Researchers test the limits of toughness in nanocomposites

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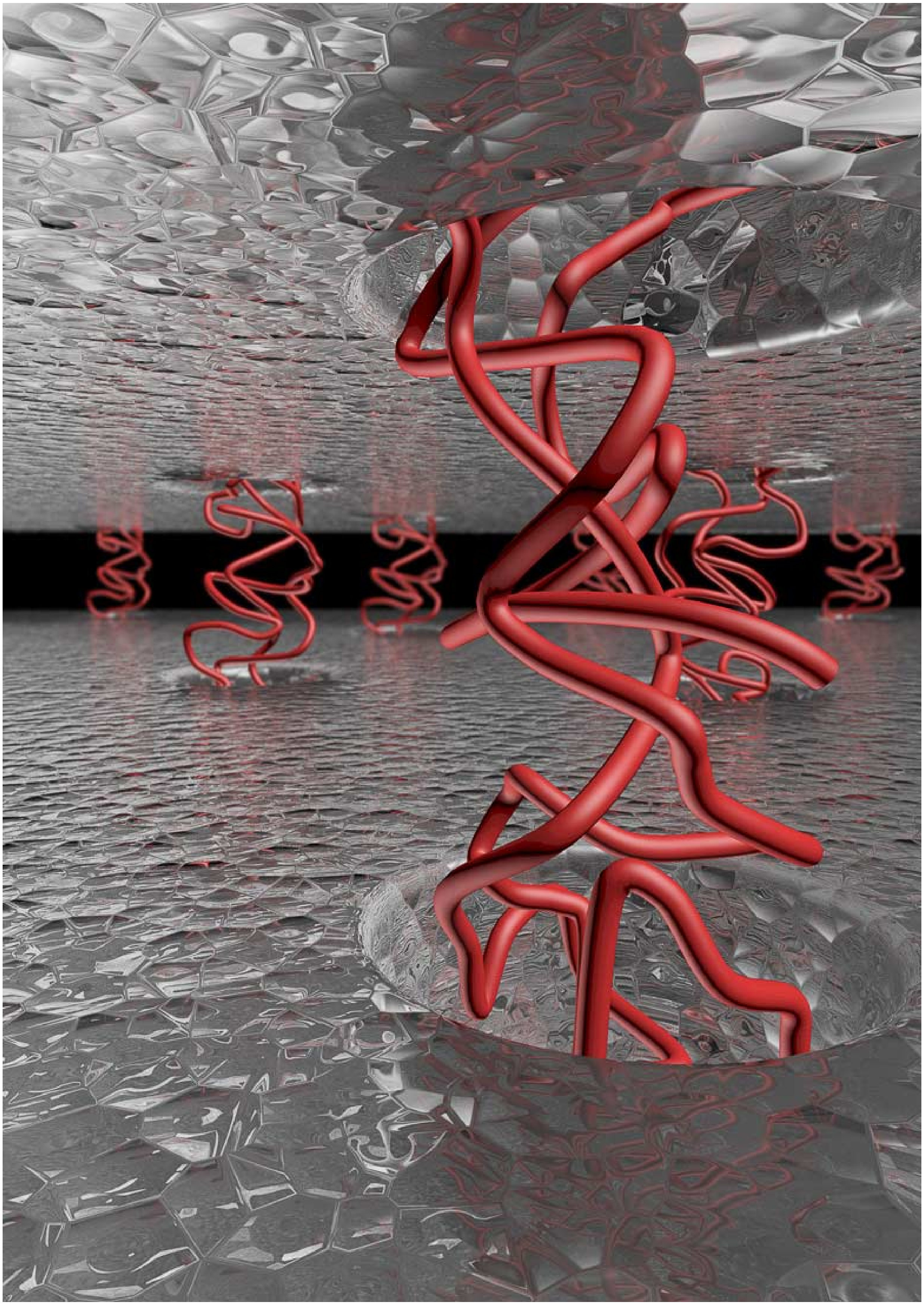

Stanford and IBM researchers inserted chain-like molecules of polystyrene – the same material in a Styrofoam coffee cup – between layers of nanocomposites to make these materials tougher and more flexible.

