



# Meeting Scene...

Presented by the Materials Research Society (MRS)  
and the European Materials Research Society (E-MRS)

**2011 E-MRS Spring Meeting**  
**MRS/E-MRS Bilateral Conference on Energy**

A Publication of the  
Materials Research Society  
*Advancing materials. Improving the quality of life.*

May 9-13, 2011  
Nice, France

## MEETING DAY 2, Tuesday, May 10



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Tuesday was another great day at the E-MRS 2011 Spring Meeting in the beautiful city of Nice, France. The weather was great, the sun was shining, but most of the attendees spent the day in darkened rooms watching presentations of the latest advances in their field of interest in materials science. Who could ask for anything better? Once again, the highlight was the Key Lecture of the E-MRS/MRS Bilateral Conference on Energy, this one given by Harry Atwater of the California Institute of Technology. The exhibitors were ready with a smile at their booths, prepared to talk about their latest products, gather some leads, and perhaps make a few sales. All 27 symposia had a full slate of speakers, and usually a full audience to listen to them. Sometimes it was standing room only, with crowds flowing out the door--one true sign of a successful meeting! .



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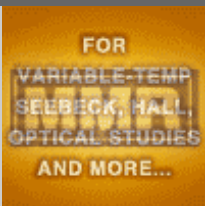
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### Contents

- [Bilateral Energy Conference Key Lecture](#)
- [Bilateral Energy Conference Technical Talks](#)
- [Technical Talks from Other Symposia](#)
- [Scanning the Meeting](#)

### **Other Links of Interest**

- [EMRS 2011 Spring Meeting Web site](#)
- [EMRS 2011 Spring Meeting Program](#)



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### ■ Bilateral Energy Conference Second Key Lecture

**New Photonic Materials and Device Designs for Solar Energy Conversion**  
Harry Atwater, California Institute of Technology



In the second Key Lecture of the E-MRS/MRS Bilateral Energy Conference, Harry Atwater of the California Institute of Technology argued for the development of lightweight, flexible solar energy conversion devices with at least 18% module efficiency as essential to meeting the goal of a \$1 per watt solar energy cost. Only fifty cents of that dollar per watt can go to the actual solar conversion module, he said; the rest must go to the balance of systems costs. All of the heavy materials that go into making rigid solar devices quickly blow the fifty cent budget for the modules, leading to his call for lightweight and flexible devices.

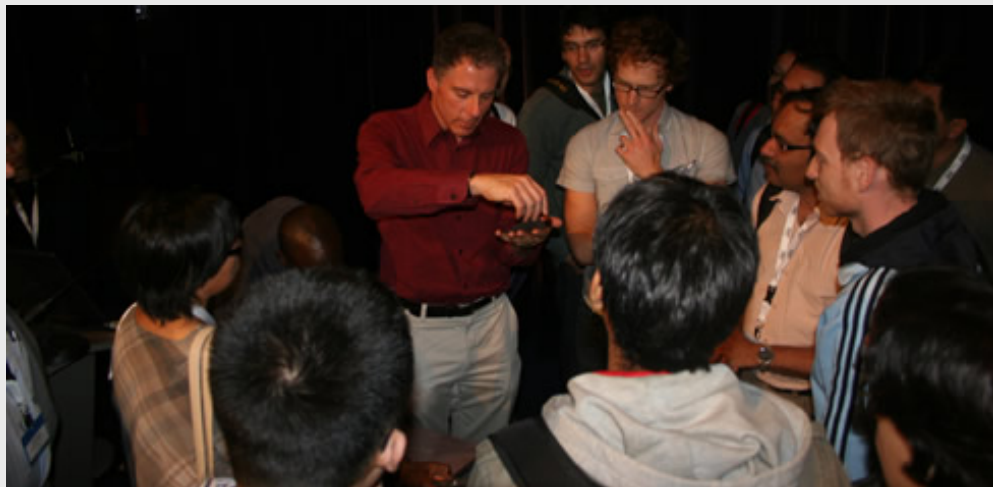
Atwater proposed two possible materials systems that could meet these criteria: (1) III-V sc-Compound films, and (2) an sc-Si wire array. In the first category, AltaDevices already makes thin film GaAs solar cells with 27.6% efficiency, but Atwater thinks the future lies in the second category. He waved in the air a sample of a flexible, peel-off, wafer-scale

(150-mm diameter) polymer made of embedded Si nanowire arrays and called it “the most promising polymer solar cell.” The absorption (approximately 96% in the mid-visible range with dielectric scattering and a back-reflector) and quantum efficiency (greater than 0.90 internal quantum efficiency throughout most above-bandgap wavelengths) of this large-scale Si nanowire array is comparable to high quality Si wafers.

