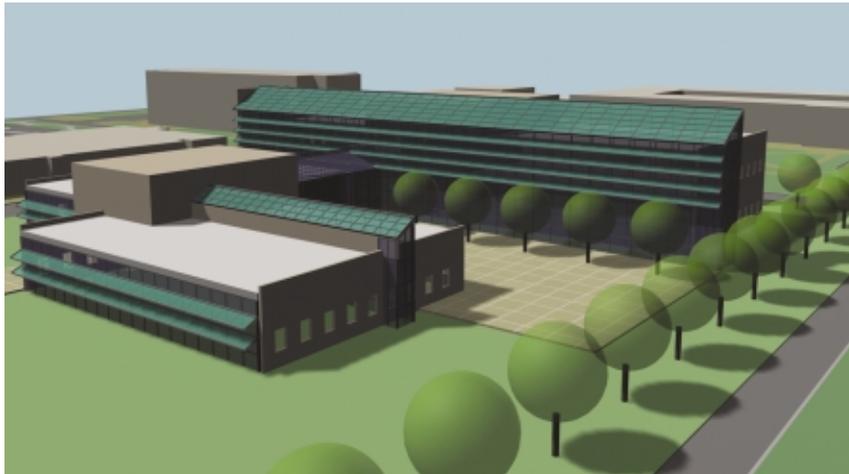
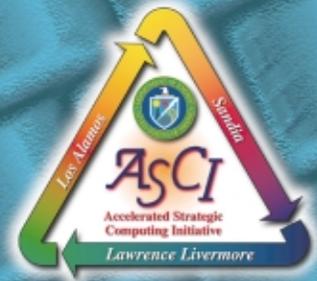


ASCI UPDATE

April 2001



Conceptual drawing of the 70,400 gsf. DISL facility.

DISL Brings State of the Art to Distributed and Distance Computing

Modeling and simulation are shortening the time for hardware delivery required by stockpile stewardship, but advances in distributed computing and information sciences are also needed to take the next steps. To help fill these needs, ASCI is sponsoring the design and construction of a new facility that will provide the nuclear weapons complex (NWC) with a more effective distributed and distance computing capability. The Distributed Information Systems Laboratory (DISL), to be constructed at Sandia's California site by 2003, is part of the ASCI strategy for an integrated modeling and simulation-based environment.

DISL will bring together essential technologies needed to create a distributed information systems infrastructure that will link the NWC. The new facility will house computing testbed environments and labs to develop secure, high-performance networking and visualization and collaboration technologies that will enhance design and manufacturing productivity environments. DISL will provide collaborative work environments necessary to successfully research, develop, and deploy distributed computing and visualization solutions for the NWC.

Research in DISL will focus on distributed systems and visualization, networking, information security, and development of collaborative technologies. Research and development workspace and laboratories will include specialized networking research labs and a next-generation visualization design center. DISL will also house weapons design project teams who will work in systems engineering, design definition, structural and thermal analysis and other areas. The goal is to provide ASCI technologies to design teams that will enable them to enhance weapons design and manufacturing capabilities.

With its capacity to support both unclassified and classified work, DISL will be easily accessible to visitors and on-site personnel. Its two-story, 70,400 gross-square-foot design will feature an infrastructure designed to improve teaming and interaction with simulation and experimental results, and features built in to allow for future upgrades as technologies are developed. Equipment available to 130 employees and approximately 50 visiting researchers includes advanced visualization systems, enhanced video conference equipment, network and communication systems, and collaborative environments.

In the News...

ASCI's Problem Solving Environment and Distance and Distributed Computing and Communication programs completed their level-one milestone reviews at LLNL during the week of April 9.

An updated ASCI Program Plan has been completed and will be published in May.

Who's Who in ASCI Simulation and Computer Science...

PROBLEM SOLVING ENVIRONMENT

Thuc Hoang
NSNSA PSE Program Manager
thuc.hoang@ns.doe.gov

Steve Louis, LLNL
Lawrence Livermore National
Laboratory
stlouis@llnl.gov

Jeff Brown
Los Alamos National Laboratory
jeffb@lanl.gov

Mike Koszykowski
Sandia National Laboratories
mikek@sandia.gov

ASCI Lends Expertise to Corrosion Issues in Microelectronics

Materials and process computation and modeling efforts at Sandia National Laboratories develop computer models of materials and processes. The models are used to help researchers understand microstructures that link processing to performance. The Accelerated Strategic Computing Initiative (ASCI) corrosion project is part of a laboratory-wide corrosion initiative integrating computational and experimental work to understand corrosion issues in microelectronics. Corrosion is the most common source of materials-related significant finding investigations (SFIs) in the stockpile. Currently, these problems are addressed with a combination of engineering judgement and ad hoc experimental studies. The goal of the corrosion initiative is to develop a science-based modeling toolset to perform more quantitative analysis of corrosion issues. The modeling tools are also needed to correctly use the results of accelerated aging experiments to predict lifetimes of weapons under operational conditions. Finally, such a toolset will help the stockpile life extension program by identifying potential corrosion-related failures and providing an engineering tool to design more corrosion resistant replacements.

