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From lignin to spruce: Poromechanical upscaling of wood strength

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ABSTRACT

Wood strength is highly anisotropic, due to the inherent structural hierarchy of the material. In the framework of a combined random-periodic multiscale poro-micromechanics model, we here translate compositional information throughout this hierarchy into the resulting anisotropic strength at the softwood level, based on "universal" elastic properties of cellulose, hemicelluloses, and lignin, and on the shear strength of the latter elementary constituent. Therefore, derivation of the elastic energy in a piece (representative volume element – RVE) of softwood, stemming from homogeneous macroscopic strains prescribed in terms of displacements at the boundary of the RVE and from pressure exerted by water filling the nanoporous space between the hemicelluloses-lignin network within the cell walls, with respect to the shear stiffness of lignin, yields higher order strains in the lignin phase, approximating micro-stress peaks leading to local lignin failure. Relating this (quasi-brittle) failure to overall softwood failure (or strictly speaking, elastic limit of softwood) results in a macroscopic microstructure-dependent failure criterion for softwood. The latter satisfactorily predicts the biaxial strength of spruce at various loading angles with respect to the grain direction. The model also predicts the experimentally well-established fact that uniaxial tensile and compressive strengths, as well as the shear strength of wood, depend quasi-linearly on the cell water content, but highly nonlinearly on the lumen porosity.

INTRODUCTION

It is well accepted that changes in lumen porosity, as well as such in cell wall composition are the key factors governing wood strength magnitude and anisotropy. However, what remains a matter of discussion is how wood strength is functionally dependent on the aforementioned key factors. In this context, correlations between respective experimental data are often expressed in terms of empirical relations [1,6,13]. However, such relations are, as a rule, restricted in applicability and reliability, since they do not explicitly consider the mechanical behavior of the complex hierarchical microstructure of wood, which underlies the aforementioned correlations. As a remedy, we here aim at predicting relationships between porosity/composition and strength (i.e. brittle ultimate strength and yield limit in case of ductile behavior) in a micromechanical framework including random as well as periodic homogenization techniques [12,14].

THEORY AND EXPERIMENTAL VALIDATION

By combining a recently developed poroelastic multiscale model for softwood [2,7] with a *von Mises*-type failure criterion for lignin, we derive a species and specimen-specific multiscale model for lignin-related elastic limits in softwood (see figure 1). This model rests on "universal", tissue-independent elasticity properties of the elementary constituents of wood, given in table I, and on a shear strength value for lignin of 14.3 MPa, the reaching of which is identified as (lower bound for) overall failure. We use quadratic strain averages to assess the loading state and possible failure of lignin. The quadratic average of the equivalent deviatoric strain can be suitably estimated in the framework of the poroelastic multiscale model by equating two representations of the elastic energy density in a wood tissue, which are formulated in terms of microscopic and macroscopic strains and elastic properties, respectively, and by deriving the resulting relation with respect to the shear modulus of lignin.

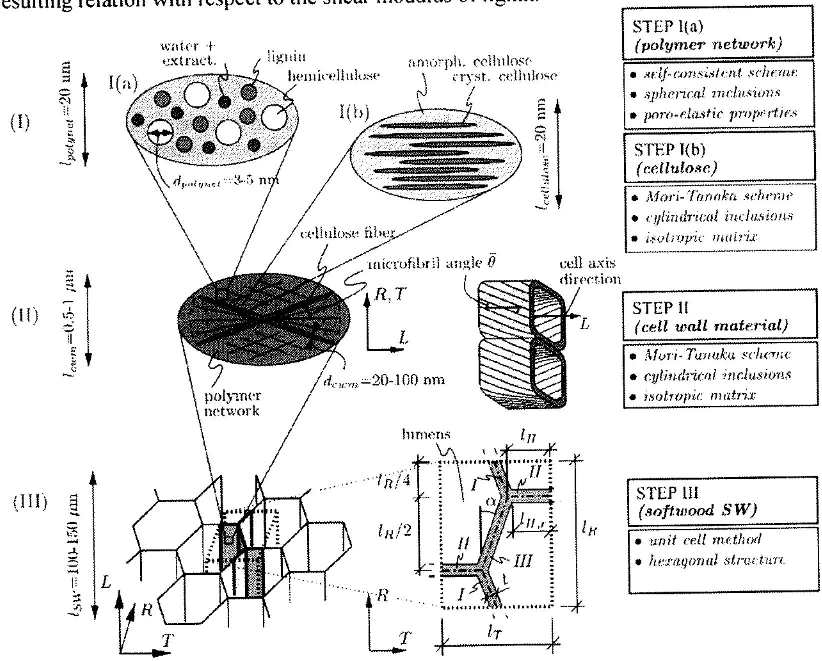

Figure 1: Four-step homogenization scheme on three hierarchical levels, with base frame for definition of stiffness tensors: *L* (longitudinal) marks direction parallel to grain, and all directions in the plane spanned by *R* (radial) and *T* (tangential) are perpendicular to the grain [2].

