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Modeling of the Primary Plant Cell Wall in the Context of Plant Development

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Abstract

The plant cell wall is a complex material made of polysaccharides, proteins, ions and water. As an external envelope around the cell it resists the internal turgor pressure. During plant cell growth, the cell wall material must yield to allow the cell to expand in a controlled spatial and temporal pattern. Modeling this behavior has been approached via a variety of techniques ranging from continuum mechanics to atomistic models, whilst at an intermediate scale, mesoscopic models attempt to consider the mechanical behavior of individual polymers and linkages while simplifying molecular structures to relevant properties. In this review an overview is provided over recent modeling approaches focusing on the primary plant cell wall.

Keywords

primary plant cell wall; cellulose; polysaccharides; plant growth; mechanical modeling; atomistic modeling; continuum mechanics; multiscale modeling

Key Concepts

- Modeling the plant cell wall assists in understanding plant cell growth and plant morphogenesis.
- The plant cell wall consists of structural polysaccharides such as cellulose, hemicelluloses, and pectin arranged into an oriented network, as well as proteins, ions, and water.
- Different quantitative modeling strategies that can be applied to modeling of the plant cell wall include continuum mechanics, mesoscopic models, atomistic models, and multiscale modeling.

Introduction

Plant cells are surrounded by a relatively stiff envelope, the cell wall. This extracellular matrix is made mostly of polysaccharides. The cell wall determines the mechanical properties of a plant tissue and hence influences the functionality of plant organs. The mechanical properties of the plant cell wall determine the behavior and quality of plant-based materials such as the suitability of different

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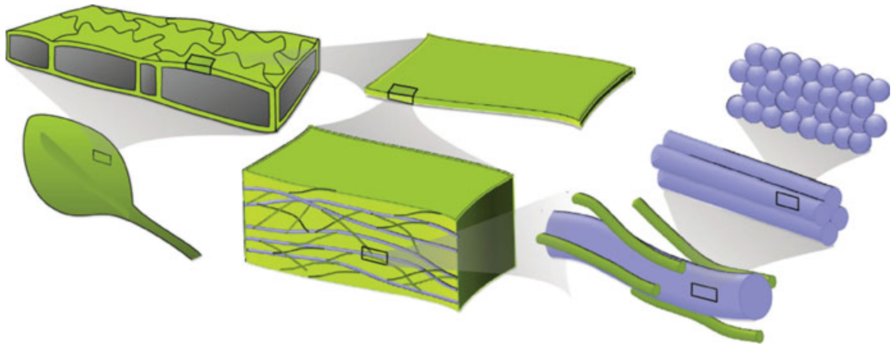

Fig. 1 Hierarchical structure of the plant cell wall. The material can be considered as a homogeneous solid or as a mixture of its components. The *rectangle* indicates an area of interest, depicted with increasing resolution in the various panels. Microfibrils are depicted in *purple*; matrix components including hemicellulose links between microfibrils are drawn in *dark green*. Polysaccharides are polymers consisting of individual sugar molecules (depicted as *spheres*)

wood types for construction, the texture and digestibility of plant-based food items, and, of increasing importance, the ease of conversion of plant materials to biofuels. For multiple reasons it is therefore important to understand the mechanical behavior of the plant cell wall and the influence of the individual components and how they are linked to this behavior. Modeling of plant architecture at multiple scales, including that of cell wall structure, is covered in an excellent and extensive book chapter by Rey et al. (2011). The modeling approaches described in that chapter pertain to mature, fully differentiated tissue and cellular architecture, and consequently the focus is primarily on secondary plant cell walls and on the mechanical principles governing the behavior of plant organs and tissues under external load application. By contrast, here modeling approaches developed in the context of developmental processes will be highlighted, i.e., processes that involve cellular growth and expansion and thus the deformation of the primary plant cell wall.

Plant cells are generated in tissues with high mitotic activity, the meristems. The products of cell division are typically small, on the order of 10–20 μm. During differentiation, plant cells grow significantly in size. The growth of plant cells entails a stretching of the cell wall which is driven by the hydrostatic pressure inside the cell, the turgor. Turgor is generated by the uptake of water which in turn is driven by a differential in osmotic pressure between the inside and the outside of the cell. The amount of stretching (strain) that a section of cell wall undergoes under the effect of turgor depends on the thickness of the wall, cellular geometry, and the mechanical properties of the wall material. Cell wall assembly and regulation of the mechanical properties of the cell wall therefore influence the development and differentiation of individual plant cells, which in turn affects both their neighboring cells and the tissue morphology as a whole. Unlike animal cells which are very flexible since they are only surrounded by the plasma membrane, cellular morphogenesis in plant cells is therefore controlled in time and space by processes that occur at the outside of the plasma membrane, in the cell wall (Geitmann and Ortega 2009; Mirabet et al. 2011). Since plant cell growth only occurs in cells (or cellular regions) with primary cell wall, the following sections pertain to this particular cell wall material.

