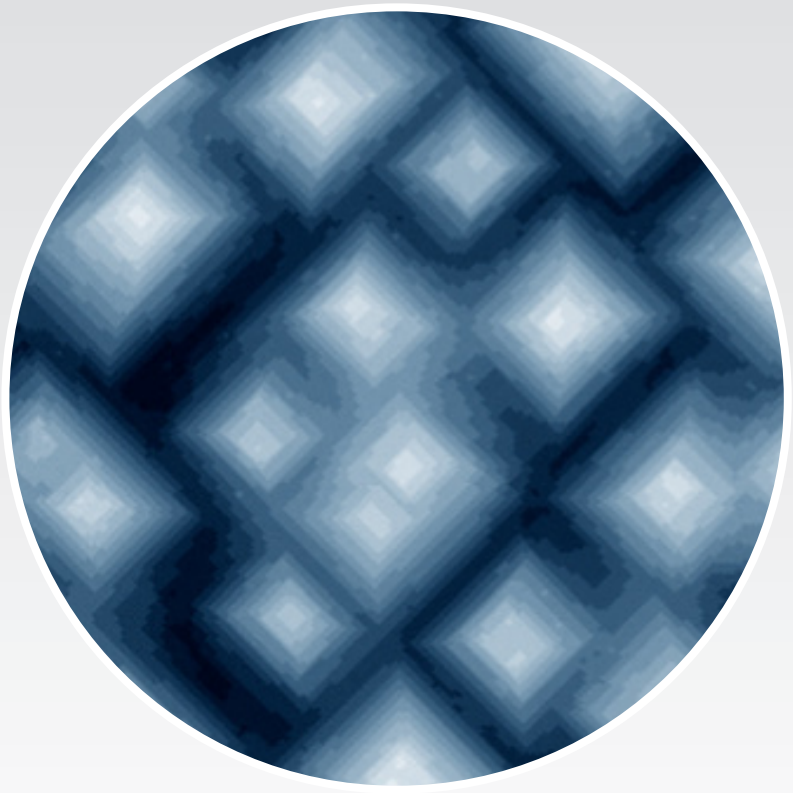
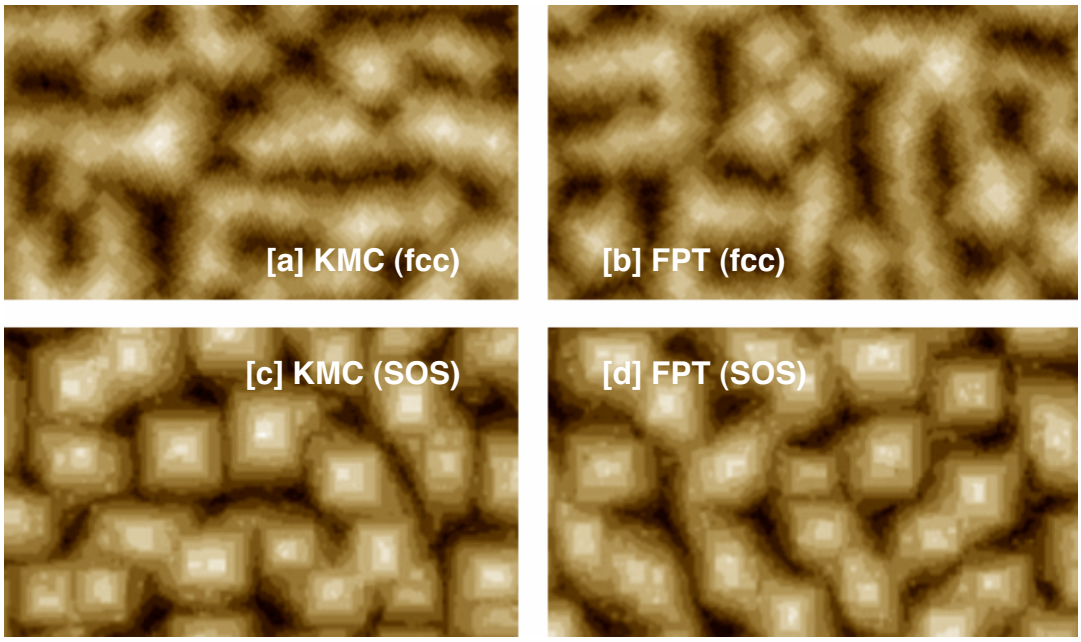


Jacques Amar accessed Ohio Supercomputer Center systems to investigate a new mathematical approach that accelerates some complex computer calculations used to simulate the formation of micro-thin materials.

