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Skin Deep: Highlights of NREL Surface Analysis PV Research

S. Asher, J. Pankow, C. Perkins, R. Reedy, G. Teeter, and M. Young

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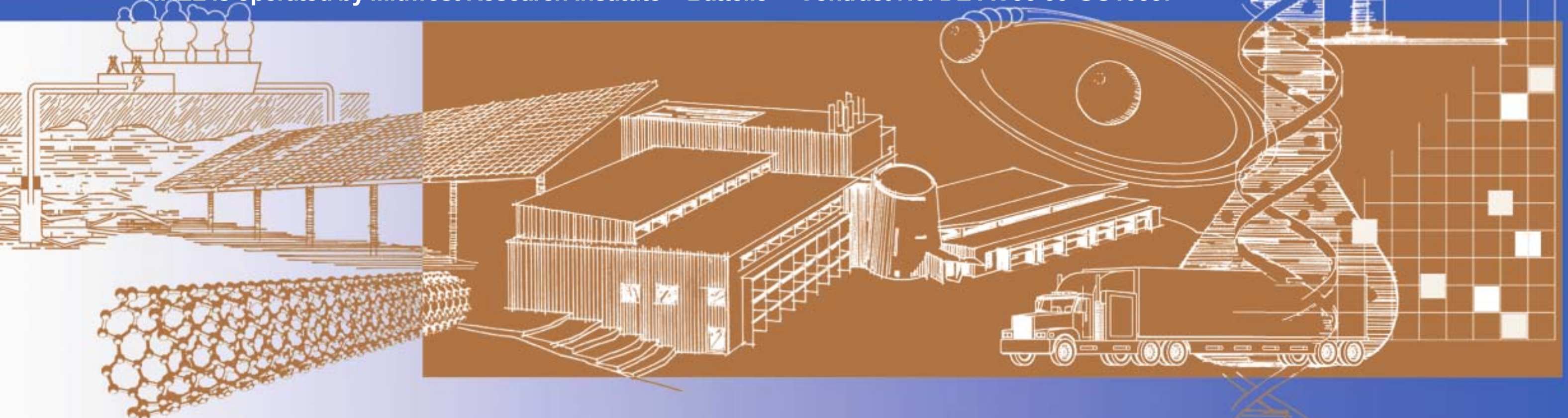

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Skin Deep: Highlights of NREL Surface Analysis PV Research

Sally Asher, Joel Pankow, Craig Perkins, Robert Reedy, Glenn Teeter, and Matt Young
National Renewable Energy Laboratory, Golden, CO, sally_asher@nrel.gov

ABSTRACT

The Surface Analysis project provides measurement support and leadership for collaborative research activities involving surface chemistry and physics in all areas of the PV program. Significant results from the past fiscal year include the following: i) *in-situ* XPS, UPS, and AES studies of chemical-bath exposure of CIGS surfaces demonstrated that Group-III elements are preferentially removed from the surface, that type conversion of the surface occurs, and that the addition of a surfactant improves CdS deposition and thus device performance; ii) XPS studies of polyethylene terephthalate (PET) candidate backsheet materials have shown that plasma exposure prior to oxide-barrier deposition results in the formation of low-molecular-weight fragments that result in the formation of a weak interfacial layer that fails during damp-heat exposure; iii) an empirical relation was derived for the source geometry that leads to optimal film-thickness uniformity in rotating-substrate physical-vapor deposition (PVD) systems; and iv) PVD flux-distribution calculations were performed to develop a novel method for combinatorial thin-film synthesis.

