Multi-scale finite element model for a new material inspired by the mechanics and structure of wood cell-walls

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A B S T R A C T

This paper proposes a fully coupled multi-scale finite element model for the constitutive description of an alumina/magnesium alloy/epoxy composite inspired in the mechanics and structure of the wall of wood cells. The mechanical response of the composite (the large scale continuum) is described by means of a representative volume element (RVE, corresponding to the intermediate scale) in which the fibre is represented as a periodic alternation of alumina and magnesium alloy fractions. Furthermore, at a lower scale the overall constitutive behavior of the alumina/magnesium alloy fibre is modelled as a single material defined by a large number of RVEs (the smallest material scale) at the Gauss point (intermediate) level. Numerical material tests show that this new composite maximises its toughness when the hierarchical design of wood cellulose fibres is replicated. The above results provide for the first time new clues into the understanding of how trees and plants optimise their microstructures at the cellulose level in order to absorb a large amount of strain energy before failure. These findings are likely to shed more light into natural materials and bio-inspired design strategies, which are still not well-understood at present.

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1. Introduction

Wood microstructure can be understood as the result of an optimisation process developed by nature over millions of years. One of its main features is its hierarchical nature distributed across multiple spatial scales. This important feature has been widely investigated over the last few years by means of multi-scale finite element models in the context of elastic response (Holmberg et al., 1999; Hofstetter et al., 2005; Qing and Mishnaevsky, 2009, 2010), and recently in the context of irreversible behavior (Saavedra Flores et al., 2011), bringing substantial progress to the understanding of this material.

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, at several scale levels, is the inspiration of new strategies to design more advanced materials. This relatively new field of bio-inspired materials has received considerable attention from scientific communities in recent years (Broedling et al., 2008; Fratzl and Barth, 2009; Luz and Mano, 2009; Bonderer et al., 2008; Stanzl-Tschegg, 2011). Nevertheless, despite the considerable effort devoted to this study, and particularly to the study of wood across different scales, little is currently known about the development of new bio-inspired materials.

In an attempt to exploit further the structural and mechanical concepts involved in wood cells, we investigate in this paper the non-linear mechanical response of a new wood-inspired composite by means of a fully coupled multi-scale finite element model in the context of large strains. By replicating the hierarchical design of cellulose fibres in wood cells, this new
The composite is characterised by alumina/magnesium alloy fibres embedded in an epoxy matrix. In the present multi-scale framework, the large scale continuum is represented by the composite, whose constitutive response is defined by a Representative Volume Element (RVE), corresponding to the intermediate scale. Furthermore, the fibres are represented by a periodic alternation of alumina and magnesium alloy fractions, whose overall constitutive behaviour is modelled as a single material defined by a large number of RVEs, i.e., the smallest scale, at Gauss point (intermediate) level. This bio-inspired strategy is suggested by the strong influence of the proportion of volume fractions of crystalline and amorphous cellulose on the overall mechanical behaviour of wood cells.

The paper is organised as follows. Section 2 presents a brief review of wood cell-wall mechanics. Section 3 describes the basis of the homogenisation-based multi-scale theory at large strains. The bio-inspired strategy adopted for the design of the new composite is detailed in Section 4. The finite element modelling of the new material is presented in Section 5. The potential failure mechanisms in the composite and considered in this investigation are described in Section 6. Section 7 shows the numerical results obtained from the present multi-scale model. Finally, Section 8 summarises our main conclusions.

2. Mechanics and structure of wood cell-wall

Microscopically, wood is composed mainly by an arrangement of long slender tubular cells, oriented nearly parallel to the axis of the stem and firmly cemented together, with dimensions and shapes variable within a tree and among species. The walls of these wood cells contain three major chemical constituents: cellulose (representing the fibre), hemicellulose and lignin (representing the matrix). These constituents form a spatial arrangement called microfibril (Dinwoodie, 1981) which can be represented as a periodic unit building block of rectangular cross-section with infinite length (see Fig. 1a). Cellulose, hemicellulose and lignin constitute approximately 30%, 30–35% and 35–40%, respectively, of the total volume of wood substance in compression wood cells (Timell, 1982, 1986). The cellulose is a long polymer organised into periodic crystalline and amorphous regions along its length and called crystalline–amorphous cellulose core (Saavedra Flores et al., 2011) as shown in Fig. 1b. This periodic arrangement is further covered with an outer surface made up of amorphous cellulose (Xu et al., 2007). The length and width of the cellulose crystallites can be taken as 36.4 nm and 3.2 nm, respectively (Andersson et al., 2004; Andersson, 2006). Donaldson and Singh (1998) obtained an average thickness of cellulose of 3.6 nm, which included the crystalline core and the outer amorphous surface sheeting.

The (volumetric) degree of crystallinity is defined as the ratio between the volume of crystalline cellulose and the total volume of cellulose. Newman and Hemmingson (1990) specified a value of 0.54 for the cellulose crystallinity of Pinus radiata trees. Sivonen et al. (2002) studied the cellulose crystallinity in earlywood and latewood cells of Scots pine trees and determined a variation between 0.51 and 0.55. Andersson et al. (2004) indicated a fraction of crystallinity for the cellulose fibres of Scots pine and Norway spruce between 0.49 and 0.60, with an average value of 0.52. Later, Newman (2004) reported a cellulose crystallinity index in the range of 0.486–0.541, for different Pinus radiata trees, with a mean value of 0.515. In his study, this range of crystallinity was observed regardless of the different cell types analysed (earlywood, latewood, compression wood, opposite wood, juvenile and mature wood).

