PS10.11.08 QUANTITATIVE NANO DiffRACTION FROM CARBON NANO TUBES. J. M. Cowley, Department of Physics and Astronomy, Arizona State University, Tempe, AZ 85287-1504, USA.

Electron diffraction patterns obtained with coherent electron beams less than 1 nm in diameter may now be recorded digitally by use of a CCD detector and quantitative structural analyses may be made of small regions such as portions of the walls of carbon nanotubes. It has been known theoretically for a long time that, for coherent diffraction with a small beam, the diffraction pattern from single-walled nanotubes and clusters of single-walled nanotubes are of interest in this connection because their curved walls have polygonal cross-sections and are of interest in this connection because their curved walls have polygonal cross-sections. Observations on diffraction pattern asymmetries may thus be used to deduce information on the curvature of nanotube, or nano-particle, walls in regions where the structure is less obvious such as at the ends of nanotubes and at bends in the walls. Diffraction patterns from single-walled nanotubes and clusters of single-walled tubes are more difficult to record because the scattering is very weak, but can give valuable information on the helicity of the tubes, the regularity of the packing of the clusters and the deformations associated with tube bending.


The crystallographic analysis of the C₆₀ molecules orientational ordering in a crystal structure and there influence on the features of diffraction pattern was carried out. The different leaves of correlation's between symmetry axes of icosahedral molecule and cubic lattice are considered. It established the magnitudes of rotation angles (44.47° and 75.83°) by transition from face-centered (Pm3) to primitive (Pm3, Pn3, Pn3) cubic structure. The result used for analysis of possible orientational ordering models, including modulation structure and discrete orientational glass.

The next interesting problems is the peculiarities of diffraction picture and its variations near the order-disorder phase transition. We have analyzed the Fourier image of the C₆₀ molecules and its superposition with Lane interference function. For disordered state the Fourier image defined the good visibility of diffraction pattern only by small range of angle and also the special extinction by condition N+k²=4n². For the "freezing" structure, including all variations of orientational ordering by lower temperature and possible other structure transformations, the image is a quite differ. The spherical symmetry of Fourier image is lost and as following the local maxima are raised by large diffraction angle. The comparison of calculated diffraction distributions and the experimental data are discussed.

PS10.11.10 STRUCTURE OF THE C₆₀-TMPD NEW COMPLEX. V. V. Gritsenko, O. A. Dyachenko, V. A. Nadtochenko, Institute of Chemical Physics in Chernogolovka, RAS, Chernogolovka, Moscow region, 142432 Russia.

The crystal structure of a C₆₀-TMPD (1) (TMPD — N,N,N',N'-tetramethylparaphenylene diamine) new complex with charge transfer was studied by X-ray analysis. The charge transfer is confirmed by IR-spectrum data. The red shift for the number of vibrational modes, especially for the 1428 cm⁻¹ mode, is observed in IR-spectra, which corresponds to a partial charge transfer from the amine molecule to C₆₀. The X-ray structural data also testify to the charge transfer in I: the TMPD molecules is flat, that pointing to the molecule charging.

It is shown that there are fullerene layers between which the TMPD molecules are arranged in the crystal structure. The shortened contacts of the C₁₋C₂ type (3.21(2)—3.32(1)Å) are discovered between TMPD and fullerene (Fig. 1). Such contact shortening is obviously based upon the donor-acceptor interaction of TMPD with C₆₀. The presence of the shortened C₁₋C₂ contacts accounts for the relative ordering of the fullerene in the structure I.

![Fig. 1](image-url)