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Biochemical Composition and Mechanical Behavior of the Primary Plant Cell Wall

The primary cell wall is a complex composite material of fibrous and matrix-like components (Fig. 1). The fibrous component consists primarily of cellulose microfibrils – long, more or less crystalline polymers made of β-1,4-linked glucan chains. The matrix is formed by hemicelluloses, pectins, structural proteins, ions, and water (Ivakov and Persson 2012). Because of their high tensile resistance and filamentous shape, cellulose microfibrils confer anisotropy to the cell wall material. A section of cell wall with preferential net orientation of the microfibrils behaves anisotropically in response to a tensile load. This means that the section deforms less easily in the direction parallel to the fibrils than in the direction perpendicular to them. Although the preferential orientation of cellulose microfibrils is a crucial determinant for anisotropy (Schopfer 2006), other factors such as the degree of cross-linking and crystallinity and the length of the individual microfibrils influence the mechanical properties of the microfibril component of the cell wall material (Geitmann and Ortega 2009).

The microfibrils are linked by hemicellulose molecules. These connect the microfibrils into a network and might also function as a matrix filling the space between microfibrils. Hemicelluloses include several different types of polymers, for example, xylans, xyloglucans, and (gluco) mannans, which are characterized by a backbone of β-1,4-linked sugars with an equatorial linkage configuration. The type and abundance of hemicelluloses, and the number and organization of cross-links with the microfibrils, thus influence the overall mechanical behavior of the cell wall and are subject to enzymatic modulation (Scheller and Ulvskov 2010).

Another important matrix component is pectin. Among the different pectic polysaccharides are homogalacturonan, xylogalacturonan, apiogalacturonan, rhamnogalacturonan I, and rhamnogalacturonan II, which occur in varying composition depending on plant species, cell type, and developmental stage (Caffall and Mohnen 2009). An interesting feature of pectin in the context of developmental regulation is the fact that its mechanical properties change depending on the degree of methyl-esterification, since acidic pectins are readily gelated by calcium ions and thus become stiffer. This allows the plant cell to modulate the mechanical behavior of a pectinaceous wall. The growing and non-growing regions of growing cells or of meristematic tissues are therefore characterized by different degrees of pectin methyl-esterification (Palin and Geitmann 2012).

The deformation of the plant cell wall by turgor-induced tensile stress can be elastic or plastic, depending largely on the amount of strain and the nature of the stretched wall material. Elastic deformation is reversible and does not lead to cell growth. This type of deformation occurs, for example, in the walls of stomatal guard cells under changing turgor conditions. Cell growth on the other hand requires plastic or viscoplastic deformation, meaning that the deformation is permanent even after removal of the deforming load. Typically this entails a reorganization of the molecular bonds, for example, by breakage and new formation of links between cell wall polymers or unfolding of curled polymers. In other words, and to more accurately express causality of this process, growth is enabled by the breakage of links between cell wall polymers (Schopfer 2006). Experimentally, the behavior of cell wall material under load application can be determined by tensile testing, a micromechanical experiment that can be applied to entire tissues or individual cells (Burgert and Fratzl 2007; Cosgrove 2005; Geitmann 2006). This type of experiments can be used both to determine the input parameters for mechanical models and to evaluate the validity of predictions made by such models.

Modeling the behavior of the plant cell wall under stress is not a simple task since it is a hierarchically built structure and its "deformation" involves a variety of processes such as breakage

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of linkages and stretching of polymers. Moreover, the wall consists of multiple layers that may behave differently depending on their chemical composition and anisotropy. The mechanical behavior of the different polymers composing and linking these layers differs depending on their chemical nature, spatial arrangement, and length. Each of these polymers is linked to several others, and the mechanical behavior of the links depends on their nature and the local conditions (e.g., pH, hydration). The mechanical deformation or stretching of the wall entails breaking and reformation of links, sliding of polymers against each other, slippage, uncoiling, and stretching of individual molecules (Boyer 2009; Cosgrove 2005). This means that there are numerous degrees of complexity in the biological reality of the plant cell wall and choices need to be made when establishing a quantitative mechanical model.

Different Modeling Strategies

The behavior of the plant cell wall has been addressed using a variety of modeling approaches that were chosen to answer different questions. At the basis of each quantitative or mechanical model is a conceptual model that provides a framework for which quantitative relationships are developed. The present review focuses on the quantitative types of modeling approaches that have been developed to understand the functioning of the primary cell wall during plant development.

Importantly, a quantitative model has to be constructed at the same spatial scale as that of the question to be both useful and efficient in terms of computation times and the quality of the predictions that are delivered. Very roughly, modeling of the mechanical behavior of a complex material such as the plant cell wall can be approached either through continuum mechanical approaches, through atomistic modeling, or by some intermediate type representing a mesoscopic approach. A continuum mechanics approach is based on the equations of mass, momentum, and energy conservation together with constitutive relations to determine the behavior of the material under the effect of a deforming load. In continuum mechanics models of the plant cell wall, individual molecules such as polymers, their different behaviors, and their connections are not considered or are simplified significantly. Similarly, if the test object is a tissue rather than a single piece of cell wall, any higher-scale organization such as the cellularity is often neglected, and the entire mass of cells forming a tissue is considered to be a homogenous material. This simplification neglects cellular geometry (i.e., the presence of the aqueous, pressurized protoplast or gas-filled intracellular spaces) and any differences in material properties between the different layers of the cell wall proper and the cell-cell linkages formed by the middle lamella. In many cases this type of simplified approach is sufficient to answer the type of question posed (Bruce 2003; Geitmann and Ortega 2009) whereas in others cellularity and variations in material properties are recognized to play an important role for the overall mechanical behavior of the tissue (Rey et al. 2011).

