Simulation of one-dimensional van der Waals heterojunction formed by a carbon nanotube embedded into MoS$_2$ nanotube

D.A. Timkaeva
Laboratory of Diffusion Processes, Ulyanovsk State University, Russia
E-mail: dianatimkaeva@mail.ru

Abstract. The concept of van der Waals (vdW) heterostructures provides a wide range of possibilities of combining two-dimensional (2D) layered materials for heterogeneous integration at atomic level without the constraint of lattice matching. The resulting structures exhibit unique physical properties and are promising for nanoelectronic and photonic applications. Recently, the concept of vdW heterostructures has been extended to 1D materials, and coaxial heteronanotubes have been synthesized. In the present work, we simulate a one-dimensional vdW heterojunction based on a carbon nanotube (semiconducting or metallic) embedded into a uniaxial MoS$_2$ nanotube. Using first-principles methods, electron difference density and transmission spectra are calculated for two vdW junctions at room temperature. The considered systems can serve as a nanodiode with controlled width of a space charge region.

1. Introduction
Vertical heterostructures based on 2D materials can be combined from one atom thick layers. Due to strong covalent bonds inside layers and weak vdW interaction between them, there is no the atomic interdiffusion. As a consequence, vdW heterostructures have atomically regulated interfaces, and the constraint of lattice matching is removed. The recent paper [1] reported on the extension of the vdW heterostructures concept to 1D materials. Coaxial single-crystal layers of hexagonal boron nitride (BN) and molybdenum disulfide (MoS$_2$) crystals were grown on single-walled carbon nanotubes (SWCNTs). They have chosen SWCNT as a basic tube because it is one of the best-studied 1D systems and can be obtained with controlled geometry [2, 3]. Metallic or semiconducting SWCNT may serve as the electrode or channel for a tubular device [1]. The authors of [1] declare the absence of correlation between structures of inner and outer nanotubes. The requirement of a threshold diameter for MoS$_2$ nanotubes is not applicable. The obtained 1D heterostructures are of interest from fundamental point of view [1, 4, 5, 6] and for application in nanodevices. Possible applications of such heteronanotubes include nanotransitors [1], optical antennas [7], microsupercapacitors [8], thermoelectric devices [9, 10], etc. As is known, the development of nanoantennas for the infrared and visible frequency ranges of electromagnetic radiation is associated with the problem of a rectifier (diode) operating at higher frequencies without large power losses. These losses usually limit the possibilities of the pn junction. In recent work [11], we considered a CNT-based hybrid diode in which a junction is created by a combination of doping with a transverse electric field produced by a charged gate electrode. The implementation of such a device is based on a shielding approximation, which suggests
that the properties of the left and right electrodes can be described by solving the problem for fully periodic cell. Using first-principle semi-empirical methods, it was determined that using the doping level and gate potential, capacitance of this diode can be varied in a controllable manner. In this report, we present the simulation results for a 1D vdW heterojunction formed by SWCNT embedded into a uniaxial molybdenite (MoS$_2$) nanotube. Metal dichalcogenide (MX$_2$) nanotubes are one-dimensional quantum systems with a wide bandgap. Unlike nanoribbons, they do not have rough edges with dangling bonds and are characterized by higher thermodynamic stability.

2. 1D van der Waals heterojunction MoS$_2$–CNT

MX$_2$ nanotubes in combination with carbon nanotubes are promising for applications in nanoelectronics and photonics [4]. In contrast to [4], where Schottky diodes MX$_2$ CNTs with a contact at the edges of nanotubes are studied, we consider a 1D vdW heterojunction formed by the SWCNT inserted inside MoS$_2$ nanotube. The simulation in [5] indicates an inhomogeneous distribution of the space charge region (SCR) in the Schottky junction with a tendency to charge transfer from metal and chalcogen atoms to carbon atoms. Figure 1 shows a simulated nanodiode based on a 1D vdW heterostructure MoS$_2$-CNT. Using the density functional theory (DFT) based method implemented in the QuantumATK package, electron difference density, electrostatic difference potential and projected local density of states are calculated. The right panel in figure 1 demonstrates the corresponding projected local density of states for this junction. We observe the distortion of bands corresponding to formation of SCR.

We used the DFT method inside GGA with functional parameterized Perdew-Burke-Ernzerhof (PBE) in the QuantumATK software. The periodic and semi-infinite electrodes are constructed by internal routines of the QuantumWise ATK tool which recognize the principal layers from the left/right side of the central region and repeat them accordingly. The electrodes in ATK are modeled as perfect leads. In our paper, we consider a 1D van der Waals heterocontact formed by the embedding of nanotubes. The presented structure can be divided into three areas: central area, where the transition is created, and areas of the left and right electrodes which are modeled as ideal leads.

From electron difference density (figure 2,a,b), one can see that SCR is located near the SWCNT surface over the length of vdW junction. This confirms the tendency mentioned above and it is in accordance with [4]. Electrostatic difference potential is shown in figure 2,c,d. The transmission spectra and IV curves were calculated using the method of nonequilibrium Green functions (NEGF) implemented in the QuantumATK package.
Figure 2. Calculated electron difference density (a,b) and electrostatic difference potential (c,d) for 1D vdW heterojunction MoS$_2$ - CNT(9,9).

