

Interface Characterization of Ohmic Metal Contacts to NanoCarbon Diamond Films via Photoemission

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1. Abstract

Ohmic metal contacts to n-type diamond have historically posed a challenge to the fabrication of diamond devices, due to the formation of a rectifying Schottky barrier, which increases contact resistance and limits the scope of practical devices. However, ohmic contact to nitrogen-doped, n-type nanostructured carbon (nanoCarbon) films have been demonstrated in previous work [1], and confirmed in this work, progressing towards the integration of devices utilizing n-type diamond for power electronics. Yet, the Ohmic contact mechanism is unclear.

In this work, the ohmic contact mechanism of ~400 nm thick nanoCarbon films with nitrogen incorporation on the order of $\sim 2 \times 10^{20} \text{ cm}^{-3}$, grown via microwave plasma-enhanced CVD on (100) and (111)-oriented IIa diamond substrates, were investigated via photoemission, and ohmic n-type contact properties were confirmed via Hall Effect measurements. Titanium and molybdenum layers were deposited on nanoCarbon/IIa-(100) and nanoCarbon/IIa-(111) films, respectively, and each metal/nanoCarbon interface was characterized via X-ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS), Transmission Electron Microscopy (TEM), and Raman Spectroscopy. The photoemission data were used to determine the Schottky barrier height (SBH), valence band maximum at the surface with respect to the Fermi level (VBM), and work function of the surfaces.

From UPS, the nanoCarbon/IIa-(100) and nanoC/2a-(111) surfaces displayed an initial work function of 3.7 eV and 4.0 eV, and a VBM of 1.8 eV and 1.7 eV, respectively. Deposition of molybdenum and titanium on nanoCarbon/IIa-(100) and nanoCarbon/2a-(111) surfaces induced changes in the work function of +0.6 eV and +0.7 eV, respectively, as well as a change in the VBM of +0.1 eV and -0.3 eV, respectively. The n-type Schottky barrier height was determined to be $\Phi_B = 3.7 \text{ eV}$ and $\Phi_B = 4.1 \text{ eV}$ for the titanium-nanoCarbon/IIa-(100) and molybdenum-nanoCarbon/IIa-(111) interface, respectively.

Evidence of sp^2 bonding in the nanoCarbon from Raman spectroscopy is used to propose a mixed-phase band diagram with states in the gap to understand the ohmic contact mechanism, given the SBH: Hopping-type conduction occurs near the Fermi level through theorized π^* -bonded states for tetrahedral amorphous carbon with nitrogen incorporation. Such states reduce the effective n-type SBH and mediate ohmic n-type conduction into the nanoCarbon. In future work, the interface between nanoCarbon films and phosphorous-doped diamond substrates will be characterized as a strategy to enable ohmic contact with phosphorous-doped diamond.

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3. References

[1] Evangeline Amonoo, Vishal Jha, Trevor Thornton, Franz A. Koeck, Robert J. Nemanich, Terry L. Alford, Ohmic contacts to nitrogen-doped nanocarbon layers on diamond (100) surfaces, *Diamond and Related Materials*, Volume 135, 2023, 109832, ISSN 0925-9635, <https://doi.org/10.1016/j.diamond.2023.109832>