In atomistic modeling, information about individual atoms is included and thus modeling even a single molecule or polymer already requires significant amounts of computational capacity. While this approach allows questions such as the twisting of a single microfibril to be addressed, it is typically too detailed and computationally expensive to be useful to understand the mechanical behavior of the cell wall at the time and length scales that are biologically relevant to plant cell growth. In between the atomistic and macroscopic scales lies a continuum of mesoscopic scales that offer the possibility to simplify while still considering the role of individual macromolecules. A typical approach would be coarse-grained models. Coarse graining consists of replacing an atomistic description of a macromolecule with a description of lower resolution by averaging or smoothing away fine details (Fig. 2). This simplification may simply remove certain degrees of

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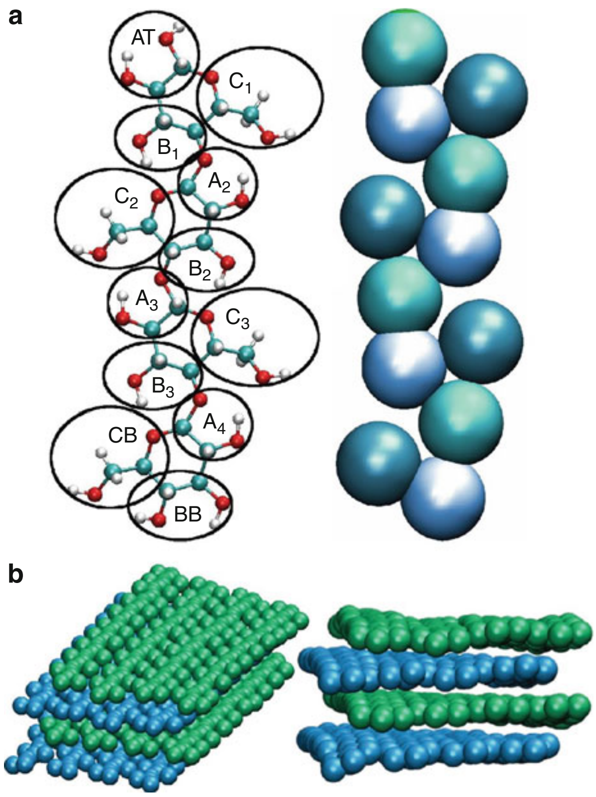

Fig. 2 Coarse-grained model of cellulose. (**a**). Atomistic structure of cellotetraose with definition of the coarse-grained beads. Each glycan is represented with three beads (*A*, *B*, *C*) with the second letters distinguishing top (*T*) and bottom (*B*). (**b**). Snapshots of the molecular dynamics simulation of a coarse-grained cellulose crystal seen from different angles (Figures modified after Bu et al. (2009) and Hynninen et al. (2011), generously provided by Michael Crowley, Penn State University)

freedom (e.g., vibrational modes between two atoms), or several atoms in the molecule may be replaced by a single particle. In a polysaccharide, this could, for example, be the representation of the individual sugar monomers as single particles in the model. The degrees of accuracy and resolution used depend on the questions to be answered with the respective model.

A modeling approach does not necessarily need to be confined to a single scale. The hierarchical organization of atoms making sugar groups which in turn form polymers that are arranged in layers forming the walls of individual cells combined to make a plant tissue invites multiscale modeling approaches. In a multiscale approach, material properties or system behavior on one level is calculated using information or models from different levels. Such an approach would have the aim to integrate the different approaches detailed above. In the following sections, several types of quantitative modeling approaches to describe the mechanical behavior of the primary plant cell wall in plant development are examined, without any attempt to be comprehensive.

The Lockhart Equation and Its Successors

The best established models of plant growth can be traced back to Lockhart who first described the elongation of a cylindrical cell, which only expands along its longitudinal axis, as is typically the case for the cells of the plant root and shoot (Lockhart 1965a, b). It consists of two coupled

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equations: a mechanical response of the cell wall to the turgor pressure combined with the regulation of this internal pressure via water movement. The mechanical stretching of the cell wall in response to the tension induced by the turgor pressure is described via a constitutive law, viz.,

$$(\mathrm{d}L/\mathrm{d}t)/L = m(P - Y) \text{ for P > Y},$$

$$(\mathrm{d}L/\mathrm{d}t)/L = 0 \text{ otherwise}, \tag{1}$$

where *(*d*L*/d*t)/L* is the relative elongation rate, i.e., the proportional rate of increase of an element of length *L* (which could, but is not restricted to, be the length of the cell) over time, *t*. Provided the turgor pressure, *P*, is above a yield threshold, *Y*, the cell will grow at a rate proportional to the difference between the pressure and the yield threshold modulated by the extensibility, *m*, of the wall which captures the mechanical properties. If the pressure is below the yield threshold, the response is elastic and no irreversible expansion (i.e., growth) occurs. This formulation is equivalent to treating the cell wall as a Bingham fluid – a viscoplastic material that behaves as a rigid body at low stresses but flows as a viscous fluid at high stress.

