Multi-scale simulations of metal-semiconductor contacts for nano-MOSFETs

M. Aldegunde, S. P. Hepplestone*, P. V. Sushko* and K. Kalna
Electronic Systems Design Centre, College of Engineering, Swansea University,
Swansea SA2 8PP, Wales, United Kingdom. E-mail: m.a.aldegunderodriguez@swansea.ac.uk
*Department of Physics and Astronomy and London Centre for Nanotechnology,
University College London, London WC1E 6BT, United Kingdom

Metal-semiconductor contacts are integral components of electronic devices. With continuous scaling to nanometre dimensions, the carrier transport through the contacts can be a limiting factor in the performance of these devices. Therefore, the accurate modelling of the transport through the metal-semiconductor interfaces is key to the development of novel nanoscale semiconductor devices, such as the next generation of III-V based transistors [1]. We have developed a multi-scale simulation methodology using first principles atomic scale calculations and a semi-classical transport framework [2] that will allow for device simulations.

We first characterise the atomic structure and electronic properties of the metal-semiconductor interface using density functional theory (DFT) simulations. From these we extract position dependent values for parameters relevant to semi-classical simulations, such as electron effective mass, band gap and electron affinity. These are then mapped into a 3D self-consistent finite element ensemble Monte Carlo (MC) [3] simulations which are enhanced with a WKB tunnelling model [4] injecting/removing particles through the Schottky barrier at the vicinity of the metal-semiconductor interface.

A schematic of this two-level hierarchical method is shown in Fig. 1. The tunnelling probability is evaluated for every particle reaching a classical turning point. To avoid the burden that a full 3D modelling of the tunnelling would impose in a 3D self-consistent MC simulation, we use the following simplification. First, the shortest tunnelling path is found from the classical turning point. We extract the conduction band edge along this line and calculate the tunnelling probability for the longitudinal energy of the particle. Fig. 2 shows an example for a benchmark system, a Mo/n^+-GaAs interface, comparing the tunnelling probabilities, using NEGF and WKB approches, obtained for the conduction band edges from classical simulations and from simulations mapping properties from DFT calculations. MC self-consistent simulations can take into account the interplay between physical phenomena such as the shift of the conduction band edge, the dependence of the effective masses of the electrons on the distance from the interface, electron-electron interactions and image charge effects. In our MC simulations, we intrinsically include long range electron-electron interactions and static image charge effects via the solution of 3D Poisson equation at every time step.

For the benchmark system we first simulate a Mo/GaAs (100) heterostructure consisting of 5 monolayers of Mo and 8 bilayers of GaAs using DFT with the PBE density functional and PAW pseudopotentials, as implemented in VASP [5]. From these simulations, the relaxed atomic structure and layer averaged projected density of states (LPDOS) were produced as shown in Fig. 3. The LPDOS shows band gap narrowing and the presence of the metal induced gap states at both the Ga-and As-terminated interfaces. From the LPDOS in Fig. 3, the variations of the conduction and valence band edges are transferred into the 3D MC simulations. For the MC simulations, we have used a Mo/n^+-GaAs interface with n-type doping of 5×10^{19} cm^{-3}. We scale the material parameters close to the interface to reproduce the same conduction and valence band in a classical equilibrium simulation (Fig. 4). These parameters are then used in the doped Mo/n^+-GaAs. Fig. 5 shows the band diagram and WKB tunnelling probability. The simulations with and without position dependent parameters are also depicted. The increase in the tunnelling

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probability induced by the band gap narrowing leads to a reduction in the resistivity by more than one order of magnitude, from 2.1×10^{-8} to 4.7×10^{-10} Ω cm^2.

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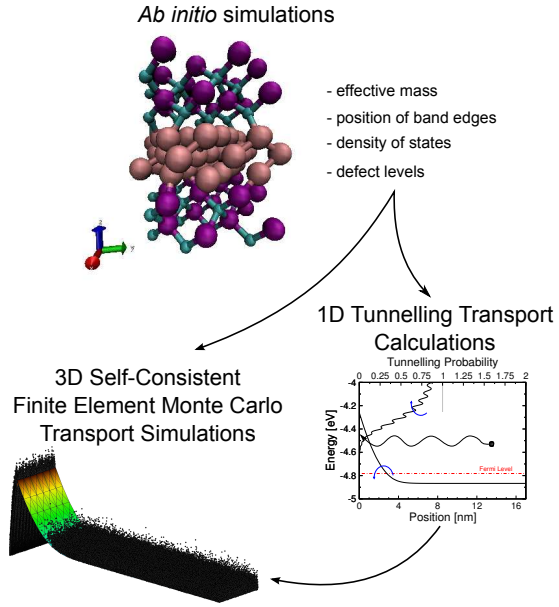

Fig. 1. Schematic representation of the hierarchical approach to calculating the current through a metal-semiconductor interface.