The corrosion modeling effort currently spans from continuum-level models at the largest length and time scales to fundamental atomistic and electronic structure level modeling. To provide focus, the current effort primarily considers sulfidation of copper components. The continuum modeling is based on the GOMA code. These models treat the mass transport on the macroscopic level and track the growth of the corrosion products. The continuum level also predicts the effect of corrosion on electrical properties such as the conductivity of crucial components. This provides connections to device level simulations. The inputs needed by the continuum models are the fundamental mechanisms and the rates associated with these mechanisms. A combination of experimental data and sub-grid level modeling efforts provides this information.

One focal area of the modeling is the chemistry in ultra-thin aqueous layers. Such layers form on surfaces under normal conditions due to atmospheric humidity. The chemical properties in aqueous layers that are just a few monolayers thick differ from bulk behavior. Atomic-scale simulations are being performed to understand the chemical thermodynamics in this case. In addition, the presence of the surface strongly modifies the dynamics in the aqueous layer. Figure 1 shows simulations that demonstrate the reduction in the diffusion constant of water in the vicinity of a cuprite surface.

Another effort looks at solid-state diffusion processes in the corrosion product layers. In some cases, this process can

limit the overall growth rate. Fundamental electronic-structure-level calculations of the relevant point defect properties identify critical point defect formation and migration energies. This has resulted in a new detailed understanding of the point defect migration mechanism in the case of copper oxides. Figure 2 shows the unexpected transition state. In addition, the interaction of point defects, such as vacancies and impurities, has been computed for the copper oxides. The complex structure of a vacancy-Al complex is also shown in Figure 2. This elucidates the effect of alloying additions on diffusion. Experiments also demonstrated the role of alloying agents in strongly modifying the solid state diffusion consistent with the computational models. Other experiments have pointed out the unexpected crucial role that gas-phase mass transport plays in determining the overall growth rates in certain cases.

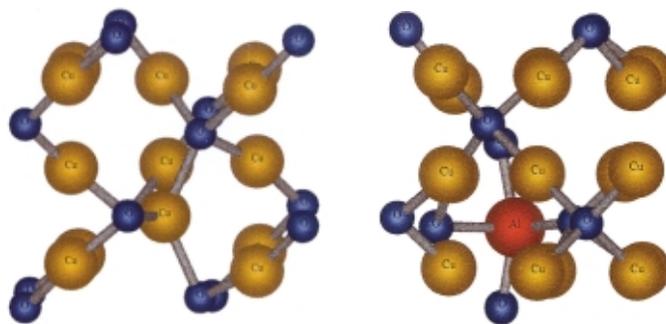


Figure 1. Molecular simulations of water diffusion near a cuprite surface.

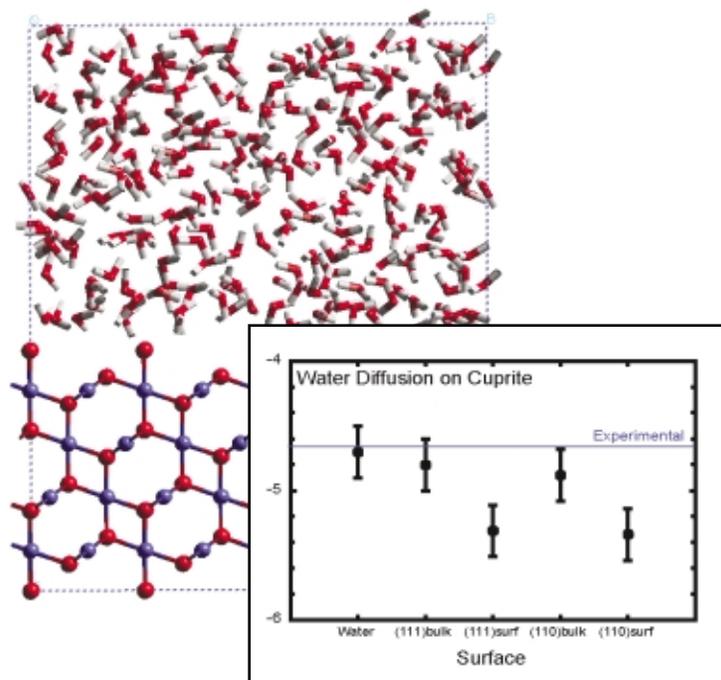


Figure 2. The structure of the transition state for vacancy migration and the structure of an Al-vacancy complex in copper oxide. These structures were determined from first-principles electronic-structure level calculations.