

Modeling the molecular structures and dynamics responsible for the remarkable mechanical properties of a plant cell wall

Anja Geitmann, Bela M. Mulder, Staffan Persson, Edgar P. Spalding*

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EVALUATION OF



Molecular insights into the complex mechanics of plant epidermal cell walls.

Zhang *et al.*

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The primary plant cell wall is a hydrated meshwork of polysaccharides that is strong enough to withstand large mechanical stresses imposed by turgor while remaining pliant in ways that permit growth. To understand how its macromolecular architecture produces its complex mechanical properties, Zhang *et al.*¹ computationally assembled a realistic network of cellulose microfibrils, hemicellulose, and pectin. The simulated wall responded to computationally applied stress like the real wall on which it was based. The model showed the location and chemical identity of stress-bearing components. It showed that cellulose microfibril interactions and movements dominated the wall's mechanical behavior, while hemicellulose and pectin had surprisingly minor effects.

EVALUATION BY



Anja Geitmann

McGill University
Plant biomechanics, plant
development, plant reproduction



Bela M. Mulder

Institute AMOLF Amsterdam; Utrecht
University
Molecular models of the plant cell
wall and cytoskeleton



Staffan Persson

University of Copenhagen
Plant cell walls, cellulose synthesis,
and the cytoskeleton



Edgar P. Spalding*

University of Wisconsin
Transport of ions including auxin,
seedling growth, and image
processing

*Corresponding author and primarily responsible for drafting the consensus evaluation:

Edgar P. Spalding (spalding@wisc.edu)

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Background

Cell walls shape plants by determining the rate and direction of cell expansion and provide structure and support to the plant body. Cell walls permit plant cells to be pressurized well beyond atmospheric pressure, which shapes their physiology. Practically, they are a source of energy and fiber.

Plant cells are “born” with a primary cell wall that continues to assemble and expand as the cell grows. It consists mostly of cellulose microfibrils, pectin, and hemicellulose polysaccharides. Somehow, these polymers combine to produce a material with remarkable mechanical properties. Just enough is known about one primary cell wall — the outer wall of onion scale epidermal cells — to make a quantitative model of the structure. A quantitative model is, at its core,

a hypothesis posed in the form of mathematical statements. If a model of the wall can reproduce the measured mechanical behavior, the information, ideas, and assumptions in the model are probably on the right track. A useful model, as opposed to a merely accurate model, leads to new insights. In this respect, Zhang *et al.*¹ were successful. Their coarse-grained molecular dynamic model identified some molecular interactions and movements that determine important aspects of the onion epidermal wall’s complex mechanical behavior. When viewed in the context of a progression of advances, this new model sets a landmark on the path to comprehension of wall structure-function relationships (Figure 1).

A major reason to seek a comprehensive understanding of the primary cell wall is that its mechanical properties control plant cell growth. In fact, an early