For plants, Harris and DeBolt (2008) reported a comprehensive study on the relative crystallinity of several plant species. Of a collection of 22 grass species, the range in the relative crystallinity was determined to be 0.511–0.585. Arabidopsis whole plant samples were measured and the value remained between 0.475 and 0.498. Furthermore, Arabidopsis plants grown to maturity were harvested and divided into roots, stems and leaves. Average values of crystallinity for stem was 0.5479, for the leaf was 0.4199 and for the root was 0.5342. In general, the lowest values (along with great scatter) were found for leaf samples, which could be attributed to their less relevant structural function.

![Fig. 1. Schematic diagram for a typical microfibril and cellulose fibre. (a) Cross-section of a representative microfibril with its fundamental constituents (Saavedra Flores et al., 2011). (b) Longitudinal section of the cellulose with its periodic crystalline and amorphous fractions.](image-url)
From the above experimental values, it is wise to assume a range of values between 0.5 and 0.55 for the cellulose crystallinity typically found in trees and plants.

Hemicellulose is a polymer with little strength under moist conditions, with a molecular structure that is partially random. Lignin is an amorphous polymer whose purpose is to cement the individual cells together. The specific orientation of microfibrils with respect to the longitudinal cell axis is called the microfibril angle (MFA).

The mechanical properties of the wood cell-wall composite and its fundamental constituents have been extensively investigated in recent years (Saavedra Flores et al., 2011; Peura et al., 2007; Keckeš et al., 2003; Salmen, 2001, 2004; Chen et al., 2004a). Fig. 2 shows the corresponding value of Young's modulus for each of the four chemical constituents in wood. The corresponding graph reveals how the stiffness in the microfibril falls abruptly from the cellulose fibre to the hemicellulose/lignin matrix.

A different trend is found for the ultimate strains of each of the constituents, varying from very low values in the crystalline cellulose to very large strains in the hemicellulose/lignin matrix. For instance, Peura et al. (2007) determined a range of maximum tensile strains in cellulose crystallites, for both juvenile and mature wood, between 0.14% and 0.40% strain. Here, we consider an average value of 0.3% strain. They also reported an elastic behaviour for this crystalline fraction.

In relation to amorphous cellulose, little information has been reported about its ultimate strain. Nevertheless, Chen et al. (2004b) 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 only 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.

Keckeš et al. (2003) showed how wood tissue and individual cells are able to undergo large deformations without damage when the main mechanism of deformation is shear in the hemicellulose/lignin matrix. This self-healing mechanism present in wood cells allows the assumption of no limit for the maximum shear strain in the hemicellulose/lignin matrix.

Since cellulose (with its crystalline and amorphous portions) is the main constituent in the wood cell-wall and is far stiffer than lignin and hemicellulose, it is assumed that the distribution of the hemicellulose and lignin in the surrounding matrix is not important (Nilsson and Gustafsson, 2007). Therefore, it is possible to adopt a single equivalent material for the description of the lignin/hemicellulose matrix based on their volume fractions and individual mechanical properties. In this paper, we choose 30% volume fraction for the whole cellulose fibre, and 32.5 and 37.5% for the hemicellulose and lignin, respectively. Thus, from Young's modulus of hemicellulose and lignin shown in Fig. 2, it is straightforward to obtain an equivalent Young's modulus $E=0.854$ GPa for the equivalent matrix. From Saavedra Flores et al. (2011) and Salmen (2004), it is also possible to determine an equivalent yield stress of $\sigma_y = 0.019$ GPa and an equivalent Poisson ratio of 0.25.

Table 1 summarises the mechanical properties of the fundamental constituents in the cell-wall. Here, a fully elastic response has been assumed for the crystalline cellulose, and an elastic-perfectly plastic behaviour for the amorphous cellulose and hemicellulose/lignin matrix.

3. Homogenisation-based multi-scale constitutive theory at large strains

The point of departure of the present family of large strain multi-scale constitutive theory of heterogenous solids is that the deformation gradient $F$ at any arbitrary point $x$ of the macroscopic continuum is the volume average of the microscopic deformation gradient field $\bar{F}_\mu$ defined over a local representative volume element (RVE). Similarly, the macroscopic or
homogenised first Piola–Kirchoff stress tensor field \( \mathbf{P} \), at the point \( \mathbf{x} \), is assumed to be the volume average of the microscopic first Piola–Kirchoff stress tensor \( \mathbf{P}_m \). For any instant \( t \), such conditions can be expressed mathematically as

\[
\mathbf{F}(\mathbf{x}, t) = \frac{1}{V_m} \int_{\Omega_m} \mathbf{F}_m(\mathbf{y}, t) \, dV
\]

and

\[
\mathbf{P}(\mathbf{x}, t) = \frac{1}{V_m} \int_{\Omega_m} \mathbf{P}_m(\mathbf{y}, t) \, dV,
\]

where \( V_m \) is the volume of the RVE with domain \( \Omega_m \), associated to the point \( \mathbf{x} \) in its reference configuration and \( \mathbf{y} \) the local RVE coordinates. Models of the present type can be found, for instance, in Miehe et al. (1999, 2002), Terada et al. (2003), Matsui et al. (2004), Mishnaevsky (2007), Giusti et al. (2009), de Souza Neto and Feijóo (2010), Michel et al. (1999), and Saavedra Flores and de Souza Neto (2010).

Further, it is possible to decompose the displacement field \( \mathbf{u}_m \) as a sum of a linear displacement \( \mathbf{F}(\mathbf{x}, t) \mathbf{y} \) and a displacement fluctuation field \( \mathbf{u}_m \). The displacement fluctuations field \( \mathbf{u}_m \) represents local variations about the linear displacement and depends on the presence of heterogeneities within the RVE.

