Collagen structure deciphered

CAMBRIDGE, Mass.—For the first time, an MIT researcher's atom-by-atom study of the deformation and fracture of collagen explains Nature's design of its most abundant protein material. It is due to the basis of the collagen structure that leads to its high strength and ability to sustain large deformation, as relevant to its physiological role in tissues such as bone and muscle. This work, likely to have wide impact on biomedical and engineering applications, appears in the Aug. 15 issue of *P. Natl. Acad. Sci. USA* (M.J. Buehler, "Nature designs tough collagen: Explaining the nanostructure of collagen fibrils").

Experiment has shown that collagen isolated from different sources of tissues universally displays a design that consists of a staggered assembly of tropocollagen molecules with lengths of approximately 300 nanometers. The reason why strands of amino acids associate to form tropocollagen molecules consistently at this length has been an unexplained phenomenon.

"Our analysis provides – for the first time – a rationalization for the distinctive design features and characteristic length scales found in natural collagen, using a theory that start at the most fundamental, atomistic scale," says Professor Buehler, Principal Investigator at the Atomistic Mechanics Modeling Laboratory at MIT.

Buehler's work represents a breakthrough in understanding how molecular and tissue properties are linked. The smallest building blocks of collagen, called tropocollagen molecules, are five to ten times stronger than steel, while sustaining enormous tensile strains of up to fifty percent before fracture occurs. In comparison, steel typically sustains only small strains of a few percent before it breaks.

Buehler discovered that the characteristic design of collagen displays a clever strategy that enables Nature to take advantage of the nanoscale properties of individual molecules at larger scales, leading to a tough material. This is achieved by arranging tropocollagen molecules into a staggered assembly known as collagen fibrils. "The natural design represents a delicate balance between tensile forces within each tropocollagen molecule and shear forces between the molecules," says Buehler. He confirmed his theory using large-scale computer simulations that begin at the atomistic scale treating individual chemical interactions based on quantum mechanical calculations.

Previous models of collagen typically involved empirical parameters and lacked a rigorous connection between quantum chemistry, molecular structure, material properties and collagen's physiological function. Buehler's model provides a first principles based materials representation.

Collagen, an extracellular matrix protein, plays an important role in defining the infrastructure of physiologic tissues under load or strain, and is critical to tissues within the skeletal, muscular and cardiovascular networks. Improved understanding of Nature's design criteria will help guide material and biomedical engineers to develop enhanced biomimetic polymers. Buehler's work could contribute to research that may one day develop cures for collagen related diseases such as the Ehler-Danlos syndrome, joint hyperextensibility or Scurvy.

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Original publication:

Markus J. Buehler
Nature designs tough collagen: Explaining the nanostructure of collagen fibrils
P. Natl. Acad. Sci. USA, August 15, 2006

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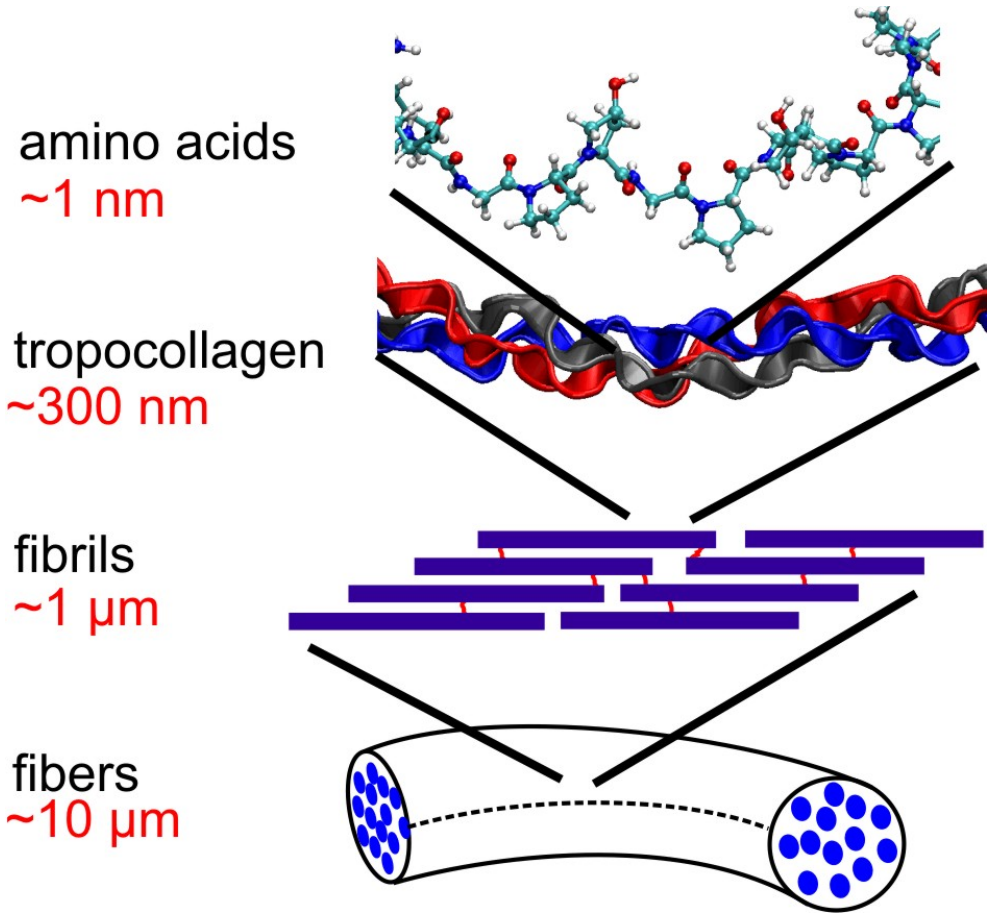

