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Effect of doping on the transport properties of single-walled carbon nanotube two probe systems

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ABSTRACT

This paper reports the doping induced negative differential resistance (NDR) in chromium substituted zig-zag (4, 0) single walled carbon nanotube (SWCNT) devices and the effect of the doping level on this property by using non-equilibrium Green's function theory formalism in combination with semi-empirical extended Huckel theory (EHT) calculations of the Atomistic Tool Kit software in device mode. The results show that the tunneling current, number of NDR peaks and the conductance increases with an increase in the level of doping. The high peak to valley current ratio (PVR) of the three proposed models are presented in the form of tables for comparative studies. The highest peak to valley current ratio of 5.70 is found in the two atom chromium doped SWCNT geometry. It is believed that the explored chromium doped CNT devices in this study will find number of applications in the future, particularly for fast switching and high speed signal processing.

1. Introduction

The outstanding fundamental properties of single walled carbon nanotubes (SWCNTs) make them promising candidates for ultimate miniaturization at the molecular level, and have the potential to find applications in high performance circuits [1–4]. Many experimental and theoretical methods have been employed in single molecular devices to induce many novel and peculiar transport properties, such as negative differential resistance (NDR) [5,6]. The discovery of NDR by Esaki in 1958 [7] has attracted a lot of interest because of its potential applications in oscillators, frequency multipliers, memory, fast switching, high speed signal processing etc. [8].

The introduction of foreign atoms brings many properties and implications in carbon nanotubes (CNTs). 3D transition metals (TMs) are frequently used to synthesize SWCNTs and can mix with nanotubes to affect their electronic and magnetic properties, which greatly expands the potential application areas of these nanostructures [9–10]. NDR in CNTs and their different mechanisms were described in recent reports [11–13]. Besides this, NDR has also been reported in nitrogen doped CNTs [14], boron nitride nanoribbons [15], parallel SWCNT contacts [16], porphyrin molecular junctions [17], carbon atomic wire-carbon nanotube junctions [18], carbon/boron nitride nanotube hetero-junctions [19], PtSi Schottky junctions [20], graphite-chain –carbon nanotube junctions [21] etc.

Recently we found that an arsenic doped two probe CNT system shows enhanced conductivity, whereas chromium doped two probe CNT system shows NDR [22]. With this encouraging report, in this work we report on the transport properties of

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chromium doped SWCNTs at various concentrations; pyridine like doping has been systematically studied using the semi-empirical extended Huckel theory (EHT). The observed NDR and its dependence on the level of doping are investigated thoroughly. In order to explain the NDR phenomena in-depth, we presented the observed values of the peak current and peak voltage of the current-voltage characteristics in the form of tables and analyzed the transmission spectrum in the range 0–2 eV The results show that all models show multiple NDR, and the number of NDR peaks depends upon the level of doping. In two atoms and four atom doped CNT devices only two NDR peaks were observed, however in an eight atom doped geometry three NDR peaks were found. Moreover, the peak to valley current ratio (PVR) shows a decreasing trend with an increase in the number of impure atoms in the configuration.

This paper is organized into four sections. Section 2 describes the details of modeling and simulation, whereas Section 3 presents the results and discussion. Section 4 concludes the paper.

2. Modelling and simulation approach

We have taken a Zig-Zag (4,0) SWCNT and doped its central region (scattering region) with chromium atoms in a pyridine line shape, as shown in Fig. 1. In the calculations the two probe system is divided into three parts: the left electrode (L), the right electrode(R) and the central scattering region. The carbon-carbon bond length was selected as 1.42 Å and the length of two electrodes was considered to be 7.10 Å for better geometric optimization. The length of the central region was considered as 25.10 Å in order to minimize the scattering losses. It was reported that the substitutional doping method shows maximum conductance due to the introduction of new electronic states near the Fermi level, as has been reported

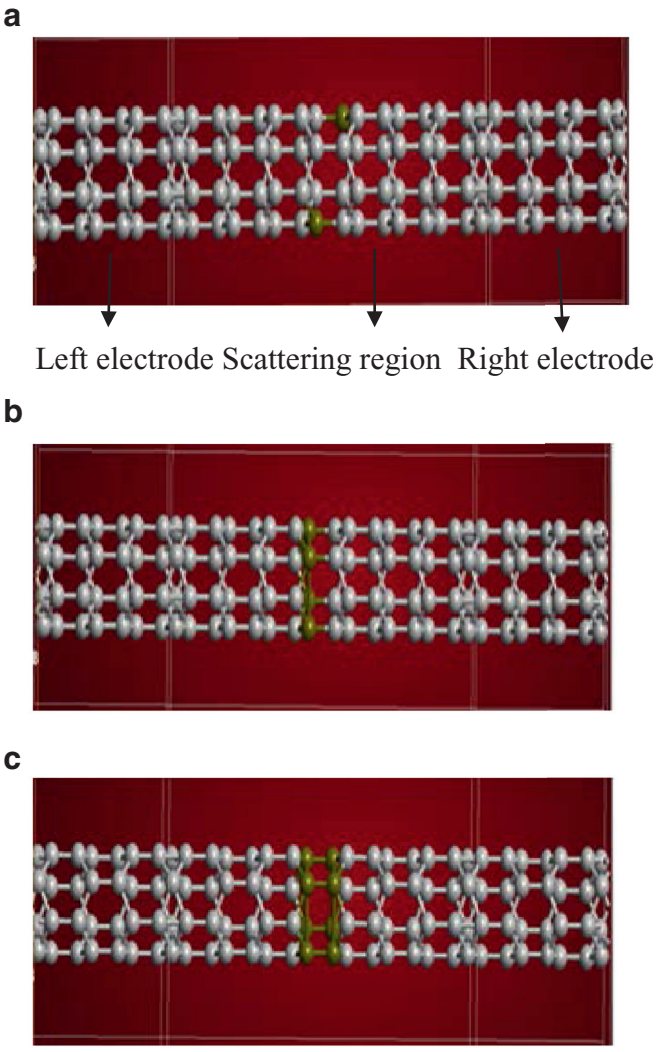

Fig. 1. The geometry of the chromium substituted zig-zag (4, 0) SWCNT devices under no bias condition: (a) two atom, (b) four atom, (c) eight atom; the pyridine dopant positions are marked in Army Green.