This model predicts very satisfactorily compression-dominated biaxial strength data for spruce (where lignin failure at the nanolevel closely indicates overall failure at the softwood level), and it gives a reliable lower bound for tension dominated biaxial strength data of spruce (where significant loads may be carried even after lignin has reached its elastic limit), see figure 2. Given these overall satisfactory predictive capabilities of the model, it offers itself for studies related to the influence of lumen porosity and loading angle on the uniaxial tensile strength, see figure 3. Corresponding predictions of uniaxial strength show a quasi-linear dependence of strength on porosity and a highly non-linear dependence on the grain angle. These general characteristics agree well with experimental observations gained over decades, which so far were frequently expressed only in terms of empirical relationships [6,8,9].

Table I: "Universal" (tissue-independent) phase properties [3].

Phase	Material behavior	Bulk modulus k [GPa]	Shear modulus μ [GPa]
Amorphous cellulose	isotropic	$k_{amocel} = 5.56$	$\mu_{amocel} = 1.85$
Hemicellulose	isotropic	$k_{hemcel} = 8.89$	$\mu_{hemcel} = 2.20$
Lignin	isotropic	$k_{lig} = 5.00$	$\mu_{lig} = 2.30$
Water + extractives	isotropic	$k_{H2Oext} = 2.30$	$\mu_{H2Oext} = 0$
		Stiffness tensor components c_{ijkl} [GPa]	
Crystalline cellulose	transversely isotropic	$c_{crycel,1111} = 34.86$ $c_{crycel,3333} = 167.79$ $c_{crycel,1313} = 5.81$	$c_{crycel,1122} = 0$ $c_{crycel,2233} = 0$

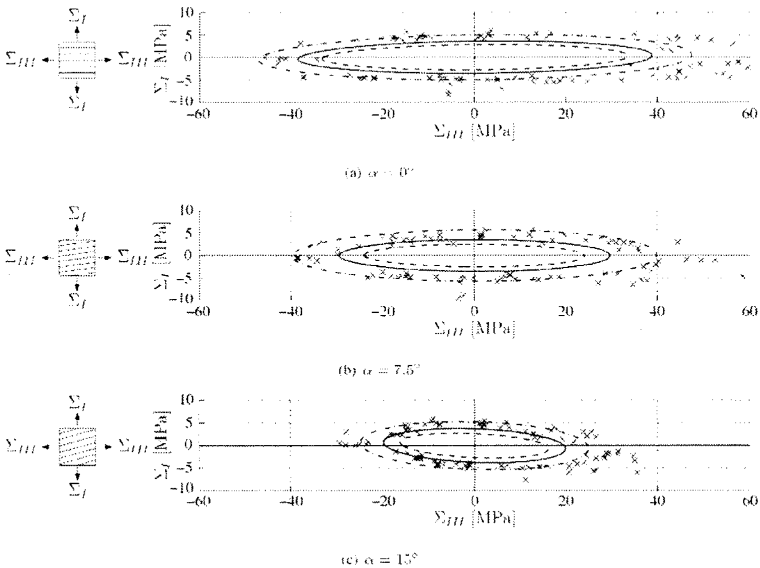

Figure 2. Results of biaxial experiments and corresponding microporomechanical predictions of plane failure surfaces at different angles α between principal loading and material directions: model predictions with mean mass density (solid line) and with maximum and minimum mass density (dashed line) of all test specimens [3].

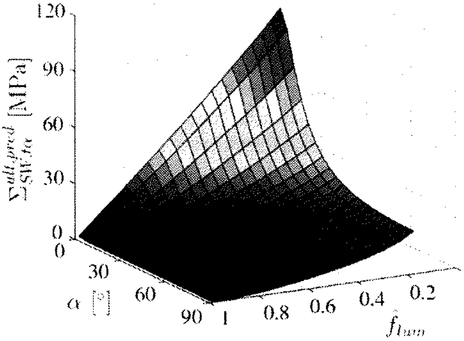

Figure 3. Model estimates for the tensile elastic limit of softwood as a function of the lumen porosity and of the loading or grain angle between principal loading and material directions, for volume fractions typical for softwood [3].