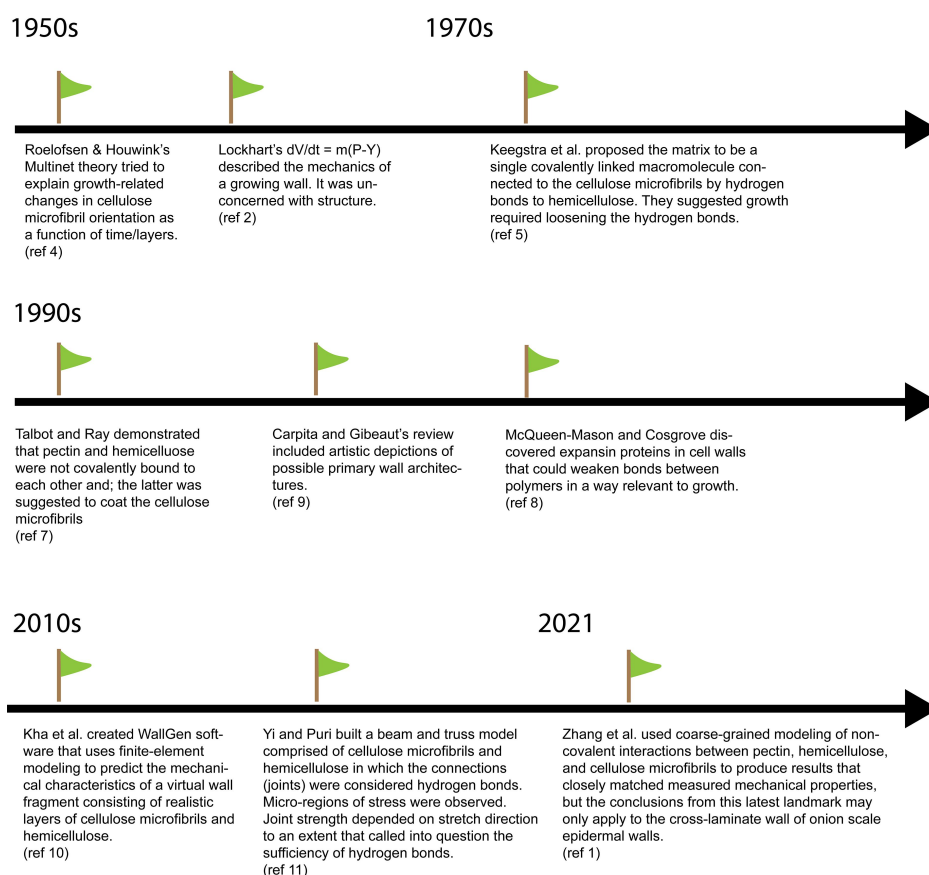


Figure 1. Landmarks along the path to a quantitative structure-function model of a cell wall

This timeline depicts some of the previous steps toward an understanding of cell wall structure-function relationships that are relevant to the Zhang *et al.*¹ landmark.

landmark on the path to comprehending the wall was Lockhart's concise model of plant cell expansion².

$$dV/dt = m(P-Y)$$

The rate of cell expansion (dV/dt) depends on the turgor pressure (P) when P is greater than a threshold pressure, Y . When P exceeds Y , wall expansion increases at a rate determined by m , the extensibility of the wall. It is now established that a plant cell pulls water in osmotically, which increases cellular volume, which increases the stress (force per unit of cross-sectional area) borne by the wall. If the stress exceeds the threshold, the wall will give way, or yield, like slipping a belt buckle to a more comfortable notch. Lowering the stress lowers the free energy of the contained water, which allows more to enter, which expands the cell, and reestablishes wall stress. This pressure-driven increase in wall size is a plastic deformation, meaning the larger size persists if you remove the force. The wall is also somewhat elastic, but the governing modulus is large, meaning that it is stiff, more like a football than a party balloon. You may have trouble thinking of an everyday material that displays such a combination of properties. For example, a bedsheet will not yield when you pull on it until it tears. Fresh pizza dough, on the other hand, will readily yield and then maddeningly spring back when you stop trying to spread it. A primary cell wall has elements of the bedsheet and the pizza dough. Somehow, cellulose microfibrils, hemicellulose, and pectin combine to make a viscoelastic material with a high tensile strength that displays a yield threshold, plasticity, and elasticity³.

The onion scale epidermal wall, which can be peeled off in strips large enough for mechanical tests and inspected by microscopy, is composed of distinct layers. The cellulose microfibrils within a layer are roughly aligned. Successive layers are slanted to form a cross-laminate structure. Cross your hands, palms-down

flat in front of you and see how your fingers form two such layers. Between the cellulose microfibrils (your fingers) are the hemicellulose and pectin. Because all components are polysaccharides bearing hydroxyl groups, the ensemble is a mosh pit of potential hydrogen bonds and other noncovalent interactions. To create a quantitative model of the structure, Zhang *et al.*¹ used detailed measurements of wall architecture made with electron and atomic force microscopy. In a systematic manner, they encoded molecular structures and properties they had reason to believe would be important into terms a computer could evaluate. They treated the polysaccharides as beads on a string, endowing each bead with some mathematically defined, physical chemistry-based propensity to interact with a nearby bead. They set chain stiffness and other parameters based on direct measurements or data-informed guesses. Then, they built a four-layered wall in equations and let it settle down. The computed equilibrium wall satisfyingly resembled high-resolution images of the onion scale epidermal wall. Now the mathematically expressed hypothesis could be tested. A tiny strip of this virtual wall was computationally 'pulled,' and the mechanical features and behaviors were computed. On the lab bench, small strips of real onion scale epidermal walls were also pulled, allowing real strains and force-relaxation curves to be measured. The real and the virtual agreed to a strikingly high degree. The model wall and the real wall displayed plasticity when stress exceeded a threshold. They both displayed elasticity, stress-dependent stiffness, and other complex mechanical nuances. The model is accurate, but is it useful?

Main contributions and importance

Zhang *et al.* did not invent major new methods or start with a novel concept. Instead, they used an existing modeling framework (coarse-grained) that

matched the scale of the operational elements (wall polymers) and, in a process familiar to material scientists, constructed a virtual wall. What makes the Zhang *et al.* project a landmark is not the approach but its accurate and insightful results. Their model identified polymer movements and interactions that are responsible for the mechanical properties and behaviors most in need of understanding. Their model shows that imposing stress causes cellulose microfibrils within a layer to align or straighten in its direction. With your crossed hands down, slightly push your elbows forward to see how your overlapping fingers make a comparable movement. As stress increases and the polymers move, some microfibrils form small bundles, like crossed wet spaghetti noodles might laterally adhere when pulled in opposite directions. When stress exceeds a threshold, the microfibrils begin to slide along each other. Thus, microfibril sliding is the basis of plastic deformation and the “straightening-to-sliding transition point marks the yield threshold.” This remarkable result shows polymer movements and interactions associated with Lockhart’s growth-controlling parameters m and Y . What was not observed, a significant stress-bearing role for hemicelluloses, is also enlightening. Even when the binding of hemicellulose to cellulose was programmatically tightened, the former did not take on a share of the load or substantively influence mechanical behavior. By applying two cycles of stress to real and simulated walls, the model produced an unexpected explanation of elasticity, again cellulose based. Apparently, bond lengths in a microfibril can increase and contract, giving its axis more of a bungee cord property than commonly believed. Because the model is based on realistic molecular-level elements, the microscopic stress and strain components can be chemically identified and located. Imagine being able to see in a strip of Velcro which of the multitude of tiny hooks was doing the fastening

