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A mathematical verification of the reinforced-matrix hypothesis using the Mori–Tanaka theory

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Abstract This article presents a theoretical verification of the reinforced-matrix hypothesis derived from tensor equations, $\sigma^W = \sigma^f + \sigma^m$ and $\varepsilon^W = \varepsilon^f = \varepsilon^m$ (Wood Sci Technol 32:171–182, 1998; Wood Sci Technol 33:311–325, 1999; J Biomech Eng 124:432–440, 2002), using classical Mori–Tanaka theory on the micromechanics of fiber-reinforced materials (Acta Metall 21:571–574, 1973; Micromechanics – dislcation and inclusions (in Japanese), pp 141–147, 1976). The Mori–Tanaka theory was applied to a small fragment of the cell wall undergoing changes in its physical state, such as those arising from sorption of moisture, maturation of wall components, or action of an external force, to obtain $\langle\sigma^A\rangle_D = \phi\cdot\langle\sigma^F\rangle_I + (1-\phi)\cdot\langle\sigma^M\rangle_{D-I}$. When the constitutive equation of each constituent material was applied to the equation $\langle\sigma^A\rangle_D = \phi\cdot\langle\sigma^F\rangle_I + (1-\phi)\cdot\langle\sigma^M\rangle_{D-I}$, the equations $\sigma^W = \sigma^f + \sigma^m$ and $\varepsilon^W = \varepsilon^f = \varepsilon^m$ were derived to lend support to the concept that two main phases, the reinforcing cellulose microfibril and the lignin–hemicellulose matrix, coexist in the same domain. The constitutive equations for the cell wall fragment were obtained without recourse to additional parameters such as Eshelby's tensor S and Hill's averaged concentration tensors A^F and A^M. In our previous articles, the coexistence of two main phases and $\sigma^W = \sigma^f + \sigma^m$ and $\varepsilon^W = \varepsilon^f = \varepsilon^m$ had been taken as our starting point to formulate the behavior of wood fiber with multilayered cell walls. The present article provides a rational explanation for both concepts.

Key words Wood cell wall · Composite material · Micromechanics · Inhomogeneities · Biomaterial

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Introduction

Softwood fiber has two main parts: a thick secondary wall and thin compound middle lamella (CML). A middle layer (S2) forms the thickest layer of the secondary wall and is reinforced with fibrous polysaccharide crystals oriented more or less parallel to the fiber axis (see Fig. 1). The orientation angle (microfibril angle; MFA) determines the mechanical properties of the softwood fibers, including the longitudinal Young's modulus,[1–3] anisotropic drying shrinkage,[4,5] surface growth stress,[6–8] and longitudinal tensile creep deformation.[9] Consequently, the S2 layer exercises an important role in determining the macroscopic properties of clear wood specimens, with the mechanical interaction between the reinforcing polysaccharides and the encrusting matrix substance ultimately controlling the material properties of the wood.

Any formulation of the material properties of a wood based on its structural hierarchy starts by considering the mechanical properties of the two-phase structure of the cell wall layer; that is, the reinforcing fibrous polysaccharide and the amorphous matrix. The reinforced-matrix hypothesis was originally proposed by Barber and Meylan[10] and provides a theoretical description of the mechanical interaction between these two phases. This model can be expressed using tensor equations:[6,11,12]

$$\sigma^W = \sigma^f + \sigma^m, \quad \text{and} \quad \varepsilon^W = \varepsilon^f = \varepsilon^m. \tag{1}$$

A physical interpretation of the tensorial quantities σ^W, σ^f, σ^m, ε^W, ε^f, and ε^m in Eq. 1 can be formulated as follows. The fibrous components of the polysaccharides are dispersed uniformly in each cell wall layer to form the framework fiber bundle. Similarly, the lignin–hemicellulose compound is diffused in each layer to provide the isotropic matrix skeleton. It is postulated that the framework bundle and the matrix skeleton occupy the same domain at the mesoscopic limit (= layer level). As a consequence, σ^W can be regarded as the stress tensor in the cell wall fragment as the whole, and σ^f and σ^m as the stress tensors in the polysaccharide framework bundle and matrix skeleton, respectively, with ε^W, ε^f, and ε^m being the respective strains.

