Non-linear optical spectroscopy study of plant cell walls – New opportunities and challenges

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Plant cell walls (often called as lignocellulosic biomass) consist of crystalline cellulose microfibrils and amorphous matrix polymers. The crystallographic information of the unit cell for the isolated and purified cellulose I-alpha and I-beta crystals provided foundations for understanding molecular interactions and packing between cellulose chains. However, little is known about how crystalline cellulose is assembled and integrated with matrix polymers in intact plant cell walls, bacterial pellicles, and animal tissues. This question could be addressed by vibrational sum-frequency-generation (SFG) spectroscopy which measures non-linear optical responses of noncentrosymmetric media. In 2011, we have reported that SFG can selectively detect crystalline cellulose in woody cell walls without spectral interference from non-cellulosic components [A. L. Barnette, et al. *Biomacromolecules***2011**, 12, 2434-2439]. Since this first report, there have been significant advances in how SFG signals can be interpreted in terms of crystal structure of cellulose and mesoscale hierarchical ordering of crystalline cellulose domains in biomass. This talk will present new insights in understanding SFG responses of plant cell walls and show how SFG can be used to obtain structural information relevant to biomass deconstruction and conversion.