Applied Mathematical Modelling 38 (2014) 3958–3967

Contents lists available at ScienceDirect

Applied Mathematical Modelling

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

Mathematical modelling of the stochastic mechanical properties of wood and its extensibility at small scales

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

[a] Departamento de Ingeniería en Obras Civiles, Universidad de Santiago de Chile, Av. Ecuador, 3659 Santiago, Chile
[b] Institute for Risk and Uncertainty, School of Engineering, University of Liverpool, Brownlow Hill, Liverpool L69 3GH, United Kingdom
[c] Aeronautics and Astronautics, University of Southampton, Southampton SO171BJ, United Kingdom
[d] Civil and Computational Engineering Centre, College of Engineering, Swansea University, Singleton Park, Swansea SA2 8PP, United Kingdom
[e] Department of Metallurgy and Materials, The University of Birmingham, Birmingham B15 2TT, United Kingdom

ARTICLE INFO

Article history:
Received 19 May 2013
Received in revised form 2 December 2013
Accepted 21 January 2014
Available online 31 January 2014

Keywords:
Wood
Multi-scale modelling
Stochastic properties
Finite elements

ABSTRACT

This paper investigates the relation between the uncertain mechanical properties of wood and its extensibility at the ultrastructural scale. A statistical approximation to the output of a multi-scale constitutive model is adopted to predict the extensibility of wood in the presence of parametric uncertainty. By means of this procedure, a very large number of computationally intensive fully-coupled multi-scale simulations are avoided. Following this approach, four different micromechanical parameters are chosen to assess their influence on the extensibility of the material under tensile loading conditions. These are the degree of cellulose crystallinity, the ultimate strain and Young's modulus of the hemicellulose–lignin matrix, and the thickness of the amorphous cellulose layer which covers the periodic crystalline portions of cellulose. We believe that a better understanding of the mechanisms of deformation and extensibility in wood and in natural materials can pave the way for the development of new strategies to design more advanced materials in engineering structures.

1. Introduction

One of the most outstanding characteristics of wood materials is their hierarchical nature distributed across five different spatial scales [1], from sub-micrometer dimensions to macroscopic levels. This important feature has been the focus of intense research over the last few years by means of multi-scale models.

Holmberg et al. [2] studied its mechanical response by means of a homogenisation-based multi-scale procedure. In their study, they considered the effects of growth rings, irregularities in the shape of wood cells and anisotropy of the material. Hofstetter et al. [1,3] suggested five elementary phases for the mechanical characterisation of wood. These were hemicellulose, lignin, cellulose, with its crystalline and amorphous portions, and water. Later, Qing and Mishnaevsky [4–6] investigated the influence of microfibril angles, the shape of cells and wood density on the elastic properties of wood. Rafsanjani et al. [7] investigated the hygro-mechanical behaviour of growth rings. They compared successfully their numerical predictions with experimental data. A description of wood failure at the ultrastructural scale was proposed by Saavedra Flore et al. [8] and Saavedra Flores and Friswell [9] by means of non-linear multi-scale models. They suggested that for initial microfibril

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

http://dx.doi.org/10.1016/j.apm.2014.01.002
0307-904X/

angles (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, 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 inelastic deformation of the amorphous cellulose portion.

To date, most of the works on multi-scale modelling of wood have been restricted to deterministic studies. However, it is a fact that the fundamental constituents of wood show a significant scatter in their mechanical properties and microstructure [10]. Very recently, an investigation of the influence of the stochastic micromechanical properties of wood on its extensibility was carried out [11]. The central idea of this work was to understand how the MFA is related to the maximum extensibility when uncertain properties are considered. The authors suggested a maximisation of the extensibility for initial MFAs between 50° and 55°, regardless of the natural randomness found typically in the microstructure of wood.

In this work, we extend the above study. We describe in detail the mathematical framework adopted to quantify the uncertainty present in the micromechanical properties of wood and we explore how the perturbation of these parameters affects the extensibility of the material. In particular, we explore the impact of the uncertainty present in the degree of cellulose crystallinity, in the ultimate strain and Young's modulus of the hemicellulose–lignin matrix, and in the thickness of the amorphous cellulose layer which covers the periodic regions of crystalline cellulose.

