First MRS Workshops Cover Tribology and Advances in Thin Film Simulations and Experimental Verification

At the inaugural Materials Research Society (MRS) Workshops held June 20–25, 1999, in San José, California, materials researchers enjoyed the opportunity to focus on issues surrounding the fields of tribology and advances in thin film simulations and experimental verification, as they identified research directions and challenges. The topics, each receiving three days of focused and interactive exploration, were presented in a series of invited talks by key players in the field, interspersed with discussion periods and poster sessions that facilitated interaction among the participants. Attendees further enjoyed ample opportunity to network over meals and coffee breaks at the Fairmont Hotel where the sessions were held. From surface science to geology and from mathematics to industrial materials processing, the defining interdisciplinarity of MRS was a strong element of the workshops. The focused sessions without competing activities gave coherence to the workshop, which allowed discussions to grow and new ideas to simmer and gel.

In the first workshop held Sunday through Tuesday on **Tribology on the 300th Anniversary of Amontons' Law**, organized by Michael D. Drory (Timken Aerospace-MPB) and Mark O. Robbins (Johns Hopkins University), 40 scientists convened for an interdisciplinary meeting with their colleagues from industry, universities, and national laboratories. One of the founding concepts of tribology is Amontons' Law, stated in 1699, that friction force is proportional to load. This provided a central theme to discuss friction and wear problems on scales ranging from the atomic to geologic, and to incorporate nearly all classes of materials, from liquid lubricants to quasicrystals.

At the atomic level, experimental talks described new measurements of friction between surfaces with controlled geometry, orientation, and surface chemistry. Simulation talks described detailed mechanisms of boundary lubrication by grafted hydrocarbon films and suggested a possible origin for the widespread observation of static friction. Calculations and measurements at intermediate length scales exposed the role of plastic and viscoelastic deformation below the contact in determining the area of contact and frictional dissipation.

At the macroscopic scale, talks provided new understanding of the flow of sand, and the complex distribution of contacts between macroscopic surfaces (see Figure 1) and their evolution with

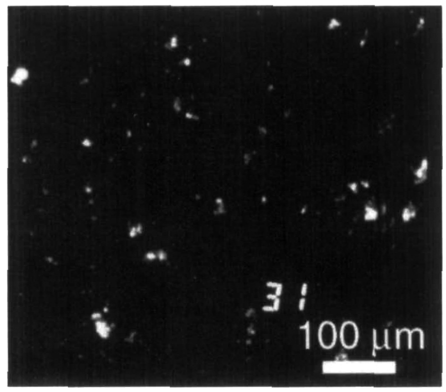

Figure 1. Photomicrograph shows areas of intimate contact (bright spots) between abraded acrylic and soda-lime glass at 10 MPa pressure. This technique is used to study the evolution of contacts in order to understand friction between rock faces in geologic systems and its role in earthquakes. (Courtesy of J.H. Dieterich, U.S. Geological Survey, Menlo Park, California.)

time, pressure, and velocity. The relation to the stick-slip motion that produces squeaks in hinges and earthquakes in geological faults was described.

The broad variety of techniques used to explore tribology is driven by the need to understand the complex interactions of multiple interfaces and materials that may limit the performance of engineering systems. Some of the examples that were described are demanding applications in space-flight hardware and magnetic storage devices (disk drives).

Most attendees were present for the full three-day span. This enabled discussions to grow and build on earlier developments. During a wrap-up session at the end of the Workshop, participants identified themes that cut across the topic and strove to connect the disparate perspectives from research at different length scales. Three hundred years later, the many complex phenomena that lead to the successes and failures of Amontons' Law are becoming clearer, but continue to challenge materials scientists.

The **Advances in Thin Film Simulations and Experimental Verification Workshop**, held Wednesday through Friday and organized by Harry Atwater (California Institute of Technology), George Gilmer (Lucent Technologies), Imran Hashim (Applied Materials), and Paco Leon (Intel Corporation), gathered 80 researchers from universities, industry, and national laboratories. The workshop brought together researchers working on the most advanced aspects of simulation with mathematicians and industrial practitioners, in the hope that all would be informed by the mixture of theoretical, computation, and experimental perspectives.

Most of the talks were related to the semiconductor industry, although some applications from the disk drive and other industries were also represented. Special emphasis was placed on the areas of metallization and plasma etch modeling.

