Composite Structures 108 (2014) 212–222

Contents lists available at ScienceDirect

Composite Structures

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

Investigation on the extensibility of the wood cell-wall composite by an approach based on homogenisation and uncertainty analysis

E.I. Saavedra Flores [a,*], F.A. DiazDelaO [b], M.I. Friswell [c], R.M. Ajaj [d]

[a] Departamento de Ingeniería en Obras Civiles, Universidad de Santiago de Chile, Av. Ecuador 3659, Santiago, Chile
[b] School of Engineering, University of Liverpool, Liverpool L69 3GQ, United Kingdom
[c] Civil and Computational Engineering Centre, College of Engineering, Swansea University, Singleton Park, Swansea SA2 8PP, United Kingdom
[d] Aeronautics and Astronautics, University of Southampton, Southampton, UK, SO171BJ

ARTICLE INFO

Article history:
Available online 7 September 2013

Keywords:
Wood
Multi-scale analysis
Uncertainty analysis
Ultrastructure
Finite elements
Gaussian process

ABSTRACT

This paper investigates the extensibility of the wood cell-wall composite in the presence of parametric uncertainty by means of a multi-scale finite element approach. Normally, the three fundamental phases in wood, that is, cellulose, lignin and hemicellulose, present considerable scatter in their microstructure and mechanical properties. Nevertheless, by considering uncertainty in their properties, a significant computational cost is added to the solution of a large set of realisations represented by expensive fully-coupled multi-scale analyses. In order to tackle this high cost, we build a statistical approximation to the output of the computer model. Following this strategy, several micromechanical parameters are perturbed to study their influence on the extensibility of the material under tensile loading conditions. By reducing the cost of performing uncertainty analysis of the homogenised mechanical response, we are able to estimate the 5-th, 50-th, and 95-th percentile of the ultimate tensile strains of the material. We contrast our numerical predictions with experimental data, finding a good agreement for a wide range of initial microfibril angles.

1. Introduction

Wood microstructure can be understood as the result of an optimisation process developed by nature over hundreds of millions years of evolution. One of its main features is its hierarchical nature distributed across multiple spatial scales, from submicrometer dimensions to macroscopic scales. This important feature has been widely investigated by means of computational multi-scale constitutive models.

In the context of elastic response, several works have been reported. Holmberg et al. [29] studied the mechanical behaviour of wood by means of a homogenisation-based multi-scale procedure, incorporating growth rings, irregularity in the shape of cells and anisotropy in the layered structure of cell-walls. Hofstetter et al. [28] suggested five elementary phases for the mechanical characterisation of wood. These were hemicellulose, lignin, cellulose, with its crystalline and amorphous portions, and water. They proposed a multi-scale model and validated their numerical predictions with experimental data. Qing and Mishnaevsky Jr. [51,52] proposed a model taking into account several scale levels and investigated the influence of microfibril angles, shape of the cell cross-section and wood density on the elastic properties of wood. Rafsanjani et al. [55] investigated the hygro-mechanical behaviour of growth rings by means of the computational homogenisation of wood at two scales. They found a good agreement when compared their numerical predictions with experimental data. Later, Rafsanjani et al. [53,54] suggested that the layered architecture of the wood cell-wall composite enhances the anisotropy in swelling behaviour of honeycomb-type microstructures with irregular configuration while regular honeycombs show isotropic behaviour.

Simplified models have also been proposed to predict the mechanical response of the wood cell-wall under axial straining [1,24,32]. In addition, phenomenological constitutive models have also been used for the modelling of wood materials [45,47,69].

In the context of non-linear irreversible response taking place at several scales, Saavedra Flores et al. [62] showed that one important mechanism of local failure in the wood cell-wall composite under tension is the inelastic yielding of the amorphous portion of cellulose fibres. This work [62] was restricted to the assumption of initial microfibril angles (MFAs) close to 45°. A similar modelling framework was adopted to investigate the development of a new material inspired by the mechanics and structure of wood cell-walls [64]. Very recently, Saavedra Flores and Friswell [65] extended the above description of failure for a wider range of MFAs. Here, they suggested that for initial MFAs smaller than 30°, the dominant mechanism of failure is related to the axial tensile straining of the crystalline cellulose, and that for very large MFAs,

* Corresponding author. Tel.: +56 (2) 27182803.
E-mail address: erick.saavedra@usach.cl (E.I. Saavedra Flores).

0263-8223/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.compstruct.2013.08.034

over 70°, the prevailing failure mode is associated with the tensile rupture of the matrix due to the separation of cellulose fibres. For intermediate values of MFA, between 30° and 70°, the failure mechanism is associated with the plastic deformation of the amorphous cellulose portion.

Normally, the fundamental constituents of wood (represented by cellulose, with its crystalline and amorphous fractions, hemicellulose and lignin) show a significant scatter in their mechanical properties and microstructure. It is interesting to note however, that despite the natural randomness found in the different tissue types of a tree, and also among the different species of trees, wood seems to be always optimised from a structural point of view. Taking into account the above observation, it is highly relevant to investigate how the material uncertainty present in wood at smaller spatial scales affects its mechanical response, and particularly its extensibility, at higher uncertthierarchical levels. We remark here that, from an engineering point of view, one of the most important consequences in fully understanding the mechanical behaviour of wood, and in general natural materials, is the inspiration of new strategies to design more advanced composite materials.