By taking into account the Hill–Mandel Principle of Macro-homogeneity (Hill, 1965; Mandel, 1971), which requires the RVE body force and external surface traction fields to produce no virtual work (de Souza Neto and Feijóo, 2006, 2010), the equilibrium equation for the RVE can be reduced to

\[
\int_{\Omega_m} \mathbf{P}_m(\mathbf{y}, t) : \nabla \mathbf{\eta} \, dV = 0,
\]

with \( \mathbf{\eta} \) representing the virtual kinematically admissible displacements field of the RVE.

In order to make problem (2) well-posed, a set of kinematical constraints upon the selected RVE is required. In what follows, the choice of this set will coincide with the widely used Periodic boundary displacement fluctuations model, typically associated with the modelling of periodic media. Here, the fundamental kinematical assumption consists of prescribing identical displacement fluctuation vectors for each pair of opposite points \( \{\mathbf{y}_+, \mathbf{y}_-\} \) on the RVE boundary \( \partial \Omega_m \), such that:

\[
\mathbf{u}_m(\mathbf{y}_+ + t) = \mathbf{u}_m(\mathbf{y}_- - t) \quad \forall \{\mathbf{y}_+, \mathbf{y}_-\} \in \partial \Omega_m.
\]

With the RVE response described by a generic local dissipative constitutive theory, the microscopic first Piola–Kirchoff stress tensor \( \mathbf{P}_m \) is a functional of the history of \( \mathbf{F}_m \). This can be symbolically expressed as

\[
\mathbf{P}_m(\mathbf{y}, t) = \Psi_m(\mathbf{F}_m, \mathbf{y}),
\]

where the functional \( \Psi_m \) associated with point \( \mathbf{y} \) maps the deformation gradient history, \( \mathbf{F}_m \), up to time \( t \), into the first Piola–Kirchoff stress tensor \( \mathbf{P}_m \) of time \( t \). In view of the decomposition of the displacement field \( \mathbf{u}_m \) and the constitutive assumption (4), the expression of the virtual work principle in (2) can be expressed as

\[
G(\mathbf{F}, \mathbf{u}_m, \mathbf{\eta}) \equiv \int_{\Omega_m} \Psi_m\{[\mathbf{F}(\mathbf{x}, t) + \nabla \mathbf{u}_m(\mathbf{y}, t)]^t\} : \nabla \mathbf{\eta} \, dV = 0,
\]

where we have defined \( G \) as the large strain virtual work functional. Eq. (5) defines the microscopic equilibrium problem stated as follows: Given the history of the macroscopic deformation gradient \( \mathbf{F} = \mathbf{F}(\mathbf{x}, t) \), at a point \( \mathbf{x} \) of the macro-continuum, find a microscopic displacement fluctuation field \( \mathbf{u}_m \), such that for each instant \( t \), Eq. (5) is satisfied for any virtual kinematically admissible displacements field \( \mathbf{\eta} \) (de Souza Neto and Feijóo, 2010).

For further details about multi-scale modelling techniques and homogenisation theory in non-linear periodic media, we refer, for instance, to Pellegrino et al. (1999) and Feyel and Chaboche (2000, 2001, 2003).

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### Table 1
Summary of the mechanical properties of the crystalline/amorphous cellulose and hemicellulose/lignin matrix.

The units for Young’s modulus \( E \) and yield stress \( \sigma_y \) are GPa. These properties have been obtained from Saavedra Flores et al. (2011), Salmén (2001, 2004), Chen et al. (2004a,b), Peura et al. (2007), and Keckeš et al. (2003).

<table>
<thead>
<tr>
<th>Constituent</th>
<th>( E )</th>
<th>( v )</th>
<th>( \sigma_y )</th>
<th>( \varepsilon_{us} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystall. cellulose</td>
<td>134*</td>
<td>0.3</td>
<td>–</td>
<td>0.003</td>
</tr>
<tr>
<td>Amorph. cellulose(^a)</td>
<td>10.42</td>
<td>0.23</td>
<td>0.104</td>
<td>0.10–0.15</td>
</tr>
<tr>
<td>Hemicel./lignin matrix(^b)</td>
<td>0.854</td>
<td>0.25</td>
<td>0.019</td>
<td>–</td>
</tr>
</tbody>
</table>

\(^a\) Young’s modulus is specified for the longitudinal axis of the cellulose fibre.

\(^b\) No hardening has been assumed during plastic yielding.
4. Bio-inspiration

In this section we explore the design of a new alumina/magnesium alloy/epoxy three-phase composite when some of the structural and mechanical concepts involved in wood cells are exploited further. Under natural conditions, compression wood cells are characterised by a low content of cellulose, which results in low overall stiffness, and by large MFAs that vary substantially under tensile loading. These features allow compression wood tissue to be very compliant, developing large amounts of strain before reaching failure. Reiterer et al. (1999) have also suggested that one of the main reasons for larger fibrillar angles in the wood cell-wall is the optimisation of extensibility. Thus, we choose compression wood cell-wall as the inspiring material in order to endow this new composite with these particular features. Consequently, the volume fractions adopted for the constituents in the new composite are taken from the relative contents of cellulose, hemicellulose and lignin in compression wood, based on the results reported by Timell (1982, 1986) (refer to Section 2).

