Transitions between states of matter: It's more complicated, scientists find

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The seemingly simple process of phase changes—those transitions between states of matter—is more complex than previously known, according to research based at Princeton University, Peking University and New York University.

Their study, which appears in the journal *Science*, reveals the need to rethink one of science's building blocks and, with it, how some of the basic principles underlying the behavior of matter are taught in our classrooms. The researchers examined the way that a phase change, specifically the melting of a solid, occurs at a microscopic level and discovered that the transition is far more involved than earlier models had accounted for.

"This research shows that phase changes can follow multiple pathways, which is counter to what we've previously known," explains Mark Tuckerman, a professor of chemistry and applied mathematics at New York University and one of the study's co-authors. "This means the simple theories about phase transitions that we teach in classes are just not right."

According to Tuckerman, scientists will need to change the way they think of and teach on phase changes.

The work stems from a 10-year project at Princeton to develop a mathematical framework and computer algorithms to study complex behavior in systems, explained senior author Weinan E, a professor in

Princeton's Department of Mathematics and Program in Applied and Computational Mathematics. Phase changes proved to be a crucial test case for their algorithm, E said. E and Tuckerman worked with Amit Samanta, a postdoctoral researcher at Princeton now at Lawrence Livermore National Laboratory, and Tang-Qing Yu, a postdoctoral researcher at NYU's Courant Institute of Mathematical Sciences.

"It was a test case for the rather powerful set of tools that we have developed to study hard questions about complex phenomena such as phase transitions," E said. "The melting of a relatively simple atomic solid such as a metal, proved to be enormously rich. With the understanding we have gained from this case, we next aim to probe more complex molecular solids such as ice."

The findings reveal that phase transition can occur via multiple and competing pathways and that the transitions involve at least two steps. The study shows that, along one of these pathways, the first step in the transition process is the formation of point defects—local defects that occur at or around a single lattice site in a crystalline solid. These defects turn out to be highly mobile. In a second step, the point defects randomly migrate and occasionally meet to form large, disordered defect clusters.

This mechanism predicts that "the disordered cluster grows from the outside in rather than from the inside out, as current explanations suggest," Tuckerman notes. "Over time, these clusters grow and eventually become sufficiently large to cause the transition from solid to liquid."

Along an alternative pathway, the defects grow into thin lines of disorder (called "dislocations") that reach across the system. Small liquid regions then pool along these dislocations, these regions expand from the dislocation region, engulfing more and more of the solid, until the entire system becomes liquid.

This study modeled this process by tracing copper and aluminum metals from an atomic solid to an atomic liquid state. The researchers used advanced computer models and algorithms to reexamine the process of phase changes on a microscopic level.

"Phase transitions have always been something of a mystery because they represent such a dramatic change in the state of matter," Tuckerman observes. "When a system changes from solid to liquid, the properties change substantially."

He adds that this research shows the surprising incompleteness of previous models of nucleation and phase changes—and helps to fill in existing gaps in basic scientific understanding.

More information: "Microscopic mechanisms of equilibrium melting of a solid" *Science*, www.sciencemag.org/lookup/doi/ … 1126/science.1253810

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