SM-P022

Electrohydrodynamic 젯 프린팅 시스템을 이용한 Graphene 기반 Graphene/Ag-grid 하이브리드 투명 전극의 특성연구

박하늘[1], 조다영[1], 이혜민[1], 서기원[1], 김효중[1], 이영우[2], 김지훈[2], 김한기[1]*

[1]경희대학교 정보전자신소재공학과, [2]공주대학교 신소재공학부

본 연구에서는 Electrohydrodynamic (EHD) 젯 프린팅 시스템을 이용하여 graphene이 올려져 있는 유연성 있는 PET 기판 위에 Ag 용액을 그리드로 간격에 따라 타진하였다. Ag 그리드 간격을 200 um, 300 um, 400 um, 500 um로 증가시켰으며, 이때 UV/Vis spectrometry, four-point probe를 이용하여 전기적, 광학적 특성을 분석하였다. Graphene/Ag-grid 하이브리드 투명전극은 그리드 간격 400 um에서 21Ohm/sq.의 면저항과 550 nm에서 84.08%의 투과도를 확인하였다. 또한, graphene/Ag-grid 하이브리드 투명전극의 기계적 응력에 따른 전기적 안정성을 알아보기 위해 radius에 따른 bending, fatigue test와 twist bending, rolling test를 진행하였다. Fatigue bending은 speed 30 mm/s, outer bending radius 20 mm, inner bending radius 22.5 mm로 bending test를 5000번 진행하였으며, twist bending, rolling test를 각각 10000번 진행하였다. 이 결과를 통해 bending-release cycle 조건에서도 초기저항 대비 5% 이내의 매우 우수한 전기적 안정성을 나타냄을 확인하였다. 이러한 graphene/Ag-grid 하이브리드 투명전극의 우수한 특성을 얻음으로써, graphene 박막의 플렉시블 투명전극으로서의 적용가능성을 타진할 수 있었다.

Keywords: EHD 젯 프린팅, 하이브리드, 플렉시블 투명전극

SM-P023

First-principles Study of Graphene/Hexagonal Boron Nitride Stacked Layer with Intercalated Atoms

Dongchul Sung, Gunn Kim, Suklyun Hong*

Graphene Research Institute and Department of Physics, Sejong University

We have studied the atomic and electronic structure of graphene nanoribbons (GNRs) on a hexagonal boron nitride (h-BN) sheet with intercalated atoms using first-principles calculations. The h-BN sheet is an insulator with the band gap about 6 eV and then it may a good candidate as a supporting dielectric substrate for graphene-based nanodevices. Especially, the h-BN sheet has the similar bond structure as graphene with a slightly longer lattice constant. For the computation, we use the Vienna ab initio simulation package (VASP). The generalized gradient approximation (GGA) in the form of the PBE-type parameterization is employed. The ions are described via the projector augmented wave potentials, and the cutoff energy for the plane-wave basis is set to 400 eV. To include weak van der Waals (vdW) interactions, we adopt the Grimme's DFT-D2 vdW correction based on a semi-empirical GGA-type theory. Our calculations reveal that the localized states appear at the zigzag edge of the GNR on the h-BN sheet due to the flat band of the zigzag edge at the Fermi level and the localized states rapidly decay into the bulk. The open-edged graphene with a large corrugation allows some space between graphene and h-BN sheet. Therefore, atoms or molecules can be intercalated between them. We have considered various types of atoms for intercalation. The atoms are initially placed at the edge of the GNR or inserted in between GNR and h-BN sheet to find the effect of intercalated atoms on the atomic and electronic structure of graphene. We find that the impurity atoms at the edge of GNR are more stable than in between GNR and h-BN sheet for all cases considered. The nickel atom has the lowest energy difference of ~0.2 eV, which means that it is relatively easy to intercalate the Ni atom in this structure. Finally, the magnetic properties of intercalated atoms between GNR and h-BN sheet are investigated.

Keywords: Density Functional Theory, Graphene, hexagonal Boron Nitride (h-BN), Graphene nanoribbon (GNR)