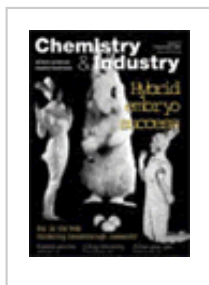


Carbon nitride solids: potential alternatives to diamond?



Chemistry and Industry

November 20, 1995 | Lieber, Charles M.; Zhang, Z. John

The development of new materials with extreme electrical, thermal and/or mechanical properties is a significant challenge to fundamental materials research. Obtaining such materials is of great importance to high-performance engineering applications ranging from microelectronics to aircraft propulsion. In this search, existing solids can often serve as a guide to the critical structural features needed to obtain desirable physical properties.

For example, the unique properties of diamond -- it is the hardest known substance, a superb electrical insulator and the best thermal conductor at room temperature -- arise from the three-dimensional network of strong, covalent bonds between the carbon atoms (see Figure 1). It is therefore reasonable to assume that materials with a relatively isotropic arrangement of short, covalent bonds should have properties similar to diamond. Cubic boron-nitride is a solid that supports this idea. It has the same structure type as diamond, but with alternating boron and nitrogen atoms replacing the carbon atoms of the diamond lattice.

A new class of materials containing only carbon and nitrogen (carbon nitride solids) can also satisfy this structure-bonding hypothesis, and could thus have diamond-like properties.[1] These materials are currently the focus of both fundamental and applied research.

Basic research exploring the synthesis and properties of carbon nitride solids is challenging the ability of chemists and material scientists to assemble new materials that, in the main, are metastable and cannot be prepared by conventional methods (since these would yield the most stable products graphite and molecular nitrogen). In addition, studies of the properties of these solids are beginning to show evidence

that these materials do indeed have some diamond-like characteristics, and thus may be useful alternatives to diamond.

Theoretical predictions

Interest in covalent carbon nitride was first stimulated by theoretical studies by M Cohen and co-workers, at the University of California at Berkeley, of a solid analogous to beta-silicon nitride: $[\text{Beta}]\text{-}[\text{C.sub.3}][\text{N.sub.4}]$, formed by replacing silicon with carbon (see Figure 2).[2] The parent $[\text{Beta}]\text{-}[\text{Si.sub.3}][\text{N.sub.4}]$, which is itself a hard material used in several demanding applications such as a wear resistant coating on bearings and a dielectric in microelectronics devices, is made up of a three-dimensional network of bonds. By replacing the Si-N bonds with shorter and stronger C-N bonds, chemical reasoning suggests that a much harder solid should result. The theoretical calculations showed that the hypothetical $[\text{Beta}]\text{-}[\text{C.sub.3}][\text{N.sub.4}]$ solid would have a large cohesive energy (the energy per formula unit binding the solid together) and should be relatively stable if formed. Furthermore, investigations of the total energy of $[\text{Beta}]\text{-}[\text{C.sub.3}][\text{N.sub.4}]$ as a function of the unit cell size indicated that this solid would be as hard as, or harder than, diamond. [2] This has clearly been a strong motivating force for experimental studies.

It is also important to consider the potential pitfalls of such calculations. ...

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