The second equation (presented here somewhat modified) captures the regulation of the turgor pressure via osmotically active solutes, such that

$$(\mathrm{d}L/\mathrm{d}t)/L = K(\Psi_o - \Psi_i) = K(\Psi_o - P + \pi), \tag{2}$$

where *K* is the hydraulic conductance of the plasma membrane, Ψ_o and Ψ_i are the water potentials outside and inside the cell, respectively, and π is the osmotic pressure inside the cell. Essentially, a difference in water potential between the inside and outside of the cell drives water movement to compensate for the changes in pressure, which are created by changes in the volume of the cell (equivalent to the relative elongation rate given the simplifying assumption of a constant cell radius).

These equations can be combined, eliminating *P*, to give:

$$(\mathrm{d}L/\mathrm{d}t)/L = mK(\Psi_o + \pi - Y)/(m + K), \tag{3}$$

which is commonly called the Lockhart equation. If *K* is much larger than *m*, which seems to be typical, then Eq. 3 reduces to Eq. 1.

To understand cell wall behavior, values for *m, Y*, and, to a lesser extent, *K* need to be measured experimentally. The challenge is that one or both *m* and *Y* may respond rapidly to changes in *P*, as well as being responsive to hormonal control through enzymatic action (or equivalent), meaning that, rather than these being fixed values for a given tissue, the expansion rate is modulated according to a set of rules that may be complex to determine (Passioura and Fry 1992).

The Lockhart equations were later expanded by Ortega to consider the three-dimensional expansion of plant cells, the elastic component of shape change, and the loss of water through transpiration (Ortega 1985, 2004). The constitutive law (1) is modified to include the elastic component of the cell wall, taking in essence a Maxwell model of the cell wall with a spring and a dashpot (a damper which resists motion via viscous friction, as seen, e.g., in the closing mechanisms which stop doors from slamming shut) in series, to become:

$$(\mathrm{dV/dt})/\mathrm{V} = \mathrm{m}\ (\mathrm{P} - \mathrm{Y}) + (1/\varepsilon)\mathrm{dP/dt} \tag{4}$$

where V gives the volume of the cell, ε is the volumetric elastic modulus, and all other variables are as previously defined. Here the cell wall can exhibit both irreversible (for stresses above the yield

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point, represented by the dashpot) and reversible (for stresses under the yield point, represented by the spring) deformations, given by the first and second terms on the right-hand side of Eq. 4, respectively. The turgor pressure regulation equation (3) is also modified to capture the loss of water via transpiration (when biologically relevant) to give

$$(dV/dt)/V = K(\psi_0 - P + \pi) - (dT/dt)/V \tag{5}$$

where T is the water volume lost through transpiration so that the equation represents both the net rate of water uptake through osmotic regulation and the rate of water loss through transpiration (first and second terms on the right-hand side of Eq. 5, respectively).

The Lockhart equation is at the basis of numerous models that attempt to explain tip growth, a very polarized process of cellular expansion in walled cells (Kroeger and Geitmann 2012b). Tip-growing walled cells such as fungal hyphae, pollen tubes, root hairs, and algal zygotes are characterized by the ability to form a cylindrical protuberance that expands only at its extreme end, the tip. Cell wall deformation is therefore spatially confined to a very small area of the cellular surface. The apical cell wall yields to the turgor pressure and new cell wall material is only delivered there. The apical cell wall matures rapidly, and once it is stiff enough to resist stretching, it forms a sleeve that generates the elongating tube. Geometrically, tip growth is therefore essentially a one-dimensional process that is amenable to modeling because of its radial symmetry (Kroeger and Geitmann 2011, 2012a). Various modeling approaches have focused either on the mechanical aspects regulating the spatial confinement of the growth process or on temporal regulation. Intriguingly, tip growth rarely occurs at a constant rate but typically displays rhythmic oscillations. These temporal changes have been modeled based on interacting feedback loops that consider a variety of parameters, focusing either on cell wall assembly driven by exocytosis and in turn controlled by transmembrane ion fluxes or on other intracellular signaling pathways. Many of these conceptual and mathematical models have been reviewed in detail (Kroeger and Geitmann 2011, 2012a; Kroeger and Geitmann 2012b; Winship et al. 2010, 2011).

Similarly the Lockhart equation is often used as the mechanical basis for more complex plant tissues modeled using a computational approach which describes individual cells surrounded by cell walls. Modeling frameworks such as the Virtual Leaf (Merks et al. 2011) incorporate biologically realistic elements such as the reaction and diffusion of chemicals, alongside cell walls which grow according to a Lockhart law to describe, for example, plant tissue growth (Merks et al. 2011) and meristem development (Hamant et al. 2008).

Continuum Mechanics Models of Growth

While the simplicity of the Lockhart/Ortega approach is attractive, providing a straightforward way to describe the mechanical responses of plants as well as to incorporate mechanics into more general models of growth, it neglects many important aspects of growth, particularly by assuming one-dimensional growth (as would be typical for a cylindrical cell in the root or shoot cortex) and neglecting much of the complexity of the cell wall. Furthermore, extensibility and yield are empirical parameters, which are difficult to relate to the intrinsic mechanical properties of the cell wall, and can change significantly depending on the geometry and scale of the system considered. Continuum mechanics models can be used to explain these additional features of plant growth, and these models use the intrinsic parameters which should (at least in theory) be measureable and do not depend on the geometry of the system in which they are measured.