Based on the natural design of wood cellulose fibres, we suggest a bio-inspired strategy to increase the toughness in this new composite. In order to endow this composite with similar mechanisms of deformation found in the wood cell-wall composite, we establish a one-to-one correspondence between each of the fundamental constituents present in wood and those existing in the new material, and therefore the role performed by each of the cell-wall constituents is replicated in the new wood-inspired material. By mimicking the natural design of the cellulose, the reinforcing fibre of the new composite is assumed to be made up of two phases. Here, the main feature of the stiff crystalline cellulose fibre in the wood cell-wall material is replicated in the new composite by adopting a very stiff elastic material as one of the phases in the fibre. Motivated by the very low ultimate strain reported in the crystalline cellulose (refer to Section 2), we choose alumina to become the very stiff elastic portion of fibre, whose maximum tensile strain of 0.3% (Bansal, 2005) coincides with that of crystalline cellulose. Young’s modulus and Poisson ratio for alumina are 414 GPa and 0.23, respectively (Bansal, 2005).

The second phase of the fibre is assumed to have a softer elasto-plastic response similar to the mechanical response of the amorphous cellulose fraction in the cell-wall. In order to endow this new composite with similar mechanisms of deformation found in the wood cell, we keep the same ratio present in the wood cell-wall composite, between Young’s modulus of the crystalline cellulose, \( E = 134 \text{ GPa} \), and its amorphous counterpart, \( E = 10.42 \text{ GPa} \). Thus, we proceed to define Young’s modulus for the softer fraction of fibre with a value of \( E = 32.19 \text{ GPa} \), which results in the same ratio when compared to Young’s modulus of alumina, that is, \( 414/10.42 = 12.86 \). Similarly, by adopting the same yield strain \( \varepsilon_y = 0.01 \) (onset of plastic yielding) of the amorphous cellulose (Chen et al., 2004a) for the softer fraction of fibre in the present composite, we estimate a yield stress \( \sigma_y = 0.32 \text{ GPa} \).

A comprehensive search for possible candidate engineering materials with similar mechanical properties to those determined above reveals that an AM50A magnesium alloy is a suitable choice. It has Young’s modulus of 31.26 GPa (Altenhof et al., 2004) which is in good agreement with the value of 32.19 GPa. In addition, it has a Poisson ratio of 0.35 (Altenhof et al., 2004). Furthermore, for a wide range of magnesium alloys, the value of the yield stress \( \sigma_y \) varies between 0.072 and 0.383 GPa (Kubota et al., 1999), which is also in agreement with the determined yield stress \( \sigma_y = 0.32 \text{ GPa} \). The ultimate tensile strain of the AM50A magnesium alloy reported in Lebeau and Decker (1999) and Avedessian and Baker (1999) is 0.20.

We note that alumina/magnesium alloy composites are important in applications in which a high stiffness/weight ratio is required (Bakkar and Neubert, 2007). Some applications can be found, for instance, in aircraft engines, power transmission housings, rotating shafts and in helicopter transmission components (Ferrando, 1989).

For the definition of the mechanical properties of the matrix, we follow the same considerations explained above. By keeping constant the ratio between Young’s modulus of the crystalline cellulose and that of the equivalent hemicellulose/lignin matrix, we estimate Young’s modulus \( E = 2.639 \text{ GPa} \) for the matrix, such that \( 414/2.639 = 134/0.854 = 156.9 \). Similar calculations lead to a yield stress \( \sigma_y = 0.059 \text{ GPa} \).

A new search for engineering materials as possible alternatives for the matrix results in epoxy as a suitable candidate. From de Kok et al. (1993), Young’s modulus and yield stress for epoxy is \( E = 2.6 \text{ GPa} \) and \( \sigma_y = 0.068 \text{ GPa} \), respectively, revealing a good agreement with those values estimated above. In addition, its ultimate tensile strain is 0.421 (de Kok et al., 1993; de Kok, 1995) when treated with functional curing agents, which is consistent with the large shear strains reported in the hemicellulose/lignin matrix before the failure of wood cells and wood tissue under straining (Kecke’s et al., 2003).

We emphasise that the natural scatter found in the mechanical properties of wood (in the crystalline and amorphous cellulose fractions and in the hemicellulose–lignin matrix) makes possible the choice of engineering materials (alumina, magnesium alloy and epoxy) whose material properties ratios may be approximated to the same ratios obtained from the literature for the wood cell-wall.

All of the material constants adopted for each of the constituents in the present composite are summarised in Table 2. By taking into consideration the morphology of the fundamental constituents in the wood cell-wall, we define the architecture of the composite. Here, we adopt the same aspect ratios found in the main constituents of wood for the suggested constituents of the bio-inspired composite. As mentioned in Section 2, the length and width of the cellulose crystallites are 36.4 nm and 3.2 nm, respectively (Andersson et al., 2004; Andersson, 2006). Therefore, inspired by these dimensions, we adopt an aspect ratio (width/length) of 3.2/36.4 for the alumina fraction. The average thickness of...
cellulose can be taken as 3.6 nm (Donaldson and Singh, 1998), which included the crystalline core and the outer amorphous surface sheeting (refer to Section 2). This results in a ratio between the width of the crystalline cellulose and the width of the entire cellulose fibre equal to $\frac{3}{2} = \frac{3}{6}$. Consequently, we assume the same proportion between the width of the alumina fraction and the whole alumina–magnesium alloy fibre. In view of the volume fraction of 0.70 for the hemicellulose–lignin matrix (refer to Section 2), we take the same value for the volume fraction of the epoxy matrix (with respect to the whole composite).

Fig. 3 shows a schematic representation of a generic composite made of a periodic alternation of stiff and soft portions of fibre, embedded in a much softer matrix. The one-to-one correspondence between the wood cell-wall and the suggested new composite is highlighted here. We note that the same aspect ratios found in the main constituents of wood have been adopted for the constituents of the bio-inspired material.

As shall be seen in Section 7, we will vary the volume fraction of alumina (with respect to the whole alumina–magnesium alloy fibre) between 0.35 and 1.0, and we will assess the impact of adopting volume fractions inspired by the degree of crystallinity typically found in trees and plants. This will constitute the main contribution of the present work.

