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Quantitative structure determination of individual carbon nanotubes using nano-area electron diffraction

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The atomic structure of a perfect single-wall carbon nanotube (SWNT) is uniquely defined by its chiral vector (*n,m*), which also determines the electronic properties of the tube. As-grown SWNTs have a dispersion of chirality and diameters; the nanotube structural energy is only weakly dependent on chirality. Hence, a critical issue in CNT applications and science study is the structure determination of a given individual tube.

Here we introduce a technique for quantitative determination of the chiral vector of individual SWNT using nano-area electron diffraction. This technique has also been applied to double-wall carbon nanotubes (DWNT) and small DWNT bundles. As shown in Fig. 1, a 50 nm parallel electron probe was obtained in a JEOL2010F transmission electron microscope and was employed to select individual SWNTs for diffraction acquisition. Recording the diffraction pattern using digital imaging plate makes the very weak diffraction features visible. Fig. 2a shows a diffraction pattern from a SWNT of a diameter of 1.4 nm which was determined to be (14,6). The equatorial oscillation (Fig. 2c) is used to determine the diameter of SWNTs and distinguish between different forms of CNTs. The chiral angle is measured from the distances between the diffraction lines to the equatorial line (Fig. 2d) using following equation:

$$\alpha = \operatorname{atan}\left(\frac{1}{\sqrt{3}} \bullet \frac{d_2 - d_1}{d_3}\right) = \operatorname{atan}\left(\frac{1}{\sqrt{3}} \bullet \frac{2d_2 - d_3}{d_3}\right).$$

The accuracy of the measurement of diameter and chiral angle are estimated to be <1% for the diameter and <0.2° for the chiral angle, which allows an unambiguous determination of the chiral vector (n, m). In addition, the measurement is not affected by the inclination of the tube. The validity of this technique is proved by kinematic simulations (Fig. 1b).

By means of this technique, the chiral vectors of individual shells in DWNTs and small CNT bundles may also be determined unambiguously. In DWNTs, the wall distance and chirality relationship were studied.

Reference:

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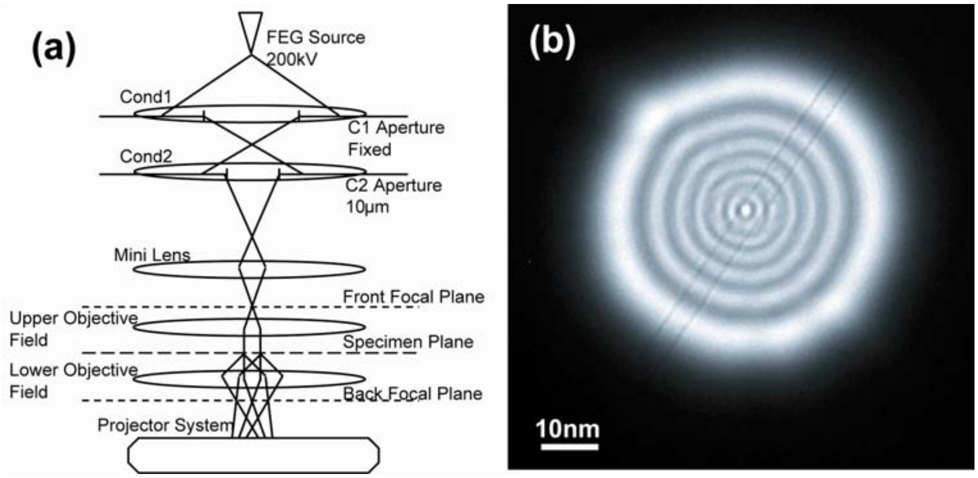

Fig. 1 (a) Schematic ray diagram of electron nano-area diffraction in JEOL2010F transmission electron microscope. A parallel beam is formed by focusing electron onto the front-focal plane of pre-objective lens. The beam size is determined by condenser aperture. (b) An image of the electron probe formed by a 10 μm condenser aperture with an individual tube illuminated. The probe current intensity is ~10^5 e/s·nm^2 with a Schottky field emission gun.

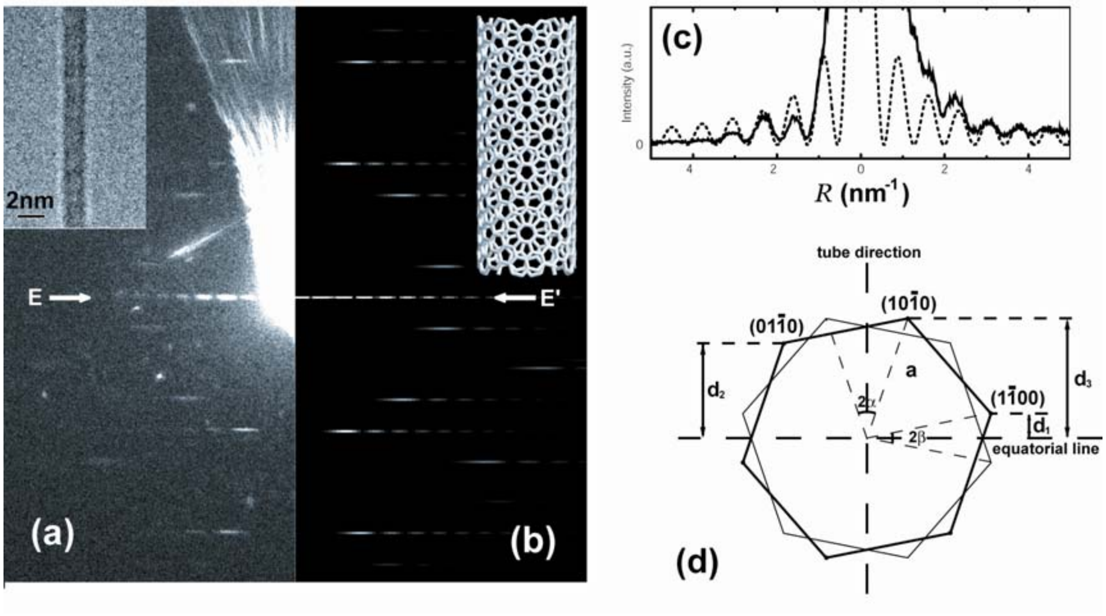

Fig. 2 (a) A diffraction pattern from an individual SWNT of 1.4 nm in diameter. The inset is a TEM image. The radial scattering around the saturated (000) is an artifact from aperture scattering. (b) A simulated diffraction pattern of a (14,6) tube. The inset is the corresponding structure model. (c) Profiles of equatorial oscillation along EE' from Fig. 2(a) and simulation for (14,6). (d) A schematic diagram of electron diffraction from an individual SWNT. The two hexagons represent the first order graphite-like $\{10\bar{1}0\}$ diffraction spots from the top and bottom of the tube.