Electrocatalytic Activity of Boron Nitride Nanosheets for Oxygen Reduction Reaction
- Theoretical and Experimental Investigations -

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Oxygen reduction reaction (ORR) is one of the most important processes in fuel cells as well as in biological system. Pt based electrocatalyst is most efficient for ORR with low overpotential. However, due to high cost, less abundance, poor stability in electrochemical environment, and still sluggish kinetics of Pt based catalysts, there are worldwide research efforts to find non-precious metal catalysts. N- and B-doped carbon materials have been demonstrated to be effective metal free ORR catalysts and one may expect the increase of ORR activity by consecutive substitution of carbon atoms in graphene by B and N atoms. In an extreme case, if all carbon atoms in graphene are substituted by B and N atoms, hexagonal boron nitride (h-BN) monolayer, which has geometric structure similar to the graphene, is obtained. Although BN is an insulator with a wide band gap (5.8eV), our recent theoretical studies showed that the band gap of h-BN monolayer can be considerably reduced by B- and N- vacancy and impurity defects as well as by interaction with Ni substrate and BN on appropriate substrates can be used as an ORR catalyst [1,2]. In the present study, ORR activity of BN nanosheets (BNNS) on Au(111) is predicted theoretically and proved experimentally.

DFT calculations for BN/Au(111) show a slight protrusion of the unoccupied BN states towards the Fermi level due to the interaction between BN and Au(111) and presence of a metastable highly activated configuration of O_2 on h-BN/Au(111) with the binding energy of -0.05 eV and stable configurations of O_2 adsorbed at the edge of the BN islands on Au(111) surface, showing the possible ORR activity of BN/Au(111).

BNNS obtained by liquid exfoliation method was placed on a substrate, Au(111) or glassy carbon, by spin coating. Figure 1 shows linear sweep voltammograms of bare polycrystalline Au (black line), BNNS/Au (red line), bare glassy carbon (GC), and BNNS deposited GC (BNNS/GC) in a rotating disk electrode (RDE) configuration in an O_2 saturated 0.5M H_2SO_4 solution at the rotation rate of

1500 rpm with the scan rate of 10 mV/s. The polarization curve of BNNS/Au clearly shows the enhancement of ORR activity compared with that at the bare poly Au. It is interesting that no ORR activity enhancement by BNNS was observed in the case of GC electrode, showing the important role of BN-substrate interaction as suggested by the theoretical calculation.

References

[1] A. Lyalin, A. Nakayama, K. Uosaki, and T. Taketsugu, Phys. Chem. Chem. Phys., 15 (2013) 2809.

[2] A. Lyalin, A. Nakayama, K. Uosaki, and T. Taketsugu, J. Phys. Chem. C, 117 (2013) 21359.

Figures

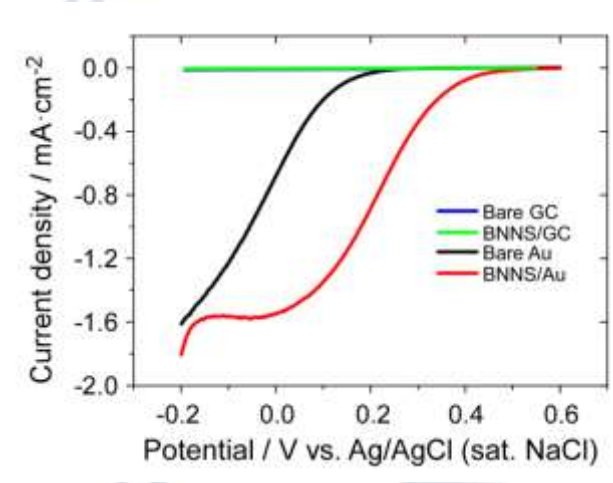

Figure 1. Linear sweep voltammograms of bare poly Au (black line), BNNS/Au (red line), bare GC (blue) and BNNS/GC (green) in an O_2 saturated 0.5 M H_2SO_4 solution. Rotation rate: 1500 rpm. Scan rate: 10 mV/s.