A Study of Field Electron Emission in a Nanoscale Air-Channel Silicon Diode

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***Abstract*—Over the past few years, the rapid progress in the field of vacuum nanoelectronics is mainly associated with the emergence of technological methods for the formation of quasi-vacuum (air) nanoscale gap between the emitter and collector (less than 100 nm). Since the probability of ionization of gas molecules on such scales is negligible, it opens up the attractive prospects of creating field-emission devices with an air channel which operate in a THz range under atmospheric conditions. In this work, we experimentally demonstrate the field-emission behavior of a silicon diode with a nanoscale air channel of about 60 nm, which was fabricated on a sapphire substrate by means of focused ion beam (FIB) etching. Based on the density functional theory (DFT) formalism, we also perform the first-principles calculations of the field-emission current in a such diode for ultra-small air-channel lengths (up to the de Broglie wavelength), where a noticeable deviation of the current-voltage (I-V) characteristics from the classical Fowler-Nordheim equation was found. The results obtained can be used for the development of high-speed solid-state nanoelectronic devices with a nanoscale air channel.**

Keywords— field electron emission, quasi-vacuum, nanoscale air-channel silicon diode, first-principles calculations, vacuum nanoelectronics

I. INTRODUCTION

Nowadays, a great attention and significant interest of researchers is paid to the development of next-generation vacuum electronics, in particular, based on diode-type and triode-type nanostructures with a nanoscale vacuum channel [1]. Such structures based on field-emission effects in a nanochannel can successfully operate in a quasi-vacuum (air) conditions (at atmospheric pressure), which eliminates the need for vacuum packaging. In the field emission mode, the transport of hot electrons from nanoscale surfaces into a vacuum makes it possible to achieve high operating frequencies (in the THz range) and stability in extreme conditions (high temperature, radiation). Recently, it was experimentally shown that the key mechanism of electron transport in metal-based air channel transistors, where the thickness of air gap is less than 35 nm, is primarily relates to the field emission effect [2]. Rather high emission currents (about 53 μA at 1 V) and stable emission (at turn-on voltage of about 0.46 V) were obtained in 10-nm air channel diode structures based on VO_2 (A) emitters [3]. The use of two-dimensional tin selenide (SnSe) as the field-emitter material made it possible to achieve high field emission stability in air-channel transistor with a channel length varied in the range from 100 nm to 6 μm [4]. Nevertheless, field-emission structures listed above have low reproducibility and high cost which is the critical issue for further commercialization of such technology. In contrast, the excellent repeatability of silicon field emitters fabricated using well-known CMOS (complementary metal-oxide-semiconductor) technology makes it possible low-cost mass production of vacuum nanoelectronic devices. As it was shown in [5], nanoscale silicon field-emission transistors can operate at a sufficiently low threshold voltage, comparable to the operating voltage of solid-state semiconductor devices. However, there are still few studies on the measurement of field-emission current in silicon nanodevices with air channel. Moreover, the field-emission current from semiconductor calculated within the traditional Fowler-Nordheim theory often do not corresponds to the experimental I-V characteristics of the field-emission at the nanoscale [6]. It determines the need to correct the theoretical formalism of the field-electron emission in the nanoscale region, according to experimental data, which can be achieved based on first-principles calculations. This paper describes the process of fabrication of nanoscale air channel silicon diode and analysis of its experimental characteristics, measured in atmospheric conditions at room temperature. First-principles calculations of the field emission current in a such silicon diode were also performed for ultra-small air channel lengths, comparable to the de Broglie wavelength, where quantum-size effects should be taken into account. Based on the obtained results, the corresponding recommendations were formulated for correcting the theoretical formalism of field electron emission in nanoscale air-channel silicon diodes.

This work was performed using the equipment of the R&D center «MEMSEC» (MIET).

II. EXPERIMENT: FABRICATION AND MEASUREMENT OF AIR-CHANNEL SILICON DIODE

The structure of a planar field-emission silicon diode was formed using FIB etching technology on the basis of a silicon-on-sapphire (SOS) substrate, where a silicon layer (Si) with a thickness of 513 nm is located below the layers of interlayer insulation and passivation. As a result of etching by FIB, two silicon blade-type electrodes (cathode and anode) were formed on a substrate, located at a distance of about 65 nm from each other, as shown in Figure 1a.

