The inner workings of sp^2 clusters in a-C:N according to UV-Vis-NIR optical analysis

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The possibility of large-scale production and low temperature deposition makes nitrogen-incorporated amorphous carbon (a-C:N) a suitable material for flexible electrodes or single-use sensors. The conduction mechanism in a-C:N thin films has been mainly attributed to sp^2 cluster size, which commonly scales linearly with the incorporation of nitrogen into the growing film. While the optical bandgap is correlated to cluster sizes, simple tools to understand the inner workings of those clusters need to be developed to further the understanding of the electrical conduction mechanism and material applications.

In this study, a-C:N thin films (~100 nm) are deposited by pulsed laser controlled cathodic arc (LaserArc) at various N_2 flow rates onto fused silica glass substrates. The optical constants, refractive index [n] and extinction coefficient [k], are solved by numerical methods from the measured reflectance [R] and transmittance [T] between 0.5 and 6.5 eV (190 and 2500 nm), which is dominated by conjugated p_z electrons within clusters of sp^2 hybridized carbon atoms. Once the optical constants are available, a variety of quantitative information is generated, such as the polarizability, and electron densities.

This study finds, that the sp^2 nature of these clusters is neither constant nor uniform as the cluster dimension changes, where larger clusters do not automatically mean greater conductance. By combining the physical density and electron density determined by optical sum rule analysis, it is shown that the number of conjugated p_z electrons per atom varies with changes in N_2 flow. Although the sum rule integration is limited by the spectral range of our spectrophotometer, the range to high energies can be extended by modeling of the measured [n,k] optical constants to capture the full electron count. Spectroscopically, we find that electrical conductivity of the material is not simply about the number of p_z electrons, but importantly about the volume that they occupy, i.e., it is about the conjugation of those sp^2 bonded carbon and nitrogen atoms.