Development of Boron Nitride-Based Composites for Enhanced Gas Sensing Applications

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Abstract

The following research focuses on the development of boron nitride-based composites engineered for the detection of carbon monoxide and carbon dioxide through changes in electrical conductivity upon gas exposure. Silver-doped boron nitride (BN/Ag) nanoparticles were synthesized and evaluated using four-point probe resistivity measurements, along with various characterization techniques.

Introduction & Background

Hexagonal boron nitride (h-BN) is a versatile material known for its excellent thermal stability, not being chemically reactive, and layered structure. BN is non-conductive, but doping BN improves conductivity and allows usage as gas sensing material.

Doping BN with metals, particularly gold, platinum, and silver, introduces new functionalities, especially in gas sensing. Doping enables improved electronic and catalytic properties, enhancing its sensitivity and selectivity to target gases, such as CO.

The present work investigates the development of doped BN nanoparticles that are received from autoclave reaction in the system BN-$AgNO_3$-PVP, which produces nanoparticles for gas sensing applications, aiming to leverage the high surface area of h-BN and the improved conductivity due to doping with silver, while using PVP as reducing agent to receive silver from the nitrate.

Methodology

To synthesize BN/Ag, boron nitride (BN) and silver nitrate ($AgNO_3$) were combined in a 1:1 molar ratio with 0.01 mmol of PVP. This mixture was placed in a 50 mL Teflon-lined autoclave containing 30 mL of N, N-dimethylformamide (DMF). The autoclave was heated to 160°C for 8 hours and left to cool to room temperature. The resulting product was washed sequentially three times with deionized water and ethanol and later dried at 80°C. DFT electronic structure calculations, optimal geometries, and dielectric functions were obtained for optimized defect *h*-BN monolayer with/without adsorbed CO using the periodic code Vienna Ab initio Simulation Package (VASP). The projector augmented-wave (PAW) pseudopotentials were used. The Kohn–Sham equations are solved using GGA under the Perdew–Burke–Ernzerhof functional form.

Data & Results

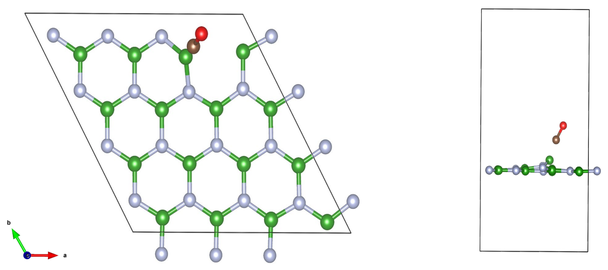

Figure 1-The top view of the DFT optimized defect h-BN monolayer with the adsorbed CO as a 4×4×1 supercell (b) its side view. Atoms are colored as follows: B, green; N, gray; C, brown; O, red. The thin black lines denote the supercell boundaries.

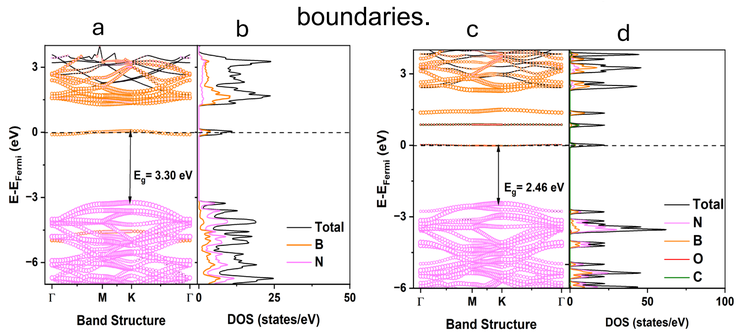

Figure 2 - (a) Electronic band structure for defect *h*-BN and (b) its densities-of-states (DOS), (c) band structure for defect *h*-BN with adsorbed CO, and (d) its DOS.

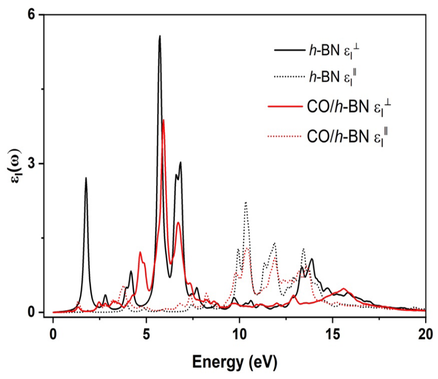

Figure 3 – The imaginary part of the dielectric function for the defect BN with and without the absorbed CO. The perpendicular and the parallel to the c-axis components are shown.