Atwater went on to review other approaches that are being investigated currently, some with great promise: single-wire radial-junction devices; GaP/Si Tandem Cells, which allow for high operating voltages; solar concentrator photovoltaics; plasmonic photovoltaics for increased light absorption; artificial photosynthesis (through highly efficient, non-biological, molecular level energy conversion



“machines”); lattice-matched and metamorphic three-junction cells; and new InAlAs-based multijunction cells that form a virtual substrate. Atwater ended his talk by discussing more basic science, asking “What kind of structure do we want for a solar cell?” A rousing question and answer session followed, after which Atwater was surrounded at the podium by scientists wishing to discuss the concepts he presented further.



## ■ Bilateral Energy Conference Technical Talks (Symposia Q to ZZ)

### Symposium R: Advances in Inorganic Materials and Concepts for Photovoltaics

#### *Spatially Ordered Conductive Quantum Dots in SiO<sub>2</sub> for Advanced Solar Cells*

Kavita Surana of CEA-LETI Minatec, Grenoble, France, and colleagues took two approaches to studying the formation and properties of Si quantum dots (QDs) on Si: (1) a single thick deposition of SiO<sub>2</sub> using plasma enhanced chemical vapor deposition on 8 in. p-type Si wafers, and (2) deposition of multiple bilayers consisting of alternating SiO<sub>2</sub> and silicon-rich oxide (SRO) layers using the same PECVD method. The single layer method produced Si QDs with diameters of 30, 50, and 75 nm; TEM results showed that order increased as the thickness of the deposited layer increased. However, current-voltage measurements on the single-layer samples revealed that current decreased with increasing layer thickness (greater order in QDs). Surana concluded that the randomness of the less ordered layer introduced conduction percolation pathways that improved conductivity. Comparing the single-layer samples with the multiple-bilayer ones, the single-layer samples had higher electrical conductivity.



#### *Plasmonic light trapping for solar cells-some design considerations*

Reducing the cost of photovoltaics is a major global initiative. Surface plasmons may be used to further increase the efficiency in solar cells and help to drive down the cost. Supriya Pillai at the University of New South Wales, Australia, has been working on doing this with metal nanoparticles on silicon solar cells. To benefit from using metal nanoparticles in solar cells, there are a number

of design considerations, including nanoparticle materials, the nanoparticle size and shape, the best place to incorporate the nanoparticles, and the thickness of a dielectric layer. Her talk covered many recommendations for these design elements based on experimental results. Silver particles were found to be optimal, with larger nanoparticles having higher polarizability and being more effective at scattering light into the solar cell. It was also noted that locating the nanoparticles on the back side of the cell, with light passing through the transparent substrate, resulted in no loss of light intensity from the presence of nanoparticles, and was more beneficial in increasing overall efficiency. Using an oxide dielectric layer before depositing the nanoparticles helped reduce losses when placed on the front side of the cell, but had little effect for the back side configuration.



### Symposium U. Nano-energy: Energy Transduction at the Nanoscale for Energy Conversion Devices.

#### *Carbon/TiO<sub>2</sub> Nanocomposite Photocatalyst for Enhanced Photocatalytic and Photoelectrochemical Applications*

Finding a suitable photocatalyst for a given application is still a challenge, said Raja Sellappan of Chalmers University of Technology in Göteborg, Sweden. His team's approach was to start with TiO<sub>2</sub>, which has a large bandgap of 3.2 eV for the anatase structure, and use bandgap engineering to optimize charge transport and surface area. They compared the properties of a fused silica substrate covered with a thin film of TiO<sub>2</sub> (25-100 nm thick) with a three-layer composite that included a 20-nm-thick layer of carbon between the fused silica and the TiO<sub>2</sub>. The TiO<sub>2</sub> deposited on graphitic carbon had a pillar morphology, which increased its surface area compared to the sample with no carbon layer. A test reaction involving these two materials as photocatalysts in the oxidation of methanol to form carbon dioxide and water showed that the three-layer fused silica/carbon/TiO<sub>2</sub> material had twice the catalytic activity of the two-layer fused silica/TiO<sub>2</sub>, probably due to the higher surface area of the three-layer composite. The researchers concluded that the enhanced photocatalytic activity was related to improved charge separation at the TiO<sub>2</sub>/C interface in the three-layer composite material.

