

Research identifies nanoscale effect of water and mineral content on bone

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University of Arkansas researchers Marco Fielder and Arun Nair have conducted the first study of the combined nanoscale effects of water and mineral content on the deformation mechanisms and thermal properties of collagen, the essence of bone material.

The researchers also compared the results to the same properties of non-mineralized [collagen](#) reinforced with carbon nanotubes, which have shown promise as a reinforcing material for bio-composites. This research aids in the development of synthetic materials to mimic bone.

Using [molecular dynamics](#)—in this case a computer simulation of the physical movements of atoms and molecules—Nair and Fielder examined the mechanics and thermal properties of collagen-based bio-composites containing different weight percentages of minerals, water and carbon nanotubes when subjected to external loads.

They found that variations of water and [mineral content](#) had a strong impact on the mechanical behavior and properties of the bio-composites, the structure of which mimics nanoscale bone composition. With increased hydration, the bio-composites became more vulnerable to stress. Additionally, Nair and Fielder found that the presence of carbon nanotubes in non-mineralized collagen reduced the deformation of the gap regions.

The researchers also tested stiffness, which is the standard measurement of a material's resistance to deformation. Both mineralized and non-mineralized collagen bio-composites demonstrated less stability with greater water content. Composites with 40% mineralization were twice as strong as those without minerals, regardless of the amount of water content. Stiffness of composites with carbon nanotubes was comparable to that of the mineralized collagen.

"As the degree of mineralization or [carbon nanotube](#) content of the collagenous bio-composites increased, the effect of water to change the magnitude of deformation decreased," Fielder said.

The bio-composites made of collagen and carbon nanotubes were also found to have a higher specific heat than the studied mineralized

collagen bio-composites, making them more likely to be resistant to thermal damage that could occur during implantation or functional use of the composite. Like most biological materials, bone is a hierarchical—with different structures at different length scales. At the microscale level, bone is made of [collagen fibers](#), composed of smaller nanofibers called fibrils, which are a composite of collagen proteins, mineralized crystals called apatite and water. Collagen fibrils overlap each other in some areas and are separated by gaps in other areas.

"Though several studies have characterized the mechanics of fibrils, the effects of variation and distribution of [water](#) and mineral content in fibril gap and overlap regions are unexplored," said Nair, who is an associate professor of mechanical engineering. "Exploring these regions builds an understanding of the structure of [bone](#), which is important for uncovering its material properties. If we understand these properties, we can design and build better bio-inspired materials and bio-composites."

More information: Marco Fielder et al. Effects of hydration and mineralization on the deformation mechanisms of collagen fibrils in bone at the nanoscale, *Biomechanics and Modeling in Mechanobiology* (2018). [DOI: 10.1007/s10237-018-1067-y](https://doi.org/10.1007/s10237-018-1067-y)

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