Figure 1: The hierarchical design of collagen. The structural features of collagen ranges from the amino acid sequence, tropocollagen molecules, collagen fibrils to collagen fibers. The new multi-scale model describes the mechanical properties of collagen fibrils using a hierarchical multi-scale scheme that starts from the atomistic level of amino acids (Figure created by M.J. Buehler / MIT).

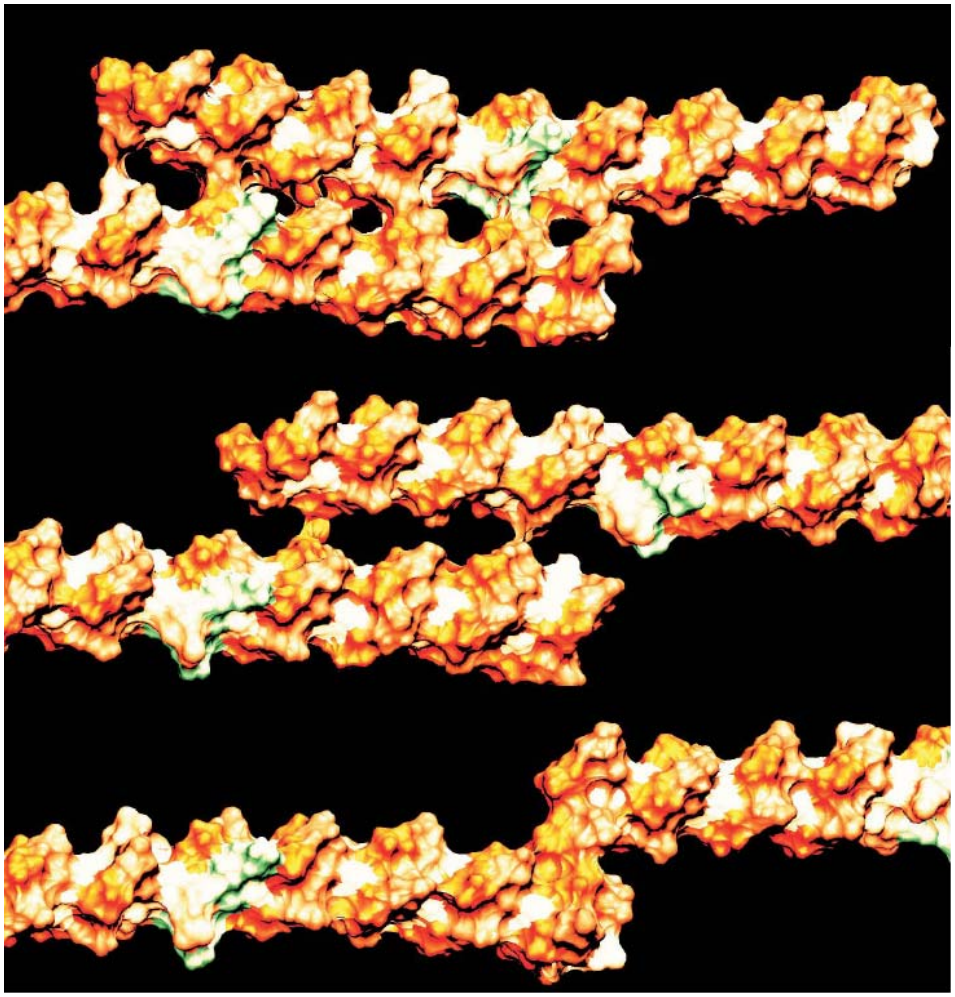

Figure 2: Shearing of two tropocollagen molecules. The figure shows the atomistic mechanisms as two tropocollagen molecules in a collagen fibril undergo microscopic shear deformation, due to macroscopic tensile loading. The