In the future, the wings of jets could be as light as balsa wood, yet stronger than the toughest metal alloys. That's the promise of nanocomposite materials.

Nanocomposites are a true example of nanotechnology. They are a special class of materials made from components smaller than one-thousandth of the thickness of a human hair. Controlling these nanometer-sized components offers countless possibilities for developing materials with unique properties.

Nanocomposites can be made flexible and strong, or resistant to heat and chemicals. Nanocomposite materials are designed to exhibit physical properties that greatly exceed the capabilities of the sum of their constituent parts.

Researchers at Stanford and IBM have tested the upper boundaries of mechanical toughness in a class of lightweight nanocomposites toughened by individual molecules, and offered a new model for how they get their toughness.

The potential applications for nanocomposites cut across many industries, from computer circuitry to transportation to athletics. They could even revolutionize spaceflight with their ability to withstand tension and extreme temperatures.

The study was published Nov. 16 in the journal *Nature Materials* by an engineering team led by Reinhold Dauskardt, a professor of materials science and engineering at Stanford, and Geraud Dubois, of IBM's Almaden Research Center. The study was sponsored by the Air Force Office of Scientific Research.

Welcome to the matrix

The nanocomposite in this study began with a glass-like molecular skeleton, called a matrix. On its own, the matrix is like a sponge, interlaced with billions of nanometer-sized pores cutting through and among its molecular structure.

"This sponge is not soft or pliable like those in your kitchen, however, but very brittle," Dauskardt said.

The researchers then infused the matrix with long, chain-like molecules of polystyrene – the same material in a Styrofoam coffee cup. The Stanford/IBM team departed from convention in the way it diffused the polymer into the matrix.

"We took these extremely large molecules, many, many times larger than the pores themselves, and confined them in these tiny spaces," Dauskardt said. "It was quite special. Typically, if you heat these molecules too much they break, but we figured out how to heat them just enough so that they diffuse uniformly into the matrix."

Molecular bridges

In the paper, the team describes a previously unknown toughening mechanism that diverges from existing understanding of how composites get their toughness, a quality defined as the ability to resist fracture.

As a composite bends, twists and stretches, the long polymers are drawn out of the confines of the pores, extending as they go.

"The molecules act like a special kind of spring – what engineers would call 'entropic springs' – to hold the composite together," Dauskardt said.

The findings do not upend existing theories so much as expand them. Conventional understanding was that the long polymers become entangled with one another to provide toughness, similar to the way the entangled fibers of a thread provide tensile strength.

In the Stanford/IBM composite, however, the polymer molecules are dispersed and surrounded by the pore walls, preventing and limiting the effect of entanglement. There had to be another explanation for the toughening effect, leading to the team's new theory of confinement-induced toughening.

"In our model, the polymer segments bridge across potential fractures, stuck inside the matrix pores to hold the material together," Dauskardt said. "If a crack were to propagate, the confined chains pull out from the pores and, collectively, elongate by large amounts to dissipate energy that would otherwise break the material."

Taking it to the limit

The amount of toughening depends on the molecular size of the polymer used in the nanocomposite and how confined the molecules are in the pores. Ultimately, however, like all things, there are limits to their toughness.

"We've shown that there is a fundamental limit that these molecules eventually reach before they break, which depends upon the strength of the individual molecules themselves," Dauskardt said.

Knowing such limits, he said, helps scientists and engineers understand exactly how tough a material might possibly be made and why – knowledge that could lead to greater advances.

"Once you understand that, there is the potential to work around these limits by controlling the way the molecules interact with the pores and preventing them from breaking," Dauskardt said. "If we can do that, then there is a real possibility of creating colossal toughening in low-density nanocomposites. That would lead to some very promising new materials."

More information: Scott G. Isaacson et al. Fundamental limits of material toughening in molecularly confined polymers, *Nature Materials* (2015). DOI: 10.1038/nmat4475

Provided by Stanford University

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