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Electronic transport properties of heterojunction Pb/Pb-Si nanochain devices

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ABSTRACT

Chemical decorated heterojunction Pb/Pb-Si nanochain devices and their electron transport properties are systematically investigated. These Pb-Si nanochain heterostructures are found to show semimetal and graphene-like properties on electronic transport. Particularly, some devices show some excellent performance with large on-off ratios, small sub-threshold swing and high peak-to-valley ratio (PVR). A link between heterojunction mode and semiconductor-semimetal-metal transformation characteristic has been built. In addition, multi-peak negative differential resistance (NDR) effect has been observed on this heterostructure. Moreover, the performance of heterojunction Pb/Pb-Si nanochain devices is observed to be effectively modulated by gate potential. These findings are very valuable for potential implications for the design of high-performance new-generation microelectronic devices.

1. Introduction

Low-dimensional nanostructures like nanowires and nanochains have received much attention for the reason that a great deal of peculiar properties have been reported before, such as optical, magnetic, electronic and so on, distinguishing from those of bulk counterparts, which lead them to hold flourishing applications in highly integrated nanodevices [1]. In particular, group *IV* element nanowires with novel properties are considered to be valuable for functional semiconductor electronic devices and their potential application. For example, group *IV* semiconducting compounds, such as PbTe and SnTe, own the special ability that makes thermoelectric direct conversion of thermal into electrical energies possibly, which is a novel renewable energy conversion method [2]. It is reported that SiC nanowires own artificial regulation property, and their band gaps have the ability to be turned fined through doping, while GeSi and SnSi nanowires show a core-shell hierarchy structure after doped [3]. By using density functional theory (DFT) calculations, Ng et al. [4] discovered that the direct gap nature of the small diameter ⟨1 1 0⟩ and ⟨1 0 0⟩ SiNWs disappears when its diameter reaches its limited size where the difference of the direct and indirect band gaps are close, showing this is the diameter size where the gap nature transition starts. Xiang et al. [5] experimentally confirmed that the performance of Ge/Si nanowires is comparable to the similar length carbon nanotube FETs and substantially exceeds silicon MOSFETs because of the change in intrinsic switching delay. In addition, Pb as an important member with tremendous characteristics which is soft, dense, ductile, easy to extract and highly malleable metal with poor conductivity has been applied in many parts of devices [6,7]. And PbSi nanowires have potential to develop into a new generation of schottky-clamped transistors [8]. Pan et al. [9] found Pb doping can be used to optimize the charge carrier concentration, which results in the decrease of the electrical resistivity and seebeck coefficient so that improving electric properties as compared to the undoped BiCuSeO. As for the electronic band structure, theoretical results demonstrated that Pb nanowires exhibit semiconducting behavior, which are useful for the electronic device [6]. On the other hand, functional electronic devices have been realized based on the Si-based nano-devices of which the carrier type and concentration can be well controlled by the doping [10].

Indeed, it is well-known that advanced device functionalities, such as modulation doping, electrical insulation, internal field generation, and charge separation, can be induced by a heterojunction, and can be used for the preparation of optoelectronic components such as diodes, light-emitting diodes, photodiodes, laser diodes, etc. [11–13]. In this context, study of group *IV* crossed nanochain heterojunctions is particularly appealing [14], because an accurate knowledge of physical mechanisms plays a crucial role in the engineering of advanced optical and electronic devices [15–18].

Here, we report on Pb-Si and Pb nanochains devices based on several novel flower-liked structure models to study the effect of the chain-

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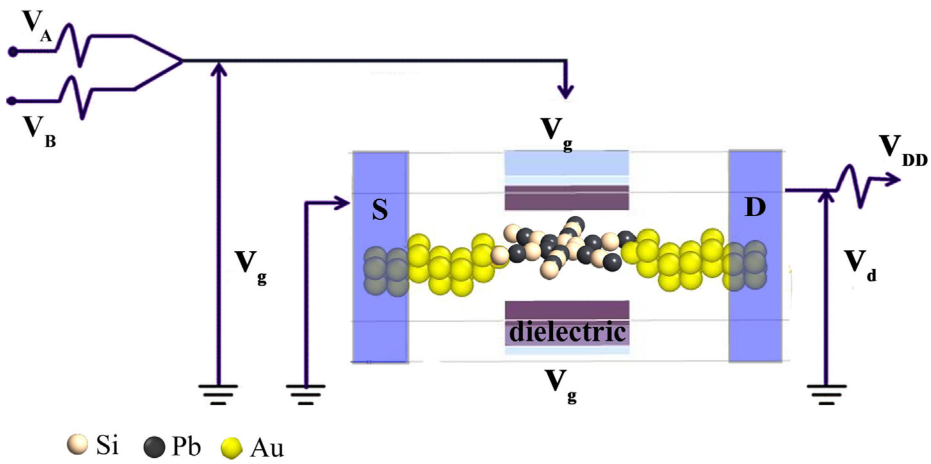

Fig. 1. Schematic of the computational model. Electrical circuit diagram of a dual input (A and B) logic gate. Between the four electrodes is the side of the calculation model (PbSi nanostructure devices). The electronic device is composed of two contacts (source and drain), a nano-device, and gate electrodes. The dielectric constant and the thickness of dielectric layers are $4\varepsilon_0$ and 4.0 Å.

