 2002; Linder and Armero, 2009; Armero and Linder, 2009; Linder et al., 2011; Linder and Miehe, 2012; Armero and Kim, 2012; Linder and Raina, 2013; Linder and Zhang, 2013; Linder and Zhang, 2014). The resulting enhanced deformation gradient, which takes failure at a material point into consideration, acts on the orientation space to compute corresponding stresses and moduli. Nonetheless, no application of the strong discontinuity approach to model failure in nonwovens at finite deformations has been proposed so far.

The outline of the rest of the paper is as follows. Section 2 presents the summary of micro and macro kinetics at finite strains with homogenized free energy response from the network model. A brief overview of the strong discontinuity approach at finite deformations in the continuum setting is presented. The effect of fiber undulation and reorientation on the bulk response of anisotropic nonwoven materials is briefly discussed. Section 3 introduces the finite element setting of the formulation where the enhanced deformation gradient, accounting for failure in the form of strong discontinuities, is linked to the homogenized bulk response to compute the Kirchhoff stresses and associated moduli, with some of the more technical results summarized in Appendix A. Experiments of nonwoven felts made of dyneema fibers (Jearanaisilawong, 2008; Chocron et al., 2008) and those made from E-glass fibers (Ridruejo et al., 2010) are finally simulated with the proposed framework in Section 4. A micromechanical tensile test is performed to compute the fracture strength of those nonwoven materials. A satisfactory quantitative comparison of the numerical and experimental results confirms the accuracy of the computed solutions and the generality of the developed methodology for modeling failure in nonwoven materials.

2. Continuum setting of failure in nonwovens through an enhanced deformation gradient

This section summarizes the key areas of Raina and Linder (2014) to introduce the concept of network model based homogenization developed for nonwovens with fiber reorientation and undulations. To introduce failure in the form of strong discontinuities in nonwovens, an enhanced deformation gradient following the developments in Armero and Linder (2008) is computed and, for the first time, linked to the homogenization procedure of Raina and Linder (2014) in this work. A step-by-step process towards a new methodology of enhanced deformation gradient driven failure in network model will be presented.

2.1. Micro–macro kinematics at finite strains

A body $\mathcal{B} \subset \mathbb{R}^{n_{\text{dim}}}$ undergoing finite strains with the motion $\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X}, t) : \mathcal{B} \times T \rightarrow \mathcal{S} \subset \mathbb{R}^{n_{\text{dim}}}$ at time $t \in \mathbb{R}_+$ is considered. Here $\boldsymbol{\chi}(\boldsymbol{X}, t) \subset \mathbb{R}^{n_{\text{dim}}}$ is a non-linear deformation map and $\boldsymbol{F} = \nabla_{\boldsymbol{X}} \boldsymbol{\chi}(\boldsymbol{X}, t) \in \text{GL}(\text{n}_{\text{dim}})$ is a deformation gradient with material points in referential and spatial configurations denoted by $\boldsymbol{X} \in \mathcal{B}$ and $\boldsymbol{x} \in \mathcal{S}$, respectively. Let $\boldsymbol{G}(\boldsymbol{X}) \in \mathcal{B}$ and $\boldsymbol{g}(\boldsymbol{x}) \in \mathcal{S}$ denote the covariant metric tensors mapping on the reference configuration and the spatial configuration at $\boldsymbol{X}$ and $\boldsymbol{x}$, respectively. The right Cauchy Green strain tensor $\boldsymbol{C}$ is subsequently given by the pull back of the spatial metric as $\boldsymbol{C} = \boldsymbol{F}^T \boldsymbol{g} \boldsymbol{F}$. For the anisotropic material under consideration, let $\Psi = \Psi(\boldsymbol{C}) = \Psi(\boldsymbol{g}; \boldsymbol{F})$ be the strain energy density per unit reference volume where the objectivity of right Cauchy Green tensor guarantees its material frame-indifference. The theory of network models (Arruda and Boyce, 1993; Wu and van der Giessen, 1993; Miehe et al., 2004; Linder et al., 2011; Tkachuk and Linder, 2012) assumes a microscopic orientation space $\mathcal{O}_0 \subset \mathbb{R}^{n_{\text{dim}}}$ at each material point $\boldsymbol{X} \in \mathcal{B}$. For two-dimensional problems of interest ($n_{\text{dim}} = 2$), an orientation space $\mathcal{O}_0$ in the reference configuration can be represented by a unit-circle. A Lagrangian unit vector $\boldsymbol{r} = \hat{\boldsymbol{r}}(\theta_0) = \cos\theta_0 \boldsymbol{e}_1 + \sin\theta_0 \boldsymbol{e}_2 \in \mathcal{O}_0 \subset \mathbb{R}^2$ is assumed to lie in the referential orientation space $\mathcal{O}_0$. This vector represents a fiber direction and is parameterized by $\theta_0 \in \mathcal{R}_\theta \in [0, \pi)$ when accounting for the symmetry across the $\boldsymbol{e}_1$-axis. A schematic illustration of the orientation space $\mathcal{O}_0 \subset \mathbb{R}^2$ with uniformly distributed unit vectors $\boldsymbol{r} \in \mathcal{O}_0$ is shown in Fig. 1. The continuous deformation gradient $\boldsymbol{F}$ maps the referential orientation space $\mathcal{O}_0 \subset \mathbb{R}^2$ to the spatial orientation space $\mathcal{O}_t \subset \mathbb{R}^2$ with $\boldsymbol{F} : \boldsymbol{r} \rightarrow \boldsymbol{t} = \boldsymbol{F}\boldsymbol{r} \in \mathcal{O}_t$ where $|\boldsymbol{t}|_{\boldsymbol{g}} = \sqrt{\boldsymbol{g}\boldsymbol{t} \cdot \boldsymbol{t}} = \bar{\lambda}$. Here, $\bar{\lambda}$ is the *macro-stretch* defined by the ratio of lengths of tangents to the material line elements in spatial and referential configuration. The *micro-stretch* λ of a single fiber is introduced based on the affine stretch assumption (Treloar and Riding, 1979) by the relation $\lambda = \bar{\lambda}$. Failure in the form of jumps in the deformation does not appear so far such that the deformation gradient $\boldsymbol{F}$ appearing above is continuous. The key aspect of this work is to introduce an enhanced deformation gradient $\boldsymbol{F}_\mu$, later in Section 2.3, based on the *strong discontinuity approach* which accounts for the jumps in the deformation and drives the orientation space $\mathcal{O}_0$.

2.2. Free energy and static equilibrium equation

Following Raina and Linder (2014), the micro–macro kinematics introduced in Section 2.1 are used next to define macro- and microscopic free energies. According to experimental investigations (Jearanaisilawong, 2008; Chocron et al., 2008; Ridruejo et al., 2010), the constituent fibers of nonwovens are linear elastic until failure. This motivates to introduce the microscopic free energy in the form of a linear spring as $\psi(\lambda) = EA\ell(\lambda - 1)^2/2$, where