I_{on} for smaller nanotubes than for larger diameter nanotubes for all three types of metal contacts. To account for their results, the researchers developed a model that "describes the CNFET as a gated nanotube channel in contact with two reservoirs that are a result of the weak coupling between the metal and the nanotube in the overlap region," thus incorporating a tunneling barrier as part of their extended SB model.

By comparing other sets of data from known reports of CNFETs fabricated from CNTs grown by arc discharge and chemical vapor deposition methods with the results of their laser-ablation-grown CNFETs, the researchers confirmed that the local contact quality is not the major contribution to the observed current variation using nanotubes of the same length and that I_{on} is independent of the nanotube growth source. The results of the extended SB model agreed well with the data from this study as well as the data from the previous experiments. Qualitative band diagrams for CNFETs further showed that the injected current decreases exponentially with increasing barrier height, which is inversely dependent on the nanotube diameter. Therefore, the researchers concluded that the variation in nanotube diameter is the main cause of the variations in current from device-to-device.

KINSON C. KAM

Heterogeneous Gold-Based Catalyst Reduces CO in Reformate PEFCs

In the past few years, the automotive industry has undertaken significant efforts to develop electric vehicles powered by polymer electrolyte fuel cells (PEFCs). These fuel cells employ an electrochemical process to oxidize H_2 while providing electricity and water as reaction by-products. The main fuel for PEFCs is either stored H_2 or a reformate fuel, which is a hydrogen-rich gas mixture obtained after conversion of an organic fuel such as natural gas in a catalytic reformer. However, the performance of PEFCs is hindered by residual CO that is usually present in reformate fuel. CO reduces the capability of the Pt anode of ionizing hydrogen, which is the start of the electrochemical process. P. Landon of Cardiff University, A.A. Herzing of Lehigh University, S.E. Golunski of the Johnson Matthey Technology Centre, and their colleagues have now developed a Au/Fe_2O_3 catalyst to remove CO from reformer fuel. They reported in the May issue of *Chemical Communications* (DOI: 10.1039/b505295p) their process of testing the catalyst in the actual conditions of temperature and gas mixture composition seen in PEFCs.

The researchers said that changes in the coprecipitation and calcination procedure influenced selectivity and performance of the catalyst. After calcination at temperatures lower than 550°C, the catalyst oxidized both H_2 and CO. Calcination for 3 h at 550°C resulted in selective oxidation of CO, and calcination at higher temperatures destroyed the catalyst activity. Transmission electron microscope observations of the catalysts obtained at the different calcination temperatures revealed extensive grain growth, suggesting that the consequent reduction of surface area is the cause of the reduction of activity at calcination temperatures higher than 550°C, said the researchers. Furthermore, Au (4*f*) x-ray photoelectron spectra for samples calcined at different temperatures revealed the formation of metallic gold particles at temperatures higher than 550°C, which are inactive for CO and H_2 oxidation, the re-

Molecular Dynamics Simulations Demonstrate Laser Healing of CNT Defects

The electronic properties of single-wall carbon nanotubes (CNTs) can be severely impaired by common structural imperfections, such as the pentagon–heptagon pair defect caused by a 90° rotation of a carbon dimer (a Stone–Wales-type transformation). Methods developed for the repair of such defects are therefore important for the pragmatic fabrication of CNTs in electronic devices. To this end, A.H. Romero of CINVESTAV, Queretaro, Mexico; M.E. Garcia of Universität Kassel, Germany, CINSaT; F. Valencia and colleagues at IPICYT, San Luis Potosí, Mexico; and H.O. Jeschke of Johann Wolfgang Goethe-Universität, Frankfurt/Main, Germany, have demonstrated with computer simulations that femtosecond laser pulses can repair atomic-scale defects in nanostructures.