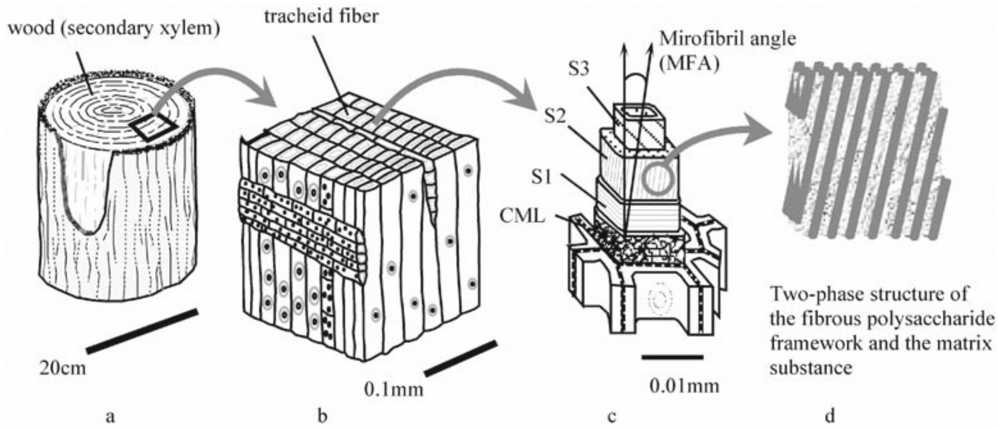

Fig. 1a–d. Structural hierarchy of wood (softwood). **a** Timber, **b** wood, **c** fiber, and **d** cell wall fragment (representative volume element)

Previously we have used both Eq. 1 and these interpretations as to the physical meanings of the tensorial quantities; that is, "the reinforced-matrix hypothesis," to develop theories to explain the MFA-dependent properties of clear wood specimens.[6,11,12] However, neither Eq. 1 nor the physical interpretations of σ^{W}, σ^{f}, σ^{m}, ε^{W}, ε^{f}, and ε^{m} have been defined in any rational manner. This article resolves this issue using the classical theory of micromechanics developed by Eshelby[13,14] and Mori and Tanaka.[15] We then compare our formulation with that of Cave[16] who proposed a constitutive relationship for the lignocellulose material of the wood cell wall, with the ultimate goal of validating the reinforced-matrix hypothesis as one of the basic theories of cell wall mechanics and physics.

Mathematical derivation of the reinforced-matrix hypothesis

Application of Mori and Tanaka's theory to two-phase structure of the cell wall

When material containing an ellipsoidal inhomogeneity is subjected to external stimulation such as heating, cooling, or external loading, a dimensional misfit can arise between the inhomogeneity and the matrix. This can induce an inhomogeneous stress disturbance inside the current inhomogeneity and in the matrix around it. Eshelby proposed an "Equivalent Inclusion Method" as a convenient way of calculating this stress disturbance, σ^{∞}.[13,14,17] His method was intended to apply primarily to the case in which an inhomogeneity exists at sufficient distance from the free surface of the material. However, in actual practice, any material has a free surface, and, furthermore, contains numerous inhomogeneities. This free surface and the neighboring inhomogeneities affect the stress field in both the current inhomogeneity and the surrounding matrix. This effect is called background stress.[15,17] Mori and Tanaka refined Eshelby's method to include the case in which the stress in the material is the background stress.[15,17]

Consider a small fragment of the secondary wall that occupies a closed domain D. First, assume that domain D is surrounded by a free surface and incurs a dimensional change on moisture sorption or substance deposition (Fragment 1). Such changes in the physical state often generate some dimensional misfit between each inhomogeneity and the matrix around it. Second, consider the case in which domain D is subjected to an external loading (Fragment 2), and in Fragment 2, assume that no physical change of state occurs except that induced by the external loading. Finally, consider a small domain D in an actual cell wall that incurs a definite external stimulation in addition to the boundary force (Fragment 3). We can now calculate the stress distribution in Fragment 3 by superposing the stress fields in Fragments 1 and 2. In either case, an infinitely long, rod-like polysaccharide microfibril embedded in the matrix substance can provide an ellipsoidal inhomogeneity with an infinitely large aspect ratio.

