

and its dependence on crystallographic orientation and surface roughness on the atomic scale. They also reveal how repeated contact between surfaces leads to nucleation and progression of damage at the nanoscopic dimensions, and why real crystals exhibit unusually high local strength for defect nucleation beneath a free surface when subjected to nanoscale contact.

With such insights gained from the bubble model, the researchers formulated a mechanistic theory for defect nucleation at surfaces during nanoindentation. The researchers have since used the bubble system to explore how defects form for a variety of surface conditions.

They have experimentally simulated the effects of atomic-level surface roughness on defect nucleation at surfaces. Although soap bubbles have long been used to study deformation of bulk metals, this work attempts the quantitative simulation of nanoscale contact deformation and defect nucleation at surfaces. By monitoring the defect nucleation characteristics in the bubble experiments as a function of surface asperity dimensions and the radius of the indenter tip, Suresh and his colleagues were also able to identify the conditions governing the nucleation of defects either at surfaces or in the interior for different local contact geometries. With the information obtained on homogeneous defect nucleation beneath the surface when the asperity dimension is comparable to or larger than the indenter tip radius, they were then able to rationalize why many metals exhibit unusually high local strengths near surfaces prior to the onset of defect nucleation during nanoindentation when the surface is penetrated by an indenter to a depth of only a few tens of nanometers.

"Our ultimate goal is to use them to predict how defects will form on the nanolevel, because such defects can affect the performance of these surfaces and nanoscale devices," said Suresh.

### LiNbO<sub>3</sub> Crystals Reduced in Vacuum Show a Photorefractive Response Time in the Order of 100 ms

Photorefractive crystals have different applications in optics including optical storage, coherent optical amplification, and phase conjugation. In many photorefractive materials, it is possible to write a holographic grating with a response time of less than a second. However, in the case of lithium niobate, the response time is slow, of the order of several minutes, in contrast with predictions from theoretical calculations. A group of researchers from Nankai University in China has demonstrated a method that

improves this condition in LiNbO<sub>3</sub>. According to their latest results published in the July 1 issue of *Optics Letters*, the application of a reducing treatment on a near-stoichiometric crystal significantly decreases its response time in the order of 100 ms.

A high-purity LiNbO<sub>3</sub> single crystal grown by the Czochralski method and with 49.6 mol% Li<sub>2</sub>O was reduced in vacuum at 950°C for 5 h. The resultant, near-stoichiometric sample had blue-shifted absorption edge as compared with the as-grown crystal. Holographic gratings were written in the sample using an argon ion laser of 514.5-nm-wavelength light at an optical intensity of ~1.6 W/cm<sup>2</sup>. Measurements of the diffraction efficiency as a function of the intensity of an incident He-Ne laser beam and the correspondent diffracted beam were performed. The diffraction efficiency quickly increased to a maximum when the experiment started and after the beams were turned off it decreased to zero as the light-induced grating decayed. The corresponding time constants for grating and dark decay were 122 ms and 182 ms. The incident light caused a temperature increase during the holographic grating that increased the dark conductivity, and also reduced the diffraction efficiency. The dependence of the diffraction efficiency with light intensity showed that the maximum value increased with increasing light intensity and the stationary value had an optimal point. Under the effect of an external electric field, the diffraction efficiency was greatly increased. In these conditions, the potential for the use of LiNbO<sub>3</sub> crystals in optical applications is significantly enhanced.

SIARI S. SOSA

### Parameter-Free Quasi-Particle Calculations Reveal CaB<sub>6</sub> as a Semiconducting Material

The materials classification of CaB<sub>6</sub> has been shifted from semi-metal to semiconductor by a group of researchers from the University of Twente, Catholic University of Nijmegen, and Eindhoven University of Technology. The most commonly accepted electronic structure model for this alkaline-earth hexaboride has been so far provided by the full-potential linearized augmented plane-wave (FLAPW) method. CaB<sub>6</sub> is classified as a semi-metal by this model, due to a small overlap between the valence and the conduction band in the  $\chi$  direction.

When CaB<sub>6</sub> is doped with minute amounts (~1%) of lanthanum, the system displays unexpected ferromagnetic behavior. This material has a particularly

high Curie temperature of 900 K. Because this is an odd behavior for a semi-metal matrix, the research team reexamined the validity of the semi-metal model for CaB<sub>6</sub>. As reported in the July 2 issue of *Physical Review Letters*, using the GW approximation (expanded Green's function and Coulomb screening in a perturbation series) and applying the quasi-particle condition, very good overall agreement with the FLAPW model was obtained. The results indicated lower electron and hole effective masses by an average of 10%. However, at  $\chi$ , the conduction band shifted upward while the valence band moved downward, opening a small bandgap of ~0.8 eV. According to the research team, CaB<sub>6</sub>, instead of being a semi-metal, is a semiconductor. The researchers reported experimental phenomena that also support this new finding. For example, resistivity in CaB<sub>6</sub> increases as the temperature decreases, which is identified as classical semiconductor behavior.

According to the researchers, ferromagnetic behavior in La-doped CaB<sub>6</sub> is especially encouraging because it opens the possibility of creating a new class of devices using magnetic semiconductors. Ca<sub>0.99</sub>La<sub>0.01</sub>B<sub>6</sub> is an especially good candidate for studies, they said, due to its room-temperature stability as suggested by the extraordinarily high Curie temperature.

JUNE LAU

### Generalized Titanate Ceramic Waste Form Developed for Processing Radioactive Waste with Various Compositions

A titanate ceramic phase assemblage has been developed to immobilize a wide range of nuclear-waste stream compositions. As reported in the May issue of the *Journal of the American Ceramic Society*, waste loadings of 42–50 wt% were achieved for a variety of waste-stream compositions, with leach rates comparable to those of reference grade Synroc C.

According to Ewan Maddrell, a research associate with British Nuclear Fuels at Sellafield, United Kingdom, the processing method that the research team used led to dissolution of significant amounts of the fuel assembly components together with the fission products. This resulted in waste streams rich in zirconium, iron, chromium, and nickel and gave rise to variable waste-stream compositions depending on the fuel assembly design of each reactor.

To reduce the large volume of highly active waste generated by the process, the researchers blended some of these waste-