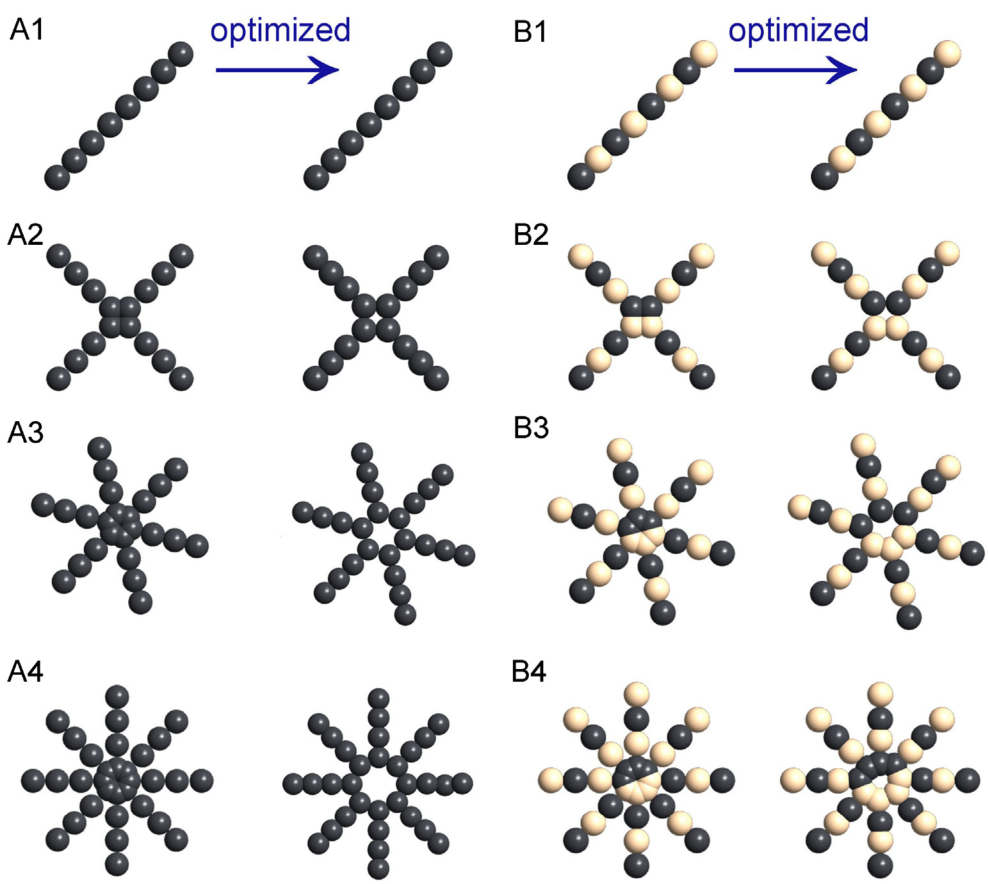

Fig. 2. Different nano-structures named Ax and Bx respectively, and their structures after optimized. The Pb and Si atoms are marked in black and yellow, respectively. All calculations are made by using the optimized structures.

chain conjunction and doping on the electronic transport properties. First principle calculation is performed in order to well understand the electronic transport properties under nanometer scale and eventually to design new materials or devices with desired characteristic.

2. Computational method

Following the Atomistix ToolKit (ATK) package, the calculations are carried out through the Non-equilibrium Green Function (NEGF) method in combination with the density functional theory (DFT) [19–21]. The Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation (GGA) is used. The k-point sampling set is $1 \times 1 \times 100$ and the energy mesh cutoff is set to be 75 Ha. An electron temperature of 300 K is adopted at Fermi distribution function. The Troullier-Martins norm-conserving pseudopotentials are employed. Considering the electrical polarized effects of atoms, the double-zeta plus polarization (DZP) basis set is used for all atoms. The geometries are modeled whining a supercell with over 14 Å of vacuum space between neighboring cells to avoid interactions between periodic images. As shown in Fig. 1, the schematic of the device is bonding chemically to two Au electrodes, serving as the central scattering region and the other is the "contacts" [22]. We also add up to four gate electrodes foursquare surrounding the nanostructure and electrically insulated from the nanostructure by oxide layers. Before calculating the electron transport properties, all structures are optimized using the quasi-Newton method until all residual forces on each atom are smaller than 0.05 eV/Å. The