5. Fully coupled multi-scale finite element model

In the present paper we propose a fully coupled multi-scale finite element model for the mechanical response of the new composite. The constitutive description of the composite, or large scale continuum, is obtained by means of a computational homogenisation of an RVE at the intermediate level (refer to Fig. 4). Furthermore, at a lower scale the fibre is represented as a periodic alternation of stiff and soft portions (corresponding to alumina and magnesium alloy fractions), whose overall constitutive behaviour is modelled as a single material defined by a large number of RVEs at Gauss point (intermediate) level. We remark that the same multi-scale framework has been adopted in Saavedra Flores et al. (2011) but to investigate the dissipative behavior of wood cell-walls.

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

Fig. 5 shows the finite element meshes adopted in the analyses. Here, we define the terms mesoscopic and microscopic finite element meshes to represent the intermediate and small material scales, respectively. Details about these RVE meshes can be found in Saavedra Flores et al. (2011). The 3-axis is related to the longitudinal direction of the alumina fibres, whereas 1 and 2-axes define the transversal directions, respectively.

### Table 2

Summary of the mechanical properties of alumina, magnesium alloy and epoxy matrix, adopted in the present multi-scale model. The units for Young’s modulus $E$ and yield stress $\sigma_y$ are GPa. These material properties have been obtained from Avedessian and Baker (1999), Altenhof et al. (2004), Bansal (2005), de Kok et al. (1993), Kubota et al. (1999), and Lebeau and Decker (1999).

<table>
<thead>
<tr>
<th>Constituent</th>
<th>$E$ (GPa)</th>
<th>$v$</th>
<th>$\sigma_y$ (GPa)</th>
<th>$\epsilon_{\text{ult}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alumina</td>
<td>414</td>
<td>0.23</td>
<td>~</td>
<td>0.003</td>
</tr>
<tr>
<td>Magnesium alloy$^a$</td>
<td>31.26</td>
<td>0.35</td>
<td>0.32</td>
<td>0.20</td>
</tr>
<tr>
<td>Epoxy$^a$</td>
<td>2.6</td>
<td>0.37</td>
<td>0.068</td>
<td>0.421</td>
</tr>
</tbody>
</table>

$^a$ An elastic-perfectly plastic behaviour has been assumed.
Alumina is modelled by means of an isotropic elastic material. Magnesium alloy and epoxy are modelled isotropically with a conventional von Mises law with no hardening. The mechanical properties of these constituents adopted in the present multi-scale framework are summarised in Table 2.

We study the new composite under approximate tensile loading conditions. Since we are interested in the constitutive response of the material, we focus our investigation to the study of the RVE at the intermediate material scale (fully coupled with the smallest material scale). By estimating a representative strain state at this scale, approximately equivalent to the actual tensile loading conditions, we can exclude from the multi-scale analyses the modelling of the large scale continuum. This approach allows us to reduce substantially CPU times and memory requirements in the finite element computations since fully coupled three-scale analyses are simplified into the analysis of two fully coupled material scales.

For compression wood cells of Norway spruce, Gindl et al. (2004) reported a MFA of $50.1^\circ$. Gierlinger et al. (2010) determined an average value of $43.51^\circ$ for the same type of cells. Similarly, Keckés et al. (2003) indicated an initial MFA of $45.7^\circ$ for compression wood cell. Consequently, an average MFA of $46.4^\circ$ will be assumed. Inspired in this feature, we adopt the same value for the angle between the longitudinal axis of the alumina fibres ($3$-axis) and the direction of the tensile loading ($Y$-axis, refer to inset in Fig. 5 for further details). In the finite element modelling, this (initial) orientation is obtained through a spatial rotation of the coordinates in the mesoscopic and microscopic meshes.

For simplicity, the constitutive response of the present composite is investigated under plane strain conditions. A rectangular element of material on the $X-Y$ plane (see inset in Fig. 5) is selected to estimate the strain state. From Saavedra Flores et al. (2011), the in-plane Poisson ratio with respect to the $X$ and $Y$-axes can be approximated by means of the expression $\nu = \frac{\cot(\alpha)}{2}$, in which $\alpha$ is the angle between the fibres and the tensile loading direction. By replacing $\alpha = 46.4^\circ$ in the above expression, we obtain $\nu = 0.9$. Therefore, the strain components $\varepsilon_{xx}$ and $\varepsilon_{yy}$ can be related through the condition $\varepsilon_{xx} = -0.9\varepsilon_{yy}$. Despite the limitation of this expression to small strains, it has shown good agreement with experimental data for different wood specimens and even for strains up to almost 20% (Saavedra Flores et al., 2011; Keckés et al., 2003). This simple equation results from the assumption of inextensible cellulose fibres in the wood cell-wall composite, and is accurate enough for initial MFAs close to $45^\circ$, when the cellulose fibres mainly undergo rotation. We remark, however that the assumption of inextensible fibres is used here only to define the macroscopic strain path to be...
imposed in the analysis of the RVE subjected to tensile loads, as an approximation to the actual (and more complex) strain path. It should be emphasised though that this assumption is not made in the constitutive definition of the fibres in the bio-inspired material. That is, in the present model the alumina and magnesium alloy fractions are modelled as deformable materials.