In Fragment 1, the stress inside an arbitrary inhomogeneity can be given as the sum of the background stress, σ_1^{b}, and Eshelby's solution, σ_1^{∞}.[15,17] In contrast, the stress in the matrix is equal to the background stress, σ_1^{b}.[15,17]

In Fragment 2, we can assume that the external loading induces a stress distribution, σ^{A}, inside the domain, where hypothetically no inhomogeneity is included. When a homogeneous stress field is disturbed by an inhomogeneity, it can be modeled by Eshelby's solution, σ_2^{∞}. According to Mori and Tanaka's theory,[15,17] the stress in each inhomogeneity is given as the superposition of the background stress, σ_2^{b}, Eshelby's solution, σ_2^{∞}, and the externally induced stress, σ^{A}. In contrast, the stress in the matrix is provided by superposition of σ_2^{b} and σ^{A}.

In Fragment 3, the stress distribution in D can be calculated by superposing the stress fields in Fragments 1 and 2; that is, $\sigma = \sigma_1^{b} + \sigma_2^{b} + \sigma_1^{\infty} + \sigma_2^{\infty} + \sigma^{A}$ inside each inhomogeneity, and $\sigma = \sigma_1^{b} + \sigma_2^{b} + \sigma^{A}$ in the matrix. If we denote $\sigma_1^{b} + \sigma_2^{b} \equiv \sigma^{b}$ and $\sigma_1^{\infty} + \sigma_2^{\infty} \equiv \sigma^{\infty}$, the stress distribution inside the small domain D becomes

$$\sigma = \begin{cases} \sigma^{b} + \sigma^{\infty} + \sigma^{A} \, (= \sigma^{F}) & (\text{in I}) \\ \sigma^{b} + \sigma^{A} \, (= \sigma^{M}) & (\text{in D} - \text{I}). \end{cases} \tag{2}$$

where I is the domain of the inhomogeneities in D, and D–I is that of the matrix. The problem now resolves itself into establishing the constitutive relationship of the small fragment of the cell wall by analyzing the behavior of σ^{b}, σ^{∞}, and σ^{A} in D.

The volume average of the internal stress distribution over domain D is given as σ^{A} (see Appendix); that is,

$$\frac{1}{D}\int_{D}\sigma dV=\frac{1}{D}\int_{D}\sigma^{A}dV\equiv\langle\sigma^{A}\rangle_{D},\tag{3}$$

where D is the volume of domain D. The above equation can be rewritten as

$$\langle\sigma^{A}\rangle_{D}=\frac{1}{D}\left(\int_{I}\sigma dV+\int_{D-I}\sigma dV\right)=\frac{1}{D}\int_{I}(\sigma^{b}+\sigma^{A}+\sigma^{\infty})dV+\frac{1}{D}\int_{D-I}(\sigma^{b}+\sigma^{A})dV,\tag{3′}$$

leading to the equation

$$\langle\sigma^{A}\rangle_{D}=\phi\cdot(\langle\sigma^{\infty}\rangle_{I}+\langle\sigma^{b}\rangle_{I}+\langle\sigma^{A}\rangle_{I})+(1-\phi)\cdot(\langle\sigma^{b}\rangle_{D-I}+\langle\sigma^{A}\rangle_{D-I}),\tag{4}$$

where ϕ ($= I/D$) is the volume fraction of the inhomogeneities in the small volume D, and $\langle\#\rangle_{D}$, $\langle\#\rangle_{I}$, $\langle\#\rangle_{D-I}$ are the integral averages of the tensorial quantities # in the respective domains. We can identify the stress $\langle\sigma^{\infty}\rangle_{I}+\langle\sigma^{b}\rangle_{I}+\langle\sigma^{A}\rangle_{I}$ with the average stress in the inhomogeneity denoted by $\langle\sigma^{F}\rangle_{I}$, with $\langle\sigma^{b}\rangle_{D-I}+\langle\sigma^{A}\rangle_{D-I}$ regarded as that in the matrix region denoted by $\langle\sigma^{M}\rangle_{D-I}$. Thus, Eq. 4 can be rewritten as

$$\langle\sigma^{A}\rangle_{D}=\phi\cdot\langle\sigma^{F}\rangle_{I}+(1-\phi)\cdot\langle\sigma^{M}\rangle_{D-I}\tag{4′}$$

