●FY2010 Yasuaki Einaga （Professor, Keio University）

Development of Innovative Technologies Using Diamond Electrodes for Improving Environment

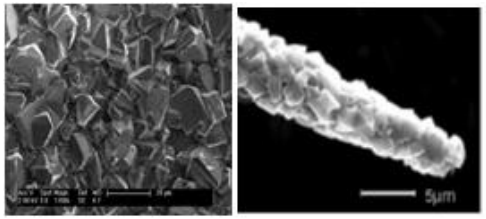
Research Project Outline (From Apr. 2011 to Mar. 2015)

Development of innovative technologies including fundamental studies on **Boron-doped Diamond (BDD) Electrodes ,**

◎To develop technologies of BDD as next generation functional materials for improving global environment.

◎To study fundamentals including physical properties of functional interfaces of BDD.

→BDD can be applied to practical devices such as electrochemical sensors, wastewater treatment systems, and carbon dioxide reduction systems.



Bonon-doped Diamond electrodes (BDD)

Research Results (FY2014)

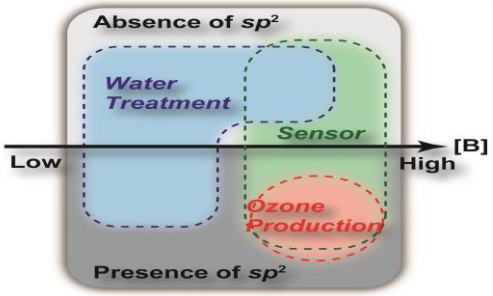
◆Tailored design for various electrochemical application

✓To design electrodes for their individual application is expected.

✓The effect of sp^2-bonded carbon impurities on the electrochemical properties of boron-doped diamond were investigated.

✓The guidelines proposed in this study can be used effectively to design electrodes according to their individual application.

Electrode design



Electrode design for applications

Physica Status Solidi (a), 211, 2709-2717 (2014).

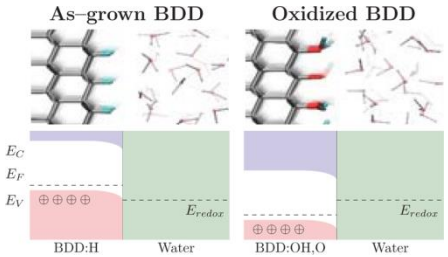
◆First principles calculation study on surfaces and water Interfaces of BDD

✓The electrochemical behavior of BDD is still challenging from a computational point of view because of the great complexity of the semiconductor/electrolyte interface.

✓Water interfaces of BDD terminated by H, O, and OH groups by using DFT-based molecular dynamics were investigated.

✓The reductive character of the H-terminated BDD is found, while the interface covered by the carbonyl oxygen is clearly oxidative.

Theoretical calculation



Electronic bands on H-BDD and O-BDD

J. Phys. Chem. C, 118, 22040-22052 (2014).