In addition, it is also reasonable to assume that the shear strains, $\gamma_{xy}$, are restrained due to the prevention of torsional rotation by the tensile testing device, that is, $\gamma_{xy} = 0$. Finally, under plane strain conditions ($\varepsilon_{zz} = \gamma_{yz} = \gamma_{xz} = 0$), the loading programme can be expressed as a strain vector $\varepsilon$ imposed on the RVE at the intermediate material scale, represented by

$$
\varepsilon = [\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \gamma_{xy}, \gamma_{yz}, \gamma_{xz}]^T = \varepsilon_{yy}[-0.9, 1.0, 0, 0, 0, 0]^T, \tag{6}
$$

in standard engineering strain array format. Static loading conditions are assumed in all of the analyses. The above expression (6) defines the (mesoscopic) strain path to be prescribed incrementally by means of a monotonically increasing strain component $\varepsilon_{yy}$. For each simulation, the strain component $\varepsilon_{yy}$ is increased from an unstressed virgin state of the RVE ($\varepsilon_{yy} = 0$), until failure in one of the constituents (alumina fibres, magnesium alloy or epoxy matrix). The mechanisms of failure considered in this investigation are detailed in the following section.

### 6. Failure mechanisms

The possible types of failure in the composite considered in this work are based on the Maximum Strain Criterion (Soni, 1983), due to its simplicity in terms of physical concept and also in terms of the material information required for its use. Since we adopt a fully coupled multi-scale finite element approach to analyse the material, the physical microscopic information, such as relative displacements, interaction among phases, localised bending of fibres, etc., can be easily retrieved. When combined with the very simple maximum strain failure criterion, this kind of modelling technique results in a very robust framework to predict the different stages of deformation and failure in the composite. In fact, the main philosophy of homogenisation-based multi-scale techniques is to adopt very simple phenomenological models at the microscopic level to obtain complex and possible intricate mechanisms of deformation at the macroscopic scale of difficult representations by means of conventional internal variable-based phenomenological models. Nevertheless, other more sophisticated failure criteria based on Continuum Damage Mechanics models (Lemaitre and Chaboche, 1990) could be adopted instead. However, the need of more experimental information for the basic constituents of wood and specific material parameters for each of these damage mechanics models makes this alternative unfeasible at present.

In this investigation, the total failure of the composite is assumed to be associated with the local failure of one of the constituents. When the strain exceeds the maximum value or ultimate strain in (at least) one of the constituents, the whole composite is assumed to reach the failure and the corresponding numerical simulation is stopped. Three possible mechanisms of failure are considered in this investigation and described as follows.

(i) **Longitudinal tensile failure in alumina:**

In this particular failure mode, the longitudinal tensile strain in the alumina fraction reaches the ultimate strain of 0.003. For each load step, the longitudinal tensile strain is computed as the change in length per unit reference length for each pair of longitudinally opposite nodes of the alumina constituent, in the microscopic finite element mesh. Refer to Fig. 6 for further details.

Since we are interested in representative quantities rather than localised maximum values, we calculate the volume average of these strains in order to obtain a representative value of the longitudinal tensile strain state, $\varepsilon_{al}$, in the material. This calculation is carried out at each microscopic finite element mesh, and then, over all the (mesoscopic) Gauss points belonging to the elements which define the homogenised material fibre, at the mesoscopic mesh level (refer to Fig. 5). This volume averaging process is possible since the strains and stresses distribution is nearly uniform.

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**Fig. 6.** Longitudinally opposite nodes considered for the calculation of $\varepsilon_{al}$ in the alumina fraction of the microscopic finite element mesh under tension.
over the whole homogenised material fibre, due mainly to the strong discrepancy in stiffness with respect to the very soft epoxy matrix.

(ii) Failure in the magnesium alloy due to accumulated plastic deformation:
Due to the rotation of the fibres, the magnesium alloy content may undergo a considerable amount of shear plastic deformation (see for instance, Fig. 7), particularly since its elastic stiffness is much smaller than that of alumina. In addition, a combination of tension and shear deformation modes, or other more complex strain paths, may increase even further the plastic strain state in the material. In order to quantify a representative plastic strain state, $\varepsilon_{\text{pl}}^{1,\text{mg}}$, for this general case, we volume average the equivalent plastic strains over all the elements which constitute the magnesium alloy fraction in the microscopic mesh (as shown in red in Fig. 7, on the left), and then, over all the Gauss points of the elements which define the homogenised material fibre, at the mesoscopic finite element mesh (Fig. 7, on the right). From the mechanical properties shown in Table 2, it is straightforward to estimate a value for the ultimate plastic strain of magnesium alloy under tensile loading. This ultimate value can be computed as $\varepsilon_{\text{pl}}^{\text{ult}} = \varepsilon_{\text{ult}} - \sigma_y/E = 0.20 - 0.32/31.26 = 0.19$. Therefore, the condition of failure is assumed to occur when the volume averaged equivalent plastic strain, $\varepsilon_{\text{pl}}^{1,\text{mg}}$, reaches the value of 0.19.

A second verification of failure is made in the outer surface of magnesium alloy which covers the inner periodic alternation of alumina and magnesium alloy. Here, the equivalent plastic strains are volume averaged over the region highlighted in pink as shown in Fig. 7, on the right. The choice of this particular region is made in view of the (possibly large) amount of tensile and shear plastic strains located at this region of the fibre. As in the previous case, the condition of failure is found when the volume averaged equivalent plastic strain, $\varepsilon_{\text{pl}}^{2,\text{mg}}$, reaches the value of 0.19.

(iii) Failure in the epoxy matrix due to accumulated plastic deformation:
As explained before, due to the misaligned orientation of the alumina/magnesium alloy fibres with respect to the tensile loading direction, the composite will tend to show large rotation of fibres and therefore, a large amount of accumulated shear plastic strains in the matrix (refer, for instance, to Fig. 7, on the right). Similarly, under tensile straining the composite may also exhibit separation of fibres which combined with the development of shear deformation may result in a worse condition. In order to quantify a representative strain state for this general condition, we calculate the volume average of the equivalent plastic strains over the red region shown in Fig. 8a. The calculation of the ultimate plastic strain in the material follows the same considerations explained before.

