Ring-shaped polymers solidify into glass, offering sustainable material potential

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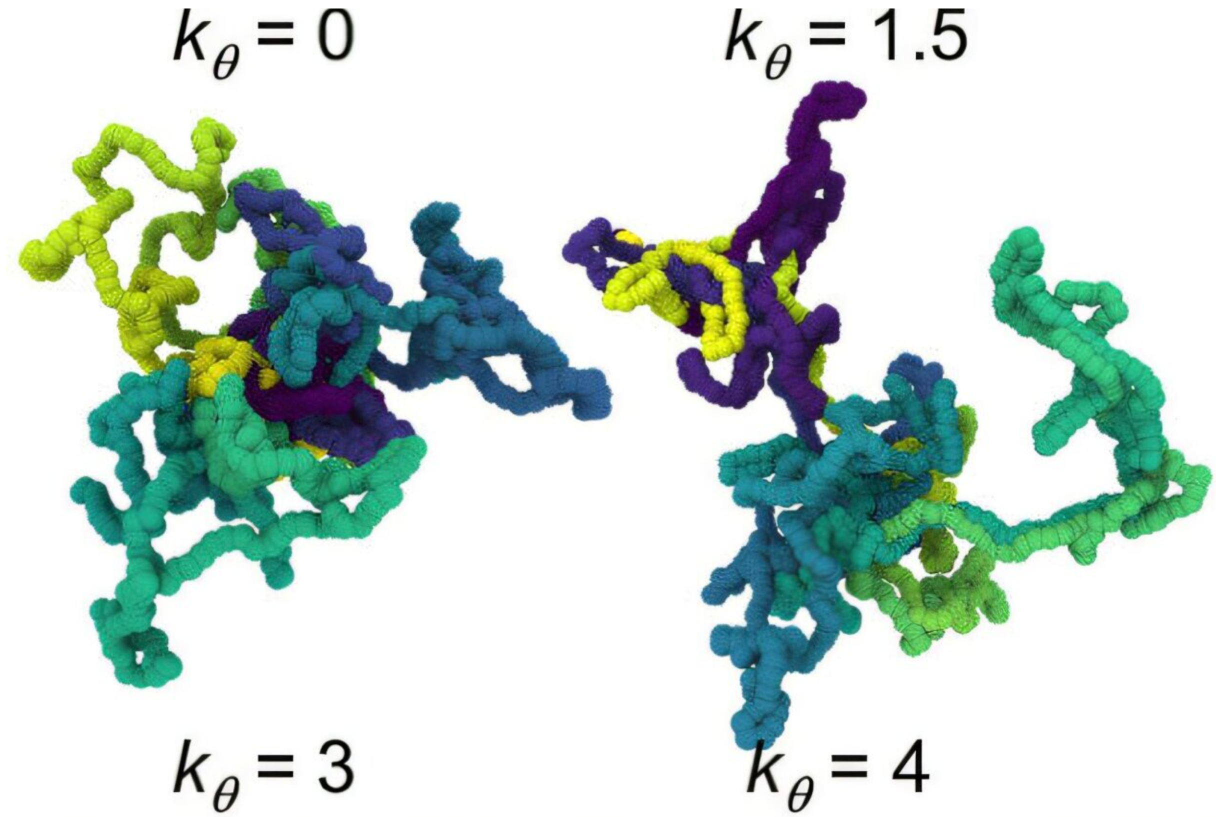

Molecular dynamics (MD) simulation snapshots of a single ring polymer conformation taken from a dense melt of N = 1,600 for the four indicated values of bending energy. Different colors indicate different parts of the same ring. Credit: *Proceedings of the National Academy of Sciences* (2024). DOI: 10.1073/pnas.2403964121

When a spider is spinning its web, its silk starts out as liquid and quickly turns into a solid that is, pound for pound, sturdier than steel. They manage to create these impressive materials at room temperature with biodegradable and environmentally friendly polymers. Materials scientists at Carnegie Mellon are studying these processes to better understand the ways biological systems manipulate polymers, and how we can borrow their techniques to improve industrial plastic processing.

One unique quality of polymers is that their molecules can have different shapes or "architectures," and these shapes can have a big impact on their material properties and recyclability. Polymer chains can form molecular strings, mesh-like networks, or even closed rings.

A new discovery about how ring-shaped polymers behave offers the potential to enable new ways for polymer scientists to design more sustainable materials. A team of researchers from Carnegie Mellon, Sandia National Laboratories, and the University of Illinois at Urbana-Champaign (UIUC) has conducted the largest simulation to date on this type of polymer and confirmed theoretical predictions, finding that the ring polymers spontaneously solidify into glass when their chains become sufficiently long.

The study, published in *Proceedings of the National Academy of Sciences*, shows how changing the shape of polymers from open strings to closed rings completely alters how the molecules pack and diffuse inside the material. The researchers found that as ring polymers become longer, separate chains become increasingly cramped together until the chains cannot move, causing the material to solidify. The simple act of changing the shape of the molecules from open strings to closed rings also changed the plastics phase from a liquid to a solid.

"We usually have to cool a sample's temperature to make molten plastic solidify, but we have found that simply changing the shape of the molecules into rings causes them to slow and vitrify into glass," said Thomas O'Connor, assistant professor of materials science and engineering at Carnegie Mellon.

O'Connor and materials science and engineering doctoral student Songyue Liu ran large-scale molecular dynamics simulations for over a year on Department of Energy supercomputers to test the theoretical predictions developed by their colleagues at UIUC. The simulations built upon previous research by the team in which they experimentally synthesized a recyclable polymer material made of pure ring polymers that unexpectedly vitrified in the lab. These new theoretical results explain this surprising behavior and will help guide the design of recyclable cyclic polymers.

The research also has implications for the behavior of biopolymer systems like folded proteins and the chromosomes that bundle and store our DNA. These biological systems adopt loopy structures similar to the ring polymers that the team explored.

"Understanding how loopy polymer structures crowd around each other and fold up is insightful for materials science, but it is also important for understanding why living systems use these structures to enable biological functions," says O'Connor. "There is potential for us to draw parallels between these disciplines to make new discoveries."

More information: Baicheng Mei et al, Unified understanding of the impact of semiflexibility, concentration, and molecular weight on macromolecular-scale ring diffusion, *Proceedings of the National Academy of Sciences* (2024). DOI: 10.1073/pnas.2403964121

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