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Theoretical study of electronic transport properties of lead nanowires doped with silicon

Lishu Zhang, Xinyue Dai, Yi Zhou, Zhenyang Zhao, Longwei Yin, Hui Li *

Key Laboratory for Liquid-Solid Structural Evolution and Processing of Materials, Ministry of Education, Shandong University, Jinan 250061, People's Republic of China

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ABSTRACT

The potential application of nanotechnology is based on the integration of microelectronic function with advanced group IV element technology, such as silicon-based field-effect transistors. In this paper we investigate theoretically the electronic transport properties of lead nanowires doped with silicon by employing molecular dynamics simulations and the non-equilibrium green function method with density functional theory frame. We observed the conductance of lead wires with silicon doping shows ballistic feature and high doping concentration wire have more intense oscillation amplitude because of the resonance transmission peak and the transmission channels. Importantly, the initial cause of negative differential resistance (NDR) effect and bonding mechanism in lead-silicon system have also given explanation.

1. Introduction

The discovery of carbon nanotubes (CNTs) in the early 1990s [1] led to an emerging concentration in exploring the promising potentials of one-dimensional (1D) nano-materials in new generation electronic devices based on their specific structural and distinct properties. To date, a large number of nano-materials have been discovered and incorporated in devices showing their potential to overtop the performance of applied technology nowadays [2–5]. For example, groups II—VI, groups III—VI, group IV and oxide–semiconductor nanowires (NWs), nanotubes (NTs), and nanoribbons (NRs), etc. Among these nano-materials, 1D group IV nanostructures have performed to be a vital member with tremendous advance in the manufacturing and utilization of their novel properties in far-ranging and amusing applications [1,6–13]. Whereas, the changeover from basic theory to production environment requires an even stronger appreciation and control at the nanoscale in morphology and composition. Miniaturized common bulk materials into the nanometre regime or new nanostructure combination can push device performance forward and open into novel discoveries. For example, the unique and interesting physical properties which is observed in 1D nanoscale materials are depending on the size and have induced emission and photon absorption, such as metal-to-insulator transition in a material [14], nanoscale avalanche photodiodes [15], and quantised or ballistic transport characteristics [16]. In addition, the increased number of transistors per area of a silicon chip in microelectronic, has brought faster performance and lower power consumption [17]. Thus far, the 1D IV family system such as nanowires provides not only a new stage for basic theoretical research but also a fresh material system for next-generation electronic devices.

Today, intensive attention has been paid to the electronic devices made by group IV elements because of their excellent semiconductor performance, especially Si-based nanodevices [6,7,12,18]. Inaoka and coworkers[12] found Pb/Si system exhibits wave length-dependent transitions from 1D to anisotropic 2D properties. Lovrinčić et al. [19] demonstrated a neoteric method to nondestructive top-contacts for microelectronics on Si with Pb evaporated on organic monolayers, who found the transport across the devices depend on the substrate orientation, explained Si(100) has the smaller distance decay parameter than Si(111). These advances are very valuable to well understand the effective methods of fabricating nanostructures combining metal lead with semiconductor silicon. However the fundamental understanding of their electronic properties which can improve device performance is still limited.

Recently, Ogloblya et al. [20] performed Keldysh non-equilibrium Green's function calculations for the conductivity of heterojunction carbon nanotube quantum dots(QD) with spin-orbital coupling and interacting leads in the presence of Coulomb repulsion. And found interesting and innovative phenomenon that the presence of the QD-lead interaction yields form a new pair of peaks in the differential conductance dependence. Whereas, chem-

* Corresponding author.
E-mail address: lihuilmy@hotmail.com (H. Li).

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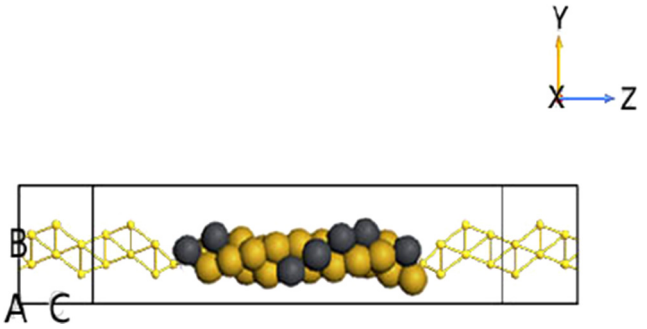

Fig. 1. The schematics of the computational models. The schematic of Pb-69%Si nanowire with the length of electrodes is 51 Å. Color coding, grey Pb, dark yellow Si. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

ical doping or alloying with other elements is rarely considered and it can provide a new route to synthesize nanowire [21], and these materials would applied in manufacturing field-effect transistors (FETs) [22–25], integrated logic circuits [26], and biosensors [27]. A previous investigation showed that it has been successful obtained n-type SiNWs by doping phosphorus in laser-assisted catalytic growth method. Zheng et al. [13] reported the first time to control growth and phosphorus doping of SiNWs, and prepare great performance n-type FETs from these nano-materials. It has been found that the phosphorous-doped SiNWs are single crystals with well-controlled diameters. All of these findings provide a new line for reversibly changing the electron transport properties of nano-electronics.

