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Protein's strength lies in H-bond cooperation

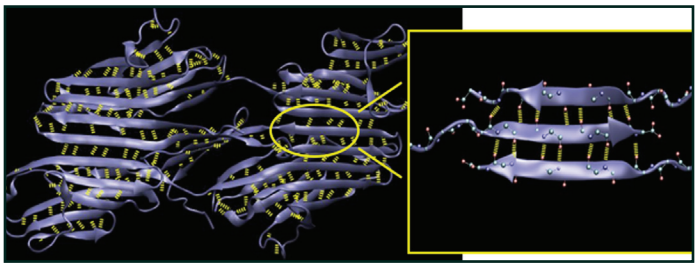
PROBLEM

The study of materials at the molecular level is important for applications in nearly every field of engineering, science and medicine. In particular, understanding the mechanics of biological materials may help engineers use the natural world as design space to develop novel materials for use in healing injury, curing disease, and building structures and devices that incorporate nanotechnology. Protein-based materials represent one such frontier.

Despite significant advancements, researchers don't understand how protein-based materials like spider silk, bone and muscle tissue can be strong, lightweight and exceptionally robust. A dense material such as steel has a crystal lattice structure held together by strong metallic bonds. Most structural proteins consist of alpha-helices or beta-sheets composed of hierarchical features that form an intriguing merger of structure and material. One very puzzling aspect is that much of a protein's secondary structure is held together by weak hydrogen bonds, which are actually 100 to 1,000 times weaker than the bonds in steel. So, what gives protein-based materials their great strength, elasticity and resilience?

APPROACH

Professor Markus Buehler combines theoretical modeling with large-scale molecular simulation implemented on supercomputers for the study of protein-based materials. The simulations play the role of virtual experiments; they include details of chemical bonding controlled by the laws of quantum mechanics, and describe a material's behavior at the atomistic level. Buehler is particularly interested in the nature of deformation, including rupture, and its consequences on tissues like bone, muscle and spider silk.



This figure shows the structure of a beta-sheet protein, Z1-Z2 telethonin complex, in the giant muscle protein titin. The inset shows the orientation of the protein backbone of three beta strands (in purple) with hydrogen bonds (yellow) holding the assembly together. Buehler and Keten found that hydrogen bonds in beta-sheet structures break in clusters of three or four, even in the presence of many more bonds.

FINDINGS

Recent research on beta-sheet proteins by Buehler and Ph.D. student Sinan Keten revealed that the strength of protein-based materials may lie in the geometric configuration of the beta strands that make up the beta sheets, which make use of small clusters of hydrogen bonds (H-bonds) working cooperatively to resist force and dissipate energy.

Proteins dominated by a beta-sheet structure fold into sheets of short, stacked parallel strands attached to one another top and bottom by a single cluster of three or four H-bonds. During molecular dynamics simulations of mechanical shear, Buehler and Keten observed that the H-bonds connecting beta strands ruptured simultaneously in clusters of three or four rather than sequentially, giving the beta sheets increased resistance to force. Further simulations demonstrated that a single bond or pair of bonds reduced strength, and that longer beta strands with more than four bonds also were significantly weaker, even though the bonds ruptured in clusters.

Buehler and Keten theorized that the geometric confinement of the bonds in these short strands governs the rupture strength. They used thermodynamics to describe how the external force changes the entropic energy of the protein's very elastic system and determined that the concurrent breaking of three to four H-bonds is an intrinsic upper limit for the uniform shear loading of H-bonds in a beta strand. They also observed a similar behavior in the same-sized H-bond clusters in alpha-helical proteins, which together with beta-sheet proteins make up the majority of all structural proteins.

IMPACT

The dominance of beta-strand length and H-bond geometric confinement in one of the two most dominant structural proteins suggests that the correlation between this geometric configuration and a protein's strength is an important evolutionary driving force behind its design. Continued research by Buehler and others may one day provide a guiding principle for the design of novel bio-inspired materials.

MORE

Buehler, the Esther and Harold E. Edgerton Assistant Professor, and Keten published a paper describing this research in the Feb. 13 online issue of Nano Letters.

The Department of Civil and Environmental Engineering at the Massachusetts Institute of Technology is dedicated to balancing the built environment with the natural world. In our research, we seek to understand natural systems, to foster the intelligent use of resources and to design sustainable infrastructure systems.

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