Engineers Provide Insight Into the Dynamics of Molecular Self-Assembly

July 5 2007

By studying how a layer of molecules grows into an ordered layer from the edge of a rectangular silicon wafer, engineers at North Carolina State University, working with researchers from the National Institute of Standards and Technology (NIST), have established the time evolution of self-propagating self-assembly fronts. The team is the first to confirm the phenomenon in a real physical system.

The NC State researchers, Dr. Jan Genzer, professor of chemical and biomolecular engineering, and Dr. Kirill Efimenko, research assistant professor of chemical and biomolecular engineering, and NIST researchers, Dr. Jack Douglas, Dr. Daniel Fischer and Dr. Frederick Phelan, examined the spontaneous assembly of organosilane molecules into a monolayer film formed on an oxidized silicon surface.

They found that if a supply of the carbon-silicon-based molecule is placed along one edge of a treated silicon wafer, under controlled conditions, the organosilane molecules spontaneously organize themselves into a well-ordered layer, creating a carpet-like layer on the silicon that advances from the edge of the wafer at a constant velocity where the ordering initiates, ultimately covering the surface at long times. By following this process using a high resolution synchrotron X-ray technique and computer simulations, the NC State/NIST team established that the propagating wavefronts did not follow the constant width predicted by the classical mean-field theory that is widely believed to govern reaction-diffusion and self-assembly processes. (A wavefront is the leading edge of a wave or line of points that have the same phase

or stage in a process.) What actually occurred is described as a “power-law broadening in time” when an autocatalyst is present.

A paper describing the research appears in the June 19, 2007, issue of the *Proceedings of the National Academy of Sciences*; the paper is also mentioned as a highlight on the journal cover.

“We found that simple diffusion is not going to explain our data; it will not govern the molecular processes involved in our experiment,” Genzer said. “So we began looking for the connection between diffusion and wavefront propagation, something the NIST team of theorists has been looking for some time.”

Propagating fronts are fueled by catalysts, which typically involve small chemical compounds that participate in the reaction and recover themselves after it. In the present case, the process may be governed by a very different type of autocatalyst, namely the system’s confinement. One of the benefits of the present set up is that the “broadening” of the front can be adjusted (and thus studied systematically) by varying the characteristics of the “building blocks,” the organosilane molecules, and the conditions under which the gradients are formed.

In addition to providing validation for simulation and theoretical predictions for precisely how these fronts should broaden, the researchers say that these results should be important to understanding self-organization in diverse other material processing and biological systems where similar fronts arise. Examples include, but are not limited to, material sciences, human health, social sciences, anthropology, and many others.

“Processes in nature follow just a few principles that apply to nanoscale, microscale and macroscale,” said Genzer. “Since pattern formation processes exist everywhere in the natural world, we believe the model

can be used to verify dynamics in other (seemingly rather unrelated) phenomena such as the spread of disease, tumor growth, wound healing, the spread of epidemics, and the spread of languages across Europe."

Source: North Carolina State University