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Ultrastructural mechanisms of deformation and failure in wood under tension

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ABSTRACT

This paper investigates the deformation and failure mechanisms of wood at the ultrastructural scale. At this level, wood is composed of a periodic alternation of amorphous and crystalline cellulose fractions, embedded in a soft hemicellulose-lignin matrix. The mechanical response of wood is calculated under tensile loading conditions by means of the computational homogenisation of a representative volume element (RVE) of material. Three potential mechanisms of failure are suggested: axial straining of the crystalline fraction of cellulose, accumulation of plastic strain in the amorphous portion of cellulose and tensile rupture in the hemicellulose-lignin matrix due to cellulose fibres separation. In order to validate the present multi-scale framework, we compare our numerical predictions for the reorientation of cellulose fibres with experimental data, finding a good agreement for a wide range of strains. Furthermore, we assess successfully our numerical predictions for ultimate strains at the instant of failure when compared to experimental values. Numerical simulations show that our model is able to provide new clues into the understanding of how trees and plants optimise their microstructure in order to develop larger strains without apparent damage. A remarkable prediction by our model suggests that the extensibility of the material is maximised for initial microfibril angles (MFA) between 50° and 55°, a range of values found typically in branches of trees, in which the extensibility is an essential requirement. These findings are likely to shed more light into the dissipative mechanisms of wood and natural materials, which are still not well-understood at present.

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 (Gibson, 2012), from submicrometer dimensions to macroscopic scales. This important feature has been a subject of intensive research over the last few years in applied and computational mechanics circles (Holmberg et al., 1999; Hofstetter et al., 2005; Hofstetter et al., 2007; Qing and Mishnaevsky, 2009; Qing et al., 2009; Qing and Mishnaevsky, 2010; Saavedra Flores et al., 2011; Qing and Mishnaevsky, 2011). Nevertheless, despite the increasing interest in this subject and the considerable effort devoted to its description, the complete understanding of the deformation and failure mechanisms of this material at very small scales, and their implications on the macroscopic response, is still an issue which remains open at present.

The constitutive description of wood at several scales has been widely investigated by means of computational multi-scale constitutive models. In the context of elastic response, several works have been presented. Holmberg et al. (1999) 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. Rafsanjani et al. (2012) investigated the hygro-mechanical behaviour of growth rings by means of the computational homogenisation of wood at two scales. Persson et al. (2000) proposed models for the stiffness and moisture-shrinkage properties of wood, encompassing from the scale of chemical constituents to growth rings. Hofstetter et al. (2005, 2007) 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 et al. (2009, 2010) 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. Recently, Qing and Mishnaevsky (2011) extended their model by incorporating progressive damage to the homogenised elasticity matrix. Sedighi-Gilani and Navi (2007)

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presented a micromechanical model to take into account damage and the influence of non-uniform microfibril angles on the stiffness of wood cells. Additional works in this field can be found, for instance, in reference Mishnaevsky and Qing (2008).

In spite of this extensive work, a review of the current literature shows that little research has been done in the context of irreversible processes and microscopic dissipative phenomena taking place in wood at several scales. In reference Saavedra Flores et al. (2011), the authors investigated the non-linear irreversible behaviour of wood cell-walls. By adopting a finite element-based computational multi-scale approach, it was shown that one important mechanism of dissipation under tensile loading is the shear irreversible deformation in the hemicellulose-lignin matrix due to the reorientation of cellulose fibres induced by their alignment with respect to the loading direction. This mechanism of deformation was observed experimentally in wood tissue and individual wood cells undergoing large shear deformations in the hemicellulose-lignin matrix (Keckés et al., 2003). These authors (Keckés et al., 2003) showed how wood tissue and individual cells are able to undergo large deformations without apparent damage and also proposed a recovery mechanism after irreversible deformation, interpreted as a *stick–slip* mechanism at the molecular level. The authors suggested that this mechanism might be mediated by hemicelluloses, but could not distinguished whether the mechanism occurs at the interface between cellulose and hemicelluloses, or between the links of hemicelluloses.

Due to its relevance in the macroscopic mechanical response of wood and wood-based materials, our main objective in this paper is to investigate the ultrastructural mechanisms of deformation and failure in wood under tensile loading conditions by means of a computational multi-scale approach. We remark here that, in reference Saavedra Flores et al. (2011), the numerical results were restricted to the assumption of undeformable cellulose fibres in the definition of the strain path imposed at the wood cell-wall scale. Such an assumption is accurate enough for initial microfibril angles close to 45°, and for small to moderate levels of strains. However, it could be questionable how accurate this approach is for very large strains and for different initial orientation of cellulose fibres in which the assumption of inextensibility is not longer valid. In this paper, however, this drawback is circumvented without need of assuming undeformable fibres. We study the local mechanisms of deformation in wood and we extend the possible modes of failure to a wide range of initial orientation of fibres. Here, we study the failure mechanisms associated with axial straining of the crystalline cellulose fraction, accumulation of irreversible deformation in the amorphous portion of cellulose and tensile rupture in the hemicellulose-lignin matrix due to cellulose fibres separation. We validate the present model by comparing our numerical predictions for the reorientation of cellulose fibres and for the strains at the instant of failure with experimental data for wood under tension.