Therefore, from Table 2, we have that $\varepsilon_{\text{pl}}^{\text{ult}} = 0.421 - 0.068/2.6 = 0.395$ for the epoxy matrix. Consequently, the condition of failure in the matrix (and therefore in the composite) is assumed to occur when the volume averaged equivalent plastic strain, $\varepsilon_{\text{pl}}^{1,\text{epx}}$, reaches the ultimate value of 0.395.

Since the stress and strain fields in this region are not clearly uniform, we proceed to average the equivalent plastic strain in a second region. Preliminary results show a large amount of accumulated plastic strains concentrated in the region close to the interface magnesium alloy–epoxy (region shown in red in Fig. 8b). As in the previous case, the condition of failure is found when the volume averaged equivalent plastic strain, $\varepsilon_{\text{pl}}^{2,\text{epx}}$, reaches the ultimate value of 0.395.

In order to obtain normalised parameters for the potential mechanisms of deformation and failure in the composite, we divide the above averaged strains by their corresponding ultimate (elastic or plastic) strains. Therefore, these new

![Fig. 7. Typical shear failure mode in the magnesium alloy and epoxy due to the rotation of the fibres. Regions in red and pink show where the equivalent plastic strains have been averaged to compute $\varepsilon_{\text{pl}}^{1,\text{mg}}$ and $\varepsilon_{\text{pl}}^{2,\text{mg}}$, respectively, in the magnesium alloy fraction. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)](image-url)
normalised strains are defined as

\[
\eta_{al} = \tau_{al}/0.003, \quad \eta_{p,1}^{al} = \tau_{p,1}^{al}/0.19, \quad \eta_{p,2}^{al} = \tau_{p,2}^{al}/0.19,
\]

\[
\eta_{p,1}^{epx} = \tau_{p,1}^{epx}/0.395 \quad \text{and} \quad \eta_{p,2}^{epx} = \tau_{p,2}^{epx}/0.395.
\]

\[\text{(7)}\]

7. Numerical results

7.1. Local mechanisms of deformation

In order to investigate the mechanical response, we explore the local mechanisms of deformation and failure in this new material under the present loading conditions. Here, we assume 35\% volume fraction of alumina with respect to the whole volume of alumina/magnesium alloy fibre. An initial orientation of fibre of 46.4° with respect to the tensile loading direction is considered in all of the analyses presented in this section.

The numerical simulation is performed by imposing the strain vector \(\varepsilon\) incrementally on the mesoscopic finite element mesh. As explained in Section 6, the strain component \(\varepsilon_{yy}\) is increased monotonically from zero until reaching the failure of any of the constituents.

The graph of Fig. 9 shows the variation of the normalised average strains in alumina \((\eta_{al})\), magnesium alloy \((\eta_{p,1}^{al} \text{ and } \eta_{p,2}^{al})\) and epoxy \((\eta_{p,1}^{epx} \text{ and } \eta_{p,2}^{epx})\), according to the strain component \(\varepsilon_{yy}\).

Fig. 8. Regions in red show where the equivalent plastic strains have been averaged in the epoxy matrix. (a) Region adopted to compute \(\eta_{p,1}^{epx}\). (b) Region adopted to compute \(\eta_{p,2}^{epx}\). (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

Fig. 9. Variation of the normalised average strains in alumina \((\eta_{al})\), magnesium alloy \((\eta_{p,1}^{al} \text{ and } \eta_{p,2}^{al})\) and epoxy \((\eta_{p,1}^{epx} \text{ and } \eta_{p,2}^{epx})\), according to the strain component \(\varepsilon_{yy}\).
value close to the failure. As anticipated in Section 6, a large amount of plastic dissipation is observed, particularly in the interface magnesium alloy–epoxy. This is shown in Fig. 10, with the contour plot of the equivalent plastic strains projected on the nodes of the mesoscopic finite element mesh, at \( e_{yy} = 0.175 \). The fact that a large accumulation of shear deformation in the matrix does not result in failure is mainly due to the large value of ultimate strain adopted for epoxy (0.421). This choice has been made here in order to develop this new material by replicating the mechanical behaviour found in wood. As commented in Section 2, a large amount of shear deformation has been reported in the hemicellulose/lignin matrix of wood cell-walls under tensile straining, with no apparent damage in the matrix (Keckés et al., 2003).

A similar trend is found for the outer surface fraction of magnesium alloy which covers the alumina/magnesium alloy core. Here however, the maximum value of the normalised average strain, \( \eta_{mg}^2 \), reaches only a value of 0.65 at \( e_{yy} = 0.175 \). For the inner portion of magnesium, the normalised value of \( \eta_{mg}^1 \) is zero up to \( e_{yy} = 0.125 \). After this value, the inelastic yielding starts to develop in the inner core, and therefore, in the whole homogenised material fibre.

Further, we explore the sequential mechanisms of deformation under tensile loading in a stress–strain curve for the same case analysed above (35% volume fraction of alumina with respect to the total volume of fibre with an initial orientation of 46.4°). The stress and strain components, \( \sigma_{yy} \) and \( \epsilon_{yy} \) (in the tensile loading direction) along with the different stages of deformation, are plotted in Fig. 11.

