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3D COMPUTATIONAL HIERARCHICAL MODEL OF WOOD: FROM MICROFIBRILS TO ANNUAL RINGS

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Abstract

Based on the structures of wood at several scale levels, a 3D hierarchical computational model of wood is developed. At macrolevel, an improved rule-of-mixture model, based on 3D orthotropic stress-strain relations and taking into account the compatibility of deformations at the interface of two phases and equilibrium of tractions at phase boundaries, is proposed for the analysis of the effect of the annual rings structure on the properties of softwood. At mesolevel, the layered honeycomb-like microstructure of cells was modeled as a 3D unit cell with layered walls. The finite element model was generated in the preprocessing FE software PATRAN using the parametric modeling technique. At submesolevel, each of the layers forming the cell walls was considered as composite, taking into account the experimentally determined microfibril angles and chemical contents. The elastic properties of the layers were determined through FEM. With the use of the developed hierarchical model, the influence of the microstructure, including microfibril angles (MFAs), the cell shape angles (CSAs) and the wood density (annual ring structure) on the elastic properties of softwood was studied. The computational results are compared with experimental data, and good agreement can be obtained.

1 Introduction

Recently, the mechanical properties and microstructure-strength relationships of wood started to attract a growing interest of researchers. The reasons for this upsurge of research activity in this area are twofold. Firstly, wood reappeared in civil industry, and the problem of prediction of strength and reliability of wooden parts more significant for practical applications. Another reason for the growing interest in the microstructure mechanical properties and -strength relationships of natural materials is called 'biomimicking'. As differed from the most of manmade materials, the strength, damage and fracture resistance of wood are by several orders higher than the strength and damage resistance of its components (cellulose, lignin). Other natural biological materials demonstrate often the extraordinary strength, damage resistance and hardness as well. The interest in the possibilities of mimicking the microstructures of biomaterials in order to design and to improve composites and other man-made materials encouraged many scientists to initiate their studies of microstructure-strength and microstructure-damage resistance relationships of biomaterials ([1]-[3]).

Following the characteristic length scales, softwood can be usually described at four different structural levels [4]. At the macroscale, it contains many annual rings, which appear as alternating light and dark rings. The lighter rings are called earlywood, characterized by cells with large diameters and thin cell walls, while the darker rings being latewood characterized by cells with small diameters and greatly thickened cell walls. At the mesoscale, it is a cellular material, built up by hexagon-shaped-tube cells oriented fairly parallel to the stem direction. At the microscale, every cell wall of wood consists of 4 layers with different microstructures and properties, which are called usually P, S1, S2 and S3, and middle layer M acts as bonding material. At the nanoscale, the S1, S2 and S3 layers in the secondary wall of a tracheid cell are built of several hundred individual lamellae with varied volume fractions and characteristic microfibril angles (MFAs).

The cellular microstructure of softwood makes it a member of the large family of foams and honeycombs. Easterling et al. [5] and Gibson and Ashby [6] modeled softwood as a honeycomb with regular hexagons, and assumed that rays cause the higher elastic modulus in the radial direction. However, Boutelje [7] studied the swelling mechanisms in pines with different densities experimentally, comparing tissue with rays and tissue without rays, and demonstrated that the anisotropy of swelling does not depend on whether the samples contain rays or not. Then, some other cellular models, irregular hexagons [8], honeycombs with cell walls being bent and stretched [9], honeycombs with the variation of the cell wall thickness [10] and so on were developed to study the elastic properties of softwood. The cellular models allow predicting the elastic properties of softwood, taking into account the mesostructure of softwood, cell shape and properties of the cells. However, Mark [11] and Bodig and Jayne [12] pointed out that the cell wall is an anisotropic material, built up as cellulose fibrils as reinforcement in the hemicellulose and lignin matrix. The cellular models did not take into account the helix structure of microfibril in the secondary layer, multilayered cell wall and annual ring structures, and they normally were applied only to the analysis of earlywood.

