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First-Principles Device Simulations of All Two-Dimensional Material Tunneling Field-Effect Transistors

Mari Ohfuchi[1] and Taisuke Ozaki[2]

[1] Fujitsu Laboratories Ltd.
10-1 Morinosato-wakamiya, Atsugi, Kanagawa 243-0197, Japan
Phone: +81-46-250-8194 E-mail: mari.ohfuti@jp.fujitsu.com
[2] Institute for Solid State Physics, The University of Tokyo
5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan

Abstract

We implemented a gate function in a general-purpose density functional theory (DFT) code to realize gate-controlled electron transport calculations, and performed first-principles device simulations of an all two-dimensional (2D) material tunneling field-effect transistor (TFET). We designed GeSe/MoS_2/VS_2 TFETs and demonstrated that a 2 nm channel length device exhibits an on/off current ratio larger than 10. This provides a powerful tool for exploring novel nanoelectronic and spintronic devices.

1. Introduction

As dimensional scaling in ultra large scale integration (ULSI) becomes increasingly difficult, the implementation of new technologies, such as novel channel materials and even non classical complementary metal-oxide-semiconductor (CMOS) like tunneling or spin devices, is expected. This shift towards equivalent scaling along with the recent requirements of various device functions make physics-based device simulation more and more important. The tight binding (TB) approximation combined with the non-equilibrium Green's function (NEGF) method and the three-dimensional (3D) Poisson equation has achieved significant results in the field of computational nanoelectronics [1,2]. The TB method, however, has some limitations because the question remains of how valid the parameters that are usually obtained from the electronic structure of bulk materials are when they are applied to nanostructures.

DFT-based electron transport calculations [3−5] provide a promising solution for first principles device simulations. Not only the electronic properties but also the stable atomic geometry can be determined without empirical parameters for any nanostructures including a hetero-interface. The spin transport calculations are also well established in the spin-polarized DFT framework [3,6] for research into spintronic applications. However, the introduction of a gate function to DFT-based electron transport calculations has been limited to a few specific cases [7,8]. In this study, we implement a gate function in general-purpose DFT-based NEGF code, OpenMX [6], by applying open boundary conditions to the 3D Poisson equation. Then we demonstrate first principles device simulations of an all 2D material TFET using the developed code. We designed GeSe/MoS_2/VS_2 TFETs and demonstrated that a 2 nm channel length device exhibits an on/off current ratio larger than 10.

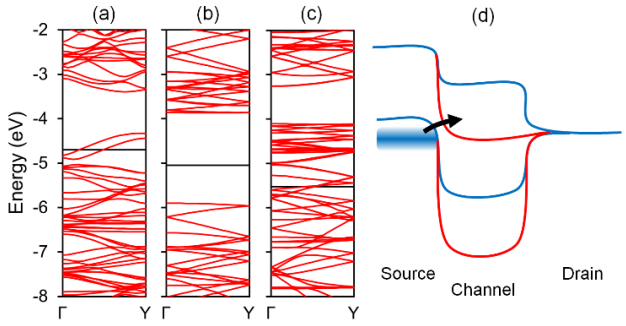

Fig.1 Energy band structures of monolayer (a) P-doped GeSe, (b) MoS_2, and (c) VS_2 sheets. (d) Schematic diagram of the predicted band alignment in the off (blue) and on (red) states for the GeSe/MoS_2/VS_2 TFET.

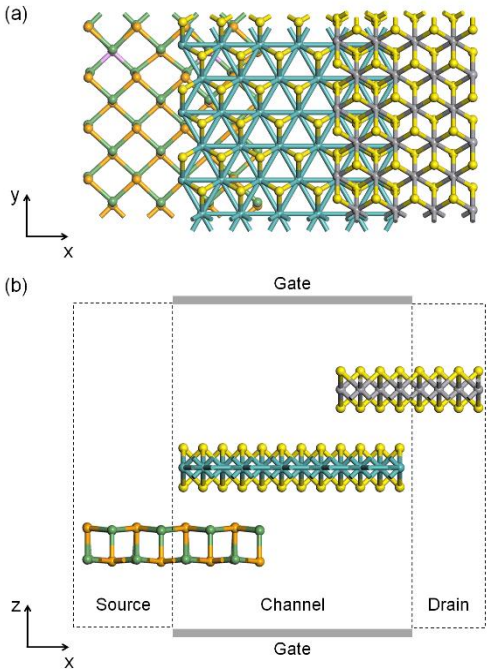

Fig.2 (a) Top and (b) side views of the atomic structure of the GeSe/MoS_2/VS_2 TFET. The green, orange, pink, blue-green, yellow, and gray spheres represent Ge, Se, P, Mo, S, and V atoms, respectively. Only atoms of the unit cell are shown in the y direction. The channel length and the distance between the double gates (gray rectangles) are 1.9 and 2.6 nm, respectively. The unit cells of the leads (broken line rectangles) are repeated for semi-infinite source and drain electrodes.

