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Thermal Properties of Carbon Nanotubes

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7.1. Introduction

The experimental observation of carbon nanotubes by Sumio Iijima in 1991 [1], sparked a significant effort in theoretical and experimental investigation of carbon nanotubes and related structures. The studies of thermal properties, although very important from fundamental and applications points of view, have received less attention in comparison with other aspects such as the electrical and mechanical properties [2–18]. This might be due to the fact that one associates the nanoscale aspect of nanotubes with quantization of transport properties which applies to electrons at room temperature. On the other hand, thermal transport involves many phonon modes and these can form a continuum at room temperature and phonon quantization manifests itself in nanotubes at very low temperatures (less than 8 K) [5]. Carbon nanotubes can be viewed as rolled-up graphene sheets and therefore one can infer their thermal properties by comparing them with graphite. Graphite has a large in-plane thermal conductivity, second only to type II diamond, and significantly lower out-of-plane thermal conductivity [19,20]. Therefore, in carbon nanotubes or nanotube ropes, one can expect very high thermal conductivity along the tube axis compared to the radial component due to the large separation between the different layers in multiwall nanotubes [22,13].

The ability to grow single-wall nanotube (SWNT) and multiwall nanotubes (MWNT) with different diameters and chiralities opens the possibility of developing materials with tailored thermal properties for different applications including thermal management, switches, and sensors. Carbon nanotubes can be added to other materials to enhance the magnitude and directionality of their thermal properties. This has motivated several groups to investigate the thermal properties of carbon nanotubes using experimental and theoretical approaches. The physical structure of nanotubes and their electrical properties are briefly discussed in Section 7.2. In Section 7.3, the theoretical analytical approaches to thermal conductivity and specific heat calculations are introduced. This is followed by a review of the recent experimental measurement of thermal conductivity of single- and multiwall nanotubes. Sections 7.4 and 7.5 focus on the molecular dynamics (MD) simulation...
approach and its application to investigation of thermal conductivity of SWNT, Y-junction nanotubes, and heat pulse propagation in SWNT.

7.2. Background

7.2.1. Physical Structure

A single-wall carbon nanotube can be viewed as a single sheet of graphite rolled up into a cylinder. Figure 7.1 shows a representation of the 2-D hexagonal plane that makes up a graphitic sheet, where the carbon atoms lie at the corners of each hexagon. In this figure, one can see that if point O is connected to point A, and point B is connected to point B', then the sheet will be rolled into a cylindrical structure. However, this is just one of many possible cylindrical orientations that can be constructed. For example, points A and B' could lay directly to the right of points O and B, respectively, which would result in a different orientation of the hexagonal rings on the face of the cylinder [22]. The chiral vector \( \vec{C}_H \) uniquely determines the physical structure of a carbon nanotube, and is perpendicular to the tube axis \( \vec{z} \). \( \vec{C}_H \) can be written in terms of the unit vectors of the hexagonal lattice,