Study takes a micro-mechanics approach to understanding how water impacts fiber-wrapped concrete structures

By Alice Waugh
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For decades, engineers have relied on an approach that looks at a material as a homogenous mass when studying the deterioration of materials in bridges, roads and dams. While useful for looking at materials on a large scale, this approach doesn't reveal much about what's happening on a much smaller physical scale.

MIT researchers have used a technique called molecular dynamics simulation to study how materials interact at the molecular level and applied it for the first time to look at how the interface between epoxy and silica –a material combination similar to those found in some civil engineering applications – changes in the presence of moisture. The researchers hope their work will serve to introduce a new analysis paradigm for structural and design engineers to use when predicting the lifespan of building components and large structures such as bridges from the molecular level upwards.

Epoxies are often used to bond concrete with fiber-reinforced polymer, a material that's sometimes wrapped around bridges and columns to increase their strength and durability. Using the classical continuum mechanics model, engineers have learned how epoxy and concrete behave as separate and homogenous materials, "but this is not sufficient to understand the fundamentals of deterioration" where the atoms in epoxy molecules interact with silica and other atoms in concrete — especially when that epoxy-concrete interface is exposed to water, said Professor of Civil and Environmental Engineering Oral Buyukozturk. He and Professor Markus J. Buehler co-authored a paper published in an April issue of the International Journal of Solids and Structures that described their use of molecular dynamics simulation to study an epoxy-silica interface from a fundamental perspective that unifies chemistry and mechanics.

Previous research has shown that the presence of moisture increases the likelihood of delamination between concrete and epoxy in situations where epoxy is used to attach fiber-reinforced polymer to concrete. Researchers had also found that the presence of water changes the way in which the interface starts to fail – moisture makes it more likely to fail because of separation of the layers of material at the interface rather than from cracking in one of the materials itself.

"When water seeps in, it changes the dynamics of the system on a molecular level, though exactly how that happens is unclear," Buyukozturk said.

The new MIT study was able to quantify the decrease of adhesive energy in the interface by examining the changes in the physical forces of attraction and repulsion between molecules in the two materials – changes that can lead to failure of the concrete-epoxy interface. When peel and shear forces were measured, the simulation showed that in a "wet" scenario, adhesive energy decreased by approximately 15 percent compared to a "dry" scenario. This reduction at the molecular scale may translate into greater reductions in large-scale structures due to interaction of local effects that significantly reduce their integrity.

"The molecular modeling result validates our hypothesis that the adhesive strength of the interface is weakened due to interaction between epoxy and water, and provides a detailed chemistry-based view on the mechanical properties of the interface," the authors wrote.

Molecular dynamics simulation was first developed in the late 1950s to study the dynamics of a system consisting of several hundred particles. The technique has been more widely applied as

computational power has increased and is now used in fields including molecular biology and protein modeling, and increasingly as a powerful tool in computational mechanics.

The continuum approach gives information about materials on a scale of millimeters to meters, while the atomistic approach used in molecular simulation is useful for studying distances of 0.1 to 100 nanometers in materials. A “hand-shaking region” where information can be exchanged between the two regions may be somewhere from 1 to 100 micrometers. The next challenge is further study of that hand-shaking region to bridge the emerging understanding of materials at the nano level with existing macro-level knowledge to improve the accuracy of predictions about the deterioration and life cycles of large civil structures.

“By advancing the understanding of civil structures from the realm of structures and materials into the domains of chemistry, physics and mathematics, molecular simulation may do for engineering analysis what the introduction of the now-standard mathematical technique of finite method analysis did for continuum mechanics four decades ago,” Buyukozturk said.

Co-authors with Buyukozturk and Buehler were graduate student Denvid Lau and recent Ph.D. recipient Chakrapan Tuakta in the CEE Infrastructure Science and Technology Group. The group is supervised by Buyukozturk, who recently received a lifetime achievement award from the Swiss Federal Research Laboratory for Materials Science and Technology for his “most valuable and sustained contributions” to materials science and engineering in the domain of civil engineering.

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