cycles. The Si/TiB_2 microcomposite Li-ion battery anode avoids mechanical failure when compared with silicon and tin-based systems such as SnFeC, Cu_6Sn_5, and SnSb systems. The latter have become of recent interest due to their high initial capacities of up to 4000 mAh/g. However, their capacities quickly drop to about 1/20 of their initial values and they suffer from cracking or crumbling caused by the large volume change in the material during repeated charging and discharging.

As described in the June issue of *Electrochemical and Solid State Letters*, the researchers used high-energy mechanical ball milling to mix and grind the two components, Si and TiB_2, into a fine micron- to nano-sized powder. Their process yielded a nanostructured material consisting of 300–3000-nm size grains composed of 3–10-nm TiB_2 crystallites and amorphous silicon. An anode fabricated using this material exhibited a stable capacity of ~400 mAh/g after 15 cycles (with a current rate of ~C/25). Phases consisting of larger particles led to materials with higher discharge capacities (726 mAh/g), but with larger losses per cycle, while materials containing smaller particles show a lower initial capacity, but with a much higher overall charge retention (<0.4% loss per cycle). The group examined the anodes using scanning electron microscopy and high-resolution transmission electron microscopy, but could not detect any cracking or other structural damage, indicating that the small TiB_2 particles reduce the stresses caused by the volume change to a tolerable level. The researchers said that these properties make the anode material a viable alternative to the currently used graphite.

ALFRED A. ZINN

Simulations Indicate That Controlled Vertical Manipulation of Individual Molecules by Scanning Probes Is Possible

The idea of controllable modifications of surface structure on the atomic scale using scanning tunneling microscopy (STM) and atomic force microscopy (AFM) has attracted considerable attention from researchers in the last decade. Manipulation of single molecules is usually classified as lateral or vertical. Lateral manipulation has been extensively studied, while vertical manipulation is now in the beginning stages of research. A group of researchers from Tel Aviv University, Israel and the Donetsk Institute for Physics and Engineering, Ukraine has proposed a method of controlled vertical manipulation of individual molecules with scanning probes. The method is based on the different probabilities of transfer of molecules to the STM tip depending on both tip velocity and the distance of closest approach to the surface. The surface–tip transfer time competes with the tip's velocity; consequently, the adsorbate cannot always follow the motion of the tip.

As reported in the June issue of *Nano Letters*, M. Urbakh of Tel Aviv and coworkers performed detailed modeling of manipulations of molecules by STM or AFM tip by using a "pick-up-and-put-down" (vertical) mode. As a result of their simulations, the researchers presented a map giving the probability of trapping a given number of particles ranging from 0 to 8 for a given driving velocity of the tip. They also calculated histograms for the number of trapped particles for various values of velocity, which indicate that picking up 1, 3, 5, or 8 particles is much more likely than picking up 4, 6, or 7 particles.

The researchers found that the number of molecules picked up by the tip can vary over a wide range, and the number of trapped molecules decreases with an increase in tip velocity. Furthermore,

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according to their simulations, trapping of different numbers of molecules occurs with different probabilities. The researchers discuss this fact in terms of the geometry of the tip. According to their modeling conditions, the most energetically preferred configurations of molecules around the tip correspond to either five particles—a tetragonal pyramid—or eight particles in which six form a hexagon in the plane of the tip and two are out of plane. The researchers said that the configurations and the number of particles are determined by the radius of the tip, molecule conformation, and the tip geometry among other factors.

The research team concluded that changing the pulling velocity enables control of the number of molecules transferred from the surface layer to the tip and vice versa.

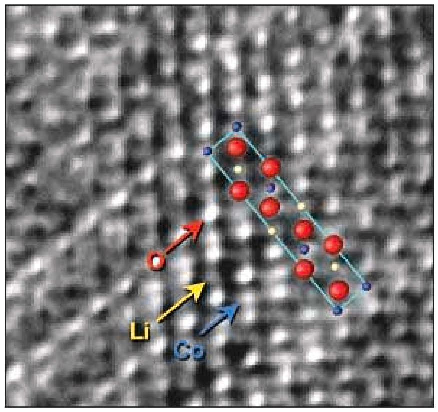
ANDREI A. ELISEEV

Focal Reconstruction Produces TEM Images of Individual Lithium Atoms

In work that could aid the development of batteries for products from laptop computers to electric cars, an international team of researchers has taken images of individual atoms of lithium, a key element in state-of-the-art rechargeable batteries.

