Cornell University
Center for Advanced Computing

CAC and Shefford Baker

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Thin Metal Films: How do They Behave?

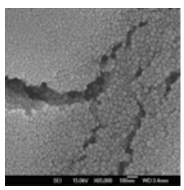
Why do thin metal films sustain much greater stresses than corresponding bulk materials?

Finding the Answer

Shefford Baker and his colleagues in Cornell's Department of Materials Science and Engineering are studying the behavior of defects in and the mechanics of thin metal films using a unique combination of experiments, modeling and simulations. CAC high-performance computing systems enable the researchers to simulate the effects of defects or "dislocations" on the mechanical behavior of the films at the atomic level.

Thin Metal Films
Thin metal films are critical components of many high-tech devices.





For example, they are used to form the microscopic conducting wires in integrated circuits; they act as optical reflecting or absorbing layers in cameras, photocopiers, and lasers; and, they are used for chemical activation in catalytic converters. In such applications, the films can develop enormously high stresses, and the device will fail if the film cracks, peels off, or simply distorts the structure to which it is attached.

Improved Research

Research Metrics

- Use "mezzo-scale" simulations: Relate defect interactions on a local scale to global behavior of a small system; allow dislocations to move and interact with each other in response to imposed boundary conditions
- Speed: Complete more complex simulations in less time using CAC systems

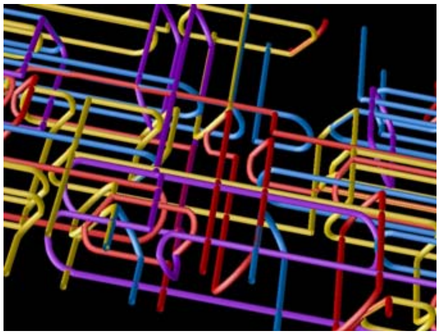
Research Challenge

Designers, for instance people creating circuit boards for computers, rely on the fact that thin films are known to be able to sustain greater stresses than corresponding bulk materials, but are hard pressed to explain the phenomenon. Shefford and his colleagues hope that in the future the knowledge that they generate will allow companies, such as chip manufacturers, to produce more reliable components.

Solution

Baker and his colleagues are using CAC high-performance computing systems to calculate the force on a dislocation due to all the other dislocations, which is an order N^2 (N being the number of calculation points), and this has to be done every step of the simulation.

Because of the amount of computation time needed per data point, researchers rely on CAC systems which allow calculations and the analysis of the data to be done in parallel.



Dislocations in thin metal films

As a first step, the researchers conducted a detailed study of interactions between pairs of dislocation. They ranked the strengths of various interactions as a function of thickness and orientation, and studied the shapes adopted by dislocations as they move and interact in a film. They then conducted simulations involving many dislocations to see how realistic dislocation structures evolve. In this work, the researchers statistically categorize interactions, hoping to gain a better understanding of which interactions are preferred in the film at various stress states and which ones are not.

In ongoing work, the researchers are building upon this study by including the effects of temperature and grain size on thin film strength. In a real film, thickness and grain size are typically smaller than the characteristic length scale of dislocation structures, so dislocations are found predominantly at grain boundaries and interfaces. These investigations will discover whether dislocations are simply stopped at the boundaries, if they can dissipate into the boundary by some mechanism, or if they can initiate deformation in adjacent volumes.

The Client

Shefford P. Baker

- Associate Professor, Department of Materials Science and Engineering, Cornell University
- Research focus on deformation mechanics in thin metal films, adhesion of thin metal films to glass, mechanical property profiling at the nanometer scale, electromigration

The Collaborative Relationship

CAC systems and staff are enabling unprecedented and detailed study of the mechanisms that control stresses and deformation in thin films metallization during thermal cycling.

“A tightly integrated program of experiments and simulations will yield many new insights into the complex relationships between defect behavior and mechanical behavior in constrained volumes that would not be found in projects focused exclusively on experiments or simulations. Although we are primarily an experimental group, the insights that we have gained by being able to run simulations has been invaluable. This is a truly interdisciplinary research that can only be accomplished by a team running experiments and dislocation simulations with the HPC systems and staff available at an exceptional facility like CAC.”

Shefford Baker
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