gen atoms—mathematical entities that assign the surface atoms the same reactivity as that of a real nanoparticle in suspension. The positions of the interior atoms were calculated with the valence force field method, which models the strength, elasticity, and direction of bonds among atoms.

Then LDA was used to determine the charge “motifs” around a number of representative atoms, including the surface pseudohydrogens. Through charge patching, the calculation is extended to include the entire nanostructure. In a final step, a “folded spectrum” method that with control size vapor 10 years ago is used to determine the material’s electronic states near the bandgap, including the highest energy state of the valence band and the lowest energy state of the conduction band (see Figure 1b).

Mapping the ways different compounds are assembled into different structures reveals the structures’ optical and electronic properties. Wang said, “The charge-patching method allows us to model thousand-atom structures with ab initio accuracy in about one hour.”

High Purity and Controllable Growth of MgB2O5 Nanowires Accomplished by CVD

Magnesium borate (MgB2O5) is a remarkable ceramic material that has been shown to be a thermoluminescent phosphor, a friction-reducing additive, and a ferroelastic material that may find application in nanocomposites, nanomechanics, and nanoelectronics. Synthesis of MgB2O5 (another form of magnesium borate) nanowires has been previously attempted by heating mixed powders of MgO, B2O3, and B with catalysts, but the result was a mixture of precursors or fiberlike agglomerates, necessitating a further purification process. Furthermore, with this kind of process, it is difficult to control size and location of the nanowires. Recently, researchers Y. Li and R.P.H. Chang of Northwestern University, and Z. Fan and J.G. Lu of the University of California, Irvine, have reported in the June 29 issue of Science [8](p. 960), J.P. Levin, G.R. Dickinson, and R.W. Trice at Purdue University observed in situ the microstructure evolution of a plasma-sprayed YSZ stand-alone tube under incremental compressive load while simultaneously viewing it in a scanning electron microscope (SEM). They found that cracks oriented parallel to the loading direction have opened, while cracks oriented perpendicular to the applied stress have partially closed up. This suggests that new cracks nucleated and then propagated parallel to the direction of the applied load.

Previous observations indicated that plasma spraying forms a microstructure dominated by lamellae with significant porosity and cracks both in and between the lamellae. The sample was prepared by plasma-spraying aluminum powder onto an alumina rod, followed by plasma-spraying a 280 µm YSZ layer. After dissolving the aluminum, the scientists obtained YSZ stand-alone tubes consisting of an yttrium-rich, nonequilibrium tetragonal zirconia phase with a bulk density of ~5.2 g/cm3 and a porosity of 15%. To measure the axial strain, two strain gauges were attached to the outer surface of the YSZ tubes, which were then placed in a load frame located inside the SEM. The samples were compressed incrementally using stress increments of ~13 MPa and 8 MPa, until fracture; SEM images were taken after each stress increment.

The stress-strain curve showed variable slope, but the researchers reported the data as having two slopes, corresponding to the two main regions. The first slope, up to stresses of 46 ± 1 MPa, had a modulus of 30 GPa; at higher stresses, a modulus of 60 GPa was measured. The region of the outer tube that was investigated by SEM had cracks of various widths and orientations: parallel, perpendicular, and off-axis with respect to the applied load.

The scientists’ observation supports the hypothesis that the increase in modulus of the material under compression was caused by cracks oriented perpendicular to the applied load that close partially or completely, thus increasing the planar density of the sample. Cracks parallel to the applied load widen as the crack faces slide relative to one another under the shear stress. The formation of microcracks was observed at approximately half the failure stress of the tube. The researchers’ observations agree with previous research done on the failure of brittle solids.

Maria Cortalezzi

Charge Transfer across Nanocrystalline Metal Oxide/DNA Interfaces Enables DNA Recognition