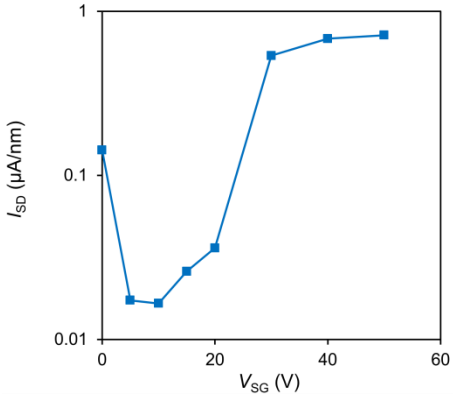

Fig. 3 I_{SD}-V_{SG} characteristics at V_{SD} = 0.1 V of the GeSe/MoS_2/VS_2 TFET.

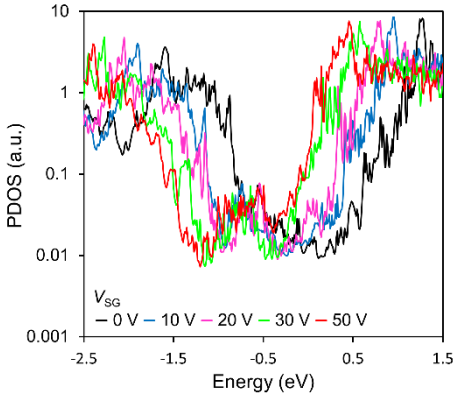

Fig. 4 V_{SG} dependence of the PDOS of the Mo atom lying in the center of the channel in the GeSe/MoS_2/VS_2 TFET (V_{SD} = 0.1 V).

2. Calculations

Design of all 2D material TFETs

In order to design all 2D material TFETs, we first examined the optimized geometry and the electronic structure of various monolayer 2D materials and the doping, and then chose monolayer P-doped GeSe, MoS_2, and metallic VS_2 as the components of the TFETs. Their energy band structures are shown in Fig.1. Assuming that MoS_2, P-doped GeSe, and VS_2 are used as the channel material, source and drain electrodes, respectively, we can predict the TFET operation as shown in Fig. 1(d) from their band alignment. Their lattices are matched with a relatively small unit cell, which is also important to reduce the computational cost in the first trial study.

The atomic structure of a GeSe/MoS_2/VS_2 TFET is shown in Fig. 2. The total number of atoms in the model amounts to 244. The source, channel, and drain monolayer materials were vertically aligned and the interlayer distance was determined to be 0.323 nm. We found that a contact length of 0.6 nm is enough for the current to flow through the contact. The channel length and the distance between the double gates are 1.9 and 2.6 nm, respectively.

Device Properties of the GeSe/MoS_2/VS_2 TFET

Fig. 3 shows the source drain current I_{SD} versus the source gate voltage V_{SG} at a source drain voltage V_{SD} of 0.1 V. We obtained a very large on current of approximately 1 μA/nm, which means the contact resistances between the layer materials are sufficiently low. We also found that the on/off ratio is larger than 10 despite the short channel length (2 nm). In order to confirm the gate control, we examined the partial density of states (PDOS) of the Mo atom lying in the center of the channel. As expected, the PDOS shifts downward as V_{SG} increases, and a decrease in the energy shift at larger V_{SG} originates from the increasing quantum capacitance of the device with increasing V_{SG}. We would be able to improve the subthreshold swing (SS) by using a high-k material as a gate dielectric that is a vacuum in the present model. We can perform such calculations in a reliable manner without any empirical parameter fitting using the developed code.

3. Conclusions

We implemented a gate function in general-purpose DFT-based NEGF code. We designed GeSe/MoS_2/VS_2 TFETs and demonstrated that a 2 nm channel length device exhibits an on/off current ratio larger than 10 using the developed code. This could be a powerful tool for exploring novel nanoelectronic and spintronic devices.

Acknowledgements

The calculations were performed on the Fujitsu FX100 and CX400 supercomputer systems at the Information Technology Center, Nagoya University.

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Appendix (Computational methods)

The DFT code (OpenMX [3,6]) that we employed uses pseudoatomic orbitals (PAOs) centered on atomic sites as the basis function set. This open-source software package provides a well-benchmarked database of pseudopotentials and PAOs for an extensive list of elements. In this study, the exchange-correlation potential was treated with both generalized gradient approximation (GGA-PBE) with van der Waals correction. For geometry optimization, we used the PAOs specified by Ge7.0-s3p3d3f2, Se7.0-s3p3d2f1, P7.0-s3p3d2f1, Mo7.0-s3p2d2f1, S7.0-s3p3d2f1, and V6.0-s3p3d2, where Ge, Se, P, Mo, S, and V are atomic symbols. The figure indicates the cutoff radius of the PAOs in Bohr. The symbol s3, for example, indicates the employment of three orbitals for the s component. For transport calculations, we reduced all PAOs to s2p2d1. The energy band occupation was smeared by the Fermi distribution function (temperature T = 300 K). The gate function was implemented by applying open boundary conditions to the 3D Poisson equation.