Panelists on Modeling of Copper Interconnect Processing directed the discussion on future technologies for the copper seed layer and copper fill. S. Rossnagel (IBM) said that although significant technical challenges have presented themselves in further scaling of copper technology, they are not hard physical limits such as those foreseen in other areas of semiconductor development, such as optical lithography and MOS device scaling. K. Takahashi (Lucent Technologies) said that although progress has been made recently in modeling the copper electroplating process, no consistent physical model is yet available to explain the role of electroplating additives in improving the fill properties of high aspect ratio features. D. Coronell (Motorola) demonstrated that advanced modeling techniques exploiting a combination of reactor scale and molecular dynamics simulations can have an impact on industrial technology development of copper interconnects (see Figure 2).

While continuum modeling approaches for thin films have been used by the semiconductor industry for over a decade, emphasis on atomistic modeling has seen

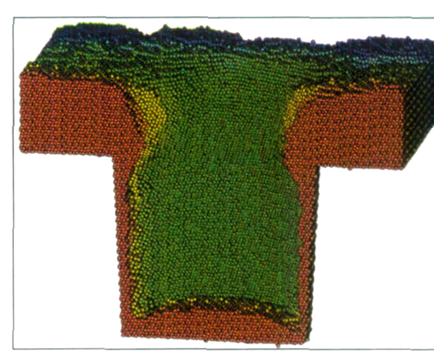

Figure 2. Three-dimensional simulation of copper seed layer step coverage over a sub-micron sized via ionized physical vapor deposition.

1999 MRS Workshop on Tribology on the 300th Anniversary of Amontons' Law

a: Mark O. Robbins of Johns Hopkins University (left) and Michael D. Drory of Timken Aerospace-MPB chair the first 1999 MRS Workshop.

b: Jacqueline Krim (North Carolina State University) describes friction of incommensurate lattices.

c: David Rigney (Ohio State University) takes questions.

d,e,f: Poster session provides opportunity for attendees to discuss the science.

g,h,i: Attendees converse over breakfast, during the workshop sessions, and over coffee breaks.

1999 MRS Workshop on Thin Film Simulations and Experimental Verification

a,b,c: Participants converse during coffee breaks, poster sessions, and over breakfast.
d,e,f: The room filled with 80 attendees to hear A. Voter (Los Alamos National Laboratory); panelists on Modeling of Copper Interconnct Processing (left to right) P. Leon (Intel and co-chair of the MRS Workshop), D. Coronell (Motorola), S. Rossnagel (IBM), and K. Takahashi (Lucent Technologies); and D. Coronell (Motorola).

a recent increase. Discussion at the Workshop showed the benefits of atomistic approaches for gaining insight into the basic processes at the evolving surface and for explaining microstructure and grain structure phenomena. However, atomistic techniques themselves—such as molecular dynamics and kinetic Monte Carlo—require further development before they can be widely used. A. Voter (Los Alamos National Laboratory) demonstrated an increase in the speed of molecular dynamics. He reported on simulations of ionized physical vapor deposition of copper with his "hyperdynamics" method that were nearly fast enough to model processes with realistic deposition rates. Molecular dynamics techniques are only as accurate as the potential functions that embody the interatomic interactions, and advances in this area were reported by D.G. Pettifor (University of Oxford). He described some work in progress on new approaches to potential functions that would rival quantum tight-binding accuracy, but with much higher speed. J. Sethian (University of California—Berkeley) reviewed the level-set method, a class of numerical techniques coming into wide use for the representation of evolving surfaces, and P. Smereka (University of Michigan) demonstrated the extension of the level-set technique to model grain growth and evolution.

Plasma etch modeling is a formidable challenge, due largely to the uncertainty of the surface environment, in which complex chemical reactions occur under the physical bombardment of ions and neutrals. H. Sawin (Massachusetts Institute of Technology) emphasized the critical role of depositing species in his model of the polysilicon etch process. His work also showed the need for simultaneous characterization of the basic processes, which his group carries out in beam experiments. D. Graves (University of California—Berkeley) reported on progress in molecular dynamics simulations of silicon etched by C–F compounds. In the panel discussion on etch simulation, discussion brought a consensus that one of the central challenges in the plasma etch area is to distill the detailed atomistic simulations into more phenomenological forms that would be suitable to model realistic industrial applications.

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