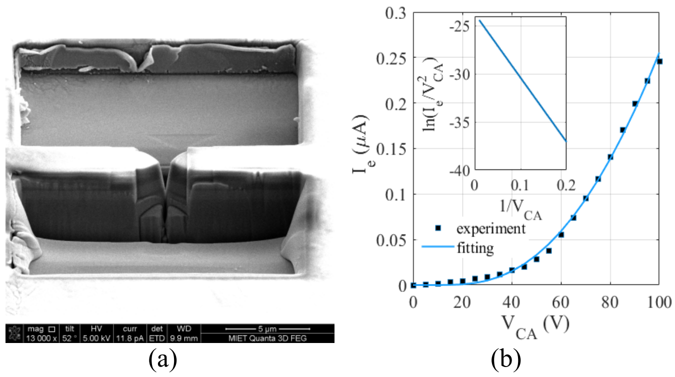

Fig. 1. (a) SEM image and (b) I-V characteristics of nanoscale air-channel silicon diode fabricated by FIB etching of SOS substrate

Figure 1b presents the I-V characteristics of the fabricated silicon diode measured under the atmospheric pressure. It follows from Figure 1b, that a field-emission current of 250 nA is reached at voltages up to 100V.

III. Theory: Simulation of Field-Emission Current in Air-Channel Silicon Diode

For the accurate simulation of field-electron emission in nanoscale silicon diode, in the case when the length of quasi-vacuum (air) gap is close to the de Broglie wavelength, first-principles quantum-mechanical calculations based on DFT method should be performed. In this work, Quantum ESPRESSO (QE) package was used to calculate the initial electronic states, where pseudopotentials and Kohn-Sham equations are explored in a self-consistent manner [7]. Field-emission current is calculated using time-dependent perturbation theory for non-zero external electric field between electrodes and the Non-Equilibrium Green Function (NEGF) formalism to describe the electron transport and inelastic scattering in the diode. In the framework of the DFT approximation, the LCAO (linear combination of atomic orbitals) method was chosen to obtain the basis of wave functions in silicon electrodes. Figure 2a illustrates the atomic structure of a silicon diode built in QE with quasi-vacuum nanogap and a radius of electrode tips equal to 1 nm. To simulate the computational mesh within the gap, we used the so-called «ghost atoms», or free orbitals, which are a set of basic wave functions with zero potential, similar to the set of wave functions of real silicon atoms of the structure.

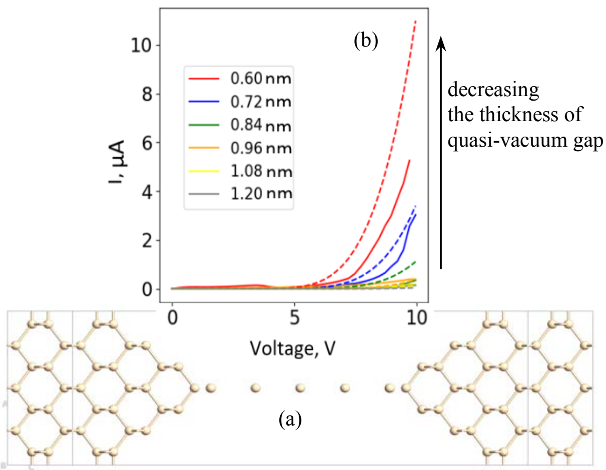

Fig. 2. (a) Atomic structure and (b) I-V characteristics of quasi-vacuum silicon diode: solid (dotted) lines – first-principles (Fowler-Nordheim) model.

To evaluate the field-emission characteristics of silicon quasi-vacuum diode, we simulated different chains of Si atoms with sizes of the quasi-vacuum gap varied from 0.6 to 1.2 nm, when the voltage between the electrodes varies from 0 to 10 V. The I-V characteristics of the diode, calculated within the framework of the first-principles model, are represented by solid lines in Figure 2b, while the dotted lines indicate the field emission current, calculated within the Fowler-Nordheim theory formalism [8]. It is easy to see that the difference in field-emission currents obtained within first-principles model and the Fowler-Nordheim theory, respectively, increases with decreasing distance between the electrodes, which is due to the influence of quantum-size effects, as it was indicated earlier in [9].

IV. Conslusions

Thus, in this work we presented a description of the technology of fabrication of a silicon diode with an air gap of about 65 nm, the I-V characteristics of which were measured under atmospheric conditions and demonstrate linear behavior in Fowler-Nordheim coordinates. At the same time, the results obtained within the first-principles theoretical approach can serve as a first step towards the consideration of field-electron emission process at the nanoscale beyond the Fowler-Nordheim theory. To describe correctly the field-emission current of air-channel silicon diode at ultra-small air gaps varied from 0.6 to 1.2 nm, quantum-size effects should be taken into account.

Acknowledgment

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