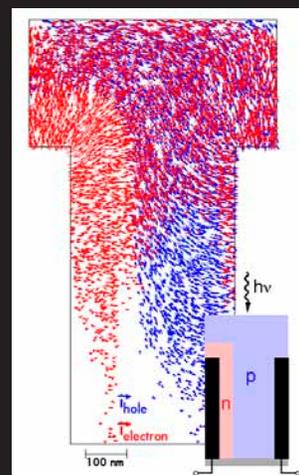


Characterization of 3D Photovoltaics

Objective

Our goal is to provide industry with test structures and models of next-generation photovoltaics, with an initial focus on cadmium telluride (CdTe) and $\text{CuIn}_x\text{Ga}_{1-x}\text{Se}_2$ (CIS or CIGS) materials. These tools will enable interpretation of measured external properties affected by three-dimension (3D) geometry, grain structure, and nanoscale phase separation, supporting improved processing and design of Second Generation (thin film) and Third Generation (nanostructured) photovoltaic devices.



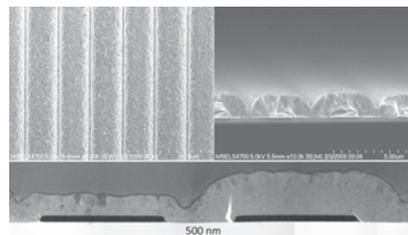
Impact and Customers

- The U.S. Photovoltaic Industry Roadmap calls for a 40-fold reduction in manufacturing costs by 2020. Thin film technologies such as CdTe and CIGS can be used on lower-cost substrates (glass, stainless steel, mylar, fabric) than the prevalent Si technology.
- Thin-film photovoltaics, particularly CdTe and CIGS, are the fastest-growing segment of the solar industry, with 43 startups in 2007 alone.
- Despite rapid growth and significant materials advantages, thin-film photovoltaics manufacturers have been hampered by manufacturing difficulties that stem from limited understanding of the detailed processing-microstructure-property relationships.
- The issues are compounded in so-called “Third Generation” devices proposed to yield enhanced efficiency and/or lower cost through the use of 3D nanoscale architectures.
- We are working with researchers in industry, national laboratories, and academia to develop experimental test structures and computational models that will lead to a better understanding of these 3D materials and microstructures and, ultimately, to improved manufacturability.



Approach

First Generation (thick layers of crystalline silicon) and Second Generation (thin films of CdTe, CIGS, and related materials) PV devices are both well established in the marketplace, with well defined techniques for fabrication and characterization. Third Generation PV encompasses a wide diversity of materials and nanostructures and commercially viable technologies and means of fabrication are yet to be determined. Many of the proposed structures have considerable microstructural variability that complicates interpretation of macroscopic device measures. The aim of this project is to develop idealized, three-dimensionally patterned templates that can serve as test structures to enable measurement of critical device and materials properties.



One of the most attractive properties of CdTe and CIGS for photovoltaic applications is their amenability to a variety of cost-effective fabrication methods, including sputtering, printing, and electrodeposition. We are developing three-dimensionally patterned photovoltaic test structures as well as fabrication processes including electrochemical deposition to enable the impact of geometry and internal defect structures on efficiency and broader photoelectrical properties to be determined.

To guide and interpret the experimental measurements we are developing models of light and charge transport within arbitrary 2D and 3D semiconductor and device geometries. These models will ultimately include the full effects of optical refraction and reflection that are relevant to all PV devices but play a particularly important role in 3D structures.

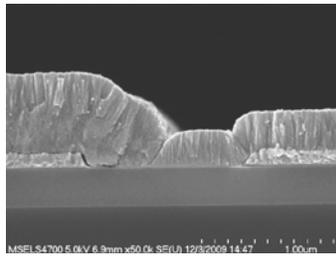
Accomplishments

In FY10 we substantially expanded our nascent effort to develop photovoltaics templates with 3D microstructures for application to 3rd Generation Photovoltaics through joint funding with NIST's CNST and EEEL from the NIST Director's Innovation in Measurement Science program. A focus of this major new effort remains developing structures with adjustable, well-defined geometries that are applicable to a broad set of materials and consistent with insightful measurements and interpretation of the properties of 3D photovoltaics.

