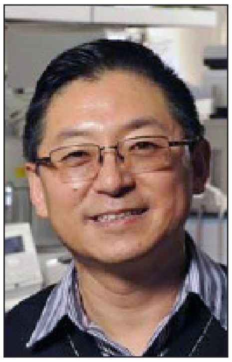
Cellulosic Revelation

Researchers Look at Molecular Structure of Biomass

Researchers at Washington State University Tri-Cities and Pacific Northwest National Laboratory (PNNL) in Richland, WA have discovered that newly-combined spectroscopy processes can reveal the differences between the inside and the outside of the molecular structure of cellulosic biomass.



Bin Yang

The researchers' spectroscopy breakthrough could lead to more efficient and economic ways to make products from cellulosic biomass, according to Bin Yang, associate professor of biological systems engineering at Washington State University Tri-Cities (*www.tricities.wsu.edu*).

Yang told *BioFuels Journal* in a telephone interview that this is the first time that researchers have been able to reveal the characteristic differences between the surface layers and the crystalline core of cellulose by the Total Internal Reflection Sum Frequency Generation Vibrational Spectroscopy (TIR-SFG-VS) and conventional SFG-VS, which together use a combination of laser and other light sources.

Understanding Biomass

Understanding cellulosic biomass at the molecular level is an important step in overcoming its resistance, or recalcitrance, to degradation so its sugars can be released for processing, Yang noted.

To understand the molecular makeup of cellulose, he stated, a new instrumental measurement was needed by combining TIR-SFG-VS and SFG-VS. The new, combined instrumental measurement has given researchers a better understanding of the differences between the surface and the core of cellulosic biomass.

"It is very important to understand the structure of cellulose so it can be broken down the right way," he said. "The spectra signatures obtained may lead to modification of the current definitions of the different types of cellulose structures. The success of this transformative discovery is significant as it enables characterizing structure and surface vibrational spectra *in situ* and in real time during cellulose biosynthesis and deconstruction for the first time."

Yang said that he and his collaborating researchers have been researching cellulosic biomass for many years. Cellu-

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lose is one of the most abundant organic compounds on Earth, Yang said, but its recalcitrance has made it difficult to process efficiently and cost-effectively.

Yang and the collaborating researchers are continuing to examine the molecular structure of biomass and will be issuing more papers on thermal and biological methods of processing cellulose using the newly-combined spectroscopy processes.

The researchers also are looking at different cellulosic biomass sources such as wood, grasses, and algae and examining how they can be broken down by thermal and biological means, Yang noted.

A paper co-authored by Yang that describes the research findings was published online March 14 in *Scientific Reports*, an online open-access journal produced by the Nature Publishing Group. The paper can be accessed at *www.nature.com/articles/srep44319*.

Hongfei Wang

Co-author Hongfei Wang, who is a former chief scientist in the physical sciences division at PNNL and who is currently a professor of chemistry at Fudan University in Shanghai, China, said cellulose is commonly known to be difficult to break down and convert into other useful products.

"Using our nonlinear vibrational spectroscopic technique, we can resolve some questions associated with the recalcitrance of cellulosic biomass and, in turn, more efficiently convert the product into a usable commodity," Wang said in a news release announcing the spectroscopy breakthrough.

Discovery's Significance

Arthur J. Ragauskas, governor's chair in bio-refining for Oak Ridge National Laboratory and at the University of Tennessee, Knoxville, said the discovery is significant because it challenges the traditional understanding of cellulose materials and provides further insight into the surface and bulk chemistry of cellulosic fibers, building on a novel spectroscopic tool to characterize such structural differences. Ragauskas is an expert on the subject, according to the news release on the research findings, but was not involved in the research.

"The discovery may lead to modification of the current definitions of the different types of cellulose structures," he said. "This discovery represents yet another instance of the importance of spectroscopic observations in transformative advances to understand the structure of the cellulosic biomass. We can use the application of this technology to fundamentally understand the conversion process of nearly every cellulose-based product in the future."

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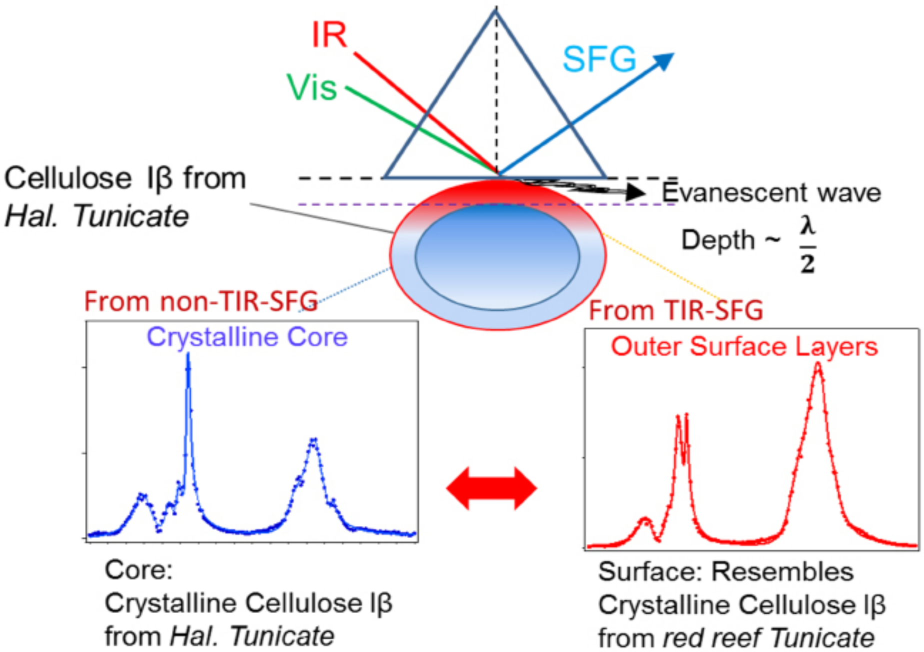
The study was a collaboration between Washington State University and the Environmental Molecular Sciences Laboratory at PNNL. It was primarily supported by a Defense Advanced Research Projects Agency (DARPA) Young Faculty Award to Yang. Ragauskas said the award was made possible because of the unique SFG capability and expertise at the Environmental Molecular Sciences Laboratory (EMSL), a national scientific user facility of the Office of Biological and Environmental Research (BER) of the Department of Energy in Richland, WA.

In addition to Yang and Wang, the research was conducted by Libing Zhang, WSU Tri-Cities biological systems engineering postdoctoral researcher; and Li Fu, William Wiley Postdoctoral fellow at the Environmental Molecular Sciences Laboratory at PNNL.

Jerry Perkins, editor



This graphic shows the measurement of the surface layer and the core of cellulose by the Total Internal Reflection Sum Frequency Generation Vibrational Spectroscopy (TIR-SFG-VS) and the conventional SFG-VS.