HISTORICAL NOTE

There is a large amount of online material on the history of nanotubes discovery (e.g. time line for nanotube research in Wikipedia). However, one interesting, but not widely known historical fact is worth to be mentioned here. The possibility of nanotubes existence was predicted with the help of computer Density Functional simulations by C.T. White (Naval Research Lab, Washington DC, USA) simultaneously with their experimental observation by S. Iijima (NEC Corporation, Tsukuba, Japan). The research of C. White was conducted in attempt to find truly metallic one-dimensional systems. Such structures should not be susceptible to Jahn-Teller distortion, which breaks symmetry of the system and opens a finite (though sometimes very small) band gap. Fifteen years later C. White privately supposed that (carbon) nanotubes are the only truly metallic 1D systems and the existence of other 1D systems is unlikely. This exceptional property of nanotubes is due to the high symmetry of nanotubes and high strength of carbon-carbon bonds, which make the temperature of Jahn-Teller transition (from distorted to undistorted state) very low. Initially C. White considered nanotubes purely hypothetical structures with low chances to be synthesized, but has reported his findings at the last day of APS March meeting in 1991 (when most attendees have already left). After that he was contacted by S. Iijima who made a report on experimental observations of nanotubes at the same conference. One of the reasons for explosive scientific interest in nanotubes was due to the existence of comprehensive theoretical explanation of nanotubes properties at the time of their observation by S. Iijima. That partly explains why multiple previous observations of nanotubes (starting in 1952; USSR) and even US patent on nanotubes synthesis (by H.G. Tennett from 1987) have not created such inter-est as S. Iijima's work.

KEY PROPERTIES OF CARBON NANOTUBES

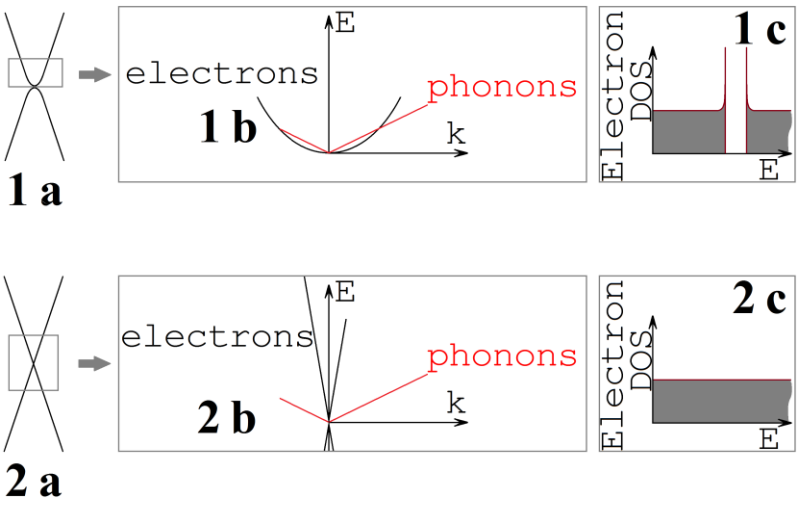
One of the most important early theoretical advances was the explanation of why CNT conductance is very stable with respect to miscellaneous distortions such as phonons and static defects. The average mean free electron path in CNT at room temperature is of the order of microns, which by far exceeds the mean free paths in nano-wires or in systems of higher dimensionality.

The absence of Jahn-Teller distortion allows bands to cross at the Fermi level (E_F). To illustrate the importance of that fact let us first consider what happened if CNTs were susceptible to Jahn-Teller distortion. Such distortion opens a band gap; electronic dispersion of above mentioned hypothetical CNT is depicted in Fig. 1a and the blowup in the vicinity of E_F is in Fig. 1b. Electron-phonon scattering must comply with energy and momentum conservation laws. Due to high strength of C-C bonds, the energy of optical phonons is rather high – about 0.15 eV. Therefore, for electrons with energies near E_F there is virtually no scattering on optical phonons, and only acoustic phonons should be considered. Dispersion of acoustic phonons can be

approximated with a linear function $\varepsilon = a|q|$ within a wide region around gamma point, where ε is the phonon energy, q is the phonon wave number, and a is a positive constant (red curve in Fig. 1b). Hence, the conservation laws are:

$$\frac{m_{eff} k_1^{\,2}}{2} + a|q_1| = \frac{m_{eff} k_2^{\,2}}{2} + a|q_2|$$
$$k_1 + q_1 = k_2 + q_2$$

