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Electronic and Structural Characterization of Diamondoid Carbon Nanothreads by Transmission Electron Microscopy

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Diamondoid carbon nanothreads are the first in a new category of one-dimensional sp^3-bonded carbon nanomaterials [1]. Recent studies have revealed single-crystalline packing of cylindrical structures into a two-dimensional pseudo-hexagonal lattice [1], [2]. These investigations reveal ~20% sp^2 bonding mixed in with the primarily diamond-like sp^3-bonded nanothreads [1]. While recent transmission electron microscopy (TEM) imaging reveals additional structural order at the nanoscale in this class of materials, the electronic and fine structure of diamondoid carbon nanothreads are completely unexplored and requires further investigation to elucidate its potential properties and illuminate the reaction mechanism [3], [4].

In this study, scanning/transmission electron microscopy (S/TEM) imaging coupled with electron energy-loss spectroscopy (EELS) is employed to examine the atomic, chemical, and electronic structure of carbon nanothreads. *Low-dose* EELS from the carbon K-edge in carbon nanomaterials reveals the bonding nature of the carbon to be primarily sp^3-bonded with hydrogen termination, as indicated by a small C=C π* peak (284 eV), a broad C-C σ* peak (290 eV), and the appearance of a C-H σ* peak (287 eV) (Figure 1a) [5]. Using S/TEM imaging and EELS this presentation will explore the beam-induced damage of the carbon nanothreads and the structural transformation of this nanomaterial as a result. Quantification of the sp^2/sp^3 ratio from our EELS measurements indicate that the nanothreads are primarily made of sp^3 bonded carbon atoms with a low sp^2 carbon content after accounting for the electron beam damage, as previously confirmed by NMR [1].

The electronic structure of the nanothreads is also probed by monochromated low-loss EELS to explore the present phonon vibrational modes in this crystal. The observed phonon modes appear at 170 meV and 370 meV which agree well with vibrational modes observed in Raman spectroscopy of bulk nanothreads (Figure 1b). In addition, this work will explore the optical band gap of the nanothreads and how it is compared with the existing calculations from ultraviolet-visible spectroscopy data [1]. Low loss EELS analysis as well as the plasmon peak also provide valuable insight on the bonding nature and the electronic structure of this nanostructure and is the key further explore potential applications of this unique carbon nanostructure.

References:
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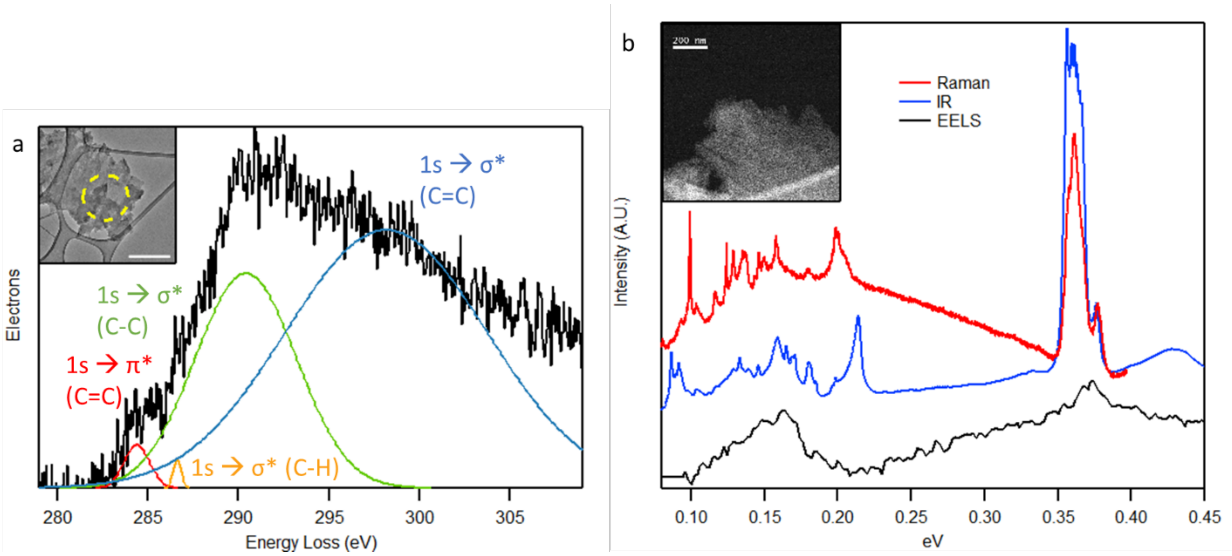

Figure 1. (a) Low-dose EELS spectrum of the carbon K-edge of carbon nanothreads with Gaussian fits of the major electronic transitions displayed. (b) Low-loss EELS spectrum of carbon nanothreads showing phonon modes compared with Raman and IR spectra of bulk nanothreads.