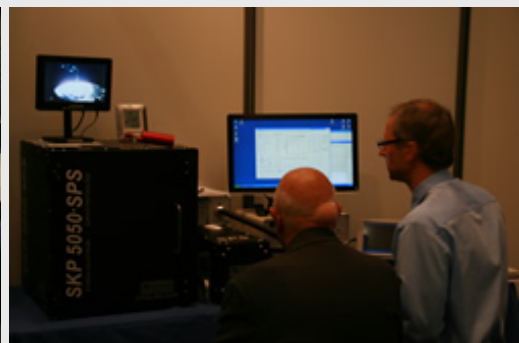


## ■ Technical Talks from Other Symposia

### Symposium A. MACAN11: Reconciling Atomistic and Continuum Approaches to Interfaces

#### *Long-term and thermal stability of organic nanowires*

The long-term morphological stability of organic semiconductor nanowires is of extreme importance for any application, considering their quasi one-dimensionality and their anisotropic index of refraction. Frank Balzer of the University of Southern Denmark used atomic force microscopy to address the long term physical and thermal stabilities of a naphthyl end-capped thiophene (NaT3) and a para-functionalized para-quaterphenylene (MOP4). During deposition, nanowires, nanoclusters, and flat islands formed on the surface. Within a few hours under ambient conditions, drastic changes in sample morphology occurred: most of the clusters vanished, and some of the wires showed strong faceting and developed breaks. By annealing the samples, the researchers identified distinct temperature regimes in which the different aggregates tended to decompose even before thermal sublimation started.



### Symposium C: Size-dependent Properties of Nanomaterials

#### *Tailoring nanocomposite properties through atomic-scale design of interfaces*

Interactions at the nanoscale lead to novel insights about the physical properties of materials, and present new opportunities for nano-mechanical, nano-electromechanical, and nano-composite applications. A tremendous amount of research is focused on the ability to control and tailor the physical properties and symmetry at the nanoscale. M.J. Demkowicz of the Massachusetts Institute of Technology presented the results of his research team's efforts to tailor the properties of metal-metal nanocomposites by controlling the nature of the interfaces. Atomistic simulation was used to understand the relationship between interface structure and interface properties, such as point

defects and impurity trapping, shear resistance, and diffusion. He cited an example of how interfaces can be used to reduce irradiation by acting as radiation sinks through induced point defects in fcc Cu and bcc Nb lattices. Demkowicz and his team also developed a base-model capable of predicting interface structures, then used it in an attempt to solve the inverse challenge of determining which structures yield interfaces with desired properties. Demkowicz concluded by indicating that the trapping and migration of vacancies, interstitials, and impurities at interfaces bears a direct relationship to the interface misfit dislocation structure. Using misfit dislocation models, certain properties of heterophase interfaces, such as the defect trapping density, may be predicted.



### Symposium D: Synthesis & Characterization of Nanoscale Multifunctional Oxide Films

#### *Raman spectroscopy of multiferroic thin films and nanostructures*

Raman spectroscopy is an excellent tool for examining properties of oxide thin films, and is complementary to other common characterization techniques such as x-ray diffraction (XRD). Vibration modes in a crystal have unique fingerprints that are highly sensitive to changes in strain, temperature, and pressure. These modes, which are probed by Raman spectroscopy, are also affected by electric and magnetic fields. Jens Kreisel of Minattec, CNRS, and the Grenoble Institute of Technology described Raman spectroscopy and then discussed three research projects highlighting unique capabilities of the technique when looking at oxide thin films. One of the projects discussed used Raman spectroscopy to study both the metal-insulator and paramagnetic-antiferromagnetic phase transitions in  $\text{NdNiO}_3$  and  $\text{SmNiO}_3$ . Raman spectroscopy was also used to study the effect of strain imposed by a PMN-PT substrate on  $\text{LaNiO}_3$  films. It was also shown that Raman spectroscopy has the capacity to reveal the strain state of  $\text{BiFeO}_3$  pillars in a  $\text{CoFe}_2\text{O}_4$  matrix deposited on a  $\text{SrTiO}_3$  substrate.



### Symposium M: X-ray Techniques for Materials Research

*High resolution reciprocal space mapping of individual grains within deforming polycrystals*  
Ulrich Lienert of the Argonne National Laboratory talked about using high-energy x-rays from the

Advanced Photon Source to map individual grains during tensile deformation. A high resolution imaging detector is placed close to the sample to provide crystal grain shape and orientation while a larger area far-field detector can reveal strain state. This can be done during the application of tensile strain to monitor sub-grain evolution. Using a grid to model the crystal grains in the sample and fitting the simulated diffraction data to the experiment allows roughly 0.1 degree accuracy in a three-dimensional grain map. The model has been successful in mapping thousands of grains.

