Twisting chemical reactions to form knots

First came spots, stripes, and swirls—patterns in the concentrations of chemical substances arising from the reaction of these chemicals and the subsequent diffusion of the products.

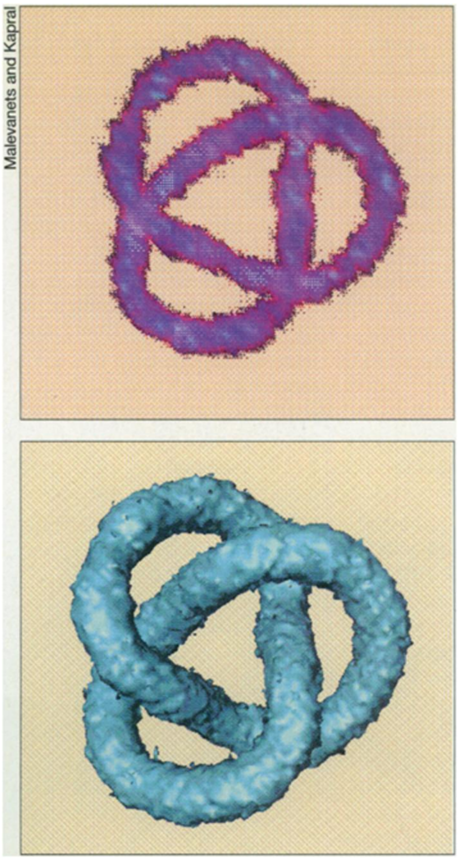
Now, chemists have shown in principle that the same type of chemical processes can generate three-dimensional patterns in the shape of loops, simple knots, and linked pairs of rings.

"We were really amazed to see them in our computer simulations," says Raymond Kapral of the University of Toronto in Ontario. "They really are stable objects." Kapral and Anatoly Malevanets report their results in the July 22 PHYSICAL REVIEW LETTERS.

A mixture of oil and water readily separates into two phases, one consisting of oil and the other of water. The same kind of separation can also occur during reactions between two chemical substances that diffuse at different rates. For example, a chemical medium can split into a phase in which the concentration of one substance is high and that of the other is low and another phase in which the situation is reversed, with a sharp boundary between the two phases.

To simulate such a reaction-diffusion chemical system in three dimensions, Kapral and Malevanets tracked the behavior of 250 billion particles representing two chemical substances. Moving about randomly, these particles collide, react, and diffuse according to a specific set of rules.

The researchers found that they could set up initial conditions to create a loop, linked rings, and trefoil and figure-8 knots.



Malevanets and Kapral

Computer simulations show that chemicals can react to produce stable patterns in which one of the reactants has a high concentration in a region shaped like a trefoil knot, pictured here in a thick layer of gel as seen from above (top) and in three dimensions (bottom).

Despite the continuing random movements of the particles involved, these patterns in the concentrations of the chemicals would remain in place, with well-defined edges.

"You can, in fact, design knots and links in these systems," Kapral says.

Small changes in the initial conditions, however, generate instabilities. For example, a concentration pattern shaped like a trefoil knot can develop fingers and knobs to become highly wrinkled.

No one has yet produced such patterns in the laboratory. Previous experiments have typically involved thin layers of gel, through which various chemicals can diffuse and react to create two-dimensional patterns (SN: 5/9/92, p. 311).

"The main complication is setting up the right initial conditions in a three-dimensional geometry," Kapral remarks. "That would take some ingenuity."

The study of the formation of knots and other structures in reaction-diffusion chemical systems is part of a larger effort aimed at understanding on a microscopic level the processes that lead to pattern formation. For example, Kapral notes, "we're looking at how fluctuations influence the patterns, either destroying or changing them." *— I. Peterson*

Nylon may take X rays into digital age

A century ago, the novelty of X rays captured the public's fancy. X-ray machines were everywhere: Anyone craving a "bone portrait" needed to go no farther than the local department store. So widespread were X rays that entrepreneurs even sold lead-lined underwear designed to protect the modest from the prying gaze of the X-ray camera.

Those early entrepreneurs would have loved a new material described in the Aug. 2 SCIENCE: X-ray-absorbing nylon. Researchers developed this material for a more high-tech purpose, however. The specially prepared nylon was created to be a key part of a system designed to make radiography—the most widely used diagnostic technique—digital. By eliminating the need for film, scientists could manipulate X-ray images by computer, send them by modem, and store them on disk—advantages shared by newer methods like magnetic resonance imaging (MRI).

The material, developed by Ying Wang and Norman Herron of the DuPont Experimental Station in Wilmington, Del., consists of tiny particles of X-ray-absorbing bismuth triiodide mixed into flexible nylon. Like many composites, this one combines the best of both compounds. Pure bismuth triiodide absorbs X rays well but is very difficult to spread into a thin film, Wang says. Nor can it handle the large electric field that would be necessary in a digital X-ray system. Nylon's properties make up for those deficiencies.

The new composite is actually a nanocomposite, which means that most of the particles are less than a billionth of a meter long. If the particles are too big—even millionths of a meter—the material loses its desirable properties and behaves more like pure bismuth triiodide.

The optimum concentration is about 50 percent bismuth triiodide by weight. "There's a natural limit, since we're basically using nylon as a solvent," Wang says. "To go beyond that limit, you have to do some more work to chemically attach the particles to the nylon."

Increasing the concentration to about 65 percent would make the X-ray absorption close to that of selenium, the best candidate material so far. Selenium, however, is toxic and can be difficult to prepare into thin films.

A digital X-ray machine that uses a nanocomposite would work something like a photocopier, Wang says. In a photocopier, a static charge is placed across a plate. The plate discharges when it's exposed to light, leaving a fine pattern of static wherever lettering or other images block the light. Powdered ink, or toner, then clings to the charges and is fused onto a piece of paper.

In a digital X-ray machine, the nanocomposite would replace the X-ray film and act like the charged plate in the photocopier. X rays passing through soft body tissue would cause the material to discharge accordingly. Some kind of electrical detection system—perhaps an array of transistors—would then transmit the remaining charge pattern to a computer.

An advantage of this system, says Clinton M. Logan of Lawrence Livermore (Calif.) National Laboratory, who is developing a different digital X-ray technique, is that the new imaging device would plug directly into existing hospital X-ray cameras. *— C. Wu*