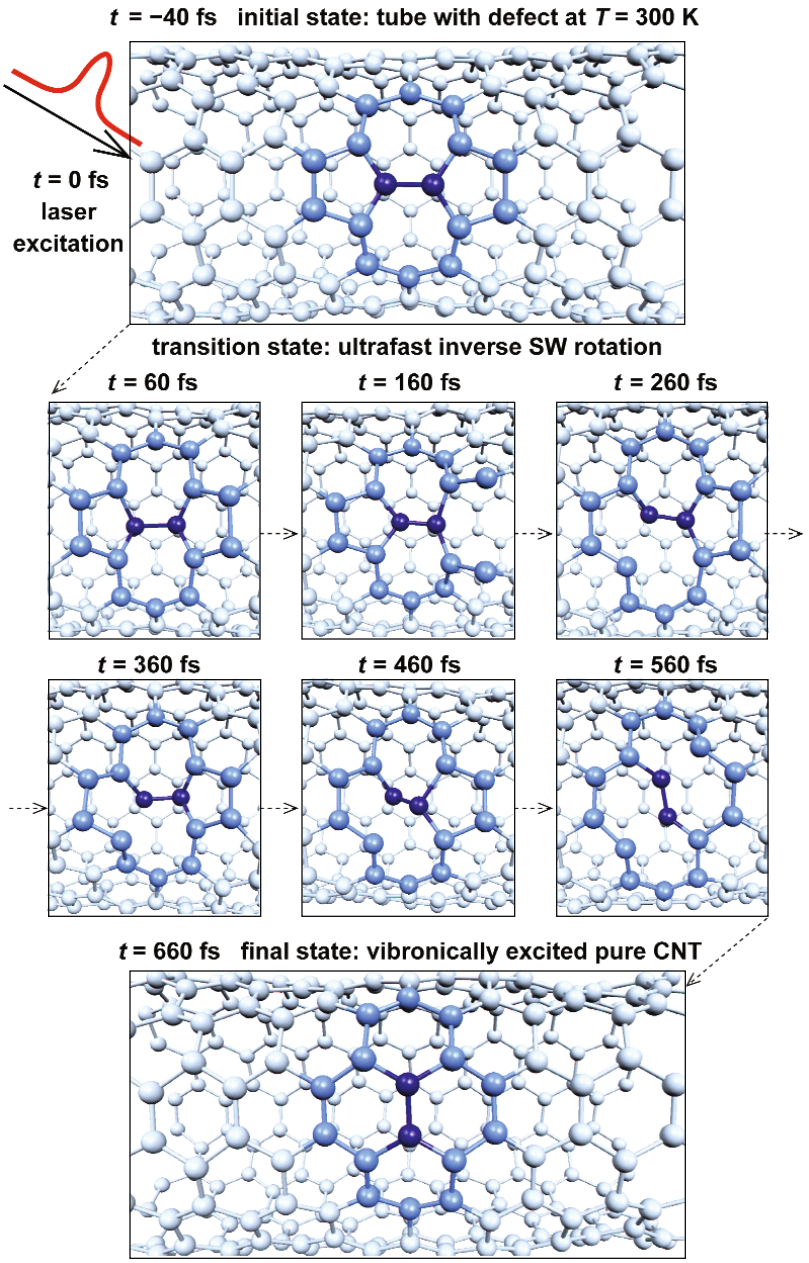

Figure 1. Simulated snapshots of the elimination of a pentagon–heptagon defect in a (7,7) carbon nanotube due to illumination with an ultrashort laser pulse. The absorbed energy induces bond-breaking processes primarily in the defect region (highlighted with darker color), making the rotation of a carbon dimer possible. Reprinted with permission from NanoLetters **5** *(2005), p. 1361; DOI: 10.1021/nl050626t. © 2005 American Chemical Society.*

As reported in the July 13 issue of *NanoLetters* (p. 1361; DOI: 10.1021/nl050626t), the researchers performed non-adiabatic tight-binding molecular dynamics simulations on (7,7) zigzag and (12,0) armchair CNTs. Using previously published parameters for this method, the only variables were the energy absorbed per atom and the type of CNT. Periodic boundary conditions were employed to simulate infinitely long CNTs with a defect density of 3%. Laser-induced structural changes were determined from simulating the dynamics of the atoms on the potential energy surface (PES), defined in terms of the electronic free energy, entropy, and temperature. Shown in Figure 1 is the simulated inversion of the generalized Stone–Wales transformation. After equilibrating the CNTs at 300 K, an ultrashort laser pulse, with a 50 fs duration and a central quantum energy of 1.96 eV, excited the system—that is, it changed the occupations of the electrons—resulting in the generation of a coherent phonon corresponding to a large-amplitude radial breathing mode during the first 400 fs. Afterwards, the PES changed by the laser pulse caused the defect's two central atoms to break their bonds with adjacent atoms. The dimer then underwent a complex motion—one component perpendicular to the CNT surface and another in the pseudo-plane of the CNT—that healed the defect.

The researchers demonstrated the universality of this mechanism by simulating the defect healing with different laser-pulse parameters and by inducing an inverse Stone–Wales transformation in a graphene sheet. The researchers said, however, that this type of dimer rotation cannot occur in C_{60}.

The researchers determined that in all their simulations, the excitation threshold for defect repair corresponded to an excitation of 7% of the valence electrons. They said that the laser pulses used to heal defects should be chosen below the laser damage threshold, which should be determined experimentally because it varies considerably with tube diameter and chirality.

STEVEN TROHALAKI

searchers reported. At temperatures of 400°C and lower, the spectra show the formation of cationic gold, which is active for the oxidation of hydrogen in the water gas-shift reaction ($CO_2 + H_2 = CO + H_2O$).

The investigators concluded that the optimal process for obtaining the selective catalyst must result in the formation of metallic gold in Fe_2O_3 particles and they established a two-stage process: 3 h at 400°C and 2 h at 550°C. The researchers demonstrated a heterogeneous catalyst that remained stable for more than 80 h of continuous use. This development, said the research team, has the potential benefit of eliminating the need for a multistage reactor currently required to eliminate CO from the reformer fuel.