A more complex group of models are the multiscale, homogenization-based models. So, Harrington et al. [13] presented a two-stage analytic homogenization scheme based on two assumptions: the softwood cell wall is a heterogeneous continuum at the nanostructural level, and the classic laminate theory can be used to determine the equivalent properties of the wall. They used this approach to determine the equivalent orthotropic elastic constants for a cell-wall lamella. Hofstetter et al. [14] developed a micro-elastic model based on a four-step homogenization scheme for softwood from a length scale of several tens of nanometers, to a length scale of around one micron, to a length scale of about one hundred microns, to a length scale of several millimeters. Further, Hofstetter et al.[15] presented a homogenization scheme containing two continuum homogenization steps (random homogenization), and one step based on the unit cell method (periodic homogenization). Homogenization-based models can take into account the microstructure of softwood, covering several orders of magnitude, from the cell wall structure, to the structure of fibers, to the macroscopic defects.

In a series of works, wood was considered as a composite at several scale levels. Combining the cellular models with the cell wall-related composite models, Astley and his colleagues [16][17] developed multi-scale models and carried out three-dimensional finite element simulations of representative sections of the softwood cell structure. They assumed that each closed cell of the cellular array contained seven composite laminated layers which are treated as a thick laminated shell through the classical laminate theory. The numerical finite element model was realized with thick composite shell elements, and used to analyze interrelationships between the macroscopic elastic properties of softwood and the local microstructural characteristics of cells such as the cell dimension, wall thickness, moisture content and microfibril angle. Bergander and Salmen [18] modeled the double radial fiber wall as a nine-layered laminate with composite cell walls, using the Halpin-Tsai model(HTM) [19] and the classical lamination theory. Composite models allow considering the structures of softwood at both meso and micro levels. As different from the homogenization-based models, the discrete multiscale continuum mechanical models permit to model damage and strongly nonlinear and time-dependent behavior of the elements of the softwood microstructures.

Qing and Mishnaevsky Jr. [20][21] modeled softwood as a cellular material with fibril reinforced, heterogeneous multiple layers under three assumptions: at the mesoscale, softwood is considered a bundle of hexagonal cells of prescribed cross-sectional tracheids with walls of constant thickness; at the microscale, the cell wall of the tracheids is represented as an elastic laminate with five layers: M, P, S1, S2 and S3; at the nanoscale, the lamellae represent fibril reinforced composites, with their own volume fractions and characteristic MFAs. Their model can be easily extended to include the micro- and nanoscale damage, and nonlinear behavior of softwood.

However, these micromechanical models of wood do not take into account the distinct softwood structure at the macrolevel,consisting of annual rings with regions of low density (earlywood) and high density (latewood). It is therefore an oversimplification to define softwood as an ideally periodical cellular structure. All of the four scale structures are important microstructural characters controlling wood properties. The models of softwoods, which take into account all the relevant levels of wood structure, should offer a better understanding of the mechanical properties and strength of wood, and allow identifying important microstructural parameters and their influence on mechanical properties.Models, which take into account alternate structure of earlywood and latewood within an annual ring, are required for the numerical analysis of the mechanical properties of softwood. Some efforts were made to develop computational models of wood, which take into account both the annual rings and cellular structure of wood. Koponen et al. ([22],[23]) developed a model consisting regularly shaped cells of earlywood and latewood (the contents of earlywood and latewood are calculated from a given wood density). They calculated the orthotropic elastic constants from model of Chou et al.[24] and shrinkage properties from Schniewind's model [25]. Modén and Berglund [26] modeled the annual ring structure as a two-phase cellular model (with homogeneous walls) which includes both cell wall bending and stretching deformation mechanisms. Kelvin model is used to calculate the tangential modulus and Voigt model is used to calculate the radial modulus. Koponen and colleagues, and Modén and Berglund applied the rule-of-mixture to calculate the moduli of softwood. However, the tractions at the phase boundaries can not be in equilibrium under Voigt stress field, while the heterogeneities and the matrix could not be perfectly bonded under the implied Reuss strains. Therefore, Qing and Mishnaevsky Jr. [27] proposed an improved rule-of-mixture (IRoM) model to study the influence of annual rings on the elastic and expansion induced by moisture of wood.

