



Meeting Scene...

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IMRC 2011 – XX International Materials Research Congress 2011

Cancun, Mexico
August 14 - 19



[Meeting Opening: Sunday, August 14, and Monday, August 15](#)



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For twenty years now, the Sociedad Mexicana de Materiales (SMM) has organized the International Materials Research Congress (IMRC) for the benefit of materials scientists from Mexico, Central and South America, and around the world. The beautiful vacation destination of Cancún provides a wonderful backdrop for this meeting of scientific minds.

MRS is pleased to once again be a co-organizer with the Sociedad Mexicana de Materiales of 10 of the 23 symposia to be held here this week. The Brazil-Mexico Nanotechnology Center is also co-organizing a symposium. With five outstanding guest speakers--Sumio Iijima, Ivan Schuller, Eduard Arzt, Dan Shechtman, and Gary D. Fullerton--and numerous invited talks, the twentieth IMRC promises to be the best ever.



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The view outside the JW Marriott hotel in Cancún, site of the XX International Materials Research Congress



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■ Opening Ceremony



(Left to right) Olivia Graeve, David Cahen, Armando Salinas, Andrea Hodge, Sergio Mejia, Mario Castro Bastos, Jim De Yoreo, Karla Smith, Jesus Gonzalez, and Jose Chavez.



Sergio Mejía of the Universidad Autónoma de Nuevo León, President of SMM, and General Chairman of the Congress, graciously welcomed everyone to the 2011 IMRC. He was quick to thank his co-chairs Andrea Hodge (University of Southern California, USA), David Cahen (Weizmann Institute of Science, Israel), and Armando Salinas (CINVESTAV-Saltillo) for all their hard work in making the meeting possible. "Thanks to them, this Congress has been growing in quantity and quality," he said. "Central and South America are now psrt of the map of materials science in the world."

MRS President Jim De Yoreo, of the Lawrence Berkeley National Laboratory, spoke of his great pleasure in the partnership between SMM and MRS, and thanked all those who had worked hard to make it a success. He announced



that after a trial period of three years of co-organizing this meeting, MRS and SMM had come to an agreement for another three years of cooperative effort.



Ing. Mario Castro Bastos, Secretaria de Infraestructura y Transporte del Gobierno del Estado, officially declared the Twentieth International Materials Research Congress open.

■ First Plenary Lecture: Sumio Iijima

Nano-carbon Materials: Their Science and Industrial Applications



Who better than Sumio Iijima, the discoverer of carbon nanotubes (CNTs) in 1991, to bring us up to date on the science and applications of CNTs and their associated materials, single walled carbon nanotubes (SWCNTs), carbon nanohorns, and graphene? Iijima, of Meijo University in Nagoya, Japan, summed up the current state of affairs early in his lecture. “It is okay for scientists to publish their results about carbon nanotubes in *Science* and *Nature*,” he said, “but in industry they keep saying, ‘Please bring me one kilogram of this material.’”

Though the field has not advanced enough to be able to supply such quantities yet, much progress has been made. Starting with early samples measuring 2 cm x 2 cm on Si that needed expensive helium gas to fabricate, laboratory scientists can now produce 50 cm x 50 cm samples on a stainless steel foil substrate using the cheaper, more readily available nitrogen gas in place of helium. One 12-meter-long reactor system can produce 600 g/day of

SWCNTs. The stainless steel foil substrate is making roll-to-roll continuous processing of SWCNTs a possibility, with the ability to reuse the substrate over and over.

Industrial applications to date include a wafer-based strain sensor made of aligned CNTs on a PDMS polymer substrate; a fully stretchable CNT rubber with 300% strain capacity, from which devices can be made in which every component, including electrodes, is stretchable; and a silicon rubber-

like SWCNT that shows no dependence of viscoelasticity on temperature over the range of 96 to 1000 °C.

Iijima next spoke about different methods of modifying SWCNTs by doping. He discussed “nano-peapods” in which SWCNTs are doped with Er and N trapped inside C₈₀ fullerene cages, and photoluminescence mapping of SWCNTs that involves inserting the organic molecule coronene into SWCNTs and observing any interaction between the molecules and the nanotubes. Doping carbon nanohorns with aggregate particles might be used for storage of fluorine gas; making fuel cells and supercapacitors; or delivery of anti-cancer drugs to a tumor, according to Iijima.