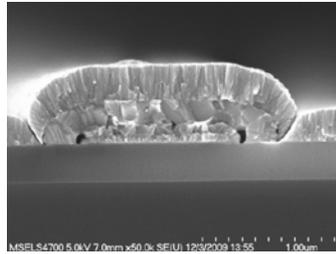
In collaboration with the CNST we have developed the capability to fabricate photovoltaic test structures using a set of interdigitated back-contact electrodes. These electrodes are used to independently electrodeposit one or more of the p- and n-type semiconductors that constitute the active device. After deposition, the same contacts are also used to extract light-generated current from the device as well as for electrical characterization.

Initial studies focused on devices composed solely of CdTe. By independently adjusting the potential of each set of electrodes, different stoichiometries were obtained, allowing the deposition of p- and n-type material from the same electrochemical bath on the two different electrodes. These structures demonstrated the proof of concept for more typical devices based on two different semiconducting materials (heterojunctions). Electrical, optical, and structural characterization was performed, in concert with the CNST and CSTL.

More recently we extended the study of these structures to include heterojunctions, which



A photovoltaic with CdTe on one platinum electrode with ITO over the entire device.



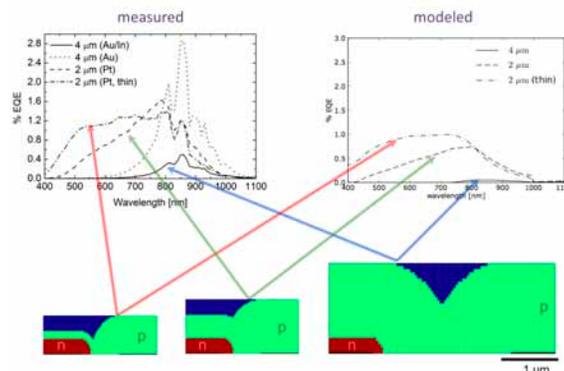
The CdTe grains coarsen during annealing

should lead to better device performance and significantly expand the range of industrially relevant materials and combinations that we can study. Thus far, we have combined our extant CdTe electrodeposition capability

with sputtered indium-tin-oxide (ITO), electrodeposited CdS, and sol-gel deposited titanium oxide.

To support this experimental effort, we have developed a photovoltaic device model that gives us complete control over geometry and microstructure. We implemented our device model in the FiPy partial differential equation solver package. This freely available package, developed within the Metallurgy Division, allows us to easily distribute our photovoltaic codes to researchers in industry and elsewhere as they are validated. Because it was designed to model phase transformations, FiPy will also allow us to examine the effect of microstructures obtained from rigorous thermodynamic and kinetic modeling.

Using an early generation model, we were able to create simulations of the external quantum efficiency (EQE) that successfully captured major trends in the measured performance of CdTe devices over a range of illuminating wavelengths for three different device geometries.



Comparison of experimental and simulated External Quantum Efficiency for different geometries

Learn More

Daniel Josell
Carlos Beauchamp
Carlos Hangarter
Albert Davydov
Abhishek Motayed (MSEL)
Nikolai Zhitenev
Behrang Hamadani
Henri Lezec
Suyong Jung (CNST)
David Gundlach (EEEL)
Lee Richter, Albert Fahey (CSTL)

Jonathan E. Guyer
 (Metallurgy Division)
 (301) 975-5329
 guyer@nist.gov
 www.nist.gov/metallurgy

Publications

Josell D, Beauchamp CR, Jung S, Hamadani BH, Motayed A, Richter LJ, Williams M, Bonevich JE, Shapiro A, Zhitenev N, Moffat TP, *Three Dimensionally Structured CdTe Thin-Film Photovoltaic Devices with Self-Aligned Back-Contacts: Electrodeposition on Interdigitated Electrodes*, Journal of the Electrochemical Society 156:H654 (2009)

Guyer JE, Wheeler D, Warren JA, *FiPy: PDEs with Python*, Computing in Science and Engineering 11:6 (2009)