The purpose of this work is to develop a model of wood, which takes into account four levels of wood microstructure (annual rings, cellular structure, multilayered cell walls, microfibril reinforced wall sublayers), which allow analyzing the effect of microstructure of softwood on its elastic properties. The annual ring structure is modeled with the use of IRoM model[27], which reflects the deformation compatibility of two phases (early and latewood) and is based on the 3D stress–strain relations. Using the 3D multiscale computational model of wood from Qing and Mishnaevsky Jr. [20][21] and combining it with the IRoM model of annual rings, we analyze the effect of microstructural parameters on softwood on the elastic properties. The model is verified by comparison with the experimental results [28] and data from the Wood Handbook [29].

2 Computational hierarchical model

2.1 Improved 3D rule-of-mixture model at macrolevel

For the micromechanical analysis, the annual ring structure of softwood can be idealized as shown on **FIGURE 1**. The unit cell of the annual ring includes earlywood and latewood regions. Each region is assumed to be homogeneous orthotropic material with coaxial principal directions.

The apparent approach for the analysis of this model is rule-of-mixture (RoM). However, the traditional RoM model has some intristic contradictions: Kelvin model is kinematically inadmissible and Voigt model is statically inadmissible for the rule-of-mixture. In order to analyze the model of bilayered unit cell from **FIGURE 1**, we develop an improved version of the rule-of-mixture approach, using the 3D orthotropic stress-strain relations. The model takes into account the constraints on the compatibility of deformations at the interface of two phases and equilibrium of tractions at phase boundaries. In **FIGURE 1**, V^L and V^E are the volume contents of reinforcement and matrix, respectively (In this paper, variables with superscripts E and L mean the properties of earlywood and latewood, respectively.). The values V^E and V^L are related by

$$V^E + V^L = 1 \quad (1)$$

To calculate the volume content of reinforcement and matrix, the relationship between the density of composite ρ and the densities of earlywood and latewood can be expressed as

$$\rho^E V^E + \rho^L V^L = \rho \quad (2)$$

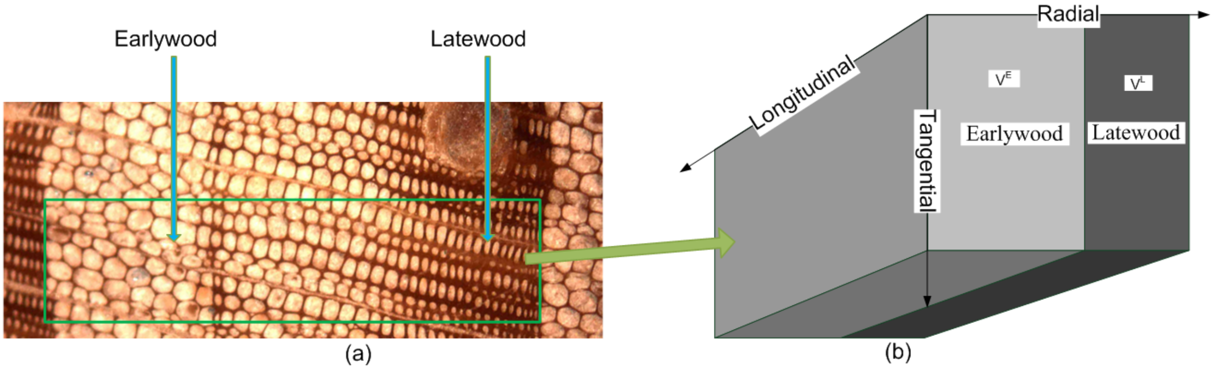

Figure 1. Schematically idealized model for annual ring structure of softwood

The Young's moduli and the Poisson's ratios along principal directions of composite can be calculated under uniaxial tension loading along the 3 principal directions, respectively. From the equilibrium conditions, the radial stresses of matrix and reinforcement should be equivalent,

$$\sigma_R^E = \sigma_R^L = \sigma_R \quad (3)$$

And from the deformation compatibility condition, the deformation of matrix and reinforcement should be equivalent in the L and T directions:

$$\begin{cases} \varepsilon_L^E = \varepsilon_L^L = \varepsilon_L \\ \varepsilon_T^E = \varepsilon_T^L = \varepsilon_T \end{cases} \quad (4)$$

