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CUBIC BORON CARBONITRIDE FOR ADVANCED ELECTRONIC APPLICATIONS TO MODERNIZING COMMUNICATION TECHNOLOGY

Whitepaper submitted to Powering the Army of the Future

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3/4/2020

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I . Proposal background and objectives

A very exciting new era of 5G communication is on the horizon with full of promises. The new wave of the technology revolution is expected to provide unique services and applications (i.e., self-driving cars and drone-based deliveries, smart homes and factories, remote medical diagnosis and surgery, and artificial-intelligence-based personalized assistants, see Figure 1). [1] Therefore, the utilization and optimization of the communication mechanisms associated with these new applications and services can be inevitable and crucial for the Army Modernization Strategy (AMS) including military use of drones and sensors, enabling superior communications to the existing technologies in terms of latency, energy efficiency, reliability, flexibility, and connection density [2].

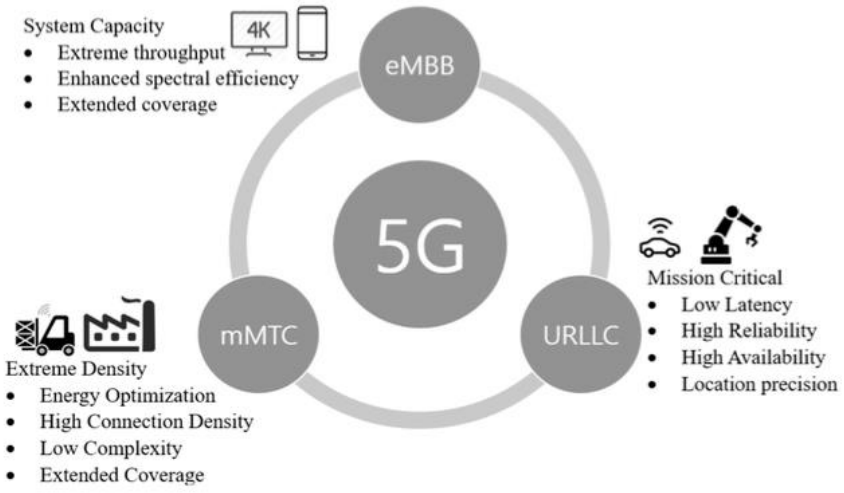

Figure 1 Future 5G features and improvement plan (Courtesy from Reference [1])

The communication devices based 5G technology are expected to operate in 3 to 300 GHz (i.e., 3 to 30 GHz for 5G small cell-phones, 30 to 300 GHz for 5G mm wave), which may result in the relatively short coverage distance (i.e., 2 meters-300 meters) due to high frequencies. Therefore, the key technology requires a significant support from advanced electronic materials to address high losses and high temperature instability occurring at high frequencies. The enabling technology that needs to be determined includes (i) low dielectric materials for dielectric resonators and (ii) magnetic materials for high frequency isolators/circulators. Here we propose to carry out a combined theory-experimental case study of diamond based compounds including cubic BCN to design low-dielectric materials relevant for 5G communication technology, which is identified as Army Priority Research Area (2. RF Electronic Materials, see Table 1).

Table 1 Army Priority Research Areas from Reference [3].

Army Priority Research Areas
1. Disruptive Energetics: Greater than 2x energetic energy over smaller footprints.
2. RF Electronic Materials: Taking advantage of optical and thermal properties of diamond materials for directed energy.
3. Quantum: Optimized information transfer, sensing, and communication with unparalleled security.
4. Hypersonic Flight: Aerodynamics, materials, and processes.
5. Artificial Intelligence: Increasing speed and agility in which we respond to emerging threats.
6. Autonomy: Maneuverability and off-road mobility of platforms.
7. Synthetic Biology: Reactive and responsive skins/spectrally selective materials/anti-materiel properties.
8. Material by Design: Protection overmatch against future threats.
9. Science of Additive Manufacturing: For next generation munitions for increased range and lethality.