Advanced Materials

Ohio's world-class polymer and advanced materials industries have long driven the state's economy, employing more than 81,000 people, according to the Ohio Department of Development. Materials researchers here are conducting ground-breaking studies of polymers and various other advanced materials, such as composites, nanomaterials, liquid crystals and bio-based materials. For example, an engineer is collaborating with industry experimentalists to study value-added composite materials. A chemist is investigating molecular systems that play a key role in drug delivery and the release of fragrances from household goods. And, a scientist is investigating how polymers age, experiencing mechanical deformation and cracks. The creation and testing of computational models through the Ohio Supercomputer Center continues to set the bar high for materials science research in Ohio, as described on the next few pages.



left: The University of Toledo's Jacques Amar leveraged Ohio Supercomputer Center systems to test an accelerated approach to simulating thin film growth. Using two different models (labeled fcc and SOS), Amar compared the regular Kinetic Monte Carlo method (figures a and c) with a first-passage-time approach coupled with the KMC method (figures b and d).

Amar's approach **speeds computer simulations** of thin film growth

Thin films are used in industry to create a variety of products, such as semiconductors, optical coatings, pharmaceuticals and solar cells. A new mathematical approach developed by Jacques Amar, Ph.D., professor of physics at the University of Toledo, accelerates some complex computer calculations used to simulate the formation of micro-thin materials.

Employing Ohio Supercomputer Center systems, Amar implemented a "first-passage time approach" to speed up simulations of materials being created just a few atoms thick. He used Kinetic Monte Carlo (KMC) methods to simulate the molecular beam epitaxy (MBE) process, where metals are heated until they transition into a gaseous state and then reform as thin films by condensing on a wafer in single-crystal thick layers.

"One of the main advantages of MBE is the ability to control the deposition of thin films and atomic structures on the atomic scale in order to create nanostructures," explained Amar. *"The KMC method has been successfully used to carry out simulations of a wide variety of dynamical processes over experimentally relevant time and length scales. However, in some cases, much of the simulation time can be 'wasted' on rapid, repetitive, low-barrier events."*

While a variety of approaches to dealing with the inefficiencies have been suggested, Amar settled on using a first-passage-time (FPT) approach to improve KMC processing speeds. FPT, sometimes called first-hitting-time, is a statistical model that sets a threshold for a process and then estimates certain factors, such as the probability that the process reaches that threshold within a certain amount time or the mean time until which the threshold is reached.

"In this approach, one avoids simulating the numerous diffusive hops of atoms, and instead replaces them with the first-passage time to make a transition from one location to another," Amar said.

In particular, Amar and his colleagues targeted two atomic-level events for testing the FPT approach: edge-diffusion and corner rounding. Edge-diffusion involves the "hopping" movement of surface atoms – called adatoms – along the edges of islands, which are formed as the material is growing. Corner rounding involves the hopping of adatoms around island corners, leading to smoother islands.

Amar compared the KMC-FPT and regular KMC simulation approaches using several different models of thin film growth: Cu/Cu(100), fcc(100) and solid-on-solid (SOS). Additionally, he employed two different methods for calculating the FPT for these events: the mean FPT (MFPT), as well as the full FPT distribution.

Amar's FPT-KMC approach accelerated simulations by a factor of approximately 63 to 100 times faster than the corresponding KMC simulations for the fcc(100) model. The SOS model was improved by a factor of 36 to 76 times. For the Cu/Cu(100) tests, speed-up factors of 31 to 42 and 22 to 28 times were achieved, respectively, for simulations using the full FPT distribution and MFPT calculations. ■

Project lead: Jacques Amar, University of Toledo
Research title: First-passage-time approach to kinetic Monte Carlo simulations of metal (100) growth
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Web site: astro1.panet.utoledo.edu/~jamar/ph/jga.html