work. Color-mapping these stress points onto the realistic tangle of wall polymers produces a striking, insightful visual.

Elements of preceding landmarks can be seen in the successful Zhang *et al.* model. Some are highlighted in [Figure 1](#). The alignment of cellulose microfibrils in different layers of walls, and the effects of growth on them, was the main interest of Roelofsen and Houwink’s Multinet Theory⁴, proposed when microfibril orientation was mainly inferred from optical birefringence and before electron microscopy was standard. The chemical composition and linkages of the non-cellulosic (matrix) polysaccharides became better understood as biochemical methods for wall deconstruction and analysis advanced. At first, evidence indicated that pectin was covalently linked to the hemicellulose and the latter to cellulose by hydrogen bonds that may be weakened to promote wall yielding⁵. Fry proposed that hemicellulose tethered cellulose microfibrils together and these tethers should be enzymatically cleaved to permit wall yielding⁶. Talbot and Ray demonstrated that the classes of polymers were mostly not covalently linked⁷. Rather than tethers bearing the load, noncovalent interactions between hemicellulose-coated cellulose microfibrils, they suggested, could govern the mechanical behavior. The importance of hydrogen bond-based interactions was raised to the fore by the discovery of expansin proteins that weaken them⁸. Even elements of previous, somewhat speculative, artistic depictions of interwoven polymers⁹ can be discerned in the Zhang *et al.* molecular model.

None of the landmarks in the top two rows of [Figure 1](#) were quantitative models (mathematical statements of hypotheses) relating structure to function but rather conceptual models meant to help us understand cell wall behavior intuitively, given

increasingly detailed descriptions. Not until the 21st century was enough known or methods sophisticated enough to combine molecular, architectural, and functional information together in the form of equations^{10,11}. The Zhang *et al.* report is the latest and most successful attempt to do so. It establishes a landmark on the path to understanding a remarkable and important biomaterial. But already since its publication, more detailed visualizations of the cellulose microfibril orientations in the onion scale epidermal wall layers have been achieved with cryo-electron tomography and ion-beam milling¹². Such new information will enable tests of the hypotheses and assumptions encoded in the Zhang *et al.* model, which will advance us toward the next landmark.

Open questions

All successful research leads to a desire for more information. Readers of Zhang *et al.* may wonder to what extent the model will apply to other types of plant primary cell walls. Will it be possible to learn about walls that are not as obviously multi-cross laminate? What makes cellulose sliding an irreversible (plastic) deformation? The measured and modeled cells have ceased growth. Can the insights gained from this system be translated to growing walls? The effects of proteins were not included in the model but expansins are thought to affect wall properties by affecting some of the noncovalent associations the model indicates are critical. Several other protein and enzymatic functions also likely contribute importantly to wall characteristics. Can the model be augmented to include the action of proteins? If measurements show effects of realistic changes in H^+ and Ca^{2+}

concentrations, could the model indicate their modes of action? Would the matrix polysaccharides play a bigger role if they had not been represented only as a simple xyloglucan and homogalacturonic acid? If the matrix polysaccharides do not contribute significantly to mechanical properties, what is their role in the wall? What are the prospects of similarly studying a non-epidermal primary wall?

Conclusion

An architecturally and molecularly realistic primary plant cell wall, assembled in the framework of a coarse-grained molecular dynamic model, produced mechanical properties essentially like measurements of the real wall on which it was based. The model provided molecular-level insights. It showed that plasticity (key to cell expansion) and a yield threshold (a potential expansion control parameter) are largely attributable to cellulose microfibrils reorienting to align with the stress, a tendency for microfibrils to adhere to each other in small bundles as stress increases, and then to sliding of the laterally adhering microfibrils. At least in an onion scale epidermal wall, cellulose interactions and movements are the principal determinants of major mechanical properties. There was surprisingly little contribution to mechanical properties from the hemicellulose and pectin components of the wall. When new hypotheses about wall structure-function relationships are posed and tested, limitations in the model may emerge. Additional polysaccharide diversity, inorganic components such as Ca^{2+} and H^+ , and wall regulating proteins may need to be incorporated to refine and expand the model.

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