a group at the Institut für Theoretische und Angewandte Physik (ITAP) of Stuttgart University carried out a demonstration run with over five billion particles. With 512 processing nodes and a total memory of 256 GB, the program IMD (ITAP Molecular Dynamics) performed a simulation with 5,180,116,000 particles.

The atoms, interacting via Lennard-Jones potentials, were placed in a cubic fcc lattice cell with an edge length of 1540 atom distances or 0.42 μm (for Al). This means that the simulations are arriving at scales comparable to the wavelength of visible light and to the width of the conductor paths of the computer. Six time steps were carried out and took a computer time of 2,328 s. According to the researchers, 223 time steps would require about a day, a typical simulation more than a month. The real challenge, they said, is the output data which cannot be stored directly but has to be analyzed parallel to the simulation.

IMD is a software package designed to perform classical molecular dynamics simulations on massively parallel computers. The interactions are not limited to pair potentials. The program permits embedded atom potentials, three-body potentials, and anisotropic Gay-Berne-potentials. In addition to the common thermodynamic ensembles, a number of boundary conditions are implemented enabling the program to deform a sample, to stress load it, or to simulate shock waves.

AFM Applied in Molecular-Scale Flattening of DAST Crystals

Due to their nonlinear optical properties, certain organic crystals are useful in applications such as ultrahigh-speed signal detection and integrated circuit diagnosis. While the polishing of these soft organic crystals is required for optimizing light transmittance, the usual polishing and cutting techniques are often insufficient for flattening these materials. A research group from the Institute for Chemical Reaction Science at Tohoku University and the Intelligent Cosmos Research Institute has invented a molecular-scale polishing method utilizing atomic-force microscopy (AFM). As reported in the August 1 issue of *Optics Letters*, ion pairs of the 4-dimethylamino-N-methyl-4-stilbazolium tosylate (DAST) crystal may be removed by applying some force to the AFM cantilever tip.

Single DAST crystals were grown from seed crystals by lowering the temperature of a solution saturated with DAST. The flattening of the (001) surface was performed by the scanning action of the AFM. "When the force applied to an AFM tip is larger than that of the interlayer bond, the layer(s) that are exposed on the surface will be removed," the scientists reported. An approximately 10 nN force was applied to the tip (with a tip curvature of 20 nm) during the scan. Three stepped terraces appeared after the first five scans, and another five after eight scans. The average step height was approximately 0.9 nm. This is a good agreement with the interlayer distance of 0.893 nm. The scientists generated a terrace area of 250,000 nm^2. A few existing terrace steps are not expected to contribute significantly to optical transmission loss.

A friction-force microscope (FFM) was used for characterizing the resulting DAST crystal. Topography photos indicate that terrace regions are indeed very flat, with a roughness of 0.12 nm rms. These results show that the AFM may be used as a polishing tool and that this technique shows promise for other organic crystals similar to DAST.

JUNE LAU

Minimization of Diffuse Scattering Reduces Resistivity of Thin Copper Films

Low resistivity values of 2–2.2 μΩ cm have been observed for copper films as thin as 30–40 nm, comparable to the mean free path (mfp) of electrons in copper. A team of researchers at Rensselaer Polytechnic Institute (RPI) reports that the deposition of copper thin films in an argon atmosphere containing 3 vol% hydrogen followed by a low temperature anneal considerably improves the conductivity of the films.

As semiconductor devices continue to shrink, the dimensions of the interconnect metals reach values comparable to the mfp of electrons. This results in a drastic increase in resistivity, which is attributed to diffuse electron scattering by surfaces. Passivation or tailoring of the surfaces that results in an increase of the elastic scattering component should therefore decrease the resistivity.

"Our experiments were designed to find conditions that may lead to a passivation of surfaces and thereby decrease the resistivity of thin copper films (30–50 nm). Earlier studies by Ficalora have indicated that sputter-depositing Cu in hydrogen lowered the as-deposited resistivity of Cu films that were greater than 100 nm in thickness. Ficalora has also shown that electromigration testing in hygrogen ambients caused significant improvements in the electromigration lifetimes of Au interconnects," said S.P. Murarka, professor of materials science and engineering at RPI.

As reported in the September issue of *Electrochemical and Solid-State Letters*, the scientists investigated films between 10 and 200 nm in thickness prepared by dc magnetron sputter deposition of copper. Substrates were *p*-type silicon with a uniform 50 nm thermally oxidized layer. The copper depositions were carried out in pure argon or in argon with 3 vol% hydrogen and annealed in high vacuum or in an argon atmosphere with 3% hydrogen at 300°C. The films that were prepared in the hydrogen-containing atmosphere showed a resistivity that was on average 10% lower than for films prepared in pure argon, and the resistivity at 39 nm thickness was estimated to be 2–2.2 μΩ cm. The resistivity of the films deposited in pure argon could be decreased by 10–30% by annealing in vacuum or Ar/H_2. The use of Ar/H_2 gave 2–5% lower resistivity values than the vacuum treatment.

"The role of hydrogen in affecting the resistivity of as-deposited films is not clear yet," said Anupama Mallikarjunan, a graduate student in Murarka's group. "It seems to passivate the electron-scattering defects including surfaces, enhancing the overall mobility across the film."

Another factor, according to the researchers, could be that hydrogen scavenges the chamber of impurities like oxygen, water, and nitrogen. Another group at RPI is currently working on *in situ* experiments in ultrahigh vacuum chambers to address these issues.

CORA LIND

High-Valence Cations Improve Hydration Resistance of MgO-CaO Materials

Improving the hydration resistance of magnesite and dolomite materials has important implications for the ceramics industry, particularly in the refractories sector where MgO-CaO bricks are often used to line basic open hearth furnaces. Research reported in the July issue of the *Journal of the American Ceramic Society* reveals that the addition of tri- and tetravalent cations in small proportions can improve hydration resistance by producing vacancies in solid solutions of CaO and MgO, and by substituting cations that are less prone to hydration.

Researchers at the East China University of Science and Technology in Shanghai and the Anshan Institute of Iron and Steel Technology pressed and fired high-density briquettes of flotation magnesite and dolomite doped with 0.5% (cation basis) of various monovalent to tetravalent cations. Dopants included NaF, NaCl, CaF_2, $MgCl_2$, Al_2O_3, Cr_2O_3, Fe_2O_3, TiO_2, and ZrO_2. Briquettes fabricated from analytically pure MgO and CaO were included

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