Here k is the wave number of electron, and indexes 1 and 2 denote respectively initial and final states. For any k_1 and q_1 these two equations always have non-trivial solutions with $k_1 \neq k_2$ and $q_1 \neq q_2$, i.e. conservation laws do not prohibit electron-phonon scattering.



Density of electronic states in 1D systems exhibits van-Hove singularities at the bands inflection points, including band edges. Figure 1-c schematically depicts two such singularities near E_F. The rate of elastic scattering on static random uncorrelated defects (e.g. potential distortion imposed by a substrate supporting CNT) is proportional to the fourth power of DOS (as is explained in Challenge Problem for CNT - /topics/CNTBandsChallengeProblem). Hence the presence of even small band gap near E_F substantially deteriorates conductance of 1D system due to both elastic and inelastic scattering.

In the absence of Jahn-Teller distortion bands cross each other. That makes the dispersion linear (Figs 2a-b). The conservation laws

$$bk_1 + a|q_1| = bk_2 + a|q_2|$$
$$k_1 + q_1 = k_2 + q_2$$

have only trivial solution $k_1 = k_2$ and $q_1 = q_2$ for $a \neq b$ (for CNT $a << b$), which means the scattering on acoustic phonons in metallic CNTs is prohibited to the first order. The DOS in the vicinity of E_F is constant and small (just one open conduction channel), which makes elastic scattering on static defects low, and gives rise to extremely robust conductance and long electron mean free path.

All metallic CNT's have two dispersion branches crossing the Fermi energy, each brunch corresponds to one conductance quanta for a given spin. Quantum conductance in 1D periodic structures follows from the trivial identity:

$$1 = \left|\frac{\partial \varepsilon}{\partial k}\right| \left|\frac{\partial \varepsilon}{\partial k}\right|^{-1} = \hbar v \; DOS\left[\varepsilon\right],$$

where v is group velocity of electron. As it is demonstrated in [/topics/CNTBandsProblems Problem 4], in the nearest neighbor π-orbital tight-binding approximation the value of v at E_F is the same for all metallic CNTs. That means the larger is the diameter of CNT, the smaller is the density of states in the energy window near E_F where only two conduction channels are available. Therefore conductance robustness in CNTs with respect to distortion potential is a trade of the two factors. CNT diameter increase reduces DOS in the two-band conduction window and hence reduces the scattering probability. The second factor is the mechanical stability of CNT, which got compromised if the CNT diameter becomes too large. Figure 3a demonstrates critical angle for {8,8} CNT. If the bending angle is less than critical, the CNT transmission within a two-bands window near E_F remains nearly ideal (Figure 3b). Only when a kink forms (Figure 3c) and sp^2 bonding is disrupted, the transmission within a two-bands window deviates from its ideal value.