two molecules interact through a nano-scale layer of water molecules and weak interactions, including hydrogen bonds and electrostatic forces. These atomic interactions break as molecules slide on top of each other. (Figure created by M.J. Buehler / MIT using VMD.)

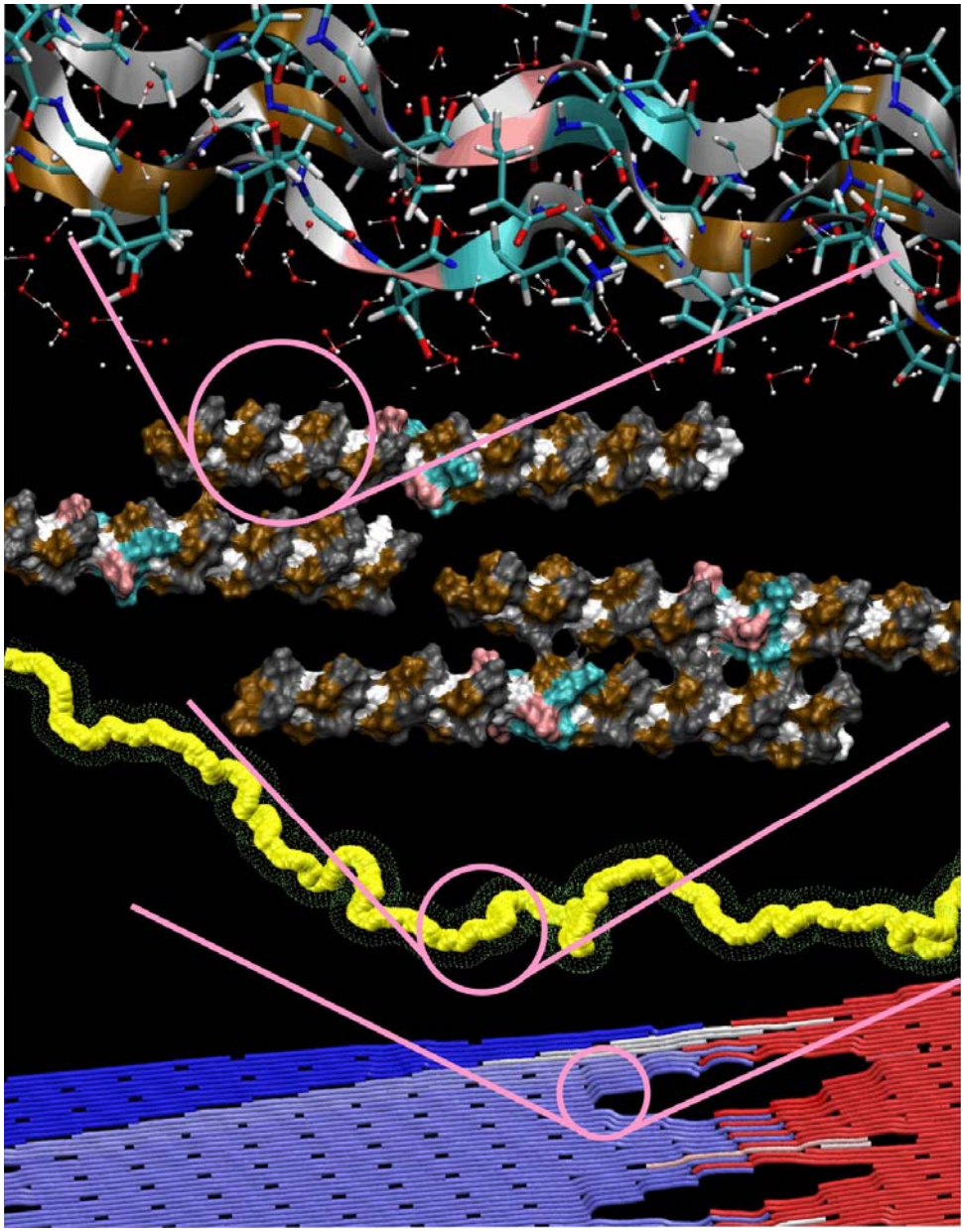

Figure 3: The hierarchical design of collagen. The figure shows snapshots of different structural features of collagen. From bottom to top: collagen fibril, single ultra-long tropocollagen molecule, assembly of tropocollagen molecules, and atomistic amino acid structure of an individual tropocollagen molecule (Figure created by M.J. Buehler / MIT).