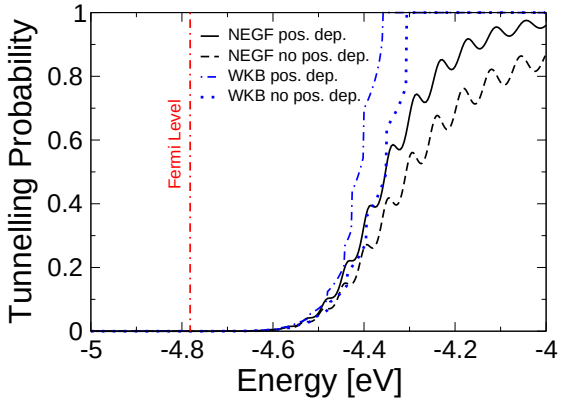

Fig. 2. Tunnelling probabilities for a 1D profile extracted from a 3D simulation of a Mo/n^+-GaAs interface. Probabilities calculated with position dependent parameters extracted from DFT and constant material parameters with both NEGF and WKB approximations are compared.

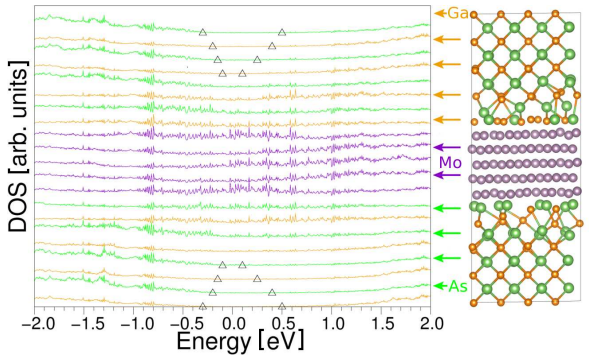

Fig. 3. Left: Projected density of states for the Mo/GaAs heterostructure. Triangles indicate the position of the conduction and valence band edges. The Fermi energy is set at 0.0 eV. Right: Atomistic structure of the supercell representing the Mo/GaAs heterostructure.

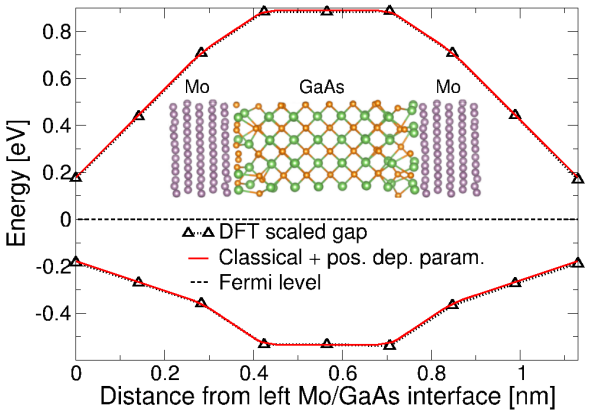

Fig. 4. Conduction and valence band edges calculated classically with the position dependent parameters (continuous red line) and extracted from the DFT simulation (black triangle dotted line) for a Mo/GaAs/Mo structure.

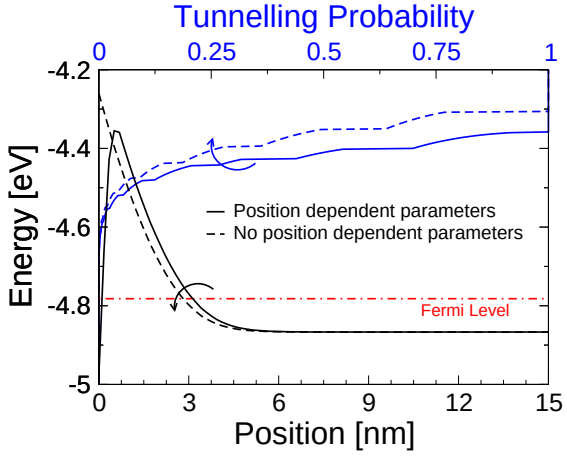

Fig. 5. Conduction band and WKB tunnelling probability of the simulated structure using position dependent material parameters (continuous line) and assuming constant bulk material parameters (dashed line).