II. Proposed research: The Quest for advanced 5G communication materials

It is well-known that inducing p- and/or n-type conduction in diamond is achievable through doping. Why is this so important? It is the common knowledge now that wide bandgap alongside with high saturated electron drift velocity and electric breakdown field makes diamond the semiconductor of choice for high-power and high-frequency electronics. What else? The temperature dependence of forward current power loss in high voltage diodes clearly demonstrates the superiority of diamond as a semiconductor of choice at elevated temperatures, which means heavy usage in development of advanced hypersonic weapons. Moreover, to enable technology for multi-domain operations with advanced communications and information processing capable of reliably functioning in variable climates such as rain, snow, hail, dust, fog, etc., a self-contained, mobile and resilient integrated sensor, communications and information infrastructure is required. Therefore, materials with advanced properties will be of paramount importance for this type of infrastructure.

Since a Schottky barrier diode, in which, if a forward voltage applied, current conduction in its forward direction is allowed, whereas reverse voltages are blocked, in reverse current discharge protection and as rectifier in power applications is already known for being able to reach nanosecond range in switching times, when based on boron doped diamond instead of SiC, without detecting any parasitic capacitances, it again suffices to state that diamond electronics is about to change (and is changing, as a matter of fact) everything in manufacturing, transportation, aerospace, power grid development and communications. All this is true also for a cornerstone of modern electronics – bipolar junction or/and field effect transistors – used as amplifiers and electrical power switches. Now, keeping in mind that everything abovementioned plus superiority in both mechanical and thermal conductivity properties is getting even more

pronounced in the case of single-crystal diamond, imagine that you are able to harness the similar treasures hidden in the single crystal of cubic (Fd-3m) boron carbonitride (BCN), which has practically identical with diamond structural, mechanical as well as electronic properties. Moreover, the tantalizing possibility of strong light-matter coupling, due to the structural presence of boron and nitrogen, potentially makes this material candidate for various applications in optics and optoelectronics, that will start replacing existing electro-optic and nonlinear optical materials in, for example, valley-optoelectronic and electrically driven excitonic light emission based devices alongside with photodetection and photovoltaic solar cells. Even though investment and unit cost is hard to presently estimate, due to nondisclosure agreement with clients that buy diamond for electronics, it is obvious that the fabrication of a, for example, all-cubic-BCN integrated circuits or microchips without contacting private companies (e.g., Akhan Semiconductors or Fraunhofer USA Center for Coatings and Diamond Technologies CCD) will be essential in dramatically increasing durability (performance in austere or hazardous environments or under shock or damage), decreasing vulnerability to attack and disruption as well as independence from commercial communications infrastructure.

A research team consists of the researchers from the University of Nevada, Las Vegas (PI, Dr. Eunja Kim) and the University of Chicago (co-PI, Dr. Sergey Tkachev) in collaboration with the researchers from Northwestern University and Lawrence Livermore National Laboratory, part of which is affiliated with the Advanced Photon Source of the Argonne National Laboratory. The team members have extensive experience to synthesize and characterize materials properties of diamond and diamond-like materials [4-5], that can be crucial to help address exactly how to fully capitalize on scientific investigation, fabrication, and understanding, subsequently, followed by prediction through experiments coupled with modeling and laser

characterization of the cubic (Fd-3m) BCN single crystal's unique electronic and photonic properties, before some commercial entity will get a technological edge over this and spread the news to the rest of the world; otherwise some foreign power will be ultimately the first to take control over this research area. Needless to say, the most accurate ways of characterizing the electronic, structural, and mechanical properties of the samples are essential to gather the necessary information to predict and to improve the performance of the devices.

III. Previous results on diamond and diamond-like materials

We have carried out theoretical studies of diamond, boron-nitride, and BC_2N samples in our previous studies that are somewhat similar in electronic and photonic properties to the proposed cubic BCN materials, demonstrating the limits and capabilities of the density-functional theory (DFT) based method to model and simulate the defects in the sample of interest prior to submitting the full proposal. Our previous DFT calculations has successfully demonstrated the predictive power as well as perform fine-tuning of theoretical modeling carried out using the VASP code.

