Modeling how thin films break up

June 19 2015, by Denis Paiste

Rachel Zucker (center), a 2015 PhD recipient in MIT's Department of Materials Science and Engineering, works with Professor Christina Scheu (left) and Alexander Müller at the Max Planck Institute for Iron Research in Dusseldorf, Germany. Scheu hosted Zucker in collaboration with the MISTI-Germany seed fund. Credit: Rachel Zucker

Excess surface energy from unsatisfied bonds is a significant driver of dimensional changes in thin-film materials, whether formation of holes, contracting edges, or run-away corners. In general, this break-up of a material is known as dewetting. Recent MIT graduate Rachel V. Zucker, who received her PhD on June 5, has developed a range of mathematical solutions to explain various dewetting phenomena in solid films.

Working with collaborators at MIT as well as in Germany and Italy, Zucker, 28, developed a model for calculating fully-faceted edge retraction in two dimensions, but she says the crown jewel of her work is a phase field approach that provides a general method to simulate dewetting.

Thin-film materials range from about 1 micrometer (micron) down to just a few nanometers in thickness. Nanometer-scale films are the basic building blocks for circuit boards in electronic and electrochemical devices, and are patterned into wires, transistors, and other components. Zucker developed models for what happens to thin films over time. "They have a lot of surface area compared to their volume, just because they are so thin, especially in one dimension, and so that can actually amount to a huge driving force for the thin film to change its shape," she says.

At MIT, Zucker was co-advised by professors W. Craig Carter and Carl V. Thompson. With dewetting, Zucker tackled one of the hard problems in materials science, Carter explains, especially with the addition of anistropic surface tension. "Equations start looking very complicated and the methods that you would you use to solve those equations start becoming more and more obscure. And so as you go down this path, you're going into terra incognita. How do you go about solving these problems?"

Dewetting of solid films looks like dewetting of a liquid—for example, water beading up on a windshield—but the material stays solid during this process. Solid-state dewetting can happen at temperatures well below the melting temperatures of the material when the film is very thin, and especially when it is patterned to make very small features like wires in integrated circuits. "Solid-state dewetting is getting to be more and more of a problem as we make things with smaller and smaller features," Thompson says.

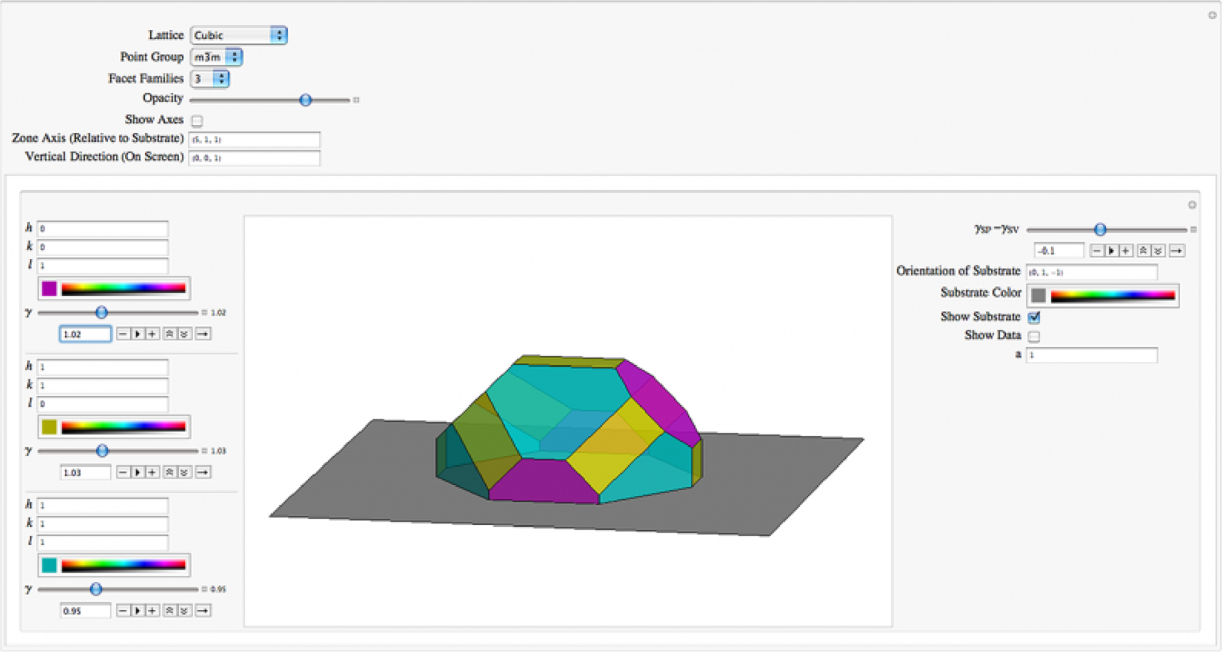
Zucker studied both isotropic materials, which exhibit the same properties in all directions, and anisotropic materials, which show different properties in different directions. Isotropic materials, which are usually glassy, are good materials to develop models, but are rarely used as engineering materials, she says. Common engineering materials such as metal, ceramic, or single-crystal thin films are usually anisotropic materials.

