Comparisons of Post-Etch Diamond XPS Analysis with Simulations

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Abstract: We report XPS measurements of amorphous layer thickness in diamond samples exposed to Ar or Ar/O_2 plasmas under variable bias and compare them to molecular dynamics simulations. Findings indicate that the density and hybridization profiles of carbon must be accounted for in order to develop an accurate picture of the surface region.

1. Introduction

Nitrogen-vacancy or NV centers are formed in diamond when nitrogen substitutions are adjacent to substitutional vacancies in the diamond lattice. This combination creates levels within the bandgap of diamond which can be excited using visible light. When used in quantum applications these excitations have the promising feature of long coherence times even at room temperatures. [1]

Unfortunately, the coherence time has been shown to be dependent upon depth beneath the surface of the diamond lattice, as well as defects and impurities near the surface. [2] To maximize coherence times, a thorough investigation of the details of plasma exposure upon the surface layer need to be conducted.

2. Methods

An ICP reactor is used to expose a nitrogen-doped diamond sample to various plasma conditions. The sample is then transferred under vacuum to an XPS system for surface analysis. This analysis is then compared against simulation results for further elucidation and validation.

The primary subject of the experiments reported here is the effect of self-bias voltage in a pure Argon plasma at 10mTorr upon amorphous layer thickness. A range of values from 100 V (sputter threshold) to 200 V were investigated.

Molecular dynamics simulations were run through the LAMMPs platform. REBO was used to determine the relevant interatomic potentials and so to provide composition details.

3. Results and Discussion

Upon exposing the sample to an Argon plasma, the XPS analysis shows that the carbon 1s peak centered at 284.5 eV develops a second peak near 283.2 eV, ascribed to carbon sp^2, i.e. carbon bound to two carbon atoms, while the main peak is the sp^3 carbon with full tetrahedral bonding. A 2-peak fit to the measured C(1s) spectrum, yields an estimated percentage of amorphous carbon averaged over the near surface region of ~3 nm, sensed with an XPS takeoff angle of 30°. Figure 1 presents this measured amorphous layer percentage as a function of bias voltage.

The simulations predict a similar upward trend in amorphous layer thickness as bias voltage increases. A more detailed comparison will be presented, utilizing computed atom densities and carbon hybridization, combined with computed electron inelastic mean-free paths. Similar measurements and simulation of the diamond surfaces after Ar/O_2 plasma etching will also be presented.

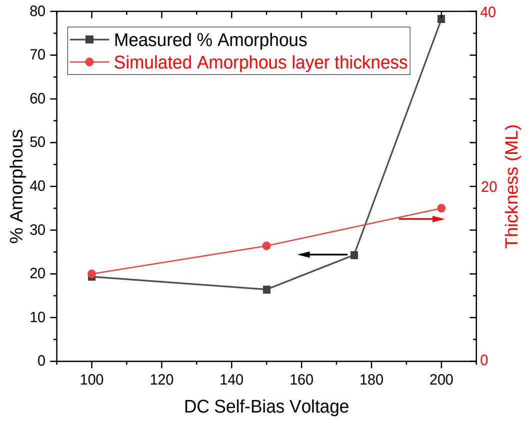

Fig. 1. Measurements of percent amorphous carbon in the near-surface region of diamond (100) surfaces, determined from the C(1s) XPS signal, after long exposures to Ar plasmas (black squares). Simulated amorphous layer thickness in monolayers (red circles), as a function of substrate DC self-bias voltage.

4. Conclusion

XPS investigations of single crystal diamond (100) after plasma exposure indicates a change in the carbon bonding near the surface. The presence of a sp^2 peak indicates the amorphization (graphitization) of the near-surface, which increases with DC substrate bias voltage, above a threshold of about 100 V, in agreement with simulations.

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References

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