According to Eshelby's equivalent inclusion method, σ^{∞} becomes uniform inside each equivalent inclusion.[13,14] It is impossible to know the distribution of σ^{b} accurately.

From Eq. 4 and following the assumption of Mori and Tanaka[15,17] that "mean field approximation" implies $\langle\sigma^{b}\rangle_{I}=\langle\sigma^{b}\rangle_{D-I}=\langle\sigma^{b}\rangle_{D}$ ($\equiv\langle\sigma^{b}\rangle$), we can obtain the formula

$$\langle\sigma^{b}\rangle=-\phi\cdot\langle\sigma^{\infty}\rangle_{I}\,(=-\phi\cdot\sigma^{\infty})$$

called the Mori–Tanaka theorem.[15] We can now estimate the value of $\langle\sigma^{b}\rangle$ from this theorem based on the value of σ^{∞}.

Deriving the equations and their physical interpretations

The constitutive equation of volume D can be derived on the basis of Eq. 4. In the past, we have used Eshelby's tensor of inhomogeneity for this purpose. In this study, however, we avoid the use of Eshelby's tensor and start with Eq. 4′.

We first introduce stress fields $\hat{\sigma}^{M}$ and $\hat{\sigma}^{F}$, and strain fields $\hat{\varepsilon}$ and $\hat{\alpha}$, defined in D as

$$\hat{\sigma}^{M}\equiv\begin{cases}\sigma^{M}\ (\text{in D}-\text{I})\\ 0\ (\text{in I})\end{cases},\quad \hat{\sigma}^{F}\equiv\begin{cases}0\ (\text{in D}-\text{I})\\ \sigma^{F}\ (\text{in I})\end{cases},$$
$$\hat{\varepsilon}\equiv\begin{cases}\varepsilon^{M}\ (\text{in D}-\text{I})\\ \varepsilon^{F}\ (\text{in I})\end{cases},\quad \hat{\alpha}\equiv\begin{cases}\alpha^{M}\ (\text{in D}-\text{I})\\ \alpha^{F}\ (\text{in I})\end{cases},\tag{5}$$

where ε^{M} and ε^{F} are the strain in the matrix and that in the polysaccharide microfibrils (= inhomogeneities), respectively. α^{M} and α^{F} are the eigen-strains generated in the respective components. These are induced by a specific change in the physical state of the cell wall, such as that resulting from water sorption, the deposition and maturation of the cell wall substance, or external loading. As a result, the dimensions of the small volume D tend to change. The tensorial quantities σ^{M}, ε^{M}, and α^{M} are defined in D – I, and σ^{F}, ε^{F}, and α^{F} in I.

In addition, we introduce tensor fields $\hat{C}^{M}$ and $\hat{C}^{F}$ defined in D to satisfy

$$\hat{C}^{M}\equiv\begin{cases}C^{M}\ (\text{in D}-\text{I})\\ 0\ (\text{in I})\end{cases},\quad \hat{C}^{F}\equiv\begin{cases}0\ (\text{in D}-\text{I})\\ C^{F}\ (\text{in I})\end{cases}.\tag{6}$$

The tensorial quantities C^{M} and C^{F} define the stiffness of the matrix substance and the crystalline polysaccharide microfibrils, respectively. These quantities do not depend on their positions within their respective domains.