2.2 Unit cells for cell wall at mesolevel

In order to analyze the wood at mesolevel (cell level), a 3D unit cell model of wood was developed as shown in **FIGURE 2**. The model generation begins with a two dimensional parametric cross section, which is used to create a solid model through extrusion along a straight line perpendicular to the section. **FIGURE 2.a** gives an example of changeable dimension variables in the cross-section, such as the cell dimension, cell shape, thickness of cell wall. As the section is swept along a straight line, solid geometry is automatically generated. When input parameters (section dimensions, sweep line length, etc.) are modified, the solid geometry is automatically updated.

The mesh shown in **FIGURE 2.b** was created with MSC/PATRAN/IsoMesh using Mesh Seeding. The finite element type is three dimensional 8-node brick element (C3D8). An ABAQUS input file has been produced through playing the PATRAN session file.

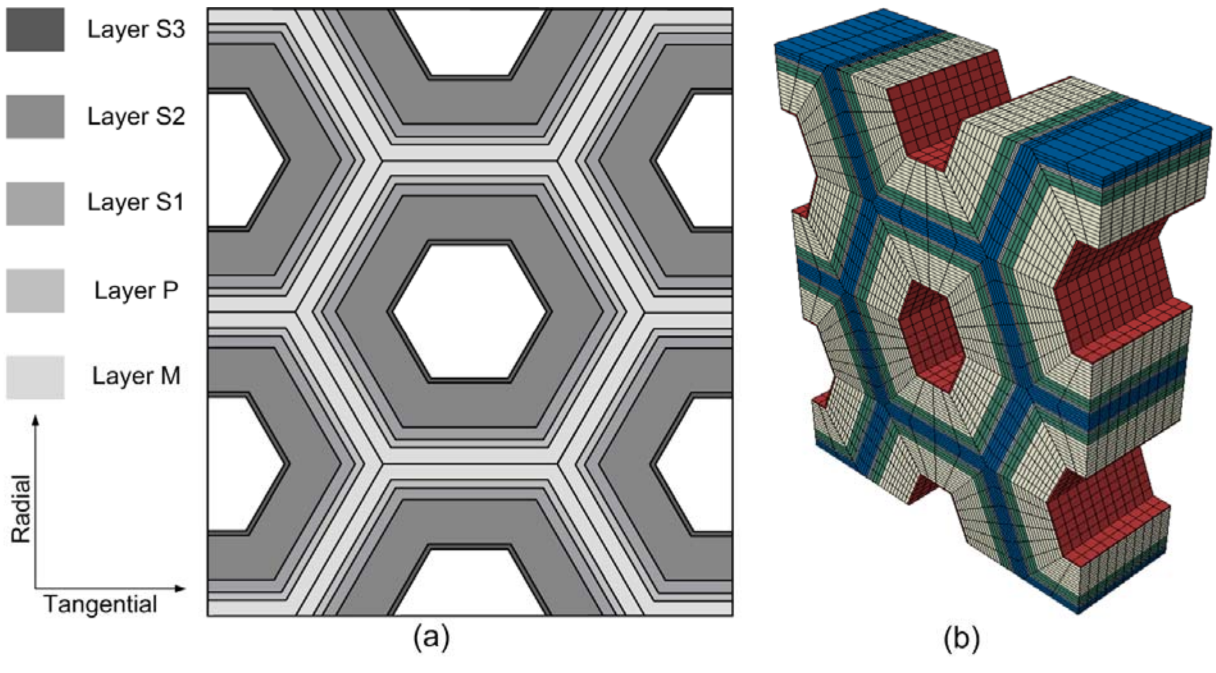

Figure 2. 3D finite element unit cell model of latewood and early

2.3 Unit cells for cell wall at submesolevel

The cell walls consist of the several sublayers (primary wall P and secondary wall S, which in turn consists of three layers S1, S2 and S3). The layer P is built a randomly distributed network of short cellulose microfibrils and is isotropic, while the secondary wall is consider as unidirectional microfibril reinforced composite and is a transversely isotropic material. Middle layer (M) is an isotropic material and acts as bonding material. The five layers differ in their thickness, their microfibril angles and the fractions of the chemical constitutes. The