The corresponding graph shows a predominantly linear response for small strains up to about 1%. After this level of deformation, an important reduction of the slope occurs. An examination of the numerical results shown in Fig. 9 reveals that this change in the slope is mainly associated with the onset of yielding in the epoxy matrix. As the deformation progresses, the alumina/magnesium alloy fibres tend to rotate and the angle between the fibres and the tensile loading axis reduces considerably. The corresponding alignment of the fibres results in the fibre reorientation-induced stiffening shown in Fig. 11. Further increase of the tensile loading results in a second important change of slope, at \( e_{yy} = 0.125 \), which is related to the beginning of plastic strains in the inner portion of the magnesium alloy, as shown in Fig. 9. We note here that little amount of plastic deformation in the inner portion of the magnesium alloy is needed to generate a noticeable change in the slope of the stress–strain curve. This is due to the large volume fraction of magnesium alloy involved in this dissipative process.

As mentioned above, the last stage of deformation occurs at \( e_{yy} = 0.175 \), when the alumina fibres begin to reach their ultimate strain, resulting in the complete failure of the composite.

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**Fig. 10.** Contour diagram of equivalent plastic strains in the mesoscopic finite element mesh at \( e_{yy} = 0.175 \).

**Fig. 11.** Typical tensile stress–strain curve for the bio-inspired material and the different stages of deformation.
7.2. Toughness as a function of alumina volume fraction: inspiration in cellulose crystallinity from trees and plants

Fig. 12 shows the stress–strain curves for different percentages of alumina volume fraction (with respect to the whole volume of fibre). For volume fractions between 35% and 100% the mechanical response is virtually the same for strains under 1%. From the numerical results, it can be concluded that up to this level of strain, the whole (alumina/magnesium alloy) fibre remains almost inextensible. The small influence of the alumina volume fraction on the overall mechanical response at lower strain levels is attributed to the large angle (near 45°) between the fibres and the tensile loading axis at this stage. Here, only a small portion of the axial load is carried by the fibre. In addition, the main mechanism of deformation in the composite is shear, localised in the epoxy matrix, due to the relative displacements among (alumina/magnesium alloy) fibres undergoing rotation and alignment in the stretching direction. Therefore, any increase of the stiffness in the fibre due to a rise in the volume fraction of alumina will not affect significantly the overall mechanical response of the composite under low strain levels since the fibre will experience predominantly changes in its orientation rather than straining along its own axis. As explained before, if the straining process continues, the corresponding alignment of fibres will result in fibre reorientation-induced stiffening, as shown in Figs. 11 and 12. Consequently, for only moderate to large strains, the choice of different volume fractions of alumina in the fibre will lead to different levels of stiffness in the material. On the contrary, for smaller strains (possible during service conditions) the amount of very stiff fraction in the fibre will have very little influence on the overall response of the material.

Fig. 12. Typical tensile stress–strain curve for the bio-inspired material with different percentages of alumina volume fraction (with respect to the whole volume of fibre).

Fig. 13. Normalised toughness in the composite for different volume fractions of alumina (with respect to the total volume of fibre). The range of crystalline volume fraction found in nature (from cellulose in trees and plants) and indicated in this figure (between 0.5 and 0.55) has been obtained from Newman and Hemmingson (1990), Sivonen et al. (2002), Andersson et al. (2004), and Newman (2004); Harris and DeBolt (2008).
Importantly, all of the curves shown in Fig. 12 have been truncated for the first failure mechanism detected in one of the constituents of the composite. For the particular loading conditions and initial orientation of fibre considered in this work, the total failure of the material coincides with the elastic failure of alumina fibres in all of these cases.

From the numerical results obtained in the present simulations, it is straightforward to calculate the area under stress–strain curves up to failure, which represents a measure of toughness or ability to absorb strain energy up to failure. Fig. 13 shows these values for volume fractions of alumina between 0.3 and 1.0. We remark that a volume fraction of 1.0 represents the composite when the whole fibre is made of only alumina, with no fraction of magnesium alloy. This particular case corresponds to the traditional engineering solution in which the fibre is made of one single very stiff material. Due to its relevance, the values shown in Fig. 13 have been normalised by the value of toughness determined for this particular case.

Remarkably, by observing Fig. 13, it is evident that the maximisation of the normalised toughness in the present bio-inspired material occurs for volume fractions between 0.5 and 0.55, the same range of experimental values found typically in trees and plants for their cellulose crystallinity (refer to Section 2 for further details). Consequently, the results shown here and obtained from the present multi-scale model, demonstrate that the choice of alumina volume fraction according to those values found in the crystalline cellulose of wood cells (bio-inspiration) results in a maximisation of toughness in this new material.

The above remarkable observation provides new clues into the understanding of how trees and plants optimise their microstructures at the cellulose level in order to absorb a large amount of strain energy before failure.

For a 50% alumina volume fraction, the graph in Fig. 13 also reveals an increase by almost 46% in the toughness of the composite, and therefore in its ability to absorb strain energy, when compared to the traditional engineering solution. We remark however that, when compared to the toughness of pure alumina, the difference becomes much more noticeable, resulting in an increase by almost 450%.

In terms of ultimate strains (and therefore in terms of ductility), the composite reaches a maximum value of 15.9% before failure (for a 50% alumina volume fraction), which represents a value 53 times greater than the maximum strain of 0.3% for alumina.

8. Conclusions

Fundamental concepts involved in wood cell mechanics have been exploited in order to design a new bio-inspired composite. A fully coupled multi-scale finite element model has been proposed to investigate the mechanical response of a new alumina/magnesium alloy/epoxy three-phase composite. Numerical results have demonstrated that the choice of the volume fraction of alumina based on those volume fractions of crystalline cellulose found typically in nature results in a maximisation of toughness in the present bio-inspired composite. An amplification by almost 450% in the toughness of the composite and an increase in its ultimate strain by 53 times has been found when compared to the corresponding values of pure alumina. The features presented above have been replicated from trees and plants and represent a natural mechanism to absorb a large amount of strain energy before the structural failure of these natural materials.

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