Using these tensors, we can formulate the generalized constitutive relationships of the matrix substance and polysaccharide microfibrils as equations of the tensor fields defined in domain D as

$$\hat{\sigma}^{M}=\hat{C}^{M}(\hat{\varepsilon}-\hat{\alpha}),\quad \hat{\sigma}^{F}=\hat{C}^{F}(\hat{\varepsilon}-\hat{\alpha}).\tag{7}$$

Taking an integral average for each equation over domain D, we obtain

$$\hat{\sigma}^{m}=\hat{C}^{m}\left(\langle\varepsilon^{M}\rangle_{D-I}-\langle\alpha^{M}\rangle_{D-I}\right),\quad \hat{\sigma}^{f}=\hat{C}^{f}\left(\langle\varepsilon^{F}\rangle_{I}-\langle\alpha^{F}\rangle_{I}\right),\tag{8}$$

where

$$\hat{\sigma}^{m}\left(\equiv\frac{1}{D}\int_{D}\hat{\sigma}^{M}dV\right)=(1-\phi)\cdot\langle\sigma^{M}\rangle_{D-I},$$
$$\hat{\sigma}^{f}\left(\equiv\frac{1}{D}\int_{D}\hat{\sigma}^{F}dV\right)=\phi\cdot\langle\sigma^{F}\rangle_{I},\tag{9}$$
$$\langle\varepsilon^{M}\rangle_{D-I}\equiv\frac{1}{D-I}\int_{D-I}\varepsilon^{M}dV,\ \alpha_{D-I}\equiv\frac{1}{D-I}\int_{D-I}\alpha^{M}dV,$$

$$\langle\varepsilon^{F}\rangle_{I}\equiv\frac{1}{I}\int_{I}\varepsilon^{F}dV,\quad \langle\alpha^{F}\rangle_{I}\equiv\frac{1}{I}\int_{I}\alpha^{F}dV,$$
$$\hat{C}^{m}=(1-\phi)\cdot C^{M},\quad \hat{C}^{f}=\phi\cdot C^{F}.\tag{10}$$

As is clear from their definitions, $\hat{\sigma}^{m}$, $\hat{\sigma}^{f}$, $\hat{C}^{m}$, and $\hat{C}^{f}$ constitute fields of uniform tensors that are defined at every point in D. From Eq. 9 and Eq. 4′, we can extract

$$\hat{\sigma}^{m}+\hat{\sigma}^{f}=\langle\sigma^{A}\rangle_{D},\tag{11}$$

provided that $\langle\sigma^{A}\rangle_{D}$ is regarded as the field of mean stress in cell wall fragment D and is identical to σ^{W} in Eq. 1.

From Eq. 9, $\hat{\sigma}^{m}$ can be taken as the stress tensor of the matrix skeleton, and $\hat{\sigma}^{f}$ as that of the polysaccharide framework bundle. Similarly, $\hat{C}^{m}$ and $\hat{C}^{f}$ are the elastic constants of the matrix skeleton and the polysaccharide framework bundle, respectively. This implies that both the matrix skeleton and framework bundle occupy an identical volume at the mesoscopic limit. This corresponds to "the idea of the coexistence of two main phases in the cell wall."

Furthermore, the two formulas of Eq. 8 can be used to model the relationships between elastic stress and stiffness in the matrix skeleton and the polysaccharide framework bundle, respectively, and these two formulas should be regarded as defining the constitutive relationships between the matrix skeleton and that of the polysaccharide framework bundle. From this perspective, we can deduce that

$$\langle \varepsilon^{M} \rangle_{D-I} - \langle \alpha^{M} \rangle_{D-I} = \hat{\varepsilon}^{m} - \hat{\alpha}^{m}, \quad \langle \varepsilon^{F} \rangle_{I} - \langle \alpha^{F} \rangle_{I} = \hat{\varepsilon}^{f} - \hat{\alpha}^{f}, \tag{12}$$

where $\hat{\varepsilon}^{m}$ is a tensor field uniformly defined at every point in D, and is considered as the strain of the matrix skeleton, and $\hat{\varepsilon}^{f}$ is that of the polysaccharide framework bundle; $\hat{\alpha}^{m}$ and $\hat{\alpha}^{f}$ are their respective eigen-strains. Because these also provide the fields of the tensors uniformly defined in D, Eq. 8 becomes

$$\hat{\sigma}^{m} = \hat{C}^{m}(\hat{\varepsilon}^{m} - \hat{\alpha}^{m}), \quad \hat{\sigma}^{f} = \hat{C}^{f}(\hat{\varepsilon}^{f} - \hat{\alpha}^{f}). \tag{8$'$}$$

