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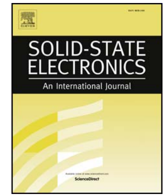

Narrowing of band gap at source/drain contact scheme of nanoscale InAs–nMOS

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ABSTRACT

A multi-scale simulation study of Ni/InAs nano-scale contact aimed for the sub-14 nm technology is carried out to understand material and transport properties at a metal-semiconductor interface. The deposited Ni metal contact on an 11 nm thick InAs channel forms an 8.5 nm thick InAs leaving a 2.5 nm thick InAs channel on a *p*-type doped ($1 \times 10^{16}\,\text{cm}^{-3}$) $AlAs_{0.47}Sb_{0.53}$ buffer. The density functional theory (DFT) calculations reveal a band gap narrowing in the InAs at the metal-semiconductor interface. The one-dimensional (1D) self-consistent Poisson-Schrödinger transport simulations using real-space material parameters extracted from the DFT calculations at the metal-semiconductor interface, exhibiting band gap narrowing, give a specific sheet resistance of R_{sh} = 90.9 Ω/sq which is in a good agreement with an experimental value of 97 Ω/sq.

1. Introduction

Metal-semiconductor contacts are essential components of many electronic devices [1]. Due to continuing scaling to nanometer dimensions, an accurate modeling of transport through metal-semiconductor contacts is the key to the development of novel nano-scale semiconductor devices [1,2] such as the next generation of III–V based transistors [3]. The III–V compounds show a large potential as a high mobility channel material to replace the current silicon (*n*-type) transistor technology in CMOS [1,2]. In addition to the high carrier mobility, they exhibit a high injection velocity resulting in reduced power dissipation at low voltage operations [3].

In this work, we present a multi-scale simulation study of a nanoscale contact combining density functional theory (DFT) calculations with solutions of 1D Poisson-Schrödinger (1DPS) equation aiming to understand a relation among contact resistance and band structure at the interface [4] relevant to the future of sub-10 nm technology [5,6].

2. Ni contact for source/drain of III-V MOSFET

A description of the self-aligned device architecture of the heterostructure used in this paper is given in Fig. 1. In practice, the nano-scale contact under study is made of Ni metal interfacing an 11-nm thick InAs layer on *p*-type doped (1×10^{16} cm^{-3}) $AlAs_{0.47}Sb_{0.53}$ (960-nm) buffer. A thermal reaction between Ni and InAs results in the formation of an 8.5 nm thick Ni_3InAs layer [5] leaving only a 2.5 nm thick of InAs acting as a channel [5].

3. Density functional theory calculation of the structure

In order to gain physical insight into carrier transport through the contact, we have employed 1DPS simulations using self-consistently [7] coupled Poisson-Schrödinger (PS) equations assuming a real-space dependent material parameters (band gap and affinity) obtained from *ab initio* density functional theory (DFT) calculations [6]. The Ni_3InAs /InAs (1 0 0) interface was modelled as a periodic heterostructure shown in Fig. 2. The DFT calculations were performed to a large size of the unit cell (consisting of 1127 atoms) using the Perdew, Burke and Ernzerhof [8] functional and the projected augmented waves method [9] using the Vienna *ab initio* simulation package (VASP) [10]. A $2 \times 2 \times 1$ Monkhorst-Pack **k**-point set was used for the calculation with a cut-off of 500 eV. The density of states (DOS) for the semiconductor segment of the structure was projected on the atomic layers of In and As [4] to create the Layered Projected Density of States (LPDOS). LPDOS is divided into sub regions, along the direction perpendicular to the contact interface. Each sub region includes all atoms of one atomic

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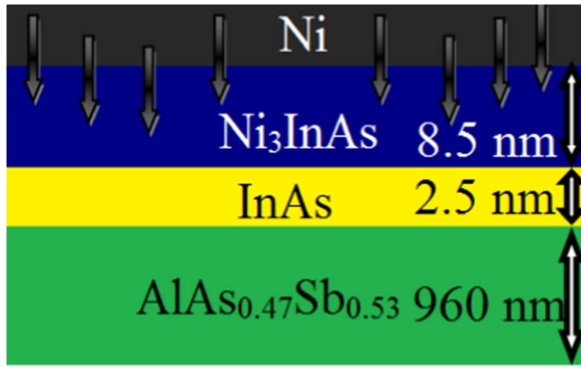

Fig. 1. Schematic of layers structure of the source/drain contact for a nano-scale InAs MOSFET. Structure has an 8.5 nm Ni_3InAs, 2.5 nm InAs, and $AlAs_{0.47}Sb_{0.53}$ buffer layers. The Ni_3InAs alloy is formed by Ni deposition on the 11 nm InAs layer. Black arrows indicate diffusion of Ni into InAs layer.

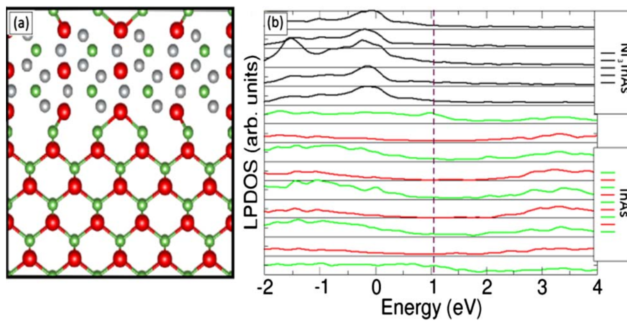

Fig. 2. (a) Atomic structure for Ni_3InAs/InAs (b) The layered projected density of states (LPDOS) for the Ni_3InAs/InAs interface calculated using VASP (PBE functional) from Ref. [6].

plane as defined in the Ni_3InAs/InAs system in Fig. 2. Then, we calculate the LPDOS as a convolution of the DOS projected on each atom assigned to the corresponding sub region. As a sequence, the total energy of the system is set to the minimum with respect to the coordinates of all atoms and the cell parameters. Fig. 2 shows the geometric structure and density of states projected on atoms of each atomic plane in the InAs/Ni_3InAs (1 0 0) heterostructure [6].