cellulose microfibrils are embedded in the hemicellulose [30]. Table 2 gives typical ultrastructural parameters of the layers [20].
As a first approximation for the elastic deformation, we model these materials as cubic unit cells (**Figure 3.a** and **b**). The logic behind this simplification is that the multireinforcement unit cells with randomly oriented short fibers and spheres show the same elastic behavior, as demonstrated by Bohm et al. [31]. In the schema of **Figure 3**, the central core, the middle layer and the outmost layer of the RVE represent microfibrils (celluloses), hemicellulose and lignin, respectively. The elastic results obtained from the cubic unit cell models (Figure 3.a-b) and from the self-consistent method (SCM) and Halpin-Tsai model (HTM)[19] are compared in Table 2, in order to validate the accuracy of the cubic unit cell methods.

The basic lamellae in S1, S2 and S3 layers are transverse elastic materials. Taking into account the periodicity and symmetry conditions, a represented volume element (RVE) has been chosen to study the elastic behaviors for these sublayers[32]. The RVE is shown in **Figure 3.c**.

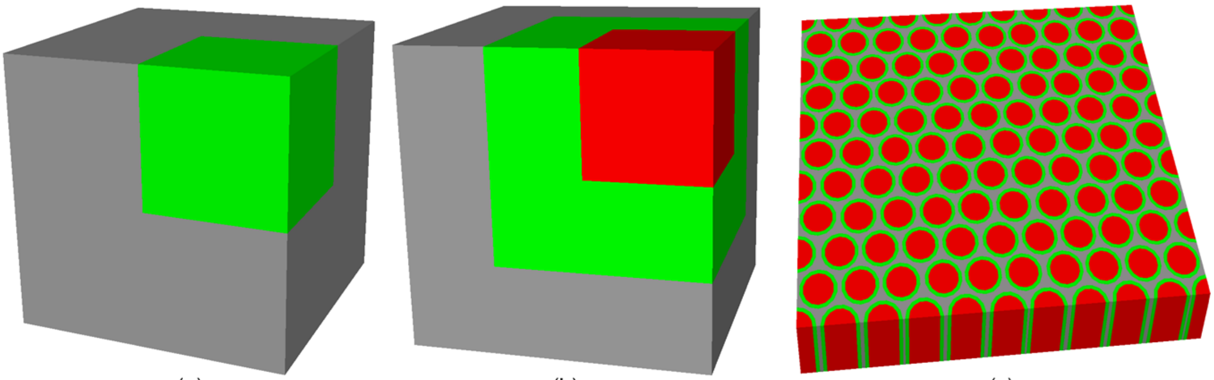

Figure 3. The homogenized procedure for the RVE of cell wall

Layer	Thickness (μm)		MFA		Chemical contents (%)		
	Earlywood	Latewood	Earlywood	Latewood	Cellulose	Hemicellulose	Lignin
M	0.5	0.5	Random	Random		38	62
P	0.1	0.1	Random	Random	12	26	62
S_1	0.2	0.3	±50-70	±50-70	35	30	35
S_2	1.4	4.0	10-40	0-30	50	27	23
S_3	0.03	0.04	±60-90	±60-90	45	35	20

Table 1 The ultrastructural parameters of the cell wall layers

	E (GPa)			υ		
Methods	FEM	HTM	SCM	FEM	HTM	SCM
Layer M	2.95	2.82	2.88	0.29	0.3	0.295
Layer P	3.81	3.97	3.79	0.26	0.28	0.285