With the behavior of the matrix skeleton on deformation being entirely consistent with that of the framework bundle, given that the matrix skeleton and framework bundle coexist in identical domain D, we obtain

$$\hat{\varepsilon}^{m} = \hat{\varepsilon}^{f} = \varepsilon^{W}. \tag{13}$$

Hence, the Mori–Tanaka theory provides both a theoretical description and a physical interpretation of Eq. 1.[15] It can be noted that $\hat{\sigma}^{m}$, $\hat{\sigma}^{f}$, $\hat{C}^{m}$, $\hat{C}^{f}$, $\hat{\varepsilon}^{m}$, $\hat{\varepsilon}^{f}$, $\hat{\alpha}^{m}$, and $\hat{\alpha}^{f}$ are the tensor fields uniformly distributed in small domain D; they were denoted in our previous articles by σ^{m}, σ^{f}, C^{m}, C^{f}, ε^{m}, ε^{f}, α^{m}, and α^{f}, respectively.[6,7,11,12] Consequently, we can obtain $\sigma^{W} = \sigma^{f} + \sigma^{m}$ from Eq. 11 and $\varepsilon^{W} = \varepsilon^{f} = \varepsilon^{m}$ from Eq. 13, which are the formulas of Eq. 1.

From Eqs. 11, 8′, and 13, we can obtain the constitutive relationship of cell wall fragment D as

$$\sigma^{W} = (C^{m} + C^{f})\varepsilon^{W} - (C^{m}\alpha^{m} + C^{f}\alpha^{f}). \tag{14}$$

This provides the starting point for analyzing the mechanical behaviors of the multilayered wood fibers.[6,7,11,12]

Simulating the behavior of the wood fiber using Eq. 14

The strains $\hat{\alpha}^{f}$ and $\hat{\alpha}^{m}$ generated in each layer of a wood cell wall tend to cause dimensional changes in each wood fiber along its length (ε_{L}) and diameter (ε_{T}). The basic formula that describes such strains can be derived from Eq. 14.[6,7,11,12] The dimensional changes in an isolated wood fiber can be simulated by using this basic formula, but with the time-dependent patterns of $\hat{\alpha}^{f}$ and $\hat{\alpha}^{m}$ optimized to obtain reasonable values of ε_{L} and ε_{T} that are quantitatively compatible with observed phenomena. We can estimate the microscopic behavior of the constituent materials on the basis of optimized values of $\hat{\alpha}^{f}$ and $\hat{\alpha}^{m}$, and hence provide one of the most important purposes of the simulation.[12]

Strictly speaking, $\hat{\alpha}^{f}$ and $\hat{\alpha}^{m}$ are the eigen-strains of the polysaccharide framework bundle and that of the matrix skeleton, respectively, and therefore do not necessarily reflect intrinsic properties of the constituent materials. In contrast, $\langle \alpha^{M} \rangle_{D-I}$ and $\langle \alpha^{F} \rangle_{I}$ give direct information on the microscopic properties of the constituent materials. The values of $\langle \alpha^{M} \rangle_{D-I}$ and $\langle \alpha^{F} \rangle_{I}$ can be estimated through simulation by first optimizing the relationship between the macroscopic strain, ε^{W} ($= \hat{\varepsilon}^{m} = \hat{\varepsilon}^{f}$), and the eigen-strains, $\hat{\alpha}^{m}$ and $\hat{\alpha}^{f}$. The behaviors of the microscopic strains, $\langle \varepsilon^{M} \rangle_{D-I}$ and $\langle \varepsilon^{F} \rangle_{I}$, can be ascertained by instrumental analysis such as X-ray diffraction.[18] From Eq. 12, we can determine the values of $\langle \alpha^{M} \rangle_{D-I}$ and $\langle \alpha^{F} \rangle_{I}$, which are the microscopic eigen-strains caused in the polysaccharide microfibril and the matrix, respectively.

