Deducing the properties of a new form of diamond

November 30 2017

Earlier this year, amorphous diamond was synthesized for the first time using a technique involving high pressures, moderately high temperatures and a tiny amount of glassy carbon as starting material. A father-son team at Clemson University has now successfully calculated a number of basic physical properties for this new substance, including elastic constants and related quantities. The results are reported this week in *Applied Physics Letters*.

Diamond is a form of pure carbon in which the atoms are arranged in a crystal lattice, with each carbon atom surrounded by four other carbons at the corners of a tetrahedron. The carbon-carbon bonds in diamond are known as sp3 bonds. The orderly arrangement of tetrahedral structures which repeats over long distances in a diamond crystal produces a hard material with high temperature stability. Diamond is thus both a valuable gemstone and a material with a variety of technological uses.

Amorphous carbon, on the other hand, has varying fractions of sp3-bonded carbon in a disordered, or amorphous, matrix. The amorphous structure produces very desirable mechanical properties. The amount of sp3 bonding in amorphous carbon is not as high as in pure diamond. A fraction of the carbon-carbon bonds are of sp2-type, found in other carbon forms such as graphite.

Sp3-bonded amorphous silicon and germanium have been known for many years and are widely used in photovoltaics, thin film sensors and transistors, and other high-tech applications. It is of great interest, then, to find ways to make amorphous diamond that retains a high fraction of sp3 bonds. While the work reported earlier this year did just that, samples are not yet widely available for testing. Preliminary tests did show that these amorphous diamonds are quite dense, optically transparent and strong.

The father-son team of Arthur and John Ballato have stepped into this knowledge gap to calculate some not-yet-measured physical properties for this new form of diamond. "We employed a modeling approach by which one can use the properties of crystalline diamond to deduce the properties of the glassy diamond analog," said Ballato. "In this work, we inferred the elastic properties of this new phase of diamond from measured properties of crystalline diamond."

The procedure they employed involves a computer model of a crystal that is computationally homogenized to create an amorphous version of the substance. The model of the crystal uses simple, classical physics and describes the carbon-carbon bonds as springs. The homogenization method employed is known as the Voigt-Reuss-Hill (VRH) technique.

Using this approach, the Ballatos computed a number of important bulk properties, including Young's modulus, Poisson's ratio and other elastic constants for the substance. They used the VRH homogenization approach in previous work to study glassy sapphire and materials of interest for use in high power lasers. The VRH method is simpler and more straightforward than sophisticated quantum mechanical methods that are also available, but the properties calculated in this work can serve as a baseline, both for more sophisticated, but expensive modeling, as well as for future experimental measurements.

More information: J. Ballato et al, Deduced elasticity of sp3-bonded amorphous diamond, *Applied Physics Letters* (2017). DOI: 10.1063/1.5005822

Provided by American Institute of Physics