Table 2 Elastic properties of layers M and P with 12% moisture content

3 Computational results and discussions

3.1 The influence of MFA in S2 on stiffness of wood

The simulation results [20] showed that the cell shape angle (CSA) has almost no influence on the longitudinal Young's moduli (E_L) of softwood. **Figure 4** illustrates the computational results of longitudinal Young's moduli for regular hexagonal cross section. From **Figure 4**, it can be seen that the Young's modulus increases with increasing the wood density (if MFA is kept constant), and decreases with increasing MFA (if the wood density is kept constant). In order to verify the model, we compared the simulations results with the experimental results from Schimleck et al. [28]. In **Figure 4**, the discrete star-points represent the experimental results from Schimleck et al., the numbers behind which indicate the MFAs. It can be seen that the developed multiscale model provides accurate estimations of longitudinal Young's moduli.

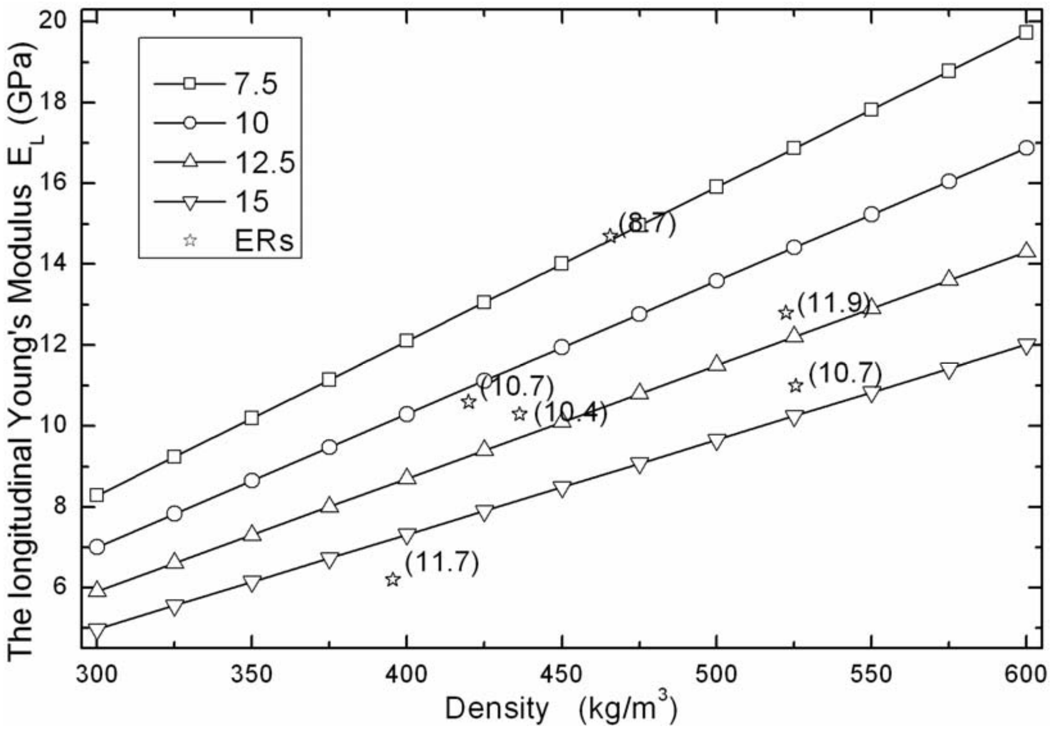

Figure 4. The longitudinal Young's moduli under different wood density and different MFAs (ERs - the experimental data from Schimleck et al. [28], the numbers behind the star-points indicate the MFAs)

3.2 Transverse anisotropy of softwood

Softwood is a highly anisotropic material [33]: the radial modulus E_R is typically 1.5-2.0 times as high as the tangential modulus E_T. The transverse anisotropy of the wood, the ratios of the Young's moduli between radial and tangential directions, should be taken into account to model the stresses accurately, especially including shrinkage and swelling behaviors of wood.

