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Engineers Discover Graphene's Weakness

In 2008, experiments at The Fu Foundation School of Engineering and Applied Science at Columbia University established pure graphene, a single layer of graphite only one atom thick, as the strongest material known to humankind. This raised a question for Chris Marianetti, Assistant Professor in Columbia Engineering's Department of Applied Physics and Applied Mathematics: how and why does graphene break?

Using quantum theory and supercomputers, Marianetti has revealed the mechanisms of mechanical failure of pure graphene under tensile stress. In a paper recently accepted for publication in the journal Physical Review Letters, he shows that, when graphene is subject to strain equal in all directions, it morphs into a new structure which is mechanically unstable.

Marianetti says this failure mechanism is a novel soft-mode phonon instability. A phonon is a collective vibrational mode of atoms within a crystal, similar to a wave in a liquid. The fact that a phonon becomes "soft" under tensile strain means that the system can lower its energy by distorting the atoms along the vibrational mode and transitioning to a new crystalline arrangement. Under sufficient strain, graphene develops a particular soft-mode that causes the honeycomb arrangement of carbon atoms to be driven towards isolated hexagonal rings. This new crystal is structurally weaker, resulting in the mechanical failure of the graphene sheet.

"This is exciting on many different levels," Marianetti notes. "Soft modes were first recognized in the 1960s in the context of ferroelectric phase transitions, but they have never been directly linked to fracture. Typically, defects in a material will always cause failure to happen prematurely, but the pristine nature of graphene allows one to test our prediction. We have already outlined some interesting new experiments to directly observe our theoretical prediction of the soft mode."

Marianetti added that this is the first time a soft optical phonon has ever been linked to mechanical failure and that therefore it is likely that this novel failure mechanism is not exclusive to graphene but may be prevalent in other very thin materials. "With nanotechnology becoming increasingly ubiquitous, understanding the nature of mechanical behavior in low dimensional systems such as graphene is of great importance. We think strain may be a means to engineer the properties of graphene, and therefore understanding its limits is critical." The research was funded by the National Science Foundation.

Marianetti's research interests lie in the use of classical and quantum mechanics to model the behavior of materials at the atomic scale. In particular, he is focused on applying these techniques to materials with potential for energy storage and conversion. Current applications in his research program range from nuclear materials such as plutonium to rechargeable battery materials such as cobalt oxides.

Marianetti received his BS and MS degrees from Ohio State University and his PhD in materials science and engineering from MIT. Before joining the faculty at Columbia Engineering, he did post-doctoral research in the Department of Physics at Rutgers University and in the Materials Chemistry Division of Lawrence Livermore National Laboratory.