4. 1D transport simulations

The source/drain (S/D) contact model used in the simulations was chosen to match the size and the composition of experimental structure made of an 11 nm thick InAs channel deposited on *p*-type $AlAs_{0.47}Sb_{0.53}$ buffer (doped to 1×10^{16} cm^{-3}) [5]. Then the Ni deposited as a metal contact on S/D followed by thermal treatment to create an 8.5 nm thick Ni_3InAs alloy, leaving only a 2.5 nm thickness of un-doped InAs layers as a device channel (semiconductor), as it shown in Fig. 1.

Due to the well-known deficiencies of DFT, the LPDOS of InAs does not reproduce a true band gap. However, the LPDOS for the Ni_3InAs/InAs atoms has a band gap which follows the same trend as seen previously for the Mo/GaAs [4].

The thicknesses of the layers in the heterostructure, doping, energy band gaps, conduction band offset, mobility, electron effective masses,

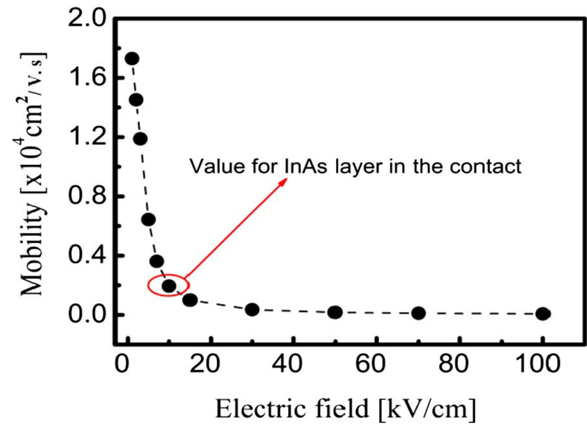

Fig. 3. Electron mobility vs. applied electric field in bulk InAs obtained from ensemble Monte Carlo simulations.

and permittivity are collected in Table 1 [11]. NiInAs is modelled assuming an InAs layer heavily doped to *n*-type concentration of 3×10^{19} cm^{-3}. This highly degenerate semiconductor mimics well the transport in NiInAs alloy exhibiting a bandgap. Note that the electron mobility in InAs has been obtained from Monte Carlo simulations as detailed in the following.

Real-space dependent semiconductor material parameters assume that the equivalent change in a position of the edge of conduction and valence bands, energy gap, band offset occurs on the Ni_3InAs/InAs interface as observed in the Mo/GaAs structure [4].

The band structure assumes that only the lowest valleys in semiconductors (InAs and $AlAs_{0.47}Sb_{0.53}$) are active in the transport through the contact which is reasonable approximation in this heavily doped structure [6]. In order to determine the mobility of InAs used then in the 1DPS simulations, we estimate the electric field first, assuming a 1 V bias applied across the contact [12]. Electric field F can be calculated as $F = V/t$ [12], where t is the thickness of a structure (11 nm InAs and 960 nm $AlAs_{0.47}Sb_{0.53}$) to get:

$F = \frac{V}{t_{(InAs+AlAsSb)}} = \frac{1V}{971\text{nm}} \approx 10\text{kV/cm}$ The electron mobility in InAs (intrinsic) plotted in Fig. 3 as a function of applied electric field has been obtained from bulk ensemble Monte Carlo simulations [13]. Details of these Monte Carlo simulations can be found in Refs. [14,15]. Fig. 3 shows that, at an electric field of 10 kV/cm, the intrinsic electron mobility of *n*-type InAs doped to 1×10^{16} cm^{-3} (nearly intrinsic) is 1960 cm^2/Vs, and 200 cm^2/Vs when *n*-type doped to 3×10^{19} cm^{-3} [16] as collected in Table 1. Finally, the electron mobility of *p*-type $AlAs_{0.47}Sb_{0.53}$ (doping concentration 1×10^{16}) used in the 1DPS is 1350 cm^2/Vs and is based on the experimental data taking into consideration the material composition of $AlAs_{0.47}Sb_{0.53}$ and carrier concentration [17].

Fig. 4a and 4b shows the conduction band, valence bands and Fermi level overlapped with electron density from the 1DPS solutions. We assume a bulk metal work function of Ni (5.01 eV) and calculate Schottky barrier height (SBH) as a potential difference between the work function and electron affinity. For the metal work function (5.01 eV) and affinity (4.9 eV) [6], the SBH was extracted as 0.11 eV. The work function dramatically affects the transport at the interface and the sheet resistance value was calculated (165 Ω/sq). When the

Table 1
InAs, and $AlAs_{0.47}Sb_{0.53}$ material parameters used in Modeling of the InAs/$AlAs_{0.47}Sb_{0.53}$ contact.

Material Thickness [nm]	*n*-type doping [cm^{-3}]	*p*-type doping [cm^{-3}]	E_G [eV]	ΔE_C [eV]	μ [cm^2/Vs]	m_e [m_0]	ε_r [ε_0]
8.5 (InAs)	3×10^{19}	1×10^{14}	0.354	−0.71	200	0.023	15.50
2.5 (InAs)	1×10^{16}	1×10^{14}	0.354	−0.71	1960	0.023	15.50
960 ($AlAs_{0.47}Sb_{0.53}$)	1×10^{14}	1×10^{16}	1.846	0.315	1350	0.088	10.95

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