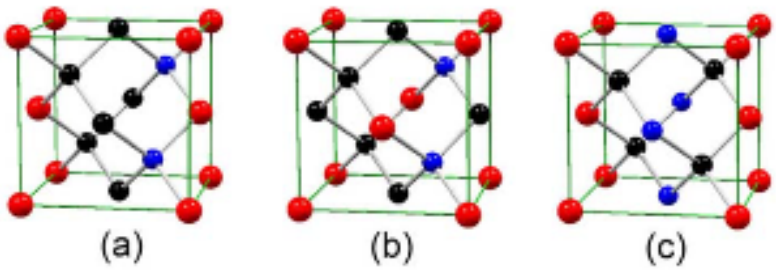

Figure 2 The cubic BC2N structures that we have found to describe the relevant phases obtained experimentally: (a) The high-density phase with C-B-N layered superstructure, (b) the high-density phase without any C-B-N layers, and (c) the low-density phase without any C–C bond. Black, red, and blue symbols are for carbon, boron, and nitrogen, respectively.

For example, as part of the effort to address the quest for a material with its material properties, including hardness, superior to diamond, three active research groups from Japan [7], the US [8], and France [9] attempted to synthesize BC_2N experimentally (see Figure 2), along with first-principles calculations to identify different cubic phases of BC_2N synthesized experimentally. [5]

As a result three distinct cubic phases of BC_2N were synthesized. With a proper choice of the supercell, cutoff energy, and sampling *k* points, three cubic phases are all found to be stable theoretically. The bulk modulus from elastic stiffness constants for each of the phases is in excellent agreement with available experimental data. All the phases are defect-free and do not possess any B–B or N–N bond. Two high-density phases with nearly degenerate energies are interpreted to represent two experimental systems of different x-ray patterns. Most of al, the high-density phases are characterized by the existence of C–C bonds, whereas the low-density phase is characterized by the absence of C–C bonds. From the calculated equation of state and the available experimental data, we show that the unique feature of each of the cubic BC_2N phases is a direct result of the corresponding local electronic structure and chemical bonding in the system. In addition, we carried out DFT calculation to benchmark the theoretical method to obtain the reliable dielectric constant of diamond. The calculated value was 5.0 which is in good agreement with experimental value of 5.7. Therefore, we plan to use the similar theoretical framework based on DFT to calculate the materials properties of and BC2N for the project. We will calculate the elastic constants and dielectric constant of various B-C-N materials to guide the experimental materials design for low dielectric materials.

IV. Relevance to the Powering the Army programs and Expected outcomes

We are convinced that it is imperative for the National Academies of Sciences, Engineering, and Medicine to take seriously abovementioned considerations, since it is a matter of national security to have an edge in thorough scientific investigation of the unique photonic, thermal and mechanical properties characteristic to the cubic (Fd-3m) BCN single crystal. We do not want our nation to be blindsided by the advances in theoretical/experimental materials design to develop new and improved materials and technologies based on cubic BCN in future, if our proposal goes unnoticed. Therefore, we are interested in submitting a full proposal to support Army multi-domain operations (MDO) in the 2035 environment, focusing on the synthesis, comprehensive investigation of this photonic material by means of single-crystal synchrotron X-ray diffraction and, thus, unambiguously establishing structure property relationships, Raman and Brillouin scattering spectroscopy, which is solely based on laser characterization/interaction with this material, Physical Property Measurement System and hardness measurement studies in combination with predictive power of computational Physics at every step of progress in experimental development in order to enable revolutionary advances in future technologies through the discovery and characterization. The proposed technology can be categorized in Tier 1–System demonstration achievable within 5years from TRL 5-7 and TRL 7-8,and an operational system acquirable by 2035.

V. Qualification and experiences of participants

Dr. Eunja Kim (PI) is a research faculty in the Department of Physics and Astronomy at UNLV. She will lead the project. She has extensive expertise and experiences to investigate materials properties crucial for energy and device applications using the density functional theory (DFT) and molecular dynamics (MD) simulations. She has published over 125

publications in high-impact journals. She has mentored several graduate/undergraduate students in the field of radiochemistry and physics, including Hispanics, African American, and Asian American students. Currently she is leading a combined computational and experimental effort to investigate the used fuel degradation funded by DOE; a PhD student and 2 undergraduate students are involved in the project.