The paper is organised as follows. Section 2 describes the stochastic microstructural parameters of wood chosen for this investigation. Section 3 reviews the multi-scale constitutive theory and the essential equations adopted to model the stochastic mechanical properties of the material at small scales. Section 4 shows the numerical results obtained from the present stochastic multi-scale framework. Finally, Section 5 summarises our main conclusions.

2. Stochastic properties of wood at the ultrastructural scale

Cellulose, hemicellulose and lignin are the three fundamental constituents of wood at the ultrastructural scale [12,13]. The cellulose is a long and stiff polymer organised into periodic crystalline and amorphous regions along its length [14], covered by an outer thin layer of amorphous cellulose [15] of thickness t_{ac}.

We note that the discontinuity of the crystalline cellulose fibres divided periodically by softer amorphous regions results in a natural composite made of shorter fibres, which allows the development of large levels of ductility in the matrix. This feature has been studied in the context of engineered short fibre reinforced metal matrix composites [16]. The (volumetric) degree of cellulose crystallinity, f_{cc}, is defined as the ratio between the volume of crystalline cellulose and the total volume of (crystalline and amorphous) cellulose.

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 [17], representing the surrounding lignin–hemicellulose matrix. These three fundamental constituents form a spatial arrangement called microfibril which is represented as a periodic unit building block of rectangular cross-section. Its specific orientation with respect to the longitudinal cell axis is called microfibril angle (MFA). Across the thickness of the cell-wall, the change of the proportion of constituents and MFA defines several layers, namely the primary (P) and the secondary (S_1, S_2 and S_3) layers. In each layer, the microfibril exists but oriented in different directions. Fig. 1 shows a schematic representation of the wood cell-wall, its primary and secondary layers and a typical microfibril, with its periodic crystalline and amorphous cellulose fractions. In this figure, the longitudinal direction of the wood cell is represented by the axis 1, and the

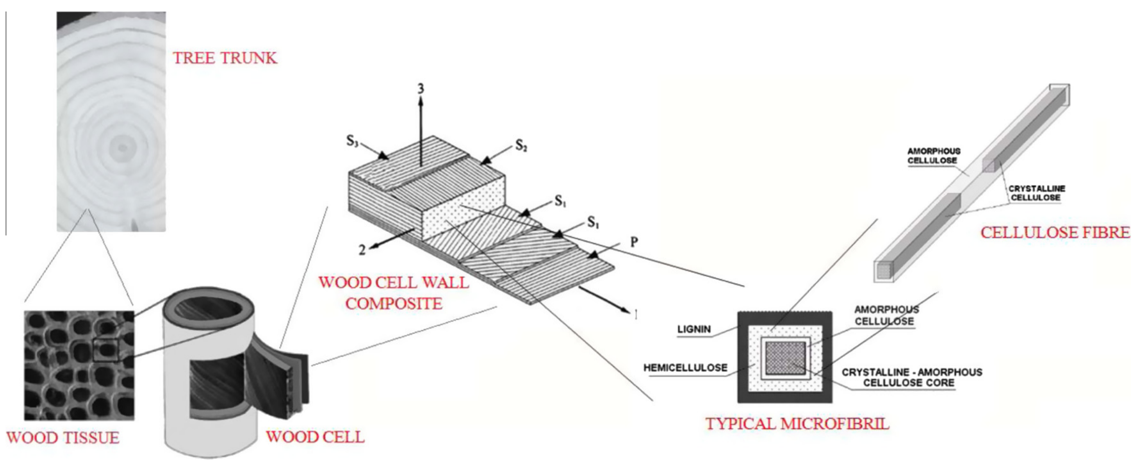

Fig. 1. Representation of the cross-section of a tree trunk [18], the wood tissue and the wood cell [19], wood cell-wall composite [20], microfibril and cellulose [8].