Zucker carried out stability analyses to understand the onset of the sometimes beautiful morphologies seen in experiments. "The big takeaway is: One, we can write down formulation of this problem; two, we can implement a numerical method to construct the solutions; three, we can make a direct comparison to experiments; and that strikes me as what a thesis should be—the complete thing—formulation, solution, comparison, conclusion," Carter says. Zucker defended her thesis, "Capillary-Driven Shape Evolution in Solid-State Micro- and Nano-Scale Systems," on April 13.

She says her breakthrough came in creating a geometric model of edge retraction. "I knew I wanted to do these stability analyses; I knew I wanted to understand the fingering instability and the corner instability, the Rayleigh instability, but I didn't know where to begin," Zucker says. When she recognized that she could generalize this geometry and use Wolfram Mathematica to handle the algebra, she was able to apply it not only to edge retraction, but also to extend it to the fingering instability and corner instability. "I'd say that was a useful insight," she adds, but notes that it came not while working, but while running during a Christmas break. "Then all of sudden it hit me," she explains.

Phase field approach

For her doctoral research, Zucker examined film break-up during dewetting based on capillary action for edge retraction and pinch-off, the fingering instability, the Rayleigh instability, and the corner instability. This capillary action occurs most dramatically at a region known as the triple line, where three phases meet, commonly the substrate, film being deposited, and atmosphere. The exception, which cannot be explained by capillary action alone, is hole formation, Zucker notes. With her phase field approach, Zucker says, "I don't have to make simplifying assumptions. I don't have to simplify the geometry, for example. It just treats the full problem. There have been I would say two previous simulation attempts, but ours is the first code that I would say is actually useful, because it's fast enough that it will run in a reasonable amount of time on a reasonable number of computer cores. So we can actually do science with it." Simulations that used to take a month on previous code can be reduced to about three days running her simulation, she explains.



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Vertical Direction (On Screen) {0, 0, 1}

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A Winterbottom shape is displayed in the WulffMaker software tool developed at MIT by materials science and engineering alumna Rachel Zucker PhD '15 and Professor W. Craig Carter. Credit: Rachel Zucker

"Rachel made very significant advances in our understanding of the fingering instability that develops along the edges of films as they undergo solid-state dewetting," Thompson says. "While people had speculated that the rims that form on these edges undergo a Rayleigh-like instability that leads to fingering, Rachel showed that a new instability she discovered, due to 'divergent retraction,' plays a dominant role. This allows better predictions of the length scales of structures that result from the dewetting process, and for how films might be modified to obtain structures with desired characteristics.

"Rachel also provided new and better explanations of the mechanisms that cause sharp corners in the edge of a retracting hole to run out ahead of other parts of the edge. Speculations in the literature focused on the role of long-range diffusion of material away from the corner, but Rachel showed that all the mass that is redistributed at the retracting tip of a corner is consumed locally in extending the length of the adjacent edges. This provided a fundamentally new way of thinking about evolution of the shapes of holes, and how that evolution might be controlled," Thompson explains.

Modeling instabilities

Zucker spent an extensive amount of time working on her doctorate in Germany, where she was hosted by Professor Christina Scheu, of the Max Planck Institute for Iron Research in Düsseldorf and the Ludwig-Maximilians University in Munich. Zucker spent about nine months in Munich followed by nine months in Düsseldorf. Zucker credits much of the code development work for phase field simulations of dewetting to Professor Axel Voigt at the Technical University of Dresden in Germany, and postdoc Rainer Backofen. She also credits Professor Francesco Montalenti at the University of Milan-Bicocca in Italy, postdoc Roberto Bergamaschini, and PhD student Marco Salvalaglio with helping her learn how to use the code. While in Germany, she has also been working on microstructural optimization for energy materials.

"I wanted to work on these surface-energy-driven problems because they are so fundamental to materials science," Zucker explains. Carter connected Zucker with Thompson, whose group had been doing experiments focused on developing a better understanding of solid-state dewetting, both in order to prevent or suppress it in some cases, and also to develop new ways to control it to make specific patterns in other cases.