1D Pb-Si nanowires have been attracting more and more attention because they have significant advantages in low-dimensional scientific research and in new nano-electronic device fabrication. Herein, Pb-69%Si and Pb-26%Si metal-semiconductor nanowires have been chosen to concentrate on their electron-transport properties by employing molecular dynamics (MD) simulations and the non-equilibrium green function (NEGF) method with density functional theory (DFT) frame.

2. Models and computational methods

In this study, the structures of nanowires are obtained by using the MATERIALS STUDIO molecular modeling software packages [28]. And the computer system we use is multiprocessor system. $A_{1,2,3}$, $B_{1,2,3}$ and $C_{1,2,3}$ are obtained according to the method presented in ref 27. In order to explore the impact of the diameter on electronic transmission properties of nanowire, we make the length of nanowires be same (34.68 Å). And the repeating units of all CNTs we used is 14, which can let us obtain the same length nanowires. In addition, we select (8,8), (10,10) and (12,12) CNTs, which is useful for getting helical and multisheel coaxial nanowires. The Forcite module is used to perform geometry optimization to obtain stable configurations. The iterative progress has been done and the number of the max iterations is 500. The universal force field parameterized for the full Periodic Table is used to model the interatomic interactions in the optimization process.

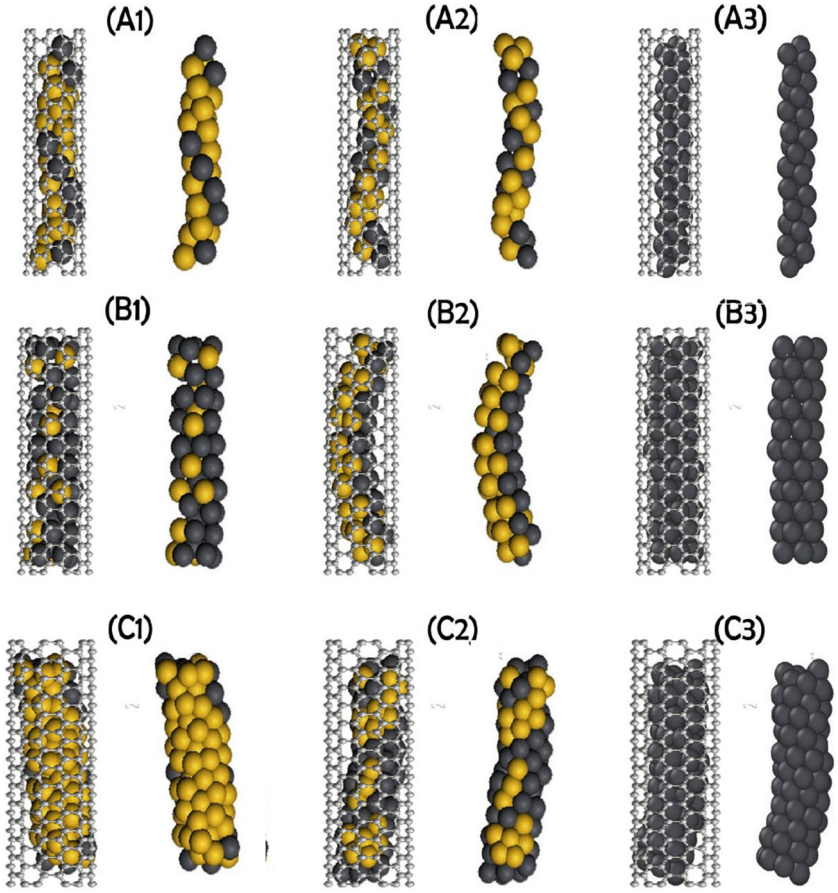

Fig. 2. The Pb-Si nanowires with different Si concentrations. (A1-A2) Nanowires with 69% and 26% Si obtained from (8,8) CNTs. (B1-B2) Nanowires with 69% and 26% Si obtained from (10,10) CNTs. (C1-C2) Nanowires with 69% and 26% Si obtained from (12,12) CNTs. A3, B3, C3 represent pure Pb nanowires consisting of 32,59 and 84 atoms. Color coding, grey, Pb; dark yellow Si. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)