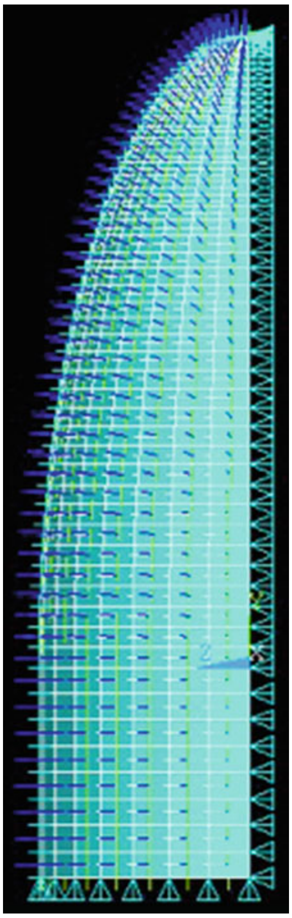

Fig. 3 Finite element model of a pollen tube showing a quarter of the tube as used in Fayant et al. (2010) (Figure prepared by Pierre Fayant)

Finite Element Models of Elastic Cell Wall Behavior

To cope with the often complex geometry of growing plant cells, finite element modeling (FEM) has been employed as a tool to predict the deformation of a geometrically complex thin-walled shell under the effect of turgor. FEM is a discretization approach based on the division of a larger structure into subdomains with the aim of producing an approximate solution. This strategy allows addressing and simplifying the calculation of geometrically complex cell shapes that are otherwise difficult or impossible to approach with conventional numerical strategies. The size of the subdomains, or finite elements, can be varied within the mesh representing the overall structure. The accuracy of the model can be increased at locations of geometrical complexity whereas the elements can be much bigger and the solutions less precise where geometry is either simple or where the anticipated load-induced behavior is more homogenous, to reduce computation time (Fig. 3). The elements composing a finite element structure can be equipped with a variety of mechanical properties, and spatial gradients are easy to implement.

Although in principle a classical continuum mechanics approach, finite element methods can be used at various length scales. This method is therefore useful for mesoscopic modeling approaches as well as for conventional continuum mechanics calculations. In an attempt to simulate the effect of single-cell ablation on the surrounding cells in the shoot apical meristem, Hamant et al. (2008) used finite element modeling to represent the cellular structure. In this model, each stretch of wall between two neighboring cells was represented as a single element and this approach allowed the authors to

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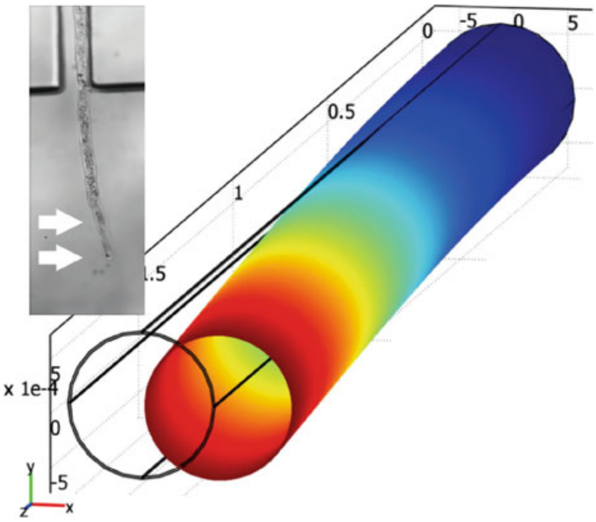

Fig. 4 Finite element model of a pollen tube bent by fluid flow using a microfluidic device for the purpose of determining the Young's modulus of the cell wall. The inset shows a micrograph of a bent pollen tube (Modified after Sanati Nezhad et al. (2013))

predict the main stress pattern resulting from the laser ablation experiments. This was informative since in the experimental situation, microtubules in the neighboring cells reoriented as a consequence of the ablation, and they did so along the stress lines predicted by the model. The finite element approach was thus useful to approximate and simulate the behavior of a plant tissue and to assess how a small-scale disturbance in the force equilibrium affects surrounding areas.

Finite element methods were also used to simulate the elastic deformation of the cell wall under a transient external load application, with the aim of extracting the mechanical properties of the cell wall in a geometrically more complex situation. The applied deformation in these situations was elastic, and typically the load consisted of a flat or stylus-like indenter directed perpendicularly to the plane of the wall (Bolduc et al. 2006; Hayot et al. 2012; Wang et al. 2006). Since much of the resistance to this type of deformation is generated by the hydrostatic pressure of the cell, the extraction of quantitative values for the cell wall properties from these measurements has profited from the finite element approach. To generate a direct tensile stress in the wall of a single cell with the aim to determine its Young's modulus (the measure of the stiffness of an elastic material), a different experimental approach was chosen in the case of the pollen tube, a very long, cylindrical cell. The cell was bent experimentally, and finite element modeling was used to calculate the properties of the cell wall from the measured bending stiffness of the cell (Fig. 4) (Sanati Nezhad et al. 2013).