Comparison with Cave's formulation

Outline of Cave's formulation

Cave is one of the pioneer researchers in cell wall micromechanics. He started his formulation with Eq. 4′[5,16] as hypothesized by Hill:[19]

$$(1-\phi)\cdot\langle \sigma^{M} \rangle_{D-I} + \phi\cdot\langle \sigma^{F} \rangle_{I} = \sigma^{W}. \tag{15}$$

Cave then introduced the constitutive relationships of two constituent materials in a shrinking cell wall fragment as[16]

$$\begin{aligned} \langle \sigma^{M} \rangle_{D-I} &= C^{M}(\langle \varepsilon^{M} \rangle_{D-I} - \langle \alpha^{M} \rangle_{D-I}), \\ \langle \sigma^{F} \rangle_{I} &= C^{F}(\langle \varepsilon^{F} \rangle_{I} - \langle \alpha^{F} \rangle_{I}). \end{aligned} \tag{16}$$

Equations 15 and 16 then yield

$$\begin{aligned} \sigma^{W} = {} & (1-\phi)\cdot C^{M}\langle \varepsilon^{M} \rangle_{D-I} + \phi\cdot C^{F}\langle \varepsilon^{F} \rangle_{I} \\ & -(1-\phi)\cdot C^{M}\langle \alpha^{M} \rangle_{D-I} - \phi\cdot C^{F}\langle \alpha^{F} \rangle_{I}. \end{aligned} \tag{17}$$

To develop this formula into the constitutive relationship of the cell wall fragment as a whole, it is necessary to relate the microscopic strains, $\langle \varepsilon^{M} \rangle_{D-I}$ and $\langle \varepsilon^{F} \rangle_{I}$, to the macroscopic, ε^{W}. Hill had introduced the following conditions on the basis of a representative volume element:[19]

$$\langle \varepsilon^{M} \rangle_{D-I} = A^{M}\varepsilon^{W}, \quad \langle \varepsilon^{F} \rangle_{I} = A^{F}\varepsilon^{W}, \tag{18}$$

where A^{M} and A^{F} are called the averaged concentration tensors and depend on the elastic constants, shapes, and contents of the components. By using this subsidiary condition, Cave developed Eq. 17 to provide the constitutive relationship,[16]

$$\begin{aligned} \sigma^{W} = {} & [(1-\phi)\cdot C^{M}A^{M} + \phi\cdot C^{F}A^{F}]\varepsilon - (1-\phi)\cdot C^{M}\langle \alpha^{M} \rangle_{D-I} \\ & - \phi\cdot C^{F}\langle \alpha^{F} \rangle_{I}. \end{aligned} \tag{19}$$

In his original report, Cave postulated $\alpha^{F} = 0$ by assuming that highly crystallized cellulose does not react with water molecules.

Comparison between Cave's formulation and the present one

To adopt Eq. 19 as the constitutive relationship for simulation, we need to provide concrete values for A^{M} and A^{F}. It is nontrivial to determine either, because little information exists on the microscopic topology of the two-phase structure. Hence, we need to assume temporizing values for these factors. Cave considered that A^{M} and A^{F} to be of minor importance by assuming, along with W. Voigt (1889), that strain is uniformly distributed in a two-phase material.[5,20] By adopting Voigt's assumption that $A^{M} = A^{F}$

= I (unit tensor),[20] Cave obtained the constitutive relationship,

$$\sigma^{W} = \left[(1-\phi)\cdot C^{M} + \phi\cdot C^{F}\right]\varepsilon^{W} - [(1-\phi)\cdot C^{M}\langle\alpha^{M}\rangle_{D-I} + \phi\cdot C^{F}\langle\alpha^{F}\rangle_{I}], \tag{20}$$

and used this equation for simulating drying shrinkage and elastic deformation of multilayered double cell walls.