1. Objectives

The primary objective of the Surface Analysis project is, *"To advance the understanding of photovoltaic materials and devices by employing state-of-the-art surface science practices and techniques to investigate surface and interfacial properties."* This is accomplished by the following: i) providing analytical support to participants in the Solar Energy Technologies Program (SETP) photovoltaics subprogram, including NREL in-house, subcontracted, and industrial researchers in all materials areas; ii) leading and facilitating collaborative research projects with researchers in the SETP to solve key problems in the development and reliability of PV materials; iii) working to advance the utility and understanding of surface-analysis measurements by improving analytical methodology; iv) developing new tools for *in-situ* study of surface and interface properties; and v) disseminating research results through publications, presentations, and regular interactions with other researchers in PV and surface-science disciplines. This project supports the goals of the SETP Multi-Year Technical Plan by conducting high-value, high-risk research that furthers the understanding of existing and emerging PV materials and devices leading to improved performance and reliability of PV. Project activities are intimately linked with the development and implementation of the Process Integration concept and the activities scheduled for the Science and Technology Facility. In addition, the project conducts research aimed at understanding sources of degradation in fielded PV modules, and studies materials and methods for improved packaging designs.

2. Technical Approach

This project uses accepted surface-science practices to obtain information about surfaces and interfaces of materials. The work is separated into three main areas: short-term support, long-term collaborative research and development, and technique development. The seven major pieces of equipment include a field-emission Auger electron spectrometer (AES) with mapping capabilities; a photoelectron spectrometer with X-ray and ultraviolet light sources (XPS/UPS); an ultra-high-vacuum (UHV) deposition chamber equipped with reflection high-energy electron diffraction (RHEED), low-energy electron diffraction (LEED), spectroscopic ellipsometry (SE), and thermal desorption mass spectrometry (TDMS); a glove box and a UHV transfer system that transforms the XPS, AES, deposition system, and glove box into a cluster tool; two dynamic secondary-ion mass spectrometers (SIMS) with ion imaging; and a static secondary-ion mass spectrometer (SSIMS) with profiling capabilities. Elemental analysis is performed with and without depth profiling by XPS, AES, and SIMS. Chemical-state analysis is performed by XPS and AES. Molecular information is obtained by XPS and SSIMS. Trace-element analysis of dopants and contaminants in materials is performed by SIMS. Quantitative analysis is performed using appropriate sensitivity factors and standards. The cluster tool is used for *in-situ* studies of surface chemistry and physics of multiple material systems via AES, XPS, UPS and TDMS. The development of the cluster tool also supports research and development for the new effort in Process Integration, including the theory and practice of integrating characterization and deposition equipment on the same platform, and the development of instrument control and acquisition software.

3. Results and Accomplishments

Researchers in the Surface Analysis project have recently commissioned a cluster tool in one of our laboratories. The tool integrates our AES and XPS analysis tools with processing and deposition tools, which allows sophisticated *in-situ* studies of the surface chemistry and physics of PV-relevant materials. Figure 1 shows a photo and a plan-view schematic of the surface-analysis cluster tool. The facilities offered by the cluster tool open new avenues for research on PV materials.

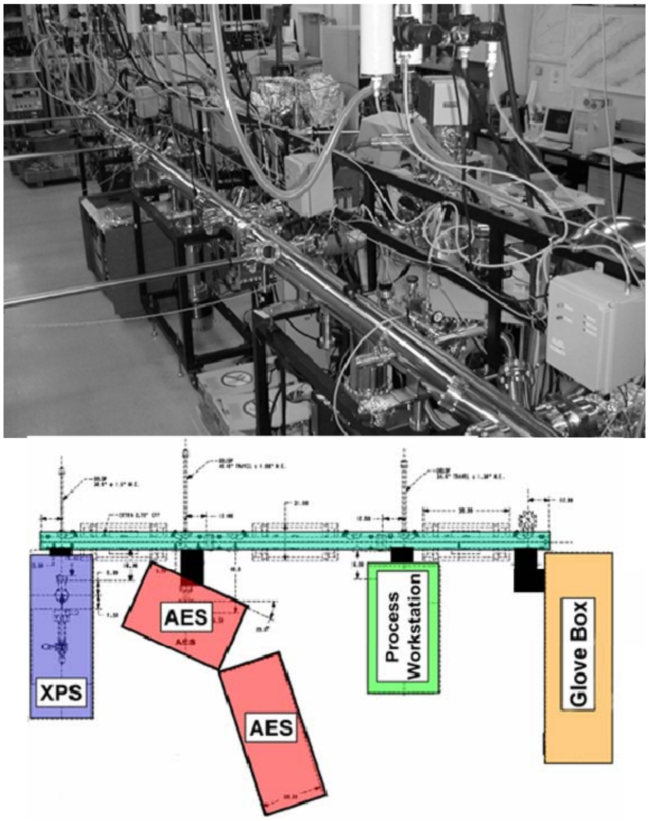

Fig. 1. Photo and schematic of the surface analysis cluster tool.

