

variables at once, or jumped from variable to variable without fully exploring any. As a result, they came up with quick, but often incomplete conclusions. "The students took a video game approach to the simulations," says Rick Borovoy, also of Apple.

Now that the Apple researchers have a better understanding of the hurdles they face,

they are at once seeking help and proposing some solutions. "We know students are amused and motivated by simulations, but we are just beginning to learn how to make simulations work in an instructional setting," Apple computer scientist James Spohrer said at the meeting. And in a nod to his audience, he added: "We are looking to

cognitive scientists to get ideas about how this can be done." Meanwhile, though, one potential solution under investigation at the company is the development of the computer equivalent of lab books to help students plot a logical course of inquiry through simulated experiments, instead of using video game tactics. ■ ANNE SIMON MOFFAT

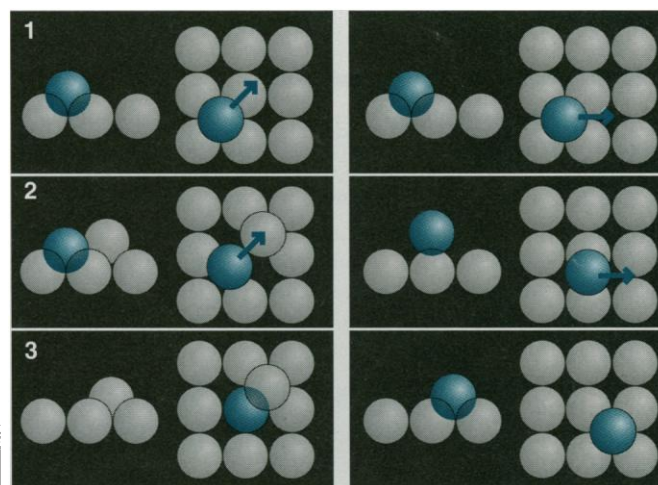
Atoms Do the Two-Step on Crystal Dance Floors

Physicists have long tended to picture an atom moving on a surface as something like a loose marble on a layer of close-packed marbles, hopping from hollow to hollow on the surface without disturbing the atoms underneath. But that's only part of the picture. Instead of hopping over a surface, it seems, an atom is often more likely to dive into it, displacing another atom, which then pops upon the surface nearby. That's the message now coming from a merger of an old microscopic technique with a theoretical analysis by physicist Peter J. Feibelman of Sandia National Laboratories.

The wanderings of a single atom might not seem to count for much. But an accurate knowledge of how atoms migrate across the topmost atomic layer of a metal is vital for understanding—and hence controlling—many basic surface phenomena. Corrosion, crystal growth, and catalysis, to name just a few, are all carried out by atoms dancing on surfaces. A refined understanding of how their dance is choreographed is also important, remarks Feibelman, "because we think it can help guide people in making materials." For example, he conjectures, a clearer picture of the dynamic behavior of atoms on surfaces could guide materials scientists who are attempting to create super-strong metallic alloys by building up atoms-thick layers of different metals.

Early hints that atoms on surfaces might not be as simple as loose marbles actually came decades ago from images made by field ion microscopes (FIMs), devices that were revealing the positions of individual metal atoms on surfaces long before the scanning tunneling microscopes now used to map atomic topography. In an FIM, a strong electric field between a sharp probe and a crystalline metal surface ionizes atoms of helium, deliberately leaked into the sample chamber, wherever the electric field is greatest—at the peaks created by atoms resting atop the crystal plane. The helium ions act as a tracer, generating an image of the peaks. And while scanning tunneling microscopes tend to drift, an FIM can repeatedly image a single patch of surface to trace the fate of atoms there.

As far back as the late 1960s, surface scientist Gert Ehrlich of the University of Illinois at Urbana-Champaign and others were using successive FIM images to show that when atoms from a vapor of one metal land in the valleys between ridges of atoms on the surface of another metal, they often burrow into a neighboring ridge, pushing atoms of the surface metal into the next valley. Feibelman's analysis shows that such behavior may be common at metal surfaces. His model, which simulates the movement of aluminum atoms across an atomically flat aluminum layer, suggests that it takes less energy—as measured by the balance of bond-making and bond-breaking—for newly arrived atoms to move by displacing an atom in the topmost layer of the crystal to a nearby site than by hopping across the surface without digging in. When an atom hops from valley to valley,



Trading places. A metal atom often migrates across a crystal by displacing an underlying atom (left) rather than hopping.

"you have to pay a toll for going over a bridge" that is higher than the cost of displacing another atom, Feibelman says.

In addition to the retrospective support from Ehrlich's work, Feibelman's model is gaining new support from FIM observations made by Feibelman's Sandia colleague, experimental physicist Gary L. Kellogg. Kellogg and others have observed platinum, iridium, and nickel atoms migrating across crystals of those metals by Feibelman's predicted exchange mode.

Feibelman's model doesn't rule out the hopping motion of the traditional picture; instead it predicts that the dominant migration pattern will vary depending on such factors as temperature, the kind of metal, and whether the wayfaring atoms move alone or in clusters. Indeed, Kellogg and his colleagues found—in keeping with Feibelman's predictions—that clusters of two platinum atoms actually migrate faster by the exchange mode than single platinum atoms do; clusters of three platinum atoms, on the other hand, migrate both by exchange and by hopping.

Ehrlich welcomes the new interest in his old observations. Together with new studies by him and others, it's leading to a much richer view of crystal growth on its atomic level, he says.

But so far the sharper picture of surface choreography applies only to metal atoms moving on metal surfaces. According to Steven George of Stanford University, who studies the surface diffusion of molecules such as carbon dioxide or hydrocarbons on metal surfaces, more complicated systems remain far out of current theoretical reach.

To be sure, Feibelman concedes, "We're just beginning to learn the rules." Subtle as these may seem, adds George, they're just what engineers will need to know as they try to design advanced new materials from the atomic level up. ■ IVAN AMATO