Simplicity is crucial to design optimization at nanoscale

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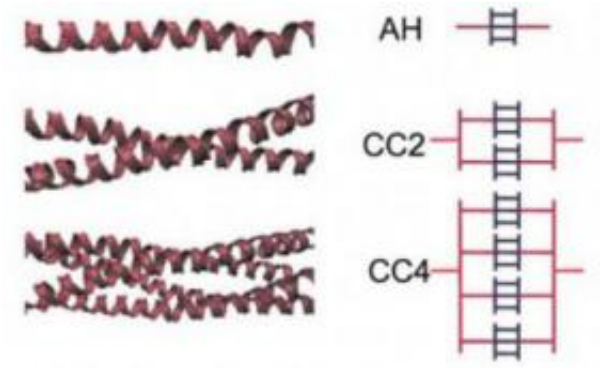

This figures illustrates the different arrangements of alpha-helical protein filaments and their schematic representation in the Buehler/Ackbarow model. Credit: Image / Markus Buehler, MIT

MIT researchers who study the structure of protein-based materials with the aim of learning the key to their lightweight and robust strength have discovered that the particular arrangement of proteins that produces the sturdiest product is not the arrangement with the most built-in redundancy or the most complicated pattern. Instead, the optimal arrangement of proteins in the rope-like structures they studied is a repeated pattern of two stacks of four bundled alpha-helical proteins.

This composition of two repeated hierarchies (stacks and bundles) provides great strength—the ability to withstand mechanical pressure without giving way—and great robustness—the ability to perform

mechanically, even if flawed. Because the alpha-helical protein serves as the building block of many common materials, understanding the properties of those materials has been the subject of intense scientific inquiry since the protein's discovery in the 1940s.

In a paper published in the Jan. 27 online issue of *Nanotechnology,* Markus Buehler and Theodor Ackbarow describe a model of the protein's performance, based on molecular dynamics simulations. With their model they tested the strength and robustness of four different combinations of eight alpha-helical proteins: a single stack of eight proteins, two stacks of four bundled proteins, four stacks of two bundled proteins, and double stacks of two bundled proteins. Their molecular models replicate realistic molecular behavior, including hydrogen bond formation in the coiled spring-like alpha-helical proteins.

"The traditional way of designing materials is to consider properties at the macro level, but a more efficient way of materials' design is to play with the structural makeup at the nanoscale," said Buehler, the Esther and Harold E. Assistant Professor in the Department of Civil and Environmental Engineering. "This provides a new paradigm in engineering that enables us to design a new class of materials."

More and more frequently, natural protein materials are being used as inspiration for the design of synthetic materials that are based on nanowires and carbon nanotubes, which can be made to be much stronger than biological materials. The work of Buehler and Ackbarow, a graduate student at the Max Planck Institute of Colloids and Interfaces in Potsdam, Germany, demonstrates that by rearranging the same number of nanoscale elements into hierarchies, the performance of a material can be radically changed. This could eliminate the need to invent new materials for different applications.

In a follow-up study, Buehler and MIT graduate students Zhao Qin and

Steve Cranford ran similar tests using more than 16,000 elements instead of eight. They found that 98 percent of the randomly arranged rope-like structures did not meet the optimal performance level of the self-assembled natural molecules, which made up the other 2 percent of the structures. The most successful of those again utilized the bundles of four alpha-helical proteins.

That analysis shows that random arrangements of elements typically lead to inferior performance, and may explain why many engineered materials are not yet capable of combining disparate properties such as robustness and strength.

"Only a few specific nanostructured arrangements provide the basis for optimal material performance, and this must be incorporated in the material design process," said Buehler.

Source: Massachusetts Institute of Technology