He finished by talking about developments in graphene fabrication and carbon nanomaterial analysis. Synthesis of large area sheets of graphene at low temperatures has been demonstrated by the production of a 30-inch (diagonal) transparent graphene sheet in a roll-to-roll process. The surface wave plasma technique also looks promising. This involves microwave-induced deposition of graphene from a volume containing a graded concentration of plasma onto a substrate. In terms of analysis of carbon nanomaterials, spherical aberration corrected HRTEM instruments are providing unprecedented structural and elemental resolution. Using single atom spectroscopy at low voltages of 30 kV, researchers can distinguish between La and Ce atoms, which are separated by just one atomic number, which Iijima called “the ultimate elemental mapping.”

Second Plenary Lecture: Ivan Schuller

Hybrid Nanostructures: Vortices, Ratchets, and Induced Phenomena



In a hilarious yet extremely informative lecture, Ivan Schuller of the University of California, San Diego, started by pulling out a camera and taking a picture of the audience, so he could determine later which of his friends were missing, he said. This surprising development was a fitting beginning to a talk that was full of scientific surprises that Schuller has participated in or learned about over his career. “If you make nanohybrids, put them next to each other, and measure them fast, you will find many surprises at the nanoscale,” he said, adding, “There is an ultrafast nanoscale technology gap.”

Characterization at the atomic level is important for Schuller because nothing is perfect or as expected, and small changes in structure can lead to big changes in properties. “If I don’t characterize a material it is perfect,” he joked. “As soon as I characterize it, it is no longer perfect.”

He focused his talk on three aspects of ultrafast nanoscale technologies: short length scales, the proximity of dissimilar materials, and the fast time response in properties that can occur under these conditions. Regarding the first of these, Schuller noted the vortices that can be created when magnetism is confined to small dimensions. The surprising thing here is that the charge can go in one direction and the spin in another. Using magnetic nanodots, researchers have created a magnetic vortex in Ni with a diameter of only 15 nm. Next, he described how by placing two ferromagnetic materials on top of a normal metal, you get what he called the “real Chesire cat effect—the smile without the cat.” In this case, a non-local spin valve effect produces a situation in which there is no current flow in the circuit, but a voltage still develops—the voltage without the current.

In terms of proximity, Schuller talked about the exchange bias effect that occurs when a ferromagnet (FM) and an antiferromagnet (AFM) are brought together. The hysteresis loop is shifted away from zero, which makes the read heads on magnetic disks possible. On cooling the FM/AFM hybrid, the magnetic moment suddenly goes in the opposite direction of the field, Schuller said.

Finally, measuring things quickly can capture phenomena never seen before, according to Schuller. He described a “pump/probe” analysis, in which you create an FM/AFM junction, pump it with a laser, and then probe the sample 60 picoseconds later. “You get a huge change in the magnetic field, which is totally unexpected,” Schuller said. If you waited until a couple hundred picoseconds to do the probing, you would miss this “induced phenomenon” entirely.



Silvery moon over Cancún

■ Technical Talks

Symposium 2: Advances in Computational Materials Science

Vibrational Spectroscopy on Metal-doped Silicon Clusters

Clusters of Si are highly reactive due to dangling bonds, Ewald Janssens of the Katholieke Universiteit Leuven, Belgium, said in an invited talk, explaining his motivation for studying the material using computational methods. He and his colleagues study the geometry of such clusters as the best way to determine their properties. They use vibrational spectroscopy and ab initio calculations for comparison, because the geometry cannot be determined using spectroscopy alone, according to Janssens. More importantly, they use “action spectroscopy,” which investigates changes in the charge state or the particle mass instead of changes in the incident light. This requires an intense, tunable IR light source, Janssens said, “because we need a lot of photons.” To date, they have determined the geometries of Si_n^+ cations with $n = 6-21$. Si_6^+ is a distorted

octahedron, Si_8^+ is an edge-capped pentagonal bipyramid, and Si_{10}^+ is a tetra-capped trigonal prism.

Beyond these basic structures, Janssens and his colleagues are interested in how they act as building blocks to create larger clusters. They add transition metals such as V or Mn, and use IR spectroscopy to determine whether the transition metal substitutes for Si on any of the sites. Of particular interest is the possibility of inserting a transition metal atom inside the Si cage, as such structures might have interesting magnetic or optoelectronic properties. The researchers have attempted to place Ti^+ , V^+ , and Cr^+ inside an Si_{16}^+ structure. To determine if this actually happens, they have developed a technique in which they use Ar as a unique structural probe of the system. Ar does not bond with Si, but it does bond with transition metals. So if they see Ar using spectroscopy, this indicates that the transition metal has substituted on the outside of

the Si cage; if there is no Ar, the transition metal may be inside the Si structure. No conclusive evidence is available to date that they have succeeded in inserting a transition metal ion, but further investigation is needed.