Molecular recognition of biological molecules has become an active area of research, partly due to the increasing importance of the fields of molecular patterning, genome sequencing, and drug recognition studies and their applications in bioelectronics. A necessary step in molecular recognition is control of the spatial positioning of the biomolecules. T. Rajh and co-workers at Argonne National Laboratory and N.F. Scherer of the University of Chicago have reported the use of TiO2 nanoparticles (5 nm diameter) in conjunction with DNA strands in the development of biosensing technology. As reported in the June 9 issue of Nano Letters (p. 1017), the researchers linked the metal oxide nanoparticles to DNA oligonucleotides by using bridging endiol ligands such as dopamine (DA). The researchers said that the oxygen-rich DA ligands bond readily to TiO2 nanoparticles smaller than 20 nm because their coordination sphere is incomplete and exhibits high affinity for the oxygen-containing ligands. Dopamine repairs undercoordination of the Ti atoms at the surface, thus forming strongly coupled conjugated structures.
Electron paramagnetic resonance (EPR) spectroscopy was used to examine the photoexcited nanostructures. Photoexcitation of structures with single-stranded DNA attached to the TiO$_2$/DA nanostructure showed the same EPR signature as for photoexcitation of the TiO$_2$/DA nanostructure alone. According to the researchers, this indicates that the charge separation in the single-stranded DNA/DA/TiO$_2$ nanostructure is terminated at the dopamine and never reaches the DNA. Double-stranded DNA/DA/TiO$_2$ nanostructures were obtained by hybridizing the attached oligonucleotides with their complementary strands. EPR studies of the double-stranded DNA/DA/TiO$_2$ nanostructures showed that charge separation into the DNA occurs.

The researchers also used silver reduction studies to confirm these results. Silver ions act as receptors for photogenerated electrons, and silver metal precipitates preferentially on the TiO$_2$ if excess electrons are available. Deposition of silver onto the TiO$_2$ was monitored for double-stranded DNA/DA/TiO$_2$, single-stranded DNA/TiO$_2$, and DA/TiO$_2$ nanostructures. More silver was found to deposit on the double-stranded structures than the other two structures, consistent with the interpretation of the EPR studies.

The researchers said that by using the interface of a nanocrystalline metal oxide semiconductor linked to a DNA molecule to probe DNA recognition, they have shown that the binding of DNA molecules to nanocrystalline metal oxide particles yields a photoelectrochemical system that can be used to perform extended pair-charge separation, a technique that finds application in constructing sensors for DNA hybridization. An important aspect of the work is that, since the nanoparticles are photoresponsive and therefore serve as a source of photogenerated charges, they can act as reporters of the electronic properties of the biomolecules. The researchers conclude that similar approaches may be used to detect DNA binding due to the change of redox properties of DNA molecules, and that the method opens doors to a new class of site-specific biomolecule electronic sensors and electronically tunable site-specific metal oxide catalysts.

Markus J. Buehler

News of MRS Members/Materials Researchers

Ronald W. Armstrong, a senior scientist in the Munitions Directorate of the Air Force Research Laboratory at Wright-Patterson Air Force Base in Ohio and professor emeritus at the University of Maryland College Park, has been honored by the Minerals, Metals, and Materials Society and the American Institute of Mining and Metallurgical Engineers for his lifetime achievement by sponsoring a symposium in his honor at the TMS 132nd annual meeting and exhibition held in San Diego, Calif. Armstrong’s main efforts involved energetic material technologies and promoting collaboration with non-U.S. governments and organizations, other services and agencies, universities, and industry, as relevant to the directorate thrusts and long-range goals of involving energetic materials and their uses.

Steven Chu, professor in the Physics and Applied Physics Departments at Stanford University, has been named director of Lawrence Berkeley National Laboratory.

Gustavo A. Cragnolino has been promoted to Institute Scientist in the Center for Nuclear Waste Regulatory Analyses at Southwest Research Institute (SwRI) by the U.S. Nuclear Regulatory Commission. The position is among the highest technical positions an SwRI staff member can attain.

Mary L. Good, dean of the Donaghey College of Information Science and Systems Engineering at the University of Arkansas, Little Rock, received the 2004 Vannevar Bush Award from the National Science Board of the National Science Foundation for her lifelong contributions to science, engineering, and technology, and for leadership throughout her multifaceted career.

Donald Paul of the University of Texas at Austin has been named a fellow of the Society of Plastics Engineers.

Xie Sishen has been appointed principal investigator of China’s National Center for Nanoscience and Nanotechnology.

The American Academy of Arts and Sciences has announced the election of 2004 fellows and foreign honorary members, including:

- A. Paul Alivisatos, professor of chemistry at the University of California, Berkeley;
- Mouni Gabriel Bawendi, professor of chemistry at the Massachusetts Institute of Technology;
- Arden L. Bement Jr., director of the National Institute of Standards and Technology;
- Murray S. Daw, R.A. Bowen Professor of Physics at Clemson University;
- Subra Suresh, Ford Professor of Engineering and department head, Massachusetts Institute of Technology; and
- Herbert Gleiter, director of the Institute of Nanotechnology, Germany.

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