smoothed and anisotropically etched samples was evident throughout a wide range of waveguide widths. According to the researchers, this smoothing technology could lead to significant improvements in practical waveguide design for optical devices.

TIM PALUCKA

Dynamics Study of Polymer Chains Shows Reduction in Atomic Diffusion Coefficients at a Free Surface

In the November 12, 2001, issue of *Physical Review Letters*, researchers from the State University of New York—Stony Brook reported the relationship between structure and dynamics of polystyrene (hPS) by dynamic secondary-ion mass spectrometry (DSIMS). Their experimental results confirmed the chain-conformation calculation at the free surface by mean-field theory.

In order to understand how the center of mass diffusion of polystyrene related to its different molecular weight as a function of distance from the vacuum interface, a special multiple-layer sample used in the DSIMS experiment was designed. It had two parts, each consisting of a 200-nm layer of matrix hPS followed by a 25-nm layer of 20% monodisperse deuterated analogue (dPS) and 80% matrix hPS. From the relationship between the concentration of the tracer polymer (hPS or dPS) volume and the distance from the free surface for the four-layer sample, the diffusion coefficients for diffusion into a semi-infinite and an infinite medium for the top layer and the middle layer were both reduced relative to the bulk value within the distance from the surface.

The researchers found that "a purely enthalpic argument" cannot explain the experimental result. They had previously reported a large slowing down of dynamics when polymer chains were oriented parallel to the surface by rubbing the surface. They then hypothesized that the stringent confinement imposed by the large surface tension at the vacuum interface was inducing the chain orientation. This type of orientation was also plausible from the theoretical work of Kurt Binder, who demonstrated that the fluctuation times at the surface of a polymer film were anisotropic—namely, those parallel to the sample surface were much faster than those in the perpendicular direction. To test this hypothesis, self-consistent field theory was used and a one-dimensional equilibrium lattice method was designed, in consideration of the small system size. This method identified the segmental distribution at the surface, that is, the number of segments a chain has near the surface as a function of its position from the surface. After comparing the theoretical calculation with the experiment results of the chain dynamics, the researchers confirmed that asymmetric segmental fluctuations at the surface resulted in decreased mobility at the surface. This result overturned the long-held assumption that a large enhancement in mobility would be found at the surface, in analogy to monomolecular systems where this effect was observed as a result of the reduced potential.

YUE HU

One-Dimensional Metallic Edge States Observed in MoS_2

Researchers at the Technical University of Denmark and the University of Aarhus have found metallic states along the edges of two-dimensional MoS_2 clusters. These edge states are a realization of one-dimensional conducting wires and have been observed in MoS_2 nanoclusters on Au(111) substrates.

M.V. Bollinger, J.V. Lauritsen, and coworkers described their results in the November 5, 2001, issue of *Physical Review Letters*. The researchers performed density functional theory (DFT) calculations on a single layer of MoS_2 and studied the edges in a model system consisting of a stripe of MoS_2 in a supercell geometry. They also reported experimental scanning tunneling microscopy (STM) images of MoS_2 nanoclusters on Au(111) substrates along with simulated STM images calculated from a Tersoff–Hamann model.

The experimental STM images achieve atomic resolution and reveal the detailed structure of these MoS_2 clusters. The images also show a brim of high conductance that extends around the edge of these clusters.

The DFT calculations for MoS_2 edges show two one-dimensional metallic states localized at the molybdenum edge. One of these states (edge state I) is localized at adsorbed sulfur dimers on this edge and is a superposition of p_x orbitals extending in two parallel chains.

To investigate whether these metallic edge states are responsible for the conducting brims seen in experiments, the researchers simulated STM images for MoS_2 stripes with and without an underlying Au(111) substrate. These calculations showed that the brim is due to the p orbital arising from the p–d bond between sulfur and molybdenum.

"The one-dimensional metallic wires existing at the edges of the MoS_2 nanoclusters may provide a template for investigating the properties of coherent electrons on this length scale," said Bollinger.

Another important consequence of this work, according to the report, is a better understanding of the catalytic properties of MoS_2. Bollinger said, "It is generally accepted that catalytically active sites of MoS_2 are localized at edges. Since the electronic structure at edges determines this reactivity, it is certainly possible the metallic edge states play an important role in this context."

CHRISTOPHER MATRANGA

Low-Temperature Aging of Zirconia Ferrules Limits Optical-Connector Reliability

The increased use of optical fibers in uncontrolled environments has recently led to research focused on the durability and reliability of interconnects. Current technology employs flat-end-face connectors where the reduction of reflected light at the fiber end is achieved by physical contact between the optical fibers secured in a stabilized zirconia ferrule. A team of researchers from the Oak Ridge National Laboratory, Rutgers University, and Bellcore in Morristown, N.J. has shown that strict polishing, which ensures physical contact, accelerates the aging of zirconia ferrules by relieving compressive stress, making the resulting phase transformation more thermodynamically favorable. This environmental-aging-induced phase transformation results in a 4–5 % increase in the unit-cell volume, leading to surface roughening and optical losses due to contact problems, thus limiting connector lifetimes.

As reported in the November 2001 issue of the *Journal of the American Ceramics Society*, the research team, led by Michael Lance, aged samples from a variety of manufacturers at temperatures from -10°C to 85°C at 95% relative humidity for 90 days. Studying the results with profilometry, optical, and interferometric microscopy, the researchers found two patterns. In some samples, they observed a significant increase in the surface roughness of polished zirconia ferrules, corresponding to a 1–2 vol% phase transformation. In other samples, they saw a flattening or deformation of the zirconia surface, corresponding to an increased volume content of monoclinic transformed zirconia, up to 40 vol%.

Raman spectroscopy equipped with a confocal aperture was used to control the sampling depth and to quantify the tetragonal–monoclinic phase transformation. They reported that the amount of transformation was lower in the vicinity of the optical-fiber-region under compression—and that transformation occurred only at the polished surface of the material. In addition, no monoclinic zirconia was found at the sides of the fer-