Lecture 4. Properties of Single-Walled Carbon Nanotube (SWCNT). Purification of SWCNTs

The purpose of the lecture: to provide information on the properties of single-walled carbon nanotube.

Expected results: be able to distinguish between the properties of single-walled carbon nanotube.

SWCNTs are endowed with exceptionally high material properties, very close to their theoretical limits, such as electrical and thermal conductivity, strength, stiffness, and low density.

Mechanical Properties

The impressive mechanical properties of SWCNTs originate from their geometrical structure and C–C bond. The carbon–carbon bond in the basal plane of graphite is one of the strongest bonds in nature. Small diameter SWCNTs are very stiff and exceptionally strong, which corresponds to having a high Young’s modulus and tensile strength. This would imply that SWCNTs are very stiff and difficult to bend. However, SWCNTs seem to be very resilient when bent and can buckle like straws without breaking and can be straightened back without any damage. Most of the materials fracture at bending due to presence of defects or dislocations, but SWCNTs have very few defects on their sidewalls, which is why they have very high mechanical properties and resilience (i.e., strain to failure).

Various efforts have been made to investigate the mechanical properties of CNTs, experimentally and theoretically. Nanotubes are the stiffest fibers, with a measured Young’s modulus of 1.4 TPa. Additionally, they have an elongation to failure of 20% to 30%, and tensile strength around 100 GPa. These values are much higher comparatively with highstrength steel (Young’s modulus ~200 GPa and its tensile strength is 1 to 2 GPa). The exceptional stiffness and strength with low density implies that CNT could be used as an ideal reinforcement in composite materials.

Specific Gravity

Specific strength of any material plays a key role in designing of structural materials. The hollow structure of CNTs makes them very light (specific gravity of 0.8), and this is very useful for a variety of lightweight high strength applications. The specific gravity of steel, on the other hand, is 7.8. Therefore SWCNTs have specific strength value at least two orders of magnitude greater than steel. Similarly, the specific strength of traditional carbon fibers (specific gravity ~1.78) is only 40 times that of steel.

Thermal Conductivity

The specific heat and thermal conductivity of CNT systems are determined primarily by phonons. Nanotubes are very conductive for phonons in their axial direction, whereas in the transverse direction their conductivity is very low. Theory predicts an unusually high value of thermal conductivity, that is, 6000 W/mK at room temperature; however thermal conductivities as high as 3000 W/mK at room temperature have been measured which is equivalent to the thermal conductivity of natural diamond and basal plane of graphite.

Electrical Conductivity

SWCNTs can either be a metal or semiconductor, depending on their diameters and helical arrangement. The condition whether a CNT is metallic or semiconducting can be obtained based on the band structure of a 2D graphite sheet and periodic boundary conditions along the circumference direction. The differences in conductivity can easily be derived from properties of the graphene sheet. It was shown that a (n, m) nanotube is metallic if $n = m$ or $(n - m) = 3i$, where i is an integer and n and m are parameters defining the nanotubes structure or chiral vector. Due to their one-dimensional nature, charge carriers can travel through nanotubes without scattering, resulting in ballistic transport. The absence of scattering means that joule heating is minimized and thus nanotubes can carry very large current densities (up to 100 MA/cm2). In addition, carrier mobility as high as 105 cm2/Vs has been observed in semiconducting nanotubes.

Purification of SWCNTs

At the time of synthesis of SWCNTs, a lot of impurities remained embedded in the material. These impurities are metallic catalyst particles, amorphous carbon, and graphitic nanoshells. Removal of these metallic impurities without degradation of the structure of CNTs is a big challenge. Several techniques have been used to purify the SWCNTs.

Acid Treatment

The treatment with different acids such as HCl and HNO3 is the simplest route to separate the transition metal from the SWCNT soot.

Air Oxidation

Oxidation of SWCNTs soot at ~350°C removes the amorphous carbon because it is unstable at this temperature, but SWCNTs are stable at this temperature.

High Temperature Annealing

For some applications of SWCNTs, such as their use as biomaterials, complete removal of metal particles is of particular importance. However, it is very difficult to achieve this by acid treatment because most of the metal particles are encapsulated by carbon layers that form a barrier to acid attack. The physical properties of carbon and metals are different at high temperature (>1400°C) under inert atmosphere. It is well known that graphite is stable even at 3000°C, whereas metal evaporates at temperatures higher than their boiling point (1300°C–1400°C). Therefore, high temperature annealing can effectively remove metal particles.