Interfacial and Processing Sciences

News Notes

May 1999

Environmental and Molecular Sciences Laboratory
Pacific Northwest National Laboratory

News Notes, established to help keep our Users and others who have had a connection with us up-to-date on activities, events, capabilities, and interesting results, including short summaries of the work of users.

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This issue includes**: Surface Tools Workshop**, **Oxide Symposium at July Users Meeting**, and **I&PS Staff in the News**

I&PS to Conduct Workshop on Surface Analysis Tools during EMSL User Meeting

A one-day workshop on Surface Analysis Methods is scheduled for **July 22, 1999**. This workshop is being scheduled in conjunction with the Environmental Molecular Sciences Laboratory (EMSL) Users Meeting on July 21 - 24, 1999. The combined workshop and Users Meeting provides an excellent way to learn about EMSL capabilities and to see some of the research being conducted.

This workshop is designed to introduce new or potential Users to several surface analysis methods including Auger electron spectroscopy, X-ray photoelectron spectroscopy, and time-of-flight secondary ion mass spectrometry. Presentations will be made by PNNL staff members responsible for instrument use. Approaches to enhancing information from the different techniques and ways to select the best approach will be discussed. Short demonstrations will be given on July 22. Longer “hands-on” demonstrations can be arranged at other times during the week of the User meeting.

The workshop is intended for new or experienced researchers wanting to know more about these tools. It should provide a good introduction for graduate students to the techniques and to EMSL.

For more information, contact Terry Law (509/376-2418) or Don Baer (don.baer@pnl.gov; 509/376-1609). If you wish to test samples or capabilities during the week of the User Meeting, please let us know of your interest, and provide information about the specimens and desired focus of experimentation.

Preliminary Schedule: Mini-Symposium on the Physics of Oxide and Chemistry of Oxide Surfaces

Because of the major focus on oxide surfaces in EMSL, the first User Meeting includes a special session on oxides on *Friday & Saturday, July 23-24, 1999.* For more information about the User Meeting see www.emsl.pnl.gov.

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July 23 AM- Plenary Session

9:00 - 10:00	V.E. Henrich (Yale University) *Metal Oxide Surfaces: Where Are We, and Where Are We Going?*
10:00 - 11:00	Structural biology speaker

11:00 - 11:30 EMSL orientation talk

July 23 PM - Clean Oxide Surfaces

1:00 - 2:00 U. Diebold (Tulane University) *Surface Preparation of Metal Oxide Single Crystals: Who Would've Thought Life is THAT complicated?*

2:00 - 2:30 S.A. Joyce (PPNL)

2:30 - 3:00 S.A. Chambers (PNNL), S. Thevuthasan (PNNL), S.I. Yi (PNNL), Y.J. Kim (Taejon University, S. Korea), J. Morais (UNICAMP-IFGW-DFA, Brazil), R. Denecke (MAX Lab, Sweden), C.S. Fadley (LBNL and UC Davis), P. Liu (Stanford U.), T. Kendelewicz (Stanford U. and SSRL), and G.E. Brown, Jr. (Stanford U. and SSRL) *Surface Structure of MBE-Grown α-Fe_2O_3(0001) and Fe_3O_4(001) by Photoelectron Diffraction*

3:30 - 4:00 M. Gajdardziska-Josifovska (U. Wisconsin), R. Plass, (U. Wisconsin), and S.A. Chambers (PNNL)

4:00 - 4:30 J. E. Jaffe (PNNL), J. A. Snyder (PNNL), Z. Lin (PNNL) and A. C. Hess (PNNL) *LDA and GGA Calculations for High-Pressure Phase Transitions in ZnO and MgO*

July 24 AM - Small Molecule Sorption and Chemistry on Oxide Surfaces

8:30 - 9:30 J.T. Yates, Jr. (University of Pittsburgh) *Chemical Bond Activation on Photochemically-Generated Sites*

9:30 - 10:00 P. Fenter (ANL), P. Geissbuhler (U. Washington), E. DiMasi (BNL), G. Srajer (ANL) L.B. Sorensen (U. Washington), and N.C. Sturchio (ANL) *Calcite-Fluid Interface Structures Probed in-situ by X-ray Reflectivity*

10:00 - 10:30 M. Gutowski (PNNL)

10:45 - 11:15 M.A. Henderson (PNNL), Sary Otero-Tapia (U. Puerto Rico) and Miguel E. Castro (U. Puerto Rico) *Electron Induced Decomposition of Methanol on the Vacuum Annealed Surface of TiO_2(110)*

11:15 - 11:45 L.Q. Wang (PNNL) *Interaction of Water with $SrTiO_3$(001)*

July 24 PM - Oxide Thin Film Growth - Bulk and Surface Properties

1:00 - 2:00 Werner Weiss (Fritz Haber Institute of the Max Planck Society) *Catalysis and Surface Chemistry on Well-Defined Epitaxial Iron Oxide*

2:00 - 2:30 Juerg Osterwalder (U. Zurich), G.S. Herman (PNNL), and Y. Gao (PNNL) *Surface Structure of CVD Grown Anatase TiO_2 by X-ray Photoelectron Diffraction*

2:30 - 3:00 S. Goss (Ohio State U.), L.J. Brillson (Ohio State U.), and S.A. Chambers (PNNL) *Geometric and Electronic Structure of MBE-Grown Al-doped TiO_2(110)*

3:30 - 4:00 J. Yu (Motorola Corporate Research)

4:00 - 4:30 R.J. Smith (Montana State U.), R. Reibel (Montana State U.), S. Thevuthasan (PNNL), and D.E. McCready (PNNL) *Preliminary Results for the Growth of Thin Oxide Layers on Zr and Ti Metal and the Measurement of Hydrogen Concentrations Using Resonant Nuclear Reaction Techniques*

I&PS Staff in the News

Catalysis Conference in C&E News

A story in a recent issue (March 29, 1999) of the American Chemical Society's Chemical and Engineering News featured the work of I&PS scientist Scott Elder. The article described the first DOE National Laboratory Catalysis Conference, which was co-organized by I&PS Interim Associate Director Chuck Peden, and held last month in Albuquerque, New Mexico. Elder's featured research is aimed at the development of new titanium dioxide (TiO_2)-based photo-catalytic materials useful for pollutant destruction and for hydrogen production from water-

splitting. Specifically, materials with enhanced sensitivity to visible light, and longer-lived photo-induced charge carriers are the goal. Elder's approach to this is to use nano-sized TiO_2 catalyst particles that are coated with a secondary oxide.

Development of Automated Nucleic Acid Processing Module Featured in R&D Magazine
Cindy Bruckner-Lea of the EMSL Interfacial and Processing Sciences directorate was one of the researchers featured in an article entitled "New Chemical Technologies Developed for Soil Testing" that was published in the April edition of *R&D Magazine*. The article describes work undertaken by Cindy and her colleagues to develop an automated nucleic acid processing module that allows concentration and purification of DNA milliliters. The concentration and purification step will be critical for applications such the environmental analysis of bacterial pathogens and the monitoring of food processing lines that require low detection limits.

Publication of Symposium Proceedings
The April edition of Surface and Interface Analysis (volume 27, number 4) featured papers from the Surface Analysis '98 conference that was held at PNNL in June 1998. Surface Analysis '98 was a Topical Conference of the American Vacuum Society (AVS) and was sponsored by AVS, PNNL, EMSL, and the Pacific Northwest Chapter of AVS. Don Baer of the EMSL Interfacial and Processing Sciences directorate and Marjorie Olmstead of the University of Washington co-chaired the conference.

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