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Linear Optical Response of Silicon Nanotubes Under Axial Magnetic Field

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We investigated the optical properties of silicon nanotubes (SiNTs) in the low energy region, $E < 0.5$ eV, and middle energy region, 1.8 eV $< E <$ 2 eV. The dependence of optical matrix elements and linear susceptibility on radius and magnetic field, in terms of one-dimensional (1-d) wavevector and subband index, is calculated using the tight-binding approximation. It is found that, on increasing the nanotube diameter, the low-energy peaks show red-shift and their intensities are decreased. Also, we found that in the middle energy region all tubes have two distinct peaks, where the energy position of the second peak is approximately constant and independent of the nanotube diameter. Comparing the band structure of these tubes in different magnetic fields, several differences are clearly seen, such as splitting of degenerate bands, creation of additional band-edge states, and bandgap modification. It is found that applying the magnetic field leads to a phase transition in zigzag silicon hexagonal nanotubes (Si h-NTs), unlike in zigzag silicon gear-like nanotubes (Si g-NTs), which remain semiconducting in any magnetic field. We found that the axial magnetic field has two effects on the linear susceptibility spectrum, namely broadening and splitting. The axial magnetic field leads to the creation of a peak with energy less than 0.2 eV in metallic Si h-NTs, whereas in the absence of a magnetic field such a transition is not allowed.

Key words: Nanostructures, semiconductors, electrooptical properties, magnetic field

INTRODUCTION

Since the discovery of carbon nanotubes (CNTs) by Ijima in 1991,[1] an extensive research field in the nanoscale has opened up due to their exceptional electronic, mechanical, thermal, and transport properties. Single-walled carbon nanotubes (SWCNTs) can be metallic or semiconducting depending on their diameter and chirality, and they are used as nanotube devices.[2,3] The existence of nanotubes of other materials, such as GaN, BN, AlN, GaS, and P, has been predicted and experimentally observed.[4,5,6,7,8,9,10,11,12,13,14]

These tubular materials also display some very interesting properties that are distinctly different from their bulk counterparts. Silicon is interesting for electronic applications in nanotechnology, so Si-based nanotubes (NTs) have been the subject of both experimental and theoretical analysis. There are several reports of fabrication of SiNTs in the laboratory.[15,16,17,18,19,20]

Several studies have also been reported on Si nanomaterials such as cluster, nanowire, and tube structures.[21,22]

Si nanotubes can be classified according to their hybridization into two categories: Si h-NTs and Si g-NTs. By rolling up a Si graphene sheet with sp^2 hybridization to form a nanotube, Si h-NTs are produced, having electronic properties similar to those of carbon nanotubes. Rolling up a sp^3 Si graphene sheet leads to Si g-NTs, which exhibit only semiconducting properties independent of their chirality. Note that the gear-like geometry is more

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