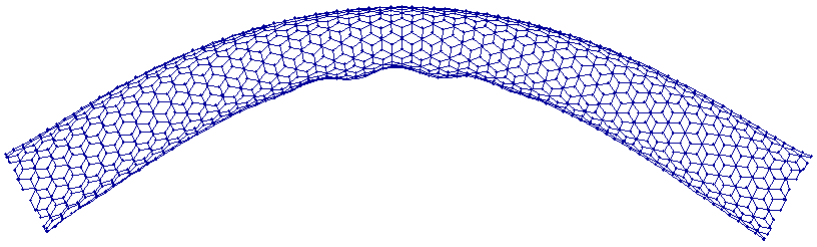


Figure 3a

{8,8} CNT bended by 56 degrees

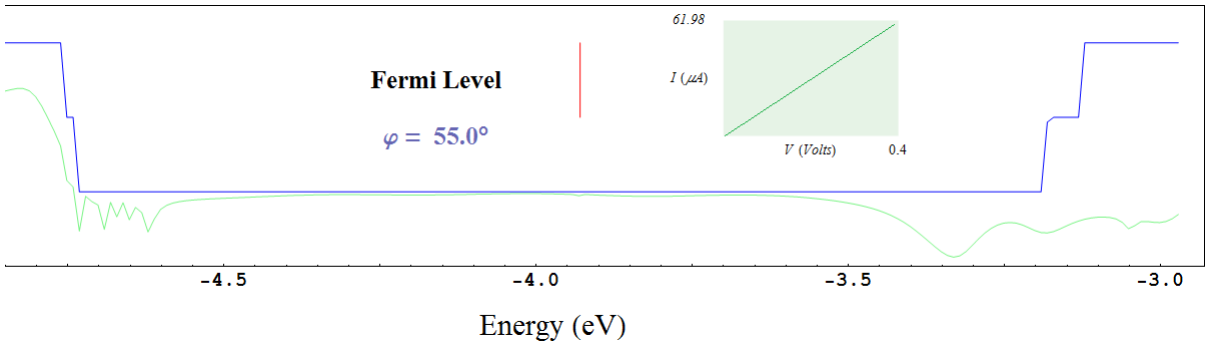


Figure 3b

Transmission for (7,10) CNT bent to 55 degrees in a Self-Consistent Environment-Dependent Tight Binding approximation.

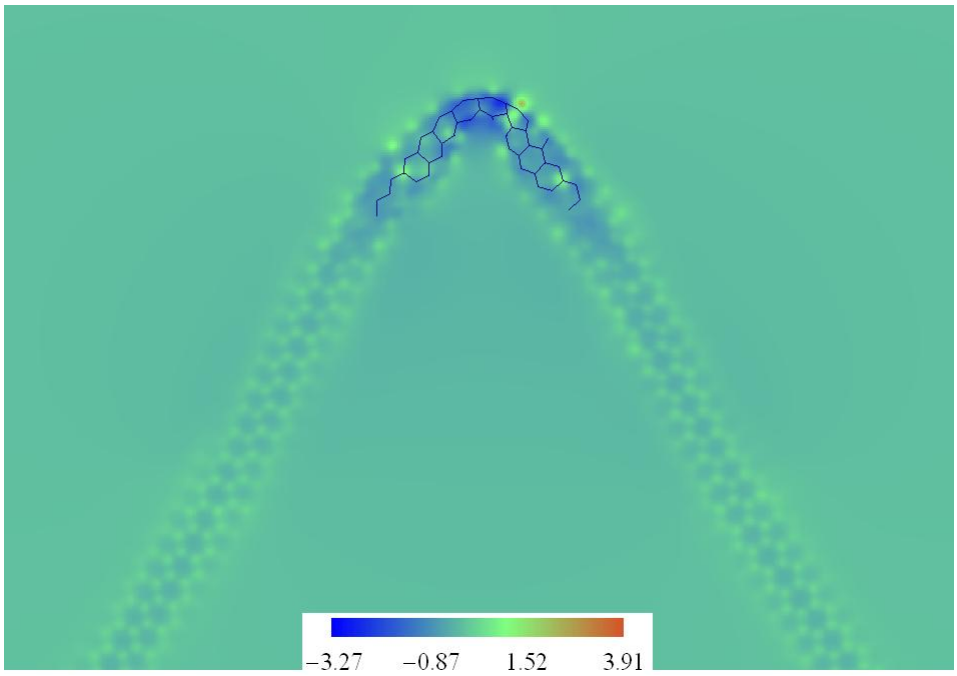


Figure 3c

Electrostatic potential in a Self-Consistent Environment-Dependent Tight Binding approximation in the plane raised above {7,10} CNT by a distance slightly exceeding its radius. Only kinked portion of CNT (solid blue lines) appears above the plane.