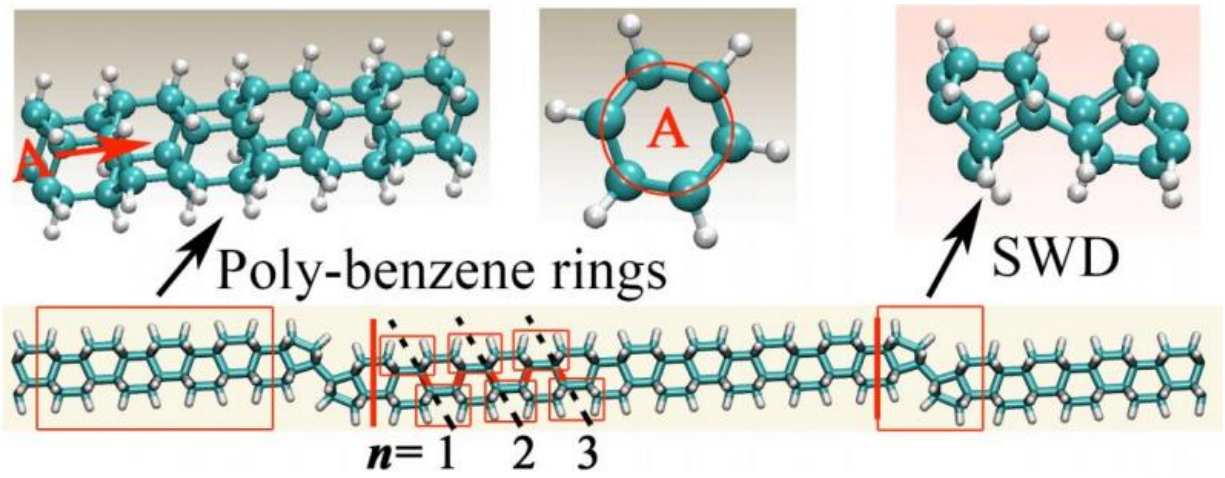
Simulation shows diamond nanothread may not have to be so brittle after all

November 23 2015, by Bob Yirka



The atomic configurations of a segment of DNT, insets show the structural representation of the poly-benzene rings and the Stone-Wales defect (SWD). Credit: arXiv:1511.01583 [cond-mat.mtrl-sci]

(Phys.org)—A team of researchers from Australia and Singapore has found via simulation that diamond nanothreads may not have to be as brittle as has been assumed. In their paper uploaded to the *arXiv* server, the team describes the simulations they created and why they believe defects found in the construction process may be the key to creating useful structures out of the material.

Last month a team of researchers at Pennsylvania State University

announced that they had created a material they called diamond nanothread—one-dimensional crystals capped with hydrogen and bonded together to form tiny chains. The results were duly noted by the scientific community, but reports by the team suggested that as the chains grew longer, they became more brittle, preventing its use in creating interesting or useful structures. They also suggested that if a way could be made to prevent the brittliing effect, it might be possible to create a thread long enough to serve as the basis for a space elevator. In this new effort, the researchers report finding a way to form similar chains that are not brittle—though their research thus far has been strictly virtual—they modeled structures on a computer, creating simulations.

In the real experiments, the researchers created the threads by exposing liquid benzene to great pressure and then slowly releasing the pressure, and that served as the starting point for the researchers looking to model the nanothreads that were produced in the earlier work. They noted immediately that different configurations could be formed depending on the ways the atoms bonded. They also noted that defects tended to appear in the chains as well, and when they did, the threads that resulted were less rigid, meaning less brittle. Taking the idea further, the team found that if they introduced such defects intentionally, they could simulate the construction of structures that were malleable.

It is not clear at this time how close the simulations would be to real-world applications, but it is likely that other teams will follow up on what was found to discern if their idea is sound, and if so, if long useful threads could indeed be created—perhaps long enough to be used for that elusive space elevator.

More information: From Brittle to Ductile: A Structure Dependent Ductility of Diamond Nanothread, arXiv:1511.01583 [cond-mat.mtrl-sci] arxiv.org/abs/1511.01583

Abstract

As a potential building block for the next generation of devices or multifunctional materials that are spreading almost every technology sector, one-dimensional (1D) carbon nanomaterial has received intensive research interests. Recently, a new ultra-thin diamond nanothread (DNT) has joined this palette, which is a 1D structure with poly-benzene sections connected by Stone-Wales (SW) transformation defects. Using large-scale molecular dynamics simulations, we found that this sp3 bonded DNT can transit from a brittle to a ductile characteristic by varying the length of the poly-benzene sections, suggesting that DNT possesses entirely different mechanical responses than other 1D carbon allotropies. Analogously, the SW defects behave like a grain boundary that interrupts the consistency of the poly-benzene sections. For a DNT with a fixed length, the yield strength fluctuates in the vicinity of a certain value and is independent of the "grain size". On the other hand, both yield strength and yield strain show a clear dependence on the total length of DNT, which is due to the fact that the failure of the DNT is dominated by the SW defects. Its highly tunable ductility together with its ultra-light density and high Young's modulus makes diamond nanothread ideal for creation of extremely strong three-dimensional nano-architectures.

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