Applied Physics A (2022) 128:391
https://doi.org/10.1007/s00339-022-05465-5

Applied Physics A
Materials Science & Processing

Effect of chirality surfaces overlap on individual carbon nanotubes resistivity

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Received: 23 October 2021 / Accepted: 7 March 2022

Abstract

Experimental results show that there are unpredicted phenomena in the resistivity behavior of nanotubes as a function of their diameter. In this paper, the electrical resistivity behavior of carbon nanotubes (CNTs) is modeled as a function of diameter (at constant temperature) based on nanotube chirality. The effect of overlap of chirality surfaces on the resistivity of individual CNTs has been investigated and showed that if the windows of hexagonal lattice of individual CNTs face each other, the CNT resistivity increases. This effect becomes weaker if the diameter of nanotube increases. The proposed theoretical model explains the behavior of electrical resistivity of CNTs as a function of their diameters caused by chirality surface overlapping effect, and the obtained results are compared with the experimental reports.

Keywords Carbon nanotubes · Chirality effect · Resistivity · Critical diameter · Lattice superposition coefficient

1 Introduction

The carbon nanotubes (CNTs) are fascinating materials inspiring many scientists in the world since their discovery by Ijima in 1991[1]. These materials have unique physical, chemical, mechanical, and thermal properties due to their characteristic properties such as cylindrical structure, nanoscale, and high length to diameter ratio. Their physical properties like electrical conductivity (determined by their chirality) and excellent mechanical properties suggest a wide area of possible applications in various technologies [2–7]. CNTs are formed through tubing of graphite Sheets with sp^2 hybridization and hexagonal lattice, which are divided into two categories: single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) [8, 9]. The nanotube is a single-walled graphene sheet that is tubed as a cylinder. By tubing the graphene sheet into a cylinder so that the beginning and the end of the lattice vector on the graphene Sheet coincide, the nanotube with the lattice vector (n, m) comes. The lattice vector specifies the chirality of the nanotube [10–13]. There are a variety of nanotubes including nanotubes with zigzag vector, armchair, and chiral [14–16]. MWCNTs consist of coaxial cylinders with a certain distance between their layers, each of which can have a different chirality [17]. The electrical properties of CNTs depend on their chirality. A SWCNT, in terms of its components (n, m), can be metal, or semiconductor with very small energy gap [18]. Ebbesen et al. [19] as well as H. Dai et al. [20] experimentally measured the dependence of electrical resistivity of individual CNTs on diameter. They showed that the resistivity of nanotubes decreases smoothly with decreasing diameter. However, in their experimental observations, they have shown the resistivity variation as a function of CNT diameter without physical justification. In this paper, the influence of different parameters such as chirality effect or phenomenon, on the resistivity of CNTs is investigated to justify these variations.

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2 Chirality effect

Two terms, chiral vector (C_h) and chiral angle (α), are used to describe the structure of carbon nanotubes. The chiral vector, also called the tubing vector, starts at the main atom and points to the next atom. The length of this vector is equal