Transport Properties of C_3N Nanoribbon-Based Nanoscale Transistors

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***Abstract*—In this paper, the transport properties of field-effect transistors based on zigzag C_3N nanoribbon saturated by hydrogen are theoretically analyzed through a multiscale simulation procedure from first-principles computation to the tight binding analysis. Density functional theory(DFT) for the electronic structure, maximally localized Wannier functions(MLWF) for the tight-binding(TB) hamiltonian, and nonequilibrium Green's function(NEGF) formalism for the transport properties. The band structure, transmission coefficient and the I-V curve are calculated. Simulation results show that zigzag C_3N nanoribbon has great transport properties.**

Keywords—C3N nanoribbons; transport properties; electron devices; nanoscale transistor; multiscale simulation flow

I. INTRODUCTION

When characteristic dimensions of transistors are going below 10 nm, fundamental limitations are emerging both in terms of manufacturing costs and device performance. To sustain Moore's law, it is essential that the transistor material and the manufacturing process should be changed. For the transistor material, using two-dimensional (2D) systems as conduction channels is definitely one of the most exciting opportunities [1]. Recently, C_3N, one graphene-like material, has been investigated. The authors have put forward the hypothesis that C_3N could be attractive for device applications such as optoelectronics [2]. Only an accurate simulation of a complete device can testified this hypothesis and satisfy experimental interest in the novel 2D materials. This task is not straightforward, however, the simulation of a device requires a preliminary characterization of the material.

In this paper, A multiscale approach based on DFT method, MLWF interpolation and NEGF formalism is performed to study the transport properties of nanoscale transistors with different channel width. All the computations are accomplished in three open packages: *VASP* for *ab initio* calculations [3], *Wannier90* for MLWF interpolation [4] and *NanoTCAD ViDES* for computing transport properties [5].

II. DEVICE STRUCTURE AND SIMULATION SCHEME

A. Device Structure

As shown in Fig. 1, the model of double-gate field-effect transistor is estabished. The channel length of the transistor is 7 nm, and the width is range from 1 nm to 2 nm, with transport of z-direction. The lengths of source and drain regions where the bias voltage is applied and current is collected are 3.5 nm, respectively. The gates are treated as ideal metal with 7 nm long. Two oxide layers made of SiO_2 are 0.5 nm thick wrap around the channel.

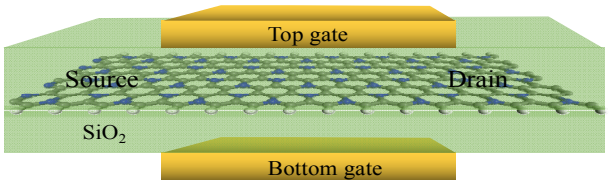

Fig. 1. Double-gate metal-oxide-semiconductor FETs based on C_3N Nanoribbon channel.

B. Simulation Scheme

Taking advantage of the high precision of DFT method in computing electronic structure and the high efficiency of TB in numerical simulation, we adopted a multiscale simulation scheme to analyse the transport properties of the transistors.

DFT method for obtaining the band structure and wave functions of the C_3N nanoribbon supercell [6]. We chose four valence bands and four conduction bands near the Fermi level contribute to the transport mostly and the related wave functions as the inputs for MLWF interpolation. For a set of N Bloch bands $\psi_{n\mathbf{k}}$, a set of N wannier functions $w_{n\mathbf{R}}$ are constructed as

$$|w_{n\mathbf{R}}\rangle = \frac{V}{(2\pi)^3}\int_{BZ}\left[\sum_{m=1}^{N} U_{mn}^{(\mathbf{k})}|\psi_{m\mathbf{k}}\rangle\right]e^{-\mathbf{k}\cdot\mathbf{R}}d\mathbf{k} \quad (1)$$

where V is a real-space unit cell volume of the crystal, k is the wave vector, BZ is the Brillouin zone over which the integral performed, $\mathbf{R}$ is Bravais lattice vector, n is the band index, and $U^{(\mathbf{k})}$ is a unitary matrix. By optimizing the $U^{\mathbf{k}}$, the MLWFs Hamiltonian retaining full first principles accuracy for the relevant electronic bands will be obtained.

We exploit the NEGF formalism to compute the currents in a complete device. The Green's function is computed as

$$G(E) = [ES - H - \Sigma_S - \Sigma_D]^{-1} \quad (2)$$

where E is the energy, S is the identity matrix, H is the Hamiltonian comes from the wannier functions interpolation. Σ_D and Σ_S are the self-energy of the drain and source

contacts, respectively. The relationship between Hamiltonian and self-energy is showed in Fig. 2.