RESULTS AND DISCUSSION

It is also interesting to discuss our modeling approach, which is based on poroelastic concentration and influence relations [3,11] relating lignin failure stresses to stresses at the macroscopic level of spruce, in view of possible nonlinearities in the macroscopic stress-strain relations prior to reaching the ultimate strength of spruce. In this context, it is beneficial to refer to four basic mechanisms in spruce behavior as discussed by Mackenzie-Helnwein et al. [10]: Upon dominant tensile loading in fiber direction, a linear elastic stress-strain regime is bounded by perfectly brittle failure (see figure 4(a)). Under these conditions, the micromechanics-predicted, lignin-failure related limit state of macroscopic stress is identical to the ultimate strength of spruce (unless additional load carrying capacity is provided by the cellulose fibers once the lignin has failed, as is reflected by the experimental points lying outside the model-predicted surfaces in figure 2(a)). The same situation is encountered upon dominant tensile loading in radial direction, see figure 4(b). Upon dominant compressive loading in fiber direction, an elastic regime pertains up to about 75% of the ultimate stress level, followed by a regime of reduced stiffness, before the sample experiences brittle failure (see figure 4(c). Also under these conditions, the micromechanics-predicted, lignin failure-related limit state of macroscopic stress is identical to the ultimate strength of spruce. Hence, in comparison to the purely elastic case, damaging processes leading to the reduced stiffnesses prior to reaching the ultimate load level do not alter the relations between microscopic failure stresses in lignin and corresponding macroscopic stress in spruce. This strongly suggests that the aforementioned damage processes are not related to lignin failure, but rather occur in terms of microcracks at the lignin-cellulose interface. Also upon dominant compressive loading in radial direction, the macroscopic stress-strain curve exhibits a nonlinear portion (see figure 4(d)). However, under these loading conditions, the micromechanics-predicted, lignin failure-related limit states of macroscopic stress relate to the elastic limit (yield limit) of the material. Hence, inelastic processes in lignin, potentially related to compaction of the polymer matrix, are key to the nonlinear regime which finally encompasses ductile material failure.

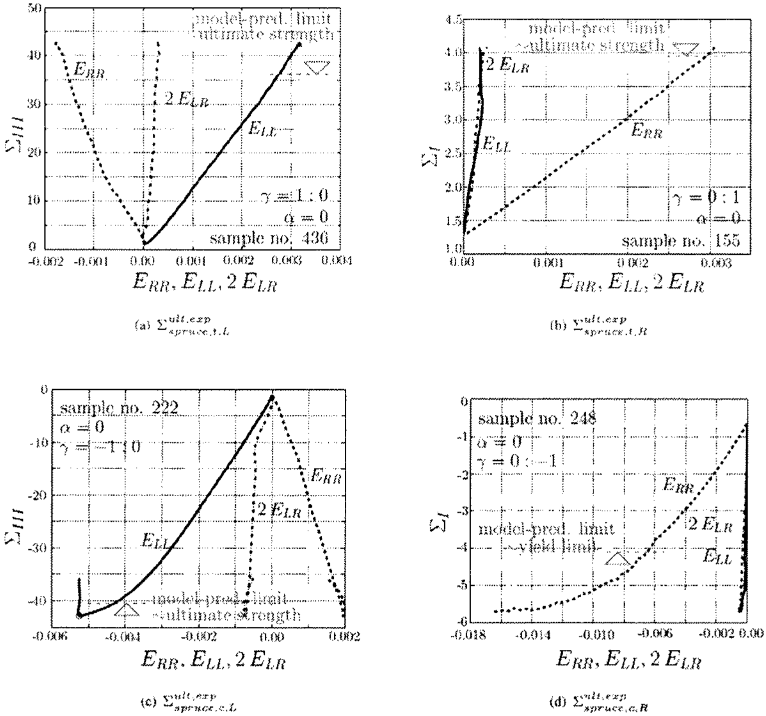

Figure 4. Typical stress-strain relationships in experiments of Eberhardsteiner [4], and corresponding model-predicted lignin failure-induced strength limits, see also figure 2(a): (a) uniaxial tension in longitudinal direction, (b) uniaxial tension in radial direction, (c) uniaxial compression in longitudinal direction, (d) uniaxial compression in radial direction [3].

CONCLUSIONS

A poroelastic multiscale model for softwood with a von Mises-type failure criterion for lignin was shown to very satisfactorily predict the biaxial strength of spruce at various loading angles with respect to the grain direction. The model also predicts the experimentally well-established fact that uniaxial tensile and compressive strengths, as well as the shear strength of wood, depend quasi-linearly on the cell water content, but highly nonlinearly on the lumen porosity. Upon dominant tensile and compressive loading in fiber direction and upon dominant tensile loading in radial direction, the micromechanics-predicted, lignin failure-related limit states of macroscopic stresses relate to the ultimate load, whereas upon dominant compressive loading in radial direction, they relate to the elastic limit (yield limit) of the material.

While the authors believe that the present model is the very first multiscale poromechanics model related to wood strength, the theoretical restriction to lignin-related elastic limits may be regarded as limitation worth to be overcome in the future: This could be done in the newly emerging field of random homogenization-based multiscale elastoplasticity [5,11].

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