Lots of interest in the poster session

Symposium 5: Advances in Semiconducting Materials

Electronic and magnetic properties of Nitrogen doping charge transfer and defects' nature in Titanium Oxide based nanostructures

A. Kassiba of the Universite du Maine in Le Mans, France, presented an innovative system aimed at improving the efficiency of photovoltaics. TiO_2 is one of the most studied systems in photovoltaics because it has characteristics well-suited for solar cells. In recent years, increasing effort has been dedicated to modifying and improving these characteristics. One method found is doping with suitable agents as N because it introduces intermediate states in the gap which can increase photo-induced efficiency.

Kassiba and co-workers proposed using a device which combines mesoporous TiO_2 and TiO_2 based-gels to obtain solar cells with high efficiency. Their strategy consisted of the investigation of properties of both components individually in order to test the efficiency of solar cells. They then investigated the properties of mesoporous TiO_2 and N-doped TiO_2 , comparing the properties of each system with and without porosity. Finally, they built their device combining the mesoporous and TiO_2 based-gels and N-doped TiO_2 . The first tests on this system did not show further improvement in efficiency. However, Kassiba points that out that this is the result of only the first test, and is hopeful that future tests will produce better results.



Learning through discussions



Symposium 6: New Catalytic Materials

Catalytic Properties of Mo-doped Pt Nanoparticles: a Computational Study

Adding Mo to Pt improves the catalytic functionality of Pt glycerol, reforming water-gas shift electrooxidation of H and other reactions. In order to understand the reaction of CO on Mo-doped Pt, A. Sumer of the Argonne National Laboratory, United States, and colleagues made an ab initio study of the electronic, structural and chemical reactivity of nanoparticles of Pt and Mo for different configurations, and then substituted atoms of Pt(Mo) by Mo(Pt). By looking at different geometric forms of Mo_n and Pt_n , they identified approximately 70 isomeric structures for sizes $n=2-$

7,13. The study of their properties is important because different geometries give rise to different electronic properties and thus catalytic reactivities. The structures of these created bimetallic clusters were then fully optimized. In total, nearly 250 isomeric and homotopic conformations were identified for sizes $n=2-7,13$. The reactivity of these particles with CO was analyzed by adding CO molecules to different sites of the particles.

Sumer also addressed coverage-induced structural change of CO on Pt_6 particles. This is important because, depending on the coverage, the structure may change during the catalytic process. They found that CO absorbs preferentially on Pt sites. One of the most interesting aspects of this process is that the reaction of CO molecules with the nanoparticles changes the magnetic states of the Pt-Mo system in such a way that the total energy of the system is reduced. This indicates that magnetic properties play a role in chemical reactivity.



Researchers take great pride in their posters

Symposium 8: Cultural Heritage and Archaeological Issues in Materials Science

New Chromatographic Investigations of Purple Archaeological Bio-material Pigments used as Biblical Dyes

In an invited talk, Zvi C. Koren of the Shenkar College of Engineering and Design, Israel, started the second session of Symposium 8 with a talk that focused on the ancient Middle East and the analysis of a purple thread fragment taken from King Herod's cloak, dated to the first century BCE.

Specifically, he spoke about the good fortune archaeologists have had in the preservation of organic materials in desert areas, such as the Judean sites of Qumran and Masada. This good fortune has allowed him to study the chemical composition of various purple dyes that have been preserved in textiles using chromatographic techniques, shedding light on the sub-species of snail that these dyes originated from. Purple dyes are especially important because they were rare pigments used only by kings, rulers, high priests, etc., back in Biblical times.

There are three purple dyes mentioned in the Hebrew Bible, Koren said: Shani, Argaman, and Tekhelet. Shani is known to come from an insect, while the other two are from the *Murex* species of snail. There are many known ritual Judaic uses of Tekhelet, so it is of particular interest to archaeologists. The dye does not exist in its purple color inside the snail. You have to expose the hypobranchial gland of the snail to air, at which point the precursor liquid turns from white to yellow to purple.

HPLC allows today's archaeologists to analyze samples of fibers micro-destructively instead of ultra-destructively, Koren said. One centimeter of a single fiber is enough to characterize the dye. In the case of the thread from King Herod's cloak, the HPLC micro-analysis (labeled somewhat anachronistically and perhaps whimsically as "King Herod's Chromatogram" by Koren) revealed it to contain a small portion of indigo, a larger portion of monobromindigo, with the greatest fraction being dibromindigo. Koren concluded that the thread was Argaman purple, not Tekhelet.