The simulation results [27] showed that the microfibril angle (CSA) has almost no influence on the transverse anisotropy of softwood. The test results of Watanabe et al. [9] shows that cell shape angle ranges from 7° to 19° for different species of softwoods. **Figure 5** illustrates the computational results of transverse anisotropy for different CSAs (CSAs θ=10°, θ=12.5° and θ=15°) and wood densities. From **Figure 5**, it can be seen that the transverse anisotropy increases with decreasing the CSA (if wood density is kept constant), and decreases with increasing wood density (if CSA is kept constant). In order to verify the model, we compared the simulations results with the experimental results from wood handbook [29]. In **Figure 5**, the discrete star-points represent the experimental results from wood handbook. One can find that the two-phase model gives more accurate results than the single-phase model.

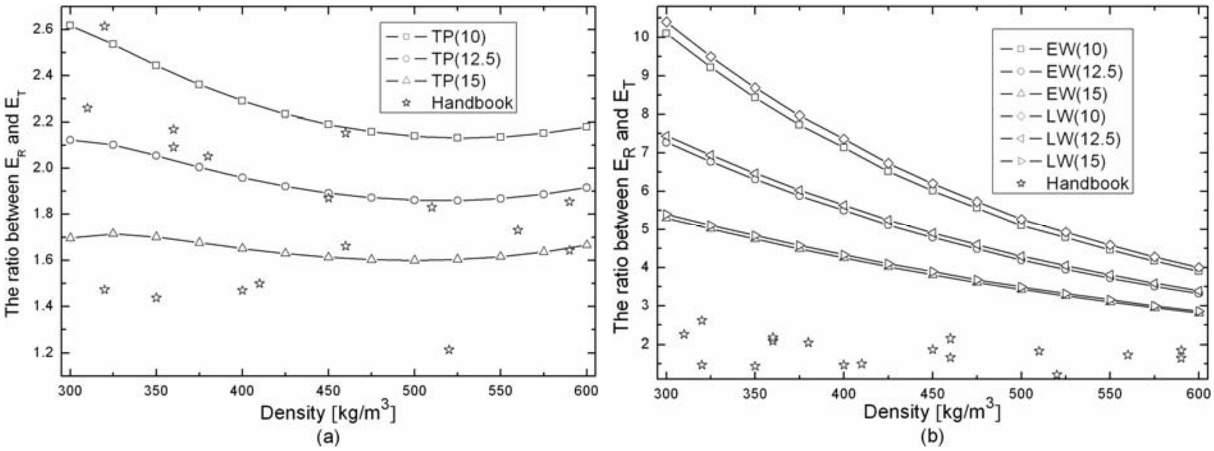

Figure 5. Transverse anisotropy of softwood with different CSAs: (a) predictions from two-phase model; (b) prediction from single model (TP – two-phase model, LW – latewood, EW – earlywood, Handbook - the data from Green et al. [29], the numbers in the brackets indicate the CSAs)

4 Conclusions

A 3D micromechanical analytical-computational model of softwood, which takes into account the wood microstructures at four scale levels, from microfibrils to annual rings, is developed. The analytical model of annual ring [27] (based on the improved rule-of-mixture model) and the computational (FE) model of the wood as cellular material with layered, nanoreinforced cell walls [20][21] are combined, in order to analyze the effect of the microstructure of wood at its properties taking into account the peculiarities of 4 levels of structure: annual rings, cellularity, multilayered cell wall, microfibrils in cell walls.

Using the combined four-level model, the effect of wood density, microfibril angle (MFA) and cell shape angle (CSA) on the elastic properties of softwood has been investigated in numerical experiments. The simulations were verified by comparison with experimental data, and a good agreement was obtained. The simulation results show that the annual ring structure has a strong influence on the mechanical properties, especially for transverse anisotropy. When compared with the single phase models, the two-phase model gives much more accurate transverse anisotropic predictions.

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