#### *X-ray diffraction peaks from correlated dislocations in epitaxial films*

Relaxation is a large concern when working with epitaxial thin films. The relaxation process can introduce both misfit and threading dislocations into the films. Vladimir Kaganar's talk described his work at the Paul Drude Institute for Solid State Electronics in Berlin on simulating the effect of dislocations on x-ray diffraction peaks of epitaxial films. One of the main goals of the simulation was to determine the degree to which the dislocation correlation affected the resulting x-ray diffraction peaks. Using a Monte Carlo technique, simulations showed that dislocation correlation can have a very strong effect on x-ray rocking curve peak width and intensity. Different dislocation types were simulated, including threading dislocations and edge dislocations. Simulated peak widths were seen to narrow by a factor of five for a moderate amount of misfit dislocation ordering.



#### **Symposium O: Bio-nanomaterials for imaging, sensing and actuating**

##### *Synthesis of PEGylated Peptidic Gold Nanorods and Their Self-organization in Solution*

Gold nanorods are a promising class of nanomaterials with potential applications ranging from surface enhanced Raman scattering and bio-imaging to bio-sensors and cancer therapy. They exhibit an intrinsic surface plasmon resonance that depends on their aspect ratio, which is important for optical materials. V. Marchi Artzner of the Université de Rennes, France, synthesized gold nanorods functionalized with small PEGylated peptides. Starting with gold nanorods, an exchange reaction between tricysteine PEGylated peptides and cetyltrimethylammonium bromide (CTAB)-protected gold nanorods (GNRs) was conducted inside an ionic exchange resin. The resulting ordering of the nanorods was clearly demonstrated by SAXS experiments and confirmed by TEM images. In addition, adjusting the amount of peptide caused a self-organization of the gold nanorods in solution, resulting in red- or blue- shifted bands.



### Symposium P: Bio-inspired and Bio-integrated Materials as New Frontiers Nanomaterials

#### *Biopolymer Mediated Syntheses of Complex Oxide Nanowires*

Simon Hall of the University of Bristol, United Kingdom, and his coworkers took a unique research path by “trying to apply bio-inspiration to superconducting materials.” They chose superconductors because they are usually made using what Hall called a “heat and beat” method, which results in irregular crystal morphologies. Because of the lack of morphological control, large angle grain boundaries act as weak links and limit the critical current density of superconducting materials. Hall’s method was to use biopolymers for templated crystallization of superconductors to see if this could bring morphological control to the process.

After dissolving chitosan from shellfish, which has a two-fold helical structure in an extended sheet-like network, Hall added YBCO superconductor precursor in sol form, expecting to get a YBCO/chitosan composite film. He was surprised to find that instead he had synthesized perfect single-crystal nanowires having lengths from 600 nm to 1 micron and widths of approximately 50 nm. Furthermore, at 10 K, these nanowires had a  $J_c$  of 0.18 MA/cm<sup>2</sup>, which is an order of magnitude better than a standard YBCO control sample whose  $J_c$  is 0.015 MA/cm<sup>2</sup>. The team repeated the process with the natural block copolymer alginate and with langasite, La<sub>3</sub>Ga<sub>5</sub>SiO<sub>14</sub>, as templates, (which Hall said no one had ever before synthesized on the nanoscale). In both cases, they synthesized single crystal nanowires of the YBCO superconductor, proving that biotemplates can indeed help to control the morphology, and sometimes the  $J_c$ , of superconducting materials.



#### *Theoretical and computational study of gold nanoparticles as heat sources for medical applications*

Ana Sofia Vila-Verde from University College, London, presented a talk on the use of gold nanoparticles for heat source applications in cancer therapy or as radiation sources for imaging. She described the idea of using organic-coated nanoparticles in the body to target specific cell types. Gold nanoparticles were chosen because they are inherently good absorbers in the IR region, are inert in air, and are easily conjugated with organic materials. Theoretical and computational methods were used on two different kinds of materials, the water-gold system and the water-thiol-gold system. In both cases, Vila-Verde explored the nanoparticle size and interface as well as the overall heat transfer. The heat transfer coefficient agreed well with experimental values, which helped to verify the validity of the computational model. The model was integrated with macroscale heat transfer equations using analytical methods, and the simplified heat conduction

equations verified the results for both systems. Vila-Verde concluded that organic coating reduces the heat transfer between gold and water, and that the dominant heat transfer mechanism depends on nanoparticle size.

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### Scanning the Meeting



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The Meeting Scene e-newsletter of the Materials Research Society (MRS) presents news from MRS and other conferences directly from the conference venue.

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