Zucker tackled various irregularities in thin-film formation, including Rayleigh instabilities, edge retraction, fingering, and corner instabilities. In the Rayleigh instability, for example, a cylinder of materials breaks up into isolated particles. The Rayleigh instability is a classical result that is now 137 years old. "Otherwise the other instabilities involved in dewetting of films haven't really been studied," Zucker says of her work. "I've done a lot of linear instability analyses to understand what wavelengths are going to be showing up in these instabilities, what length scales are we talking about and how that is connected to the film thickness."

Solid-state dewetting

The model Zucker developed for two-dimensional edge retraction for highly anisotropic, fully-faceted thin films was published in 2013 in the journal Comptes Rendus Physique ("Proceedings of Physics"). Zucker's model was largely in accordance with experiments carried out by Alan Gye Hyun Kim in Thompson's group on edge retraction of 130-nm-thick, single-crystal nickel films on magnesium oxide (MgO). Zucker was also a co-author of Kim's 2013 experimental paper in the Journal of Applied Physics. Both experiments and model showed rims form as the edges retract.

In a fully-faceted film, the crystal material has facets similar to a jewel-cut diamond. Zucker, who studied four different orientations of the crystal structure, found that the diffusivity on the facet at the top of the rim has the largest influence on retraction, followed by influences from the other facets of the material. Both experiments and the model showed retraction distances varying by up to two times, depending on the edge orientation. The model was in closest agreement with experimental results for an (001) film with an edge retracting in the (100) direction—varying by just 10 percent. However, Zucker's paper noted, the model over-estimated retraction distance for (001) film retracting in the (110) direction and underestimated distance for an (011) film retracting in the (110) direction. Zucker suggests the discrepancy between model and experiment could be accounted for by error in reported values of diffusivities for nickel facets and uncertainty about interfacial energy between the nickel film and magnesium oxide substrate. "The major factors which determine the retraction rate of a thin film, according to this model, are: the film thickness, the atomic diffusivity on the top facet and the angled facet, the equivalent contact angle of the film on the substrate, and the absolute value of the surface energy. The edge retraction distance scales with the film thickness h as h1/2," Zucker reported in "A model for solid-state dewetting of a fully-faceted thin film."

WulffMaker software

In a 2012 paper, Zucker presented a new method for finding the equilibrium shapes of faceted particles attached to a deformable surface. With Carter and three others, Zucker presented a suite of software tools to calculate these equilibrium shapes as well as for isolated particles and for particles attached to rigid interfaces. Their open-source code, WulffMaker, is available as a Wolfram computable document format file or a Mathematica notebook. It is useful for modeling Wulff shapes for engineering materials such as alumina, as well as more complicated Winterbottom and double Winterbottom shapes. While the Wulff method models the simplest case of a uniform shape attaching to a level surface, the software also incorporates a new algorithm for calculating interfaces with more complicated angles of attachment and attachment to rigid substrates. The tool could be useful for analyzing electronic and optical devices produced from materials deposited on a substrate. The software combines interface energy data with geometric shape data and so can be used in reverse to calculate interface energy for abutting materials from experimentally obtained geometric data.

"This tool introduces a new computational method for finding shapes of minimal interface energy. It also helps to build intuition about the macroscopic properties of interfaces and their interactions, and aids in the quantitative measurement of interface energy densities, given a geometry. Properties such as the equivalent wetting angle, particle contact area, total energies, and distortions to the interface surrounding the particle are displayed by the software to enable further insight and analysis," Zucker wrote in her thesis.

Teaching modules

Besides her work in creating computerized models for thin film deformation, Zucker has been working with Carter on a new format to teach materials science that Carter calls proctored scaffolding. Unlike online instruction that allows students to passively consume information by watching videos or reading text, their approach is interactive and requires critical thinking. "The student can't just skate by without doing that critical thinking," Zucker explains.

Zucker used the method, which integrates the Wolfram Language, to teach 3.016 (Mathematics for Materials Science and Engineers) two years ago while Carter was on sabbatical. She has traveled internationally with Carter to demonstrate these materials science master classes. They also made a user interface tool for content developers, to make it easier for other instructors to create Mathematica notebooks.

A native of North Carolina, Zucker completed her bachelor's at MIT in 2009, receiving an outstanding senior award from the Department of Materials Science and Engineering. Zucker starts a three-year postdoctoral fellowship in July at the Miller Institute at the University of California at Berkeley. She will be affiliated with both the mathematics and materials science departments. "I think ever since I was born I was going to be a professor," Zucker says.

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