Novel Superhard Materials and Nanostructured Diamond Composites

Benefits

The benefits of nanostructured superhard materials include

- Superior mechanical performance in hardness, toughness, strength, and wear resistance.
- High thermal conductivity, optical transparency, large band gap, and chemical inertness.

Applications

Nanostructured superhard materials may be applied in field work under extreme conditions for various Industries of the Future, including

- **Mining** and
- **Petrochemical**

In hard rock mining and petrochemical exploration, drills are often needed for boring through extremely hard formations of the Earth. Rock drill bits are equipped with teeth designed to scrape and gouge. As the geological formation becomes denser and harder, the teeth may wear down quickly, resulting in reduced drilling efficiency and thus increasing downtime and replacement cost.

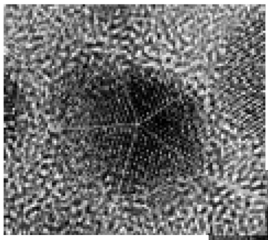
The superb thermal/optical/electronic/chemical properties also make superhard materials highly desirable in modern high-tech industrial applications as protective coatings, substrates for semiconductors, windows for optical devices, and anvils for high-pressure devices.

Novel superhard materials can provide next-generation superhard/superabrasive materials for industrial applications

Designing new superhard materials with novel properties and developing practical methods for their industrial production are the main motivations for this project. Superhard materials are normally made of light elements such as boron, carbon, and nitrogen. The intrinsically strong and directional covalent bonds of the light elements lead to tight, three-dimensional networks with extreme resistance to external shear. Novel superhard materials have become possible following the successful development of processes for producing synthetic diamonds (Bundy, et al. 1955) and cubic boron nitride (CBN) (Wentorf 1957), at high pressures and high temperatures. The design and development of novel superhard materials are aided by first-principles theory and computational simulation. Carbon nitrides (C_3N_4) and boron carbon nitrides (BC_2N, BC_4N) are deemed as the potential candidates because of the similarity of their proposed high-pressure phases in diamond crystal structure.

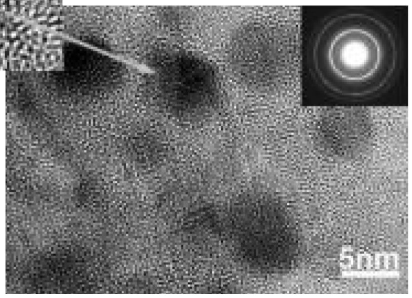
The appropriate design of nanostructured superhard composites with a strong amorphous matrix or bi-phase nanocrystalline boundaries is one of the major research focuses of the project. Nanocrystalline phases and amorphous phases enhance mechanical performance substantially (Ekimov et al. 2000). Such strengthening is caused by the decreasing number of vacancies and dislocations in crystals with diminishing sizes. In a nanostructured superhard composite, the size of the microcrack is smaller than the size of the nanocrystals, thus greatly reducing the propagation of microcracks. Grain size and phase fraction by can be controlled by changing the pressure-temperature-time conditions. Special preparation of starting materials and careful selection of catalysts/solvents will also add to the successful synthesis of nanostructured superhard composites in the B-C-N system. Future research will also be directed toward industrial application of nanostructured diamond/SiC composites and to the understanding of their mechanical properties.

Synthesis of nanostructured superhard B-C-N materials has been successful

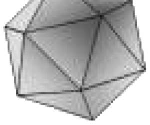


High-Resolution TEM Image and Diffraction (selected area)

BC_2N Grain Size 3~8 Nanometers



Direct View of a three-fold Symmetry Apex of a Polyhedron



Project Description

Goal: The goal of this R&D project is to synthesize novel superhard B-C-N materials and to manufacture nanostructured diamond/SiC composites. The project covers a broad research scope of high-pressure, high-temperature synthesis, property characterization, and industrial implementation. The success of this project can have significant technological impacts for future industrial applications in many fields.

Issues: The following R&D tasks, to be performed in this project, are key to the development of a manufacturing process; sample preparation; catalyst selection; property characterization; and in situ/real-time high P-T neutron/X-ray diffraction studies of phase diagrams, synthesis kinetics, and residual stress.

Approach: The successful synthesis of the superhard B-C-N materials and nanostructured diamond/SiC composites will require (a) advanced high-pressure techniques with the use of a unique Pt capsule to confine the volatile phases, (b) the effective use of suitable solvents and catalysts to promote synthesis reaction and crystallization, and (c) the appropriate selection of the composition and particular preparation of starting materials.

Systematic studies will be conducted on the correlation between hardness, elastic moduli, crystal structure, thermal stability, chemical composition, and physical properties. Particular attention will be placed on the mechanical, optical, and electronic properties, and on the potential high-tech applications of the new superhard materials.

Potential payoff: The experimental studies of novel superhard materials in the B-C-N system and of nanostructured diamond/CBN and diamond/SiC composites will provide next-generation superhard/superabrasive materials for future industrial applications. Economic and energy benefits can be achieved by the application of nanocrystalline superhard B-C-N composites to machining/cutting operations. In addition, environmental improvements can also be achieved because B-C-N composites do not need coolants for machining. Significant reduction in the numbers of "trip-out-of-hole" and "trip-into-hole" for increased drilling efficiency will also greatly reduce the risk of environmental pollution caused by oil/gas well blowouts.

Progress and Milestones

- Bulk nanostructured superhard BC_2N materials

  Following the successful synthesis of nanostructured superhard BC_2N bulks at ~20 GPa and 2200 K, characterization of superhard synthetic BC_2N samples will be analyzed by synchrotron X-ray diffraction, high-resolution transmission electron microscope (TEM), electron energy-loss spectra (EELS), synchrotron infrared (IR) spectroscopy, and Vickers indentation hardness measurements.
- Nanostructured diamond-SiC composites

  The focus is on the preparation of nanocrystalline diamond and nanocrystalline/amorphous silicon from micrcrystalline materials by ball milling. Ultrasonic disperse technology will be applied to make the homogeneous mixture of nanocrystalline/amorphous diamond and silicon powder.
- Boron suboxide

  The Vickers hardness of boron suboxide was determined and found to be very close to that of cubic boron nitride single crystals; its fracture toughness was found to be close that of diamond. Those results show that boron suboxide and its composites have great potential as new superhard materials for industrial use. The materials posses the highest hardness at high temperatures (>600 °C). This property is very important for dry high-speed cutting operations.

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