【Grant-in-Aid for Scientific Research (S)】

Broad Section D

Title of Project : Developing the lightest functional material for smart societal infrastructure

MATSUDA Iwao
(The University of Tokyo, the Institute for Solid State Physics, Professor)

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Term of Project : FY2021-2025 Budget Allocation : 80,300 Thousand Yen
Keyword : 2D material, atomic layer, borophene, borophane

【Purpose and Background of the Research】

The "monatomic layer" has the ultimate thinness as a substance, and its physical properties are not only one of the important research subjects of modern science, but also attracting attention as a next-generation device material. While research and development are being carried out worldwide centering on the representative "graphene", we have discovered the boron monatomic sheet "borophene" and HB sheet "borophane" as new monatomic layer materials. Furthermore, we have clarified that some of these substances form Dirac nodal-loop semimetal that cannot be realized with graphene and have pioneered their functionalities such as hydrogen transports (Fig. 1).

The materials are lightweight, abundant resources, and environmentally friendly. In addition, it is also theoretically predicted to have high battery performance and expected to possess the novel Dirac electronic system that has the large response in the next-generation communication band. In this research, we will clarify the low-dimensional electronic system hidden in the borophene derivatives and the physical chemistry of boron atoms. Then, we will develop the lightest functional material for smart societal infrastructure.

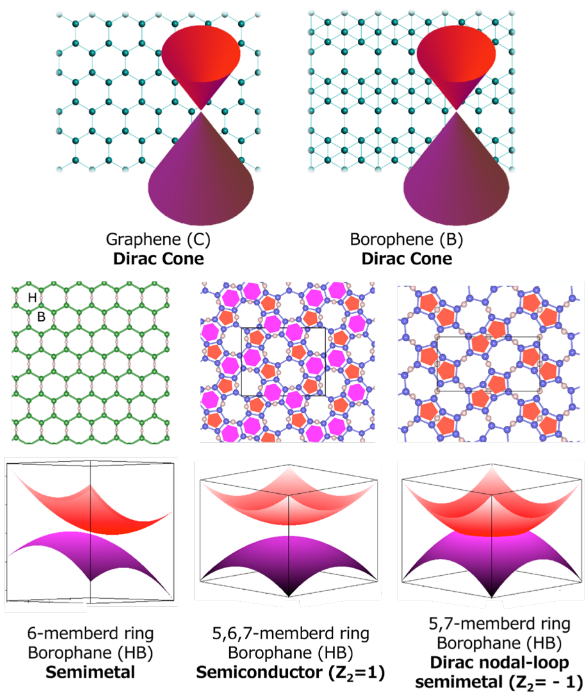

Fig. 1 Atomic structure and electronic state of light element atomic layer material. Some can be specified by the topological quantity Z_2.

【Research Methods】

In this research, we will conduct experiments on the borophene derivatives using two types of samples: a large-area synthetic sample that can be analyzed microscopically and a large-scale synthetic sample that can be easily evaluated macroscopically for practical use. Furthermore, for both, the change in electronic state under the device operating environment is observed "*operando*" together with the chemical state of boron atoms using the methods of *operando* X-ray spectroscopy that we have developed. We will comprehensively and complementarily collect material information from these measurements, clarify the origin of functionality by combining it with theoretical calculations and develop materials as smart societal infrastructure elements.

【Expected Research Achievements and Scientific Significance】

In the science and technology that supports our society, there have been promotions of the miniaturization/multi-functionalization in devices and, recently, there are also growing needs in information techniques. While such a communication network has been built between humans, it becomes necessary with things today. In the future, it will be indispensable between things. Then, the target of use will expand explosively, such as telemedicine equipment, machines in factories, livestock animals, and plants in farms. We will need a huge amount of communication elements that should be supplied from abundant material resources and be disposed with the minimum environmental load. Borophene derivative materials are requisite for such a future sustainable smart society, and this is the significance of this research.

【Publications Relevant to the Project】

- I. Matsuda and K. Wu ed., *2D boron: Boraphene, Borophene, Boronene* (Springer, 2021).
- I. Matsuda ed., *Monatomic Two-Dimensional Layers: Modern Experimental Approaches for Structure, Properties, and Industrial Use* (Elsevier, 2019).

【Homepage Address and Other Contact Information】

HP : https://imatsuda.issp.u-tokyo.ac.jp
e-mail: imatsuda@issp.u-tokyo.ac.jp