Several of the research studies from this project are discussed in more detail in other publications in this Review. The reader is referred to the following publications in this volume:

"Surfactant-assisted growth of CdS thin films for photovoltaic applications," by C.L. Perkins and F.S. Hasoon, details the effects of adding a common surfactant to the solution for chemical-bath deposition of CdS, which leads to a substantial improvement of thin-CdS/CIGS device performance.

"Plasma surface modification of polymer backsheets: origins of future interfacial barrier/backsheet failure," by J.W. Pankow and S.H. Glick, describes the chemical effects of plasma pretreatment on PET backsheet layers, and correlates the PET surface chemistry with performance of coated PET during damp-heat testing.

"Calculations of optimal source geometry and controlled combinatorial gradients in fixed- and rotating-substrate PVD systems," by G. Teeter, describes how normalized forms of conventional PVD flux-distribution formulas are used to derive the deposition geometry for optimal film-thickness uniformity for the rotating-substrate case, and how these calculations may be extended to develop a novel method for combinatorial thin-film deposition in support of the Process Integration effort.

"SIMS study of elemental diffusion during solid phase crystallization of amorphous silicon," by R.C. Reedy, D. Young, H.M. Branz and Q. Wang, studies impurity and dopant distributions during annealing, and H evolution during crystallization of a-Si. This work has enhanced the understanding of the crystallization process, leading to improved material quality.

In addition to the work discussed above, project personnel employed the cluster tool to study properties of CdTe and ZnO:N. A combined AES, XPS, and TDMS study of the Cu/CdTe system shows that the Cu + CdTe reaction obeys zero-order kinetics and forms a metastable Cu_xTe phase (with x~2). In a study of p-type ZnO:N, the cluster tool was used to study the chemical states of the nitrogen dopant. This work is the first to show that nitrogen exists in multiple chemical states in ZnO, and gives distinct identification of some of the states. It also shows that the number of N chemical states that are present in a film is determined, at least in part, by the film-growth technique. See Major FY 2005 Publications for references to these studies.

4. Conclusions

The Surface Analysis project provides high-value research and support to the DOE Solar Energy Project. Research performed by this project has a direct and substantial effect on the understanding of PV materials and devices, providing the means to advance PV technology in the marketplace.

ACKNOWLEDGEMENTS

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MAJOR FY 2005 PUBLICATIONS

C.L. Perkins, F.S. Hasoon, H.A. Al-Thani, S.E. Asher, P. Sheldon, "XPS and UPS investigation of NH_4OH-exposed $Cu(In,Ga)Se_2$ thin films," *Proc. 31st IEEE PV Spec. Conf.*, Jan. 1, 2005.

C.L. Perkins, S.H. Lee, X.N. Li, S.E. Asher, T.J. Coutts, "Identification of nitrogen chemical states in N-doped ZnO via X-ray photoelectron spectroscopy," *J. Appl. Phys.* **97** (3): Art. No. 034907. Feb. 1, 2005.

G. Teeter, "The reaction kinetics of Cu with the CdTe(111)-B surface: formation of metastable Cu_xTe (x~2)," *J. Chem. Phys.* (accepted for publication) (2005).

G. Teeter, "Physical-vapor deposition flux-distribution calculations for static and rotating substrates: derivation of the deposition geometry for optimal film-thickness uniformity," submitted to *J. Vac. Sci. Technol. A.*

G. Teeter, "Conceptual design of a deposition system for uniform and combinatorial synthesis of multinary thin-film materials via open-boat physical-vapor deposition," submitted to *J. Vac. Sci. Technol. A.*

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