In Eq. 20, the eigen-strains, $\langle\alpha^{M}\rangle_{D-I}$ and $\langle\alpha^{F}\rangle_{I}$, are unknown factors with behaviors that need to be determined from the simulation. However, it does not necessarily follow that the values of $\langle\alpha^{M}\rangle_{D-I}$ and $\langle\alpha^{F}\rangle_{I}$ in Eq. 20 will reflect the intrinsic behaviors of the constituent materials in a wood cell wall. Voigt's assumption of $A^{M} = A^{F} = I$ places an unrealistic restriction on the situation in which the elastic moduli differ between the inhomogeneity and the matrix. In contrast, the constitutive relationship (Eq. 14) describes that between macroscopic strain and stress without assuming any subsidiary conditions. By using Eq. 14 for the simulation, we can determine both values and behaviors of $\langle\alpha^{M}\rangle_{D-I}$ and $\langle\alpha^{F}\rangle_{I}$.

In our previous articles, the coexistence of the two main phases and Eq. 1 have been taken as basic premises with which to model the behavior of wood fiber.[6,7,11,12] In the present article, we offer a rational explanation for both concepts.

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Appendix

Volume average of the internal stress distribution over a small domain D as given by an externally induced stress, $\langle\sigma^{A}\rangle_{D}$

By applying Gauss' theorem for divergence and the method of integration by parts to stress field, σ, in closed domain, D, the volume average of σ in D can be calculated as

$$\frac{1}{D}\int_{D}\sigma_{ij}dV = \frac{1}{D}\int_{D}\sigma_{ik}\delta_{jk}dV = \frac{1}{D}\int_{D}\sigma_{ik}\frac{\partial x_{j}}{\partial x_{k}}dV = \frac{1}{D}\left[\int_{\partial D}\sigma_{ik}x_{j}n_{k}dS - \int_{D}\sigma_{ik,k}x_{j}dV\right], \tag{21}$$

where δ_{ij} is Kronecker's symbol, ∂D is the boundary surface of the domain D, and $n = (n_k)$ is the normal vector on ∂D. In the case when no body force acts on D, σ must satisfy the equilibrium condition in D: $\nabla\cdot\sigma$ [$\equiv \sigma_{ik,k} \equiv (\partial\sigma_{i1}/\partial x_1) + (\partial\sigma_{i2}/\partial x_2) + (\partial\sigma_{i3}/\partial x_3)$] = 0, where $\sigma_{ik}n_k$ is the boundary force that balances the external force acting on ∂D. In Fragment 1, $\sigma_{ik}n_k$ must be nil on ∂D because no external force acts on ∂D (i.e., Cauchy's boundary condition). Fragment 2 is subjected to an external force through ∂D and therefore $\sigma_{ik}n_k$ is nontrivial on ∂D. Consequently the integral on the right side of Eq. 21 becomes

$$\frac{1}{D}\int_{\partial D}[\sigma_2]_{ik}\, n_k x_j dS, \tag{22}$$

where $(\sigma_2)_{ik}$ [$= (\sigma_2^{\infty})_{ik} + (\sigma_2^{b})_{ik} + (\sigma^{A})_{ik}$] is the internal stress in Fragment 2. In addition, both Eshelby's solution σ_2^{∞} and the background stress σ_2^{b} generated in finite domain D must satisfy Cauchy's boundary condition for ∂D: $[(\sigma_2^{\infty})_{ij} + (\sigma_2^{b})_{ij}]n_j = 0$.[13,15] Therefore, $(\sigma_2)_{ik}n_k$ in Eq. 22 should be replaced by $(\sigma^{A})_{ik}n_k$ to become

$$\frac{1}{D}\int_{\partial D}[\sigma^{A}]_{ik}\, n_k x_j dS. \tag{23}$$

By applying Gauss' theorem for divergence and the method of integration by parts to stress field σ^{A}, the above integral resolves itself as $\langle\sigma^{A}\rangle$. Hence, $\langle\sigma\rangle = \langle\sigma^{A}\rangle$.