Dr. Sergey Tkachev (co-PI) is in charge of the unique synchrotron X-ray-based facility capable of thorough and unequivocal alongside with user-friendly analysis and examination, which ultimately lead to establishing the structure-property relationships in the sample as small as 5 – 7 microns at high temperature (up to 1200 degrees Centigrade) and pressures (up to 1,000,000 atmospheres) conditions, and provides a 24/7 user support for the above-mentioned operations at Argonne National Laboratory. He has published over 50 publications in high-impact journals. The resources he is using at GeoSoilEnviroCARS (The University of Chicago, Sector 13), Advanced Photon Source (APS), Argonne National Laboratory are supported by the National Science Foundation – Earth Sciences (EAR – 1634415) and Department of Energy-GeoSciences (DE-FG02-94ER14466), where the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility is operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

VI. Equipment/Capabilities:

UNLV Computational Resources The proposed computational studies will be conducted in the computer research laboratories in the department of Physics and Astronomy at UNLV. The networked computing facilities at UNLV will be used to run massively-parallel first-principles modeling calculations and molecular dynamics simulations with *ab initio* codes such as VASP,

CASTEP, Gaussian03, or CPMD to perform the work proposed in this project. The dedicated computing facility, to the UNLV co-PI (E. Kim) and her group members, consists of (i) 8 nodes, with 2 AMD 6-core CPUs per node (total of 96 cores) and (ii) 2 nodes with 4 AMD 8-core CPUs per node (total of 64 cores) running CentOS linux. This computer cluster is particularly well suited for addressing the resource-intensive nature of modeling and simulation of systems to be investigated in this project.

In addition, the National Supercomputing Center for Energy and the Environment (NSCEE) was established at the University of Nevada, Las Vegas (UNLV) in 1989 by an act of Congress of the United States of America (PL-101). In collaboration with Intel, Penguin Computing, and Switch Communications, the Cherry Creek supercomputer is now available for use. The original Cherry Creek 2.0 currently has the following capabilities: theoretical peak speed of 495 TFlops/s (Trillion Floating-Point operations per second), total Memory: 32.470 TB (TeraBytes), and total scratch storage of 46.32 TB. It is ranked 394 on the June 2015 Top 500 list (http://www.top500.org) and 186 on the June 2015 Green 500 list ((http://www.green500.org).

GSECARS provides earth, environmental and planetary scientists with access to the high-brilliance hard x-rays from the Advanced Photon Source (APS), a third-generation synchrotron light source at Argonne National Laboratory. Virtually all x-ray-based analytical instrumentation and techniques in demand by these scientists are available: (i) high-pressure/high-temperature crystallography and spectroscopy using the laser heated diamond anvil cell, (ii) high-pressure/high-temperature crystallography and imaging using the large-volume press, (iii) powder, single crystal and interface diffraction, (iv) inelastic x-ray scattering, (v) x-ray absorption fine structure spectroscopy, (vi) x-ray fluorescence microprobe analysis, that are crucial for sample synthesis and characterization to the project.

VII. References

[1] M. Ahmed Siddiqi, H. Yu and J. Joung, "5G Ultra-Reliable Low-Latency Communication Implementation Challenges and Operational Issues with IoT Devices", Electronics, 8(9), 981 (2019).

[2] Ji, H.; Park, S.; Yeo, J.; Kim, Y.; Lee, J.; Shim, B. Ultra-Reliable and Low-Latency Communications in 5G Downlink: Physical Layer Aspects. IEEE Wirel. Commun. 2018, 25, 124–130.

[3] 2019_army_modernization_strategy_final (https://www.army.mil/e2/downloads/rv7/2019_army_modernization_strategy_final.pdf).

[4] E. Kim and C. Chen, Phys. Lett. A **319**, 384 (2003).

[5] E. Kim and C. Chen, Phys. Lett. A **326**, 442 (2004).

[6] E. Kim, T. Pang, W. Utsumi, V. Solozhenko, Y. Zhao, Phys. Rev. B 75, 184115 (2007).

[7] W. Utsumi, S. Nakano, K. Kimoto, T. Okada, M. Isshiki, T. Tan- iguchi, K. Funakoshi, M. Akaishi, and O. Shimomura, Proceedings of AIRAPT-18, Beijing, China, 2001.

[8] Y. Zhao, D. W. He, L. L. Daemen, T. D. Shen, R. B. Schwarz, Y. Zhu, D. L. Bish, J. Huang, J. Zhang, G. Shen, J. Qian, and T. W. Zerda, J. Mater. Res. **17**, 3139 (2002).

[9] V. L. Solozhenko, D. Andrault, G. Fiquet, M. Mezouar, and D. C. Rubie, Appl. Phys. Lett. **78**, 1385 (2001).