All of the above examples have used the finite element approach to simulate the elastic deformation of the cell wall under a transient load. However, true growth processes have been analyzed using the finite element approach as well. To determine which distribution of mechanical properties is required to produce a cylindrical, tip-growing cell, the cell wall was represented as a mesh of finite elements that was sufficiently fine so as to represent the growing region of the cell with hundreds of elements (Fayant et al. 2010). The individual elements were then equipped with different values for the Young's modulus, expressing stiffness. Furthermore, the cell wall elements were allowed to display anisotropic behavior. A pressure was then applied to simulate the turgor and the shape of the tube resulting after the equilibration of forces was monitored. The simulations were assessed for their performance in terms of shape generation and strain profile, both based on experimental data obtained from growing pollen tubes. The predictions made by the model consisted of a spatial profile of the mechanical properties of the cell wall that would yield a cylindrical cell in the same way that the pollen tube produces its tube. Using this mechanical profile, it was then possible to identify the biochemical components in the pollen tube cell wall that are responsible for generating this gradient. It was found that the enzymatically induced maturation of pectin material plays a crucial role. The methyl-esterified versions of pectins are secreted in the apical dome, and during maturation they undergo de-esterification, a biochemical process that determines morphogenesis in this cell because it implies a stiffening of the wall and limits the further widening of the tube (Fayant et al. 2010).

Viscous Models of Cellular Growth

While the majority of the elastic models described above can effectively describe reversible shape changes which happen over a short timescale, it is difficult to capture irreversible growth behavior using such a model. This can be rectified through either incorporating an evolving reference state (i.e., stress-free configuration) or by assuming that the cell wall material behaves as a viscous/plastic material. Elastic growth models are comprehensively described in Goriely et al. (2008); therefore, the focus here is on viscous and viscoplastic models. Both approaches have merits and are somewhat analogous, and the choice of modeling framework used should depend on the biological problem considered. Treating the material as viscous is in some ways the simpler approach and benefits from using a more developed mathematical framework, producing more tractable and understandable models particularly of pure growth processes. However, when the reversible behavior of the material is important and must be captured, incorporating an evolving reference state is more appropriate.

One such model is that of Dyson and Jensen (2010), which includes the mechanical effect of the cellulose microfibrils. This model considers a cell expanding in isolation, treating the cell wall as an axisymmetric sheet with an (assumed constant) internal turgor pressure. The cell wall is treated as a fiber-reinforced viscous material, where the fibers represent the cellulose microfibrils present in the cell wall, neglecting the short-term elastic behavior and yield, but including the effect of the microfibrils which passively reorient with the cell wall material. By assuming that the cell wall is much thinner than the radius of the cell, the system of equations can be significantly simplified and shows that, provided the viscosity in the fiber direction is large compared to the viscosity of the matrix material, the radius of the cell will be conserved during growth, being constrained by the presence of the fibers. When the fibers are perfectly aligned as hoops around the cell, the model collapses to

$$(\mathrm{dL}/\mathrm{dt})/\mathrm{L} = \mathrm{PR}/(8\mu\mathrm{h}), \tag{6}$$

where μ is the viscosity of the matrix material (modified for the volume fraction of the fibers), R is the radius of the cell, and h is the thickness of the cell wall (assumed constant). Comparing Eq. 6 with Eq. 1, and recalling that Eq. 6 assumes that the yield, Y, is zero, it is seen that this model provides a more rigorous derivation of the original Lockhart model and identifies the intrinsic geometric and mechanical properties that combine to form the extensibility, m. This modeling framework can also be used to investigate how changes in fiber orientation can be mathematically described, leading to a modified Lockhart-type equation.

Similarly, Dumais et al. (2006) derive and solve an anisotropic-viscoplastic model for tip growth where the cell wall behaves as an anisotropic Bingham material, that is, as a viscous material operating above a yield threshold with a directional dependence of the mechanical parameters. They demonstrate how the mechanical parameters affect the shape of the cell and show that mechanical anisotropy is necessary to explain the patterns of wall expansion observed experimentally.

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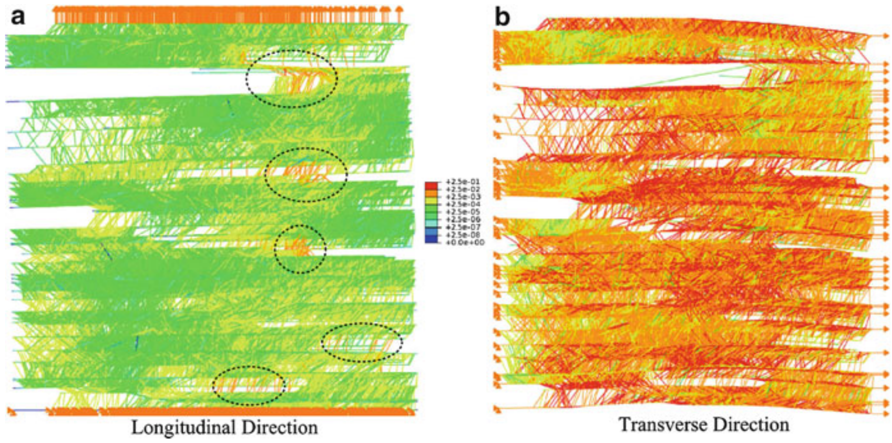