"The atomic resolution imaging of lithium atoms is a novel and significant achievement, with implications for better understanding not only of lithium-ion battery materials but of many other electroceramic materials as well," said Yang Shao-Horn, an assistant professor at the Massachusetts Institute of Technology.

Shao-Horn and colleagues M.A. O'Keefe and E.C. Nelson from Lawrence Berkeley National Laboratory used a specially modified transmission electron microscope to simultaneously resolve columns of lithium, cobalt, and oxygen atoms in the lithium battery material lithium cobalt oxide ($LiCoO_2$). They accomplished this through focal-series reconstruction of the electron wave at the specimen exit surface (see figure).



Experimental image of lithium atoms reconstructed from 20 component images obtained over a range of focus. The image shows the arrangement of lithium ions among cobalt and oxygen atoms in the battery material lithium cobalt oxide—strong white peaks occur at the positions of oxygen atom columns, strong fuzzy peaks at cobalt sites, and the weak white peaks show lithium positions. Reproduced with permission from Nature Materials ***2*** *(7) (July 2003), p. 464; © 2003 Nature Publishing Group.*

As reported in the July issue of *Nature Materials*, the researchers obtained series of 20 differently focused images of individual crystals from a $LiCoO_2$ powder sample synthesized and characterized by conventional x-ray diffraction in collaboration with colleagues L. Croguennec and C. Delmas from CNRS and the University of Bordeaux I. Using a reconstruction program and their measurements of the microscope parameters, the researchers worked backwards to assemble the focal series of images into one image that is a representation of the electron wave leaving the exit surface of the specimen. At the thin edge of a $LiCoO_2$ crystal, this reconstructed experimental image matched the image previously predicted by a simulation program.

News of MRS Members/Materials Researchers

Jeff Wadsworth Named Director of Oak Ridge National Laboratory

UT-Battelle has announced the selection of Jeff Wadsworth as director of the U.S. Department of Energy (DOE) Oak Ridge National Laboratory (ORNL). He succeeds Bill Madia, who has joined Battelle as Executive Vice President of Laboratory Operations. Wadsworth, who began his new duties on August 1, joins ORNL after years of distinguished service as a senior leader at Lawrence Livermore National Laboratory, as well as service at Battelle's world headquarters in Columbus, Ohio as a senior executive in areas such as DOE science programs, technology transfer, and homeland security.

"Jeff [Wadsworth] is an internationally respected scientist, outstanding leader, and innovator in such fields as materials science and homeland security," said Raymond L. Orbach, director of DOE's Office of Science.

Wadsworth holds BS, PhD, and DMet degrees in metallurgy from Sheffield University. In 1987, he was elected a Fellow of the American Society for Metals, and in 2000 a Fellow of The Minerals, Metals, and Materials Society. Most recently, in 2003, he was elected a Fellow of the American Association for the Advancement of Science for "distinguished contributions in developing advanced materials and superplasticity, and in determining the history and origins of Damascus and other steels, and for broad scientific leadership supporting national security."

Reza Abbaschian, Vladimir A. Grodsky Professor of Materials Science and Engineering at the University of Florida, has received the **Donald E. Marlowe** Award from the American Society for Engineering Education in recognition of his extraordinary vision and leadership in administration, education, and research, and for significant ongoing contributions to engineering education.

Kenneth T. Barry has been named President of Unaxis Semiconductors. Barry brings with him more than 15 years of global semiconductor experience.

Stephen P. Ellis, laboratory manager at Ecolochem, Inc., has been awarded a **2003 ASTM International Award of Merit** for his technical contributions to the objectives of ASTM Committee D19 on Water.

Helen Garnett, presently chief executive of the Australian Nuclear Science and Technology Organisation (ANSTO) and a representative to the United Nations International Atomic Energy Agency, has

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