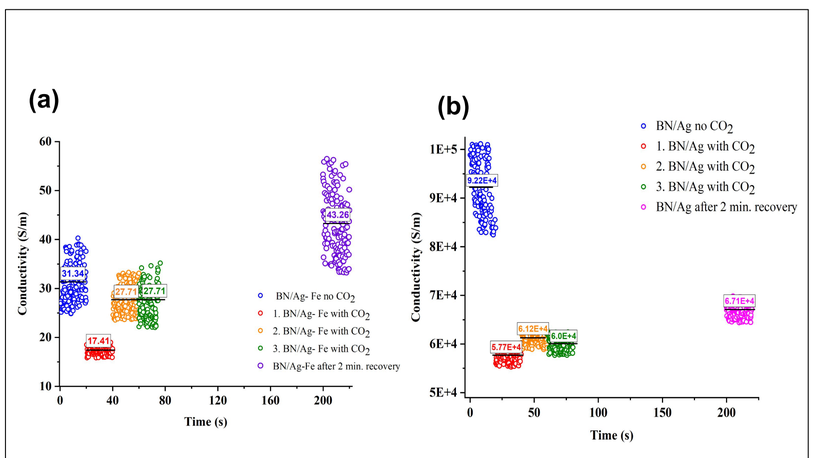

Figure 4 - (a) BN/Ag-Fe and (b) BN/Ag tested with CO2

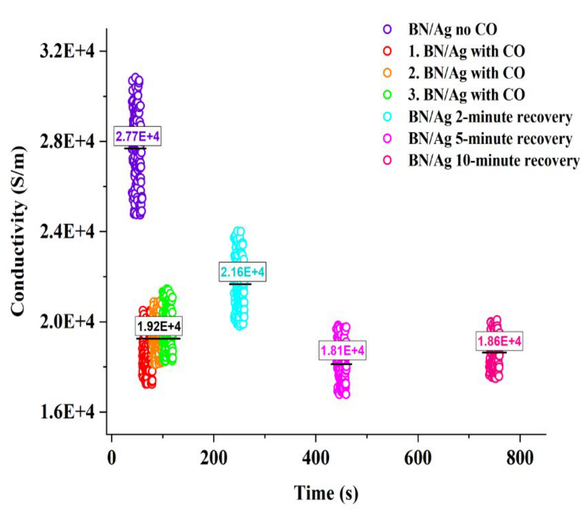

Figure 5 - (c) BN/Ag tested with CO

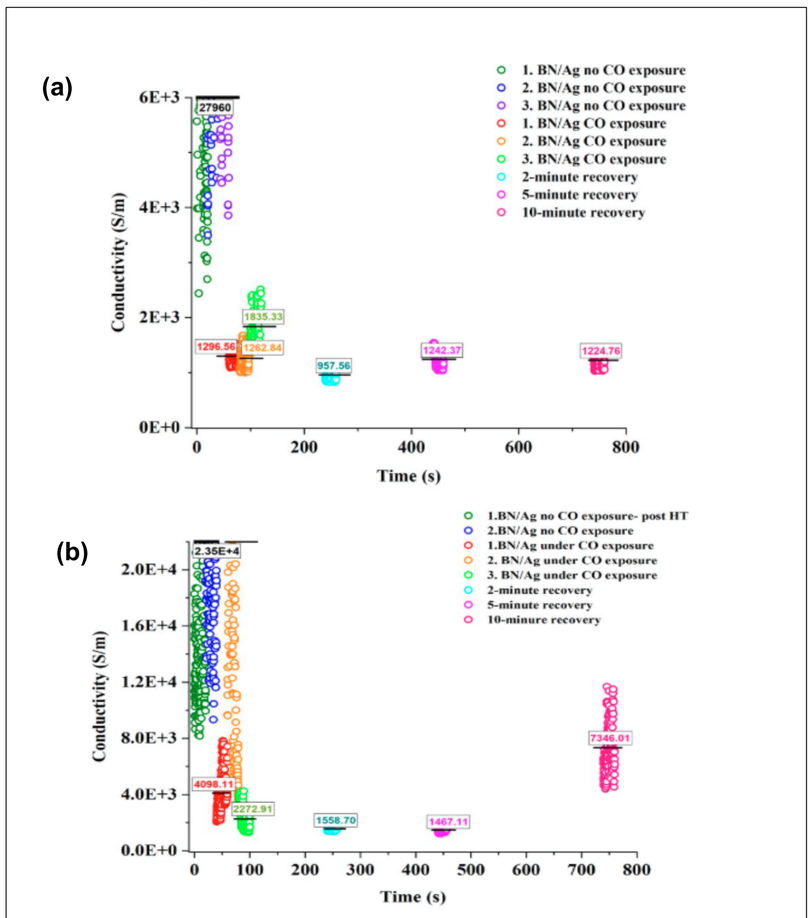

Figure 6- (a) BN/Ag testing with CO gas, (b) BN/Ag testing with CO gas after Hot plate.

Conclusions & Future Work

Computational analyses reveal that CO interactions with vacancy sites in the BN monolayer induce lattice distortions, significantly altering the material's optical and electronic properties. Figures 2–4 present the conductivity responses of BN/Ag and BN/Ag-Fe pellets upon exposure to CO and carbon dioxide (CO_2).

The BN/Ag sample exhibits a 1.6-fold reduction in conductivity immediately after CO_2 exposure, followed by partial recovery within two minutes of CO_2 removal. As for BN/Ag-Fe sample, a 1.8-fold reduction in conductivity is displayed. Under CO exposure, a similar 1.6-fold decrease in conductivity is observed; however, due to CO binding at defect sites, no initial recovery occurs until approximately 10 minutes later. To enhance the recovery rate, the BN/Ag pellet is subjected to one minute of heating on each side.

As shown in Figures 6a and 6b, the initial conductivity of the sample is 2.8 ×10⁴ S/m, which decreases to 1,224 S/m following CO exposure, with recovery occurring after 10 minutes. Heating the pellet on a hot plate restores the initial conductivity to 2.35 × 10⁴ S/m, corresponding to approximately 84% of its original value. These findings demonstrate the capability of BN/Ag for rapid and reversible detection of both CO and CO_2, underscoring its promise as an efficient gas sensing material.

Acknowledgments

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References

[1] A. Sultan, F. Mohammad, "Chemical sensing, thermal stability, electrochemistry and electrical conductivity of silver nanoparticles decorated and polypyrrole enwrapped boron nitride nanocomposite" ,*Polymer,* vol.113, 221-232 (11 pages), 2017