In figure 3, the transmission spectra for MoS$_2$ contacts with semiconducting SWCNT (14,0) and metallic SWCNT (9,9) are presented. The considered Schottky diode demonstrates higher transmittances than the MoS$_2$ - SWCNT (14,0) junction.

The current can be calculated via

\[ I = \frac{e}{\hbar} \int T(E)[f_L(E,T_L) - f_R(E,T_R)]dE \]

where \( f_L \) and \( f_R \) are electron energy distribution functions in the left and right electrodes, respectively, \( T(E) \) is a transmission spectrum calculated by the NEGF-method.

3. Summary

In the present work, we considered a one-dimensional vdW heterojunction based on a carbon nanotube (semiconducting (14,0) and metallic (9,9)) embedded into a uniaxial MoS$_2$ nanotubes. Using first-principles methods, electron difference density and transmission spectra are calculated for two vdW junctions at the room temperature. The considered systems can serve as a nanodiode with controlled width of a space charge region. Using the density functional method, such characteristics as the local state density, transmission spectra, and electrostatic potential distribution have been calculated. Examining the obtained data, it was determined that the SCR value and, therefore, the heterocontact capacity can be easily varied by selecting
Figure 3. Transmission spectrum of 1D vdW heterojunctions MoS$_2$ with CNT(9,9) (blue solid line) and CNT(14,0) (black solid line).

the diameter and chirality of the nanotubes, as well as changing the heterocontact attachment length. The considered Schottky diode demonstrates higher transmittances than the MoS$_2$ - SWCNT (14,0) junction. Considered nanodiodes based on 1D vdW heterojunction formed by SWCNT embedded into a uniaxial molybdenite (MoS$_2$) nanotube are promising for applications in nanoelectronics. Instead of the discussed ones, other variants of combined nanotubes can be used to create a heterojunction, including relatively exotic tubes such as graphenylene or octagraphene tubes [13]. The considered nanotubes effectively absorb electromagnetic waves of the visible range, and corresponding heterojunctions are promising for the development of electromagnetic radiation sensors and optical nanoantennas.

Acknowledgments
This work is supported by the Ministry of Science and Higher Education of the Russian Federation (state program 0830-2020-0009).

References
[1] Xiang, R., Inoue, T., Zheng, Y., Kumamoto, A., Qian, Y., Sato, Y., et al. (2020). One-dimensional van der Waals heterostructures. Science, 367(6477), 537-542.
[2] Dresselhaus, M. S., Dresselhaus, G., Saito, R. (1995). Physics of carbon nanotubes. Carbon, 33(7), 883-891.
[3] Bulyarskiy, S. V. (2019). The effect of electron-phonon interaction on the formation of reverse currents of pn-junctions of silicon-based power semiconductor devices. Solid-State Electronics, 160, 107624.
[4] Sengupta, A. (2017). On the junction physics of Schottky contact of (10, 10) MX$_2$ (MoS$_2$, WS$_2$) nanotube and (10,10) carbon nanotube (CNT): an atomistic study. Applied Physics A, 123(4), 227.
[5] Jariwala, D., Marks, T. J., Hersam, M. C. (2017). Mixed-dimensional van der Waals heterostructures. Nature Materials, 16(2), 170-181.
[6] Sibatov, R. T., Sun, H. (2019). Tempered fractional equations for quantum transport in mesoscopic one-dimensional systems with fractal disorder. Fractal and Fractional, 3(4), 47.
[7] Joh, D. Y., Kinder, J., Herman, L. H., Ju, S. Y., Segal, M. A., Johnson, J. N., et al. (2011). Single-walled carbon nanotubes as excitonic optical wires. Nature nanotechnology, 6(1), 51.

[8] Kitsyuk, E. P., Sibatov, R. T., Svetukhin, V. V. (2020). Memory effect and fractional differential dynamics in planar microsupercapacitors based on multiwalled carbon nanotube arrays. Energies, 13(1), 213.

[9] Blackburn, J. L., Ferguson, A. J., Cho, C., Grunlan, J. C. (2018). Carbon–nanotube–based thermoelectric materials and devices. Advanced Materials, 30(11), 1704386.

[10] Meftakhutdinov, R. M., Sibatov, R. T., Kochaev, A. I. (2020). Graphenylene nanoribbons: electronic, optical and thermoelectric properties from first-principles calculations. Journal of Physics: Condensed Matter, 32(34), 345301.

[11] Timkaeva, D. A., Sibatov, R. T. (2019, December). Simulation of quantum transport in doped carbon nanotube diode controlled by transverse electric field. Journal of Physics: Conference Series, Vol. 1410, No. 1, p. 012239.

[12] Smidstrup, S., Markussen, T., Vancraeyveld, P., Wellendorff, J., Schneider, J., Gunst, T., et al. (2019). QuantumATK: An integrated platform of electronic and atomic-scale modelling tools. Journal of Physics: Condensed Matter, 32(1), 015901.

[13] Kochaev A.I., Meftakhutdinov R.M., Sibatov R.T., Timkaeva D.A. (2020) Optical and thermoelectric properties of graphenylene and octagraphene nanotubes from first-principles calculations. Computational Materials Science (in print).