A full house for the opening ceremonies

Symposium 9: Photovoltaics, Solar Energy Materials & Technologies

Solar Cells, Assessing their Possibilities and Limits

David Cahen of the Weizmann Institute, Israel, presented a review of current types of commercial photovoltaic devices and compared their efficiencies in this invited talk. He addressed topical issues concerning photovoltaics and offered responses to common questions, such as: to what extent can we expect progress in commercial cell module efficiency? What are the possibilities for their technological application? What are the main sources of loss in photovoltaic cells? Regarding this last question, he pointed out that one of the main sources of loss comes from the absorption of photons. A way to overcome this problem lies in photon management, i.e., better use of sunlight. This possibility is being investigated in multi-bandgap and multi-junction photovoltaics. An example of one of these systems is a three junction device made of GaInP/GaAs/Ge that attains high efficiency.

Cahen also compared the maximum possible currents with experimental photocurrents in different systems. He showed that silicon has the maximum current while organic systems show the lowest currents. He concluded that to overcome efficiency losses, composite materials are worth exploring.



Exhibitors for Rubio Pharma y Asociados (left) and the International Centre for Diffraction Data

Symposium 11: Biomaterials for Medical Applications

Superparamagnetic magnetite nanoparticles, an alternative for cancer treatment

J. Santoyo-Salazar of the Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional and colleagues use ideas from materials science to address cancer treatment. Some drugs currently used in cancer treatment contain magnetic ions. The interaction between these ions and cancerous cells can be modified by manipulating the magnetic properties of these particles. The researchers explored modification of the nanoparticles' magnetic properties to investigate their reaction with, and influence on, cancer cells. The magnetic ions investigated were MFe_2O_4 nanoparticles, with $M=Fe, Zn, Co, Mg$ and magnetite. What these particles have in common is that the iron ions have different electronic configurations: Fe^{3+} and Fe^{2+} states. Due to these different states there is a net magnetic moment within the nanoparticles. The different magnetic properties of these systems were extensively examined. By applying magnetic fields,

magnetic ordering is induced in the nanoparticles. Here, the temperature is controlled by applying certain frequencies to make the particles vibrate, hence allowing them to be heated. The relation of the examined processes on enhanced drug treatment efficacy is a work in progress.

Functional Plasma Polymer Films Engineered at the Nanoscale for Biomaterial Applications

Krasimir Vasilev and his group at the University of South Australia use plasma polymerization techniques to create thin films of Ag which are used for antibacterial coatings and surface gradients. This process involves loading a film with Ag nanoparticles. Vasilev demonstrated the efficient treatment of bacteria with Ag coatings, including staphylococcus epidermidis. If bacterial infections can be treated with antibiotics, then why explore the use of Ag antibacterial coatings for the same purpose? Vasilev points to the high cost of antibiotic treatment as reason to explore alternatives. He also points out advantages of plasma polymerization techniques, such as the ability to control the amount of loaded particles, in relation to other techniques used to create thin films.



Everything under control in the registration area

Symposium 19: Advanced Electron Microscopy and Nanospectroscopy

Visualizing Alloy Fluctuations by Spherical-aberration-corrected HRTEM

Marie-José Casanove of the Université de Toulouse, France, gave an invited talk about the unexpected capabilities of spherical-aberration-corrected HRTEM to localize and quantify atoms in nanoalloys, thereby accounting for composition fluctuations. After first discussing the older methods of digital analysis of lattice images (DALI) and local composition measured by strain analysis, she said that a new technique was clearly needed.

Using an FEI Tecnai F20 HRTEM at 200 kV, fitted with a CEOS spherical aberration corrector, Casanove and her colleagues chose to examine $\text{Si}_{0.7}\text{Ge}_{0.3}$ because the material has very few defects and the two elements of the alloy are very close in atomic mass. They fabricated a controlled thickness of this alloy on an Si substrate to give them a reference region. In the HRTEM, the Si appeared as white dumbbells. In the Si substrate they observed no speckle formation, but they saw speckled regions—strong variations in brightness—in the alloy region. To determine the origins of these variations, the researchers ran a Stillinger-Weber semi-empirical potential atomic simulation and compared it with the HRTEM images. They found that the standard deviation in the mean peak intensity was much higher (19.4%) in the $\text{Si}_{0.7}\text{Ge}_{0.3}$ region than in the Si region (1.70%). This showed a clear correlation between peak intensity and the fraction of Si in an atomic column. Casanove concluded that spherical-aberration-corrected HRTEM images can be sensitive to alloy fluctuations, and that there is a clear correlation between the local composition and the image contrast.

Scanning the Meeting



ABOUT THE MEETING SCENE

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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