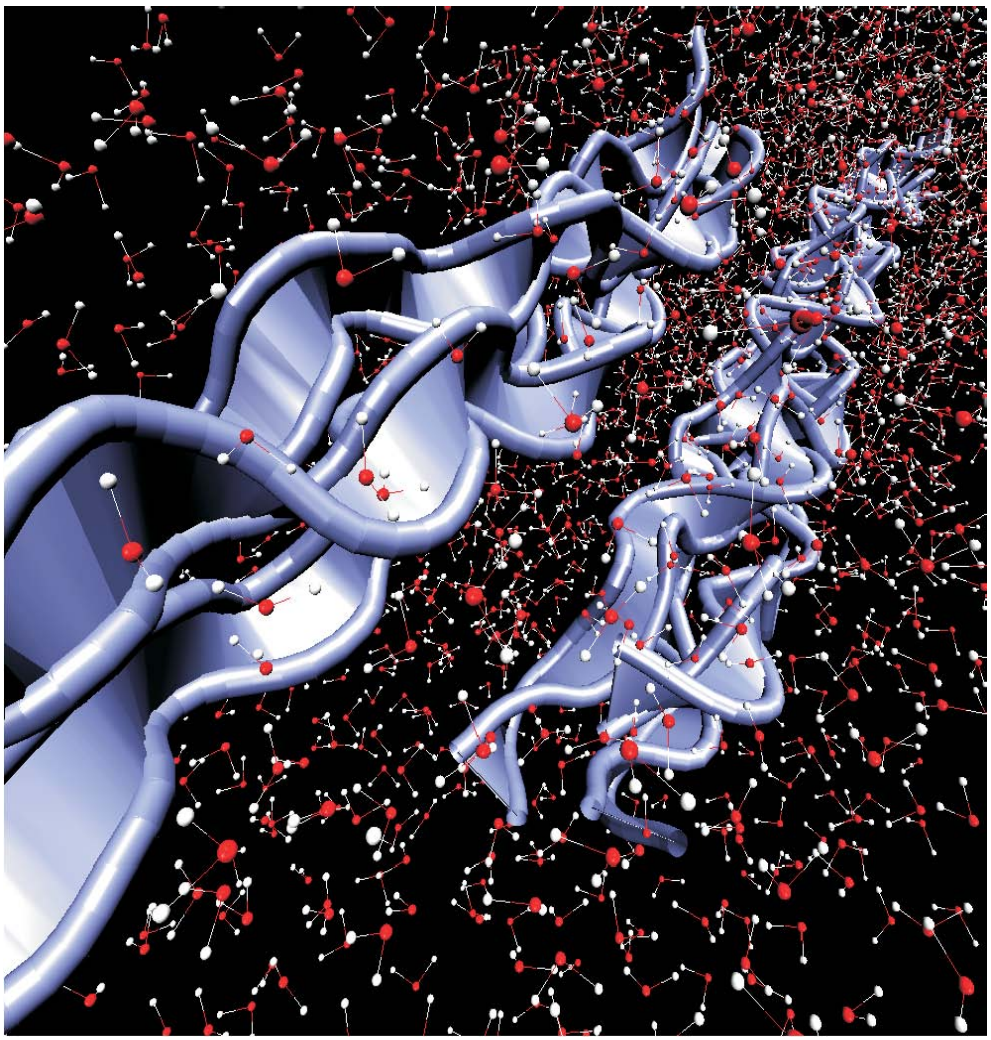

Figure 4: Shearing of two tropocollagen molecules. The figure shows the atomistic mechanisms as two tropocollagen molecules in a collagen fibril undergo microscopic shear deformation, due to macroscopic tensile loading. The two molecules interact through a nano-scale layer of water molecules and weak interactions, including hydrogen bonds and electrostatic forces. These atomic interactions break as molecules slide on top of each other. (Figure created by M.J. Buehler / MIT using VMD.)