The transmission coefficient $T(E)$ is computed as

$$T(E) = -Tr\left[\left(\Sigma_S - \Sigma_S^{\dagger}\right)G\left(\Sigma_D - \Sigma_D^{\dagger}\right)G^{\dagger}\right] \quad (3)$$

where Tr is the trace operator, $\Sigma_S^{\dagger}$, $\Sigma_D^{\dagger}$ and $G^{\dagger}$ is the conjugate transpose matrix of Σ_S, Σ_D and G respectively.

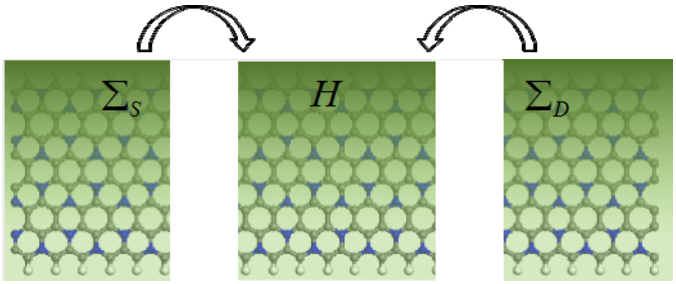

Fig. 2. The NEGF method: The device is defined by the tight-binding Hamiltonian H, which is combined with the source and drain by the self-energy Σ_S and Σ_D.

Hence, the current flowing through the device can be computed as

$$I = \frac{2q}{h}\int_{-\infty}^{+\infty} dET(E)\left[f\left(E - E_{F_S}\right) - f\left(E - E_{F_D}\right)\right] \quad (4)$$

where q is the electron charge, h is Planck's constant, E_{F_S} and E_{F_D} is the fermi level of the source and drain, respectively. Function $f(E)$ is Fermi distribution function

III. Simulation Result

The energy bands computed from DFT method and the results from MLWFs interpolation is compared in Fig. 3. The bands calculated from DFT method described in black lines are insured correct, while the results from MLWF are depicted in red circles. It can be seen that they are perfect fitted. This explains the tight-binding Hamiltonian from the Wannier interpolation has high accuracy to represent the device system.

Fig. 4 shows the transmission coefficient, and there is non-zero value, explaining that C_3N nanoribbon has great transport properties. Fig. 5 shows the currents calculated by the NEGF method. It is obvious that with a wider channel, the current will collected more.

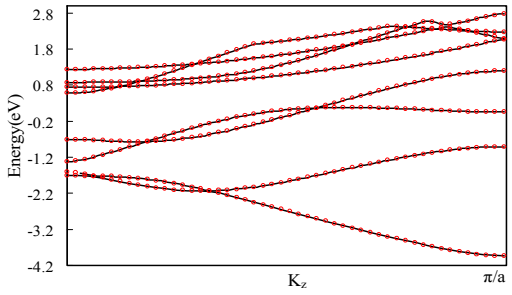

Fig. 3. Red circles: results from Wannier interpolations. Black lines: results from DFT method calculation. 0

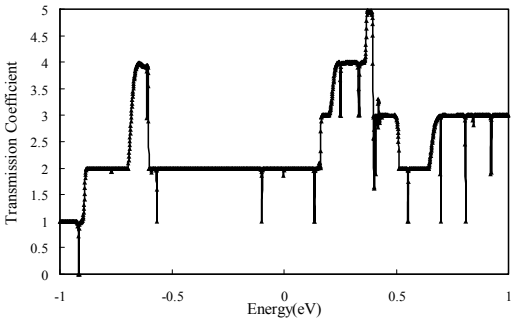

Fig. 4. The transmission coefficient calculated by NEGF method.

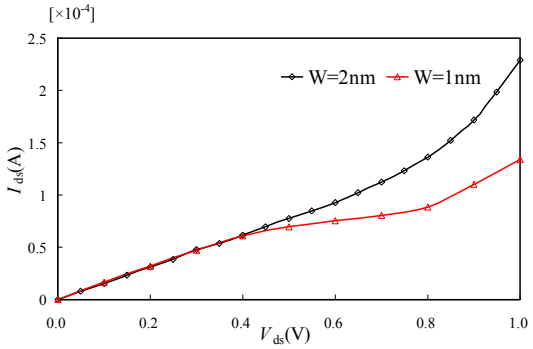

Fig. 5. Red circles: results from Wannier interpolations. Black lines: results from DFT method calculation.

IV. Conclusion

In this paper, we used a multiscale simulation approach to study the transport properties of the zigzag C_3N nanoribbon which saturated by hydrogen. Simulation results showed that zigzag C_3N nanoribbon has great conductivity. On this account, C_3N nanoribbon will be an excellent conductive material.

Acknowledgment

We would like to thank the support of Natural Science Foundation of 61522108, National Key Laboratory under Grant 614220503030317.

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