NANO HIGHLIGHT
Ideal Strength and Nanomechanics

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One strategy for strengthening materials is to refine the grain size. Using this strategy, bulk materials with grain sizes in the nanometer regime have been produced, and true to expectations, show remarkable strength (roughly a factor of five increase in comparison to their larger grained bulk counterparts). However, as grain sizes continue to shrink, the strength gains eventually give way to strength reductions. One way to stave off this reduction in strength leading to even stronger materials may be to reinforce the nanograined materials with the introduction of suitable nanostructures, for example carbon diamondoids. Consequently, we have begun to explore theoretically the mechanical properties of potential nanostructure additives.

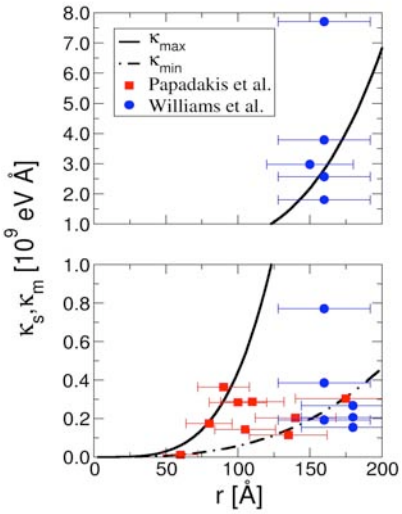

Figure 1. Bounds on torsional stiffnesses predicted by theory as compared with experiment. The theory has no adjustable parameters, and bounds all the data [2,3] (within error bars).

Our first investigations focused on the torsional properties of carbon nanotubes, largely as a model nanostructure. We computed both the ideal torsional strength and torsional stiffness of carbon nanotubes using first-principles electronic structure total energy methods and compared our results with available experiments [1]. We developed a scaling form that allowed us to *predict* the torsional stiffnesses of *all* nanotubes, and the ideal torsional strength of an entire class of nanotubes. The stiffnesses so computed agree very well with available experimental data (Fig, 1). The ideal torsional strength of a multiwalled carbon nanotube is predicted to exceed that of a similarly sized iron rod by a factor of 20.

Presently, we have turned our attention to exploring the properties of carbon based diamondoid structures. To date, we have shown that [12]-type diamondoids retain, to a large extent, the stiffness of bulk diamond. We are extending our calculations to include computation of the ideal strength of these and other diamondoid structures, and to consider the properties of diamondoids embedded within a host material (*e. g.* aluminum).

References

[1] E. Ertekin and D. C. Chrzan, "Ideal Torsional Strengths and Stiffnesses of Carbon Nanotubes." Physical Review B 72: 045425/1-5 (2005).
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