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Role of Transversal Phonon Modes in the Specific Heat Capacity of Multi-Wall Carbon Nanotubes

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Heat capacity is one of the most important properties of carbon nanotubes for applications in industry and technology. In recent years, experimental and theoretical studies have been carried out to determine the heat capacity of multi-walled carbon nanotubes (MWCNTs). In the present study, the specific heat capacity of MWCNTs was determined in terms of lattice vibrations (phonons) and free electrons. The specific heat of MWCNTs was modeled up to 200 K and deviations observed in C_v–T plots for MWCNTs are explained in terms of transversal phonon modes.

Keywords: Carbon Nanotubes, Specific Heat Capacity, Single-Wall Carbon Nanotubes (SWCNT), Multi-Wall Carbon Nanotubes (MWCNT), Longitudinal Modes, Transversal Modes.

RESEARCH ARTICLE

1. INTRODUCTION

Carbon nanotubes can be classified as single-wall (SWCNT) or multi-wall carbon nanotubes (MWCNT). An SWCNT consists of a single graphene sheet rolled up into a cylinder of 1–5 nm in diameter, whereas an MWCNT is an arrangement of coaxial tubes of graphene sheets forming a tube-like structure. Each MWCNT has 2–50 such tubes with inner diameters of 1.5–15 nm and outer diameters of 2.5–30 nm. The carbon nanotubes are several micrometers in length.[1] Recently the growth mechanism, electric field effect on growth and local buckling analysis of carbon nanotubes are study and formulized.[2–4]

Since their discovery in 1991,[5] MWCNTs have been a major driving force in the development of nanotechnology. Application of carbon nanotubes as reinforcements for composites, conducting nanowires, field emitters, and nanodevices, for instance, requires a fundamental understanding of their mechanical and physical properties.[6,7] Current intensive efforts in the fields of physics, chemistry, mechanics, and biology reflect the need for a multidisciplinary approach to nanotube research. The first theoretical study carried out by Benedict et al.[8] predicted a linear relationship between the specific heat of carbon nanotubes and temperature as long as both the nanotube diameter and the temperature are sufficiently small.[8] However, experimental measurements by Yi et al. demonstrated a strikingly linear temperature dependence of the specific heat over a large temperature range (10–300 K) and tube diameter range for MWCNTs.[9] On the other hand, because of the large diameter of MWCNTs (25–30 nm) and the presence of 15–25 multi-walls, we conclude that the specific heat capacity of MWCNTs is comparable to that of graphite, although interlayer coupling in MWCNTs is much weaker than that in graphite.[1] This weak interlayer coupling is believed to be mainly caused by the turbostratic stacking of adjacent layers.[5–10] The specific heat capacity measured by Mizel et al. for MWCNTs and ropes of SWCNTs shows a linear temperature dependence in the range 100–200 K and an approximately quadratic dependence at low temperature (<50 K).[11] Popov calculated the low-temperature specific heat capacity of MWCNTs and isolated or bundled SWCNTs using force-constant dynamic models and found that the temperature dependence changed from a square-root form to a linear form with increasing tube diameter of the system.[12] An extensive review of the thermal properties of carbon nanotubes in relation to their unusual phonon dispersion and density of states was carried out by Dresselhaus and Eklund.[13] The specific heat capacity (C_v) of carbon nanotubes has been studied up to temperatures greater than 600 K and computational results indicate that C_v shows an approximately $\sqrt{T}$ type of variation at temperatures above 600 K.[10] In the present study we modeled and calculated exactly the specific heat capacity of MWCNTs according to the equation $C_v = AT + BT$,[3] where A and B have their own meaning.[14] The specific heat capacity of electrons at low temperature is usually ignored, but in this study the specific heat capacity of MWCNTs was determined using phonon and

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