Due to the highly non-linear nature of the phenomena taking place at the ultrastructural scale, we remark that all the aspects of modelling discussed here take into account non-linear kinematics and dissipative response of the material under a large strains regime.

The paper is organised as follows. Section 2 presents a brief review of the mechanics and structure of wood at the ultrastructural scale. Section 3 reviews the adopted homogenisation-based multi-scale theory in continuum form. In Section 4, the two-dimensional multi-scale finite element model is described in detail. The validation of the model is presented in Section 5 by comparing our numerical predictions with experimental data. Section 6 shows the numerical results obtained from the present multi-scale framework. Finally, Section 7 summarises our main conclusions.

2. Mechanics and structure of wood at the ultrastructural scale

At the ultrastructural scale (Fengel et al., 1989; Harada and Côté, 1985; Neagu et al., 2006), the wall of wood cells contains three fundamental constituents: cellulose, hemicellulose and lignin. These constituents form a spatial arrangement called microfibril which can be represented as a periodic unit building block of rectangular cross-section (refer to Fig. 1).

Cellulose, hemicellulose and lignin constitute approximately 30%, 32.5% and 37.5%, respectively, of the total volume of wood substance for *compression wood* cells (Timell, 1982; Timell, 1986; Saavedra Flores et al., 2011). The cellulose is a long polymer composed of glucose units which is organised into periodic crystalline and amorphous regions along its length (Andersson et al., 2006; Haslach, 1996; Saavedra Flores et al., 2011; Smith et al., 2003) (refer to Fig. 1 for a representative portion of this periodic amorphous-crystalline cellulose arrangement). This periodic arrangement is further covered by an outer surface made up of amorphous cellulose (Xu et al., 2007). An average thickness of 3.6 nm can be considered for the (amorphous-crystalline) cellulose (Donaldson and Singh, 1998), with 3.2 nm for its internal crystalline fraction (Andersson et al., 2004). In consequence, a 0.2 nm thick layer of amorphous cellulose can be assumed at the surface of the crystalline-amorphous core. A mean length of the crystalline fraction of cellulose can be taken as 36.4 nm (Andersson et al., 2006). A length of 18.9 nm can be assumed for the amorphous cellulose between two consecutive crystalline units (Andersson et al., 2006). The (volumetric) degree of crystallinity is defined as the ratio between the volume of crystalline cellulose and the total volume of (crystalline and amorphous) cellulose. Normally, its value varies between 0.49 and 0.60 in wood cells of Scots pine and Norway spruce, with an average value of 0.52 (Andersson et al., 2004).

The Young's modulus of the crystalline cellulose in the longitudinal direction and its Poisson's ratio are $E = 134$ GPa (Salmén, 2004; Bergander and Salmén, 2002) and 0.1 (Salmén, 2004; Bergander and Salmén, 2002; Mark, 1967), respectively. The Young's modulus in the transversal direction is 27.2 GPa (Salmén, 2004; Bergander and Salmén, 2002; Mark, 1967). For latewood samples of mature wood (Norway spruce), the longitudinal tensile fracture strain reported for cellulose crystallites is 0.14% strain (Peura et al., 2007). The authors in reference Peura et al. (2007) also reported a purely elastic behaviour for this crystalline fraction. We also note that crystalline cellulose is largely impenetrable by water (Klemm et al., 1998).

The amorphous cellulose portion can be modelled isotropically due to its random molecular distribution, with a Young's modulus of $E = 10.42$ GPa and a Poisson's ratio of 0.23 (Chen et al., 2004). If we take a value for the yield strain equal to 0.01 (estimated from reference Chen et al. (2004)), we can assume a value of $\sigma_y = 0.104$ GPa for the yield stress of amorphous cellulose. In relation to the ultimate strain of amorphous cellulose, little information has been reported. Nevertheless, in reference Chen et al. (2004), the authors calculated cavity volume fractions (related to voids formation) in different amorphous cellulose models under straining, in order to estimate measures of breaking strains. By means of molecular simulations, they showed that for amorphous cellulose with 16% water, almost zero cavity volume fraction was formed for tensile strains up to 10%, and about 0.5% volume fraction for 15% strain. Since these authors related the cavity size with failure of the polymer, we can conclude that large levels of strains, possibly between 10 and 15%, are needed for the failure of the amorphous cellulose. Therefore, a value of fracture strain equal to 14% seems to be reasonable. As shall be seen later, the adoption of this value will result in numerical predictions consistent with experimental observations.