In order to investigate the extensibility of the wood cell-wall composite, we adopt a homogenisation-based multi-scale constitutive framework, along with stochastic microstructural and mechanical properties. Nevertheless, by considering uncertainty in the material, a significant computational cost is added to the solution of a large set of realisations which are represented by very expensive fully-coupled multi-scale analyses. In order to address the issue of very high computational cost, we build a less expensive surrogate of the multi-scale finite element model. Several strategies that reduce the computational cost of expensive simulators by approximating their output can be found in the literature [23,31]. A particular kind of strategy is Bayesian emulation, which consists of building a statistical approximation to the code's output.

Following this approach, we investigate the influence of several micromechanical parameters on the extensibility of the composite under tensile loading conditions. Volume fraction of the cellulose, degree of crystallinity, aspect ratio of cellulose crystallites and the Young's modulus of the hemicellulose–lignin matrix are some examples of parameters investigated in this work. We validate the present model by comparing our numerical predictions for the ultimate tensile strains at the instant of failure with experimental data. By reducing the cost of performing uncertainty analysis of the homogenised mechanical response, we are able to estimate the 5-th, 50-th, and 95-th percentile of the mechanical response without resorting to more computationally expensive methods such as a crude Monte Carlo approach for our finite element simulations.

2. Relevant micromechanical parameters in the wood cell-wall composite

2.1. Wood ultrastructure

At the ultrastructural scale, the wall of wood cells contains three fundamental constituents: cellulose, hemicellulose and lignin. The cellulose is a long and stiff polymer organised into periodic crystalline and amorphous regions along its length [3]. This periodic arrangement is further covered by an outer surface made up of amorphous cellulose [72]. Hemicellulose is a polymer with little strength built up of sugar units, with mechanical properties highly sensitive to moisture changes. Lignin is an amorphous and hydrophobic polymer whose purpose is to cement the individual cells together and to provide shear strength. Hemicellulose and lignin are typically modelled as a single equivalent material [39], representing the surrounding lignin–hemicellulose matrix. These fundamental constituents form a spatial arrangement called microfibril and can be represented as a periodic unit building block of rectangular cross-section (refer to Fig. 1). For further information about cellulose microfibrils and their applications in composite materials, we refer, for instance, to [22,25].

The specific orientation of microfibrils with respect to the longitudinal cell axis is called the microfibril angle (MFA) and is one of the most important parameters controlling the balance between stiffness and flexibility in trees. Depending on the MFA and proportion of constituents, the wood cell-wall can be divided into at least five sub-layers, from which the most important ones (from the structural point of view) are the S_1, S_2 and S_3-layers. In the S_1-layer, the MFA has been reported to be very close to 90° [8] in Norway spruce samples. In the S_2-layer, the MFA takes values normally between 10° and 40° in *earlywood* cells and between 0° and 30° in *latewood* cells [51]. In the S_3-layer, the values fluctuate between 60° and 90° for both types of cell [51]. In *compression wood* cells, the MFA varies between 50° and 60° [11].

For further information about the morphology and composition of wood at the ultrastructural scale, we refer, for instance, to [7,21].

2.2. Micromechanical parameters

In order to introduce uncertainty in the definition of the material, we propose a modelling strategy which perturbs each of the micromechanical parameters chosen for this study. As we are interested in understanding the influence of each of these parameters on the extensibility of the material, for each analysis, a single parameter is perturbed in turn within a particular range of variation. The procedure is repeated again, for a second parameter, and so on. In a final stage, all the parameters are perturbed simultaneously to obtain a realistic description of the uncertainty in the material response.

To carry out the above strategy, we choose the micromechanical parameters to be perturbed. These parameters are represented by physical properties of wood at the ultrastructural scale whose values can be considered to be distributed as a uniform random variable. The parameters are assumed to be stochastic because they are either not well-known or susceptible to considerable variations when measured experimentally. In this paper, the only parameters that are assumed to be constant correspond to the linear elastic mechanical properties of the crystalline cellulose due to the agreement found among many works [6,67], and these parameters are kept fixed during the numerical simulations (refer to [65] for

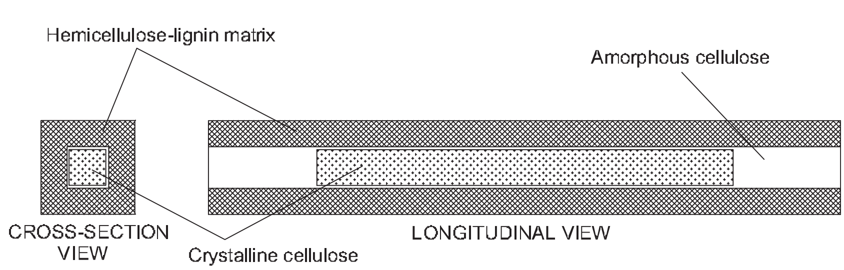

Fig. 1. Cross-section and longitudinal view of the microfibril and basic constituents [65].