Fig. 5 Wireframe network model of the cellulose microfibril – hemicellulose network by Yi and Puri (2012). Deformed shape of a network fragment when subjected to 1 % strain in the longitudinal direction (**a**) and the transverse direction (**b**). The color bar shows stresses (in MPa) in elements and joints. A longitudinal (major growth) direction deformation results in a lower stress level compared with a transverse (minor growth) direction deformation (Figure from Yi and Puri (2012) with permissions)

Microstructure Models of the Cell Wall

Rather than considering the cell wall as a continuum material with spatially averaged properties, microstructure models consider the individual polymers of the wall as elements that can behave differently and that are linked to each other to transfer forces from one element to another under tensile stress conditions. Such models allow us to make predictions about the macroscale behavior of a piece of cell wall, as well as determining how altering the microstructure, for example, through enzyme activity, affects these macroscale mechanical properties. There are significantly fewer of these models compared to the cell and tissue scale continuum mechanics models described above. Some of them are detailed below, each of which has their own merits and drawbacks. The most appropriate framework for a given situation should be selected.

Veytsman and Cosgrove (1998) consider the cell wall to be a "sticky network" and relate the elastic stress in the composite cell wall to the microfibril properties and the behavior of the hydrogen bonds between the microfibrils and the hemicellulose molecules via a thermodynamic formulation, predicting that the cell wall will creep above an elastic yield threshold. This model, however, neglects the anisotropy of the cell wall, the deposition of new wall material, and viscous stresses from hemicelluloses detachment and reattachment.

Approaches to modeling of cell wall microstructure have also been based on finite element methods, typically by considering the presence of the major elements of the load-bearing network, cellulose microfibrils, and hemicellulose linker molecules. The software WallGen (Kha et al. 2010) builds a fragment of virtual wall whose components have one-to-one spatial and mechanical correspondence with these polymers. The actual geometry of the fragment is generated by stochastic self-assembly. The model enables prediction of the effect on the anisotropy of the wall material of parameters such as microfibril orientation and the number of hemicellulose cross-bridges. While considering the mechanical properties of the individual polymers, this model does not include any description of the interaction between microfibrils and hemicellulose tethers. These cross-links in the model were therefore essentially unbreakable. A later model by Yi and Puri (2012) adopted a joint element as a linker representing these cross-links (Fig. 5). This model is hence able to accept mechanical properties for these cross-links (which were assumed to be hydrogen bonds). The effect

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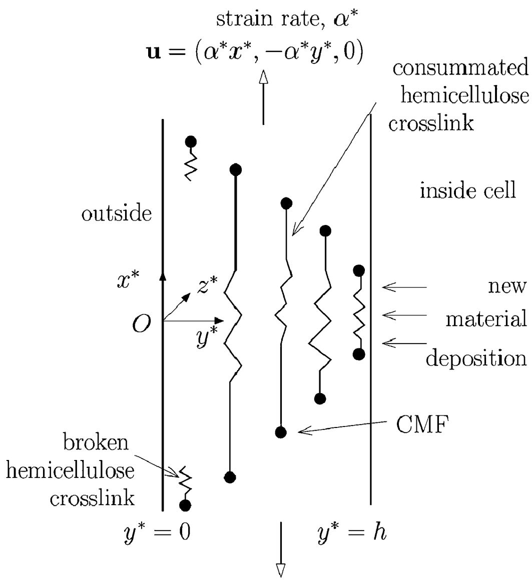

Fig. 6 Mathematical model of hemicellulose cross-link dynamics in an expanding cell wall incorporating strain-enhanced breakage and enzyme-mediated cross-link kinetics. In the cross-section of the cell wall shown here, the cellulose microfibrils are represented as black circles and lie perpendicular to the page, showing the movement of hemicellulose cross-links through the cell wall (Figure from Dyson et al. (2012) with permissions)

of matrix components such as pectin is not accounted for in the present versions of these models but will be important in future expansions of the model. Inclusion of matrix polymers is considered to be necessary to explain the viscous behavior of the growing cell wall and may be the origin of the time-dependent behavior.

Passioura and Fry (1992) derive a simple model of the dynamics of the hemicellulose network which cross-link the cellulose microfibrils, assuming uniform properties across the thickness of the cell wall. In this model, the cross-links gradually become load bearing as the cell wall stretches and they progressively detach from the cellulose microfibrils, and they also break as a function of time. Each individual cross-link behaves like a Bingham/Lockhart-type element, with a yield threshold above which the element extends irreversibly. Passioura and Fry propose a relationship between the macroscopic yield and extensibility of the cell wall segment and the microscopic yield and extensibility of the individual cross-links.

Dyson, Band, and Jensen follow a similar framework and derive a model of hemicellulose cross-link kinetics where each individual cross-link behaves as a linear spring which stretches as the cell wall expands and breaks with a strain-dependent rate (Fig. 6) (Dyson et al. 2012). The macroscopic behavior of the network can then be calculated by summing the effect of all the cross-links. The model also incorporates the effect of enzymes that remodel the hemicellulose network through breaking, reforming, and lengthening cross-links. The cell wall is considered to have constant thickness, with a continual deposition of new unstressed cross-links which are recruited to load bearing as the cell wall is stretched. The characteristic yielding behavior which is assumed in the Lockhart model is a natural output of this model, with the yield threshold found to be dependent on the properties of the hemicellulose network and with the post-yield extensibility depending on the properties of the pectin matrix. Fozard et al. (2013) incorporates this model and that by Dyson and Jensen (2010) into a vertex-element model of a plant root and include a diffusible growth inhibitor and cell division to investigate growth and bending.

