Research explains the emergence of patterns in nature

By Alice Rhein

From snowflakes to rippled beaches to cloud formations, patterns in nature are complex structures that control key material properties and biological functions. In the double helix of DNA, the pattern literally makes us who we are.

Understanding the formation of such complex morphologies and unlocking their potential depends on making efficient predictions.

Theoretical physicist Ken Elder, Ph.D., an OU professor since 1995, has devoted his research to developing methods to model patterns or non-equilibrium phenomena in materials physics. Much of his work focuses on understanding the complex spatial structures that appear following a phase change, such as when a liquid turns into a solid or when a metal transitions from a non-magnetic to a magnetic state.

The task is complicated by interactions between systems. Yet it was at one of those moments when Dr. Elder was looking for a shorter way to model a huge, difficult equation that he hit on the “phase field crystal” method of computational modeling to study pattern formation in material science.

“I was interested in adding elasticity to a particular model,” Dr. Elder says. He found that when modeling superconductivity, the patterns produced naturally incorporated elasticity. In continuing to explore this, he developed an offshoot of phase field model to include the influence of elasticity and plasticity in the formation of patterns.

Advantageously, it naturally incorporates the physics contained at the microscopic level on time scales many orders of magnitude larger than traditional atomic methods — it can be millions or billions times faster. The phase field crystal model can simultaneously model many phenomena in one situation: solidification, phase segregation, grain growth, elastic and plastic deformations, for example.

When Dr. Elder says he “stumbled into” this almost ten years ago, it was considered obscure. Now, phase field crystal model is mainstream physics. PFC models are applied to study a wide range of crystal growth phenomena such as structural defects, yield stress, fractal grow surface ordering epitaxial growth, and transition from hard, glassy material to a soft, rubbery material (glass transition).

Sessions at large conferences and whole workshops are devoted to the topic. Several of Dr. Elder’s publications, including the 2004 paper “Modeling Elastic and Plastic Deformations in Non-Equilibrium Processing Using Phase Field Crystals,” with Martin Grant of Montreal’s M University, have been cited in hundreds of other publications.

In addition, Dr. Elder and McGill professor Nikolas Provatas, Ph.D., authored “Phase-Field Methods in Materials Science and Engineering” (Wiley 2010), considered the comprehensive textbook for phase-field methodology.

“When you first discover something, it seems surprising,” he says. “The next day, you think it was obvious and don’t understand why it took so long to figure it out.”

The development of the phase field crystal method was an important step forward. However, Dr. Elder’s more recent research employs an offshoot of the method developed by researchers at the University of Illinois at Urbana-Champaign.

In this work, he studies the ordering of ultra-thin films, either one or several monolayers, on metallic surfaces. The key to understanding this and many other pattern-forming systems is to understand the boundaries, surfaces or defects that define the patterns. For example, when crystals hit each other, they form a grain boundary made up of defects or dislocations that can increase material strength.

“If you take a chunk of metal and slice it, you’ll find a very small microstructure,” he says. “The microstructure is what determines how strong the material is, and its electrical and optical properties. When you look at a pattern, it is really the boundaries between regions or defects define it. The motion and evolution of these defects is what controls pattern formation and most of my work is dedicated to understanding fundamental mechanisms behind the motion and evolution of defects.”
boundaries can often be controlled by altering the materials and conditions under which they grow, such as temperature and pressure.

From a more fundamental point of view, these films form interesting superstructures that appear as honeycomb, triangular, zigzag and stri patterns. The defects are what control the nature of the patterns. Because it is difficult to mathematically describe the motion of the defects in a simple way, Dr. Elder often uses computational methods to solve the relevant equations.

When the process of how these structures are formed is better understood, then the material properties such as strength and electrical resistance can be controlled. Developing methods to allow for the study of these processes on longer time scales would be a huge contribution to the fields of science and engineering.

In addition to his scientific research, Dr. Elder significantly contributes to teaching the next generation of physicists at OU. Several are now doctoral and post-doctoral students at top universities. His daughter, Kate, is studying mathematics and physics at McGill.

With a sabbatical in 2015-16, Dr. Elder will travel to Finland, Germany, Brazil and Budapest to visit collaborators and will give talks at several conferences in the U.S. He also plans to return to a project on state selection in non-equilibrium systems that he started 20 years ago.

“There are theories going back to the 1800s on how to determine what the lowest-energy equilibrium states are,” Dr. Elder says. “When one drives a system by continuously adding energy, it never gets to an equilibrium state. Often quite interesting steady-state patterns emerge which there are currently no exact formal methods for predicting.

“I plan to spend most of my sabbatical working on developing rigorous methods for determining state selection in such driven systems.”

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Read more about research taking place at Oakland University in the fall 2015 Research Magazine.