SIARI SOSA

Ultrafast Laser-Driven Microfocus X-Ray Plasma Source Increases Time Resolution in Diffraction Experiments

Ultrafast laser technology involves the use of a femtosecond laser, with the potential of producing laser pulses with enormous peak powers and power densities. High peak-power ultrafast laser pulses have been used at a number of facilities to generate ultrafast x-ray pulses from laser-induced plasmas. Such technology facilitates the study of very fast chemical reactions and their intermediate and transition states. When an ultrafast laser with a small spot size is applied in a diffraction experiment, the temporal resolution of the response depends on the ability to control the jitter between the x-ray pulse and the laser pulse. This is the idea behind a broadband microfocus x-ray source designed as a result of the collaboration between a research group from the Max Born Institute led by T. Elsaesser and another from the Friedrich Schiller University led by E. Förster as described in the July 1 issue of *Optics Letters* (p. 1737).

The experimental setup for the microfocus x-ray source included a 1 kHz Ti:sapphire laser source with 45 fs duration laser pulses incident upon a 20-µm-thick copper foil, which was spooled such that it could be moved with precision so that each laser pulse was incident upon a fresh surface. When the laser intensity exceeded 10^{12} W/cm^2, a high-temperature plasma developed at the target. At intensities higher than 10^{16} W/cm^2, hot electrons were created that penetrated the target, generating incoherent x-rays. Similar levels of Cu K_α flux were detected by the investigators in both transmitted and reflected directions, increasing with laser intensity to a maximum of 6.8×10^{10} photons/s, remaining stable in a 10 h span. The transmission geometry has two main advantages over the standard reflection geometry, according to N. Zhavoronkov of Max Born Institute, "The main advantages of this new setup are the possibility to determine the initial pulse time point with very good accuracy, and a significantly diminished temporal jitter, because of the novel transmission geometry introduced."

An image of the x-ray emitting area captured with a CCD and measured using a knife-edge technique gave a source diameter after deconvolution of 10 µm ± 2 µm full width at half maximum (FWHM). A more direct measurement using a toroidal Ge(444) single crystal as an x-ray focusing mirror gave a source diameter of 23 µm ± 13 µm. Such small size and accuracy for an x-ray source allows the performance of diffraction experiments with improved resolution over that obtained with traditional x-ray sources.

Using this setup to measure the response of a semiconductor placed in the transmitted beam, the duration of the x-ray pulse was estimated at no more than 500 fs from the resulting cross-correlation of the pump (laser) and probe (x-ray) pulses. This represents an improvement on time resolution for diffraction experiments, with a demonstrated increase in the Cu K_α flux. Such an advance has potential not only for x-ray microscopy, but also for phase-contrast radiography and clinical applications such as microtomography.

SIARI SOSA

Opal Strips Fabricated by Capillary-Assisted Deposition

Colloidal photonic crystals have recently attracted attention because of their ability to control light propagation. A popular method for preparing these synthetic opal photonic crystals is the self-assembly of colloidal microspheres. For advanced applications of colloidal crystals in light-controlling devices, there is a need to introduce elements of optical circuit architectures within them. As reported in the July 26 issue of *Chemistry of Materials* (p. 3809; DOI: 10.1021/cm051114i), H.-L. Li and F. Marlow of the Max-Planck-Institut für Kohlenforschung in Mülheim an der Ruhr, Germany have utilized capillary forces to fabricate alternating strips of opal from a colloidal suspension of polystyrene microspheres.

The opal strips were grown in a planar capillary cell, which was constructed by separating two parallel glass slides by a thin spacer. The bottom glass slide had a 1 mm hole, and the polystyrene microspheres were transferred to the cell by connecting this hole to a capillary tube immersed in the colloidal solution. Capillary forces assisted in delivering the suspension to the horizontal cell; the opal strips were deposited along the edges of the bottom glass slide upon solvent evaporation. By alternately dipping the capillary tube in two different solutions, the researchers were able to create up to 20 strips of opal comprising 287 nm and 345 nm polystyrene spheres. The thickness of these strips can be tuned by changing the spacer thickness, while their widths can be controlled by adjusting the polystyrene concentration and the infiltration time.

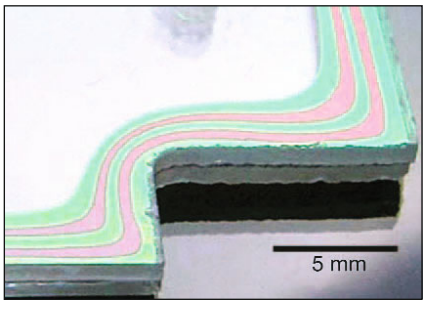

Figure 1. Alternating strip opal heterostructures obtained inside capillary cells with a special shape. Reprinted in part with permission from Chemistry of Materials ***17****(15)(2005) p. 3809; DOI: 10.1021/cm051114i. © 2005 American Chemical Society.*

These opal heterostructures exhibit multiple reflection peaks which correspond to the stop bands of the constituent opals comprising the strips. It is possible to shape the opal strips by using a non-rectangular capillary cell since the growth starts along the edge of the glass slide (see Figure 1). Marlow said that this is one of the first attempts to create bent opal strips without the use of a complicated template.

TUSHAR PRASAD