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Experiments to determine the yielding behavior of cell wall material include tensile tests during which typically a load is applied suddenly and the resulting deformation of the wall is monitored over time. Time-dependent behavior (i.e., any gradual deformation that follows the initial stretching) is interpreted as creep or viscoelastic deformation that results from the breaking of bonds. Individual breaking of bonds under the tensile load applied by the turgor is also at the basis of a physical treatment of cell wall behavior termed the loss-of-stability (LOS) model (Wei and Lintilhac 2003). However, unlike the abovementioned models, the LOS model proposes that the cell wall behaves according to the Eulerian concept of instability under gradually increasing loading conditions. With a gradual increase in internal pressure, the resulting stresses in the wall are assumed to gradually increase to a critical value, at which time LOS occurs, leading to stress relaxation in the wall. A single LOS event could essentially correspond to the breakage of the weakest/most strained individual polymer bond within the wall at a given critical pressure. The authors argue that the LOS model, but not creep/viscoelastic models, is consistent with the experimental finding that even a small reduction in turgor causes a complete arrest in cell growth.

Modeling at Atomistic Scale

For the time being, representing individual atoms within a cell wall model will remain too computationally expensive to be useful for calculations of overall cell wall deformation behavior. However, atomistic modeling has the potential to produce important data for multiscale modeling. This means that the information produced at the atom or molecular scale can be incorporated in higher-scale modeling approaches. Atomistic modeling of the plant cell wall has hitherto focused on cellulose. For example, the behavior of glucose or short polymers of cellulose has been modeled to assess how they behave in aqueous solution, in the presence of ions, or at different temperatures and to assess how enzymes bind to their surface. This includes, for example, the interaction of the carbohydrate-binding module from a fungal cellulase on the hydrophobic face of crystalline cellulose (Beckham et al. 2010) or the manner in which cellulose microfibrils twist under different conditions (Matthews et al. 2012). These types of modeling approaches were developed to determine how enzymes from fungi and other organisms degrade plants in the biosphere and to aid in designing enhanced enzymatic properties to facilitate efficient conversion of cellulose to glucose for bioenergy processes. However, similar modeling strategies will be useful to understand how endogenous enzymes and proteins interact with cell wall polysaccharides to regulate the overall mechanical properties of the wall in the context of cellular growth and expansion.

Future Directions

A number of the current challenges in plant cell wall modeling are summarized briefly below.

Modeling the plant cell wall has been undertaken with a variety of reasons in mind. Depending on the application and the question asked, the optimal approach has to be chosen. It may be intuitive to think that the more details are included in the model, the better it might represent reality. However, it must be considered that greater detail also requires a greater number of quantitative values as input parameters. If these cannot be measured experimentally, educated guesses and assumptions need to be made, the choice of which may influence the results of the simulations significantly. A model at a smaller scale is therefore not necessarily a model that produces better quality predictions. The quality of the output can only be as good as the quality of the input.

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One of the parameters required for mesoscale and for atomistic models is quantitative information about the molecular geometry of cell wall structure. This requires quantitative imaging and analysis techniques. Structural polymers such as microfibrils can be imaged and quantified relatively easily using electron microscopic techniques and atomic force microscopy and when using live imaging, with specific vital dyes or with the more recently developed click chemistry. However, the situation is much more challenging for the matrix polymers. Quantitative and true architectural information on these polymers is difficult to obtain for multiple reasons ranging from artifacts arising from sample preparation to the simple challenge of identifying polymers based on their appearance.

Some of the modeling approaches described above have incorporated the mechanics of polymer-polymer linkages. While these are based on available knowledge of the respective molecular behaviors, the complex and heterogeneous architecture of the wall may cause intermolecular bonds to behave in much more complex manner than any in vitro measured constants would reveal. Local conditions such as water content and pH may play crucial roles. In particular, incorporating the dynamics of water movement is not trivial to model.

One of the long-term goals of many modeling approaches is the integration of cell wall material behavior with biochemical and biological processes such as signaling and enzyme activity. Feedback between growth and hormone dynamics has been shown, for example, by Band et al. (2012b) who demonstrated that the dilution of the hormone gibberellin by the expansion of root cells within the elongation zone can have a significant effect on the production of downstream growth-repressing proteins such as those in the DELLA family. Coupling such a model with mechanical models for tissue growth via a mesoscale model such as that of Dyson et al. (2012) which links enzyme levels to the cell wall mechanical properties would be a significant advance and allow for a truly integrative approach (Band et al. 2012a).

Another challenge that has not been solved satisfactorily is the actual assembly process of the wall. What happens when new cell wall material is added by exocytosis? How are new cell wall polymers inserted into or added onto the existing polymer network? How does this affect existing load-bearing bonds? A number of conceptual models such as those based on the incorporation of new pectin material in the existing wall (Proseus and Boyer 2007) illustrate that producing quantitative simulations of this process is important for their validation.

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Index Terms: