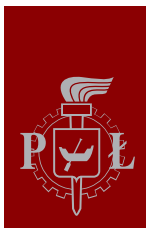

Lodz University
of Technology

CAD TOOLS

QuantumATK

Simulation of Ag–Si Metal–Semiconductor Junction

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OBJECTIVE

In this work, a simulation of the metal-semiconductor junction between silver (Ag) and silicon (Si) was realised using the QuantumATK software. This type of junction is typical of the particular family of diodes called Schottky. The objective is to investigate the response of the system under conditions of zero bias and under the application of a potential difference, with a focus on the Local Density of States (LDOS) and the transmission spectrum.

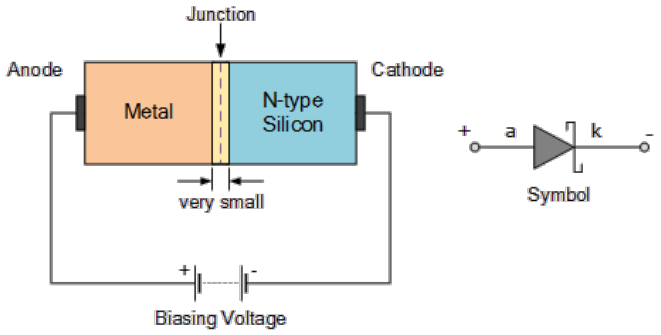

Figure 1 - Schottky Diode

1 DEVICE CONSTRUCTION

The first phase of the work involved the construction of the device from the crystal structures of the two materials involved. Both silver and silicon were modelled in their typical crystalline form.

The device structure was constructed in QuantumATK and consists of a left electrode made of silver (Ag), a central scattering region composed of Ag and Si, and a right electrode made of silicon (Si). The Ag structure was first retrieved from the materials database and cleaved along the (100) crystallographic direction using the *Surface Cleave* tool. This surface was then transformed into the left electrode through the *Electrode Builder*, with a sufficient number of atomic layers repeated along the transport direction to ensure convergence.

A similar procedure was applied to silicon: the diamond cubic structure of Si was cleaved along the (100) plane to create the right electrode. To build the central region, a silicon slab was joined with the Ag surface, and the lateral lattice constants were adjusted to ensure compatibility between the two materials. The interface spacing was manually tuned (typically 0.2–0.3 nm) to avoid unphysical overlaps or vacuum gaps. Care was taken to minimize strain at the interface by adjusting the in-plane lattice vectors, and the entire central region was built to include sufficient Ag and Si layers to preserve bulk-like behaviour away from the interface.

Before creating the final device configuration, the central region underwent structural relaxation using *OptimizeGeometry* block, where only atoms in the scattering region were allowed to relax, while electrode atoms were kept fixed to represent semi-infinite leads.

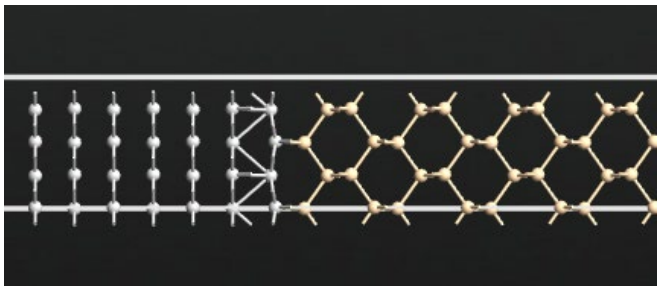

Figure 2 - Ag-Si Junction

Once relaxed, the full two-probe system was assembled using the *Device from Bulk* tool, with the relaxed Ag–Si interface as the central region, flanked by the Ag left electrode and the Si right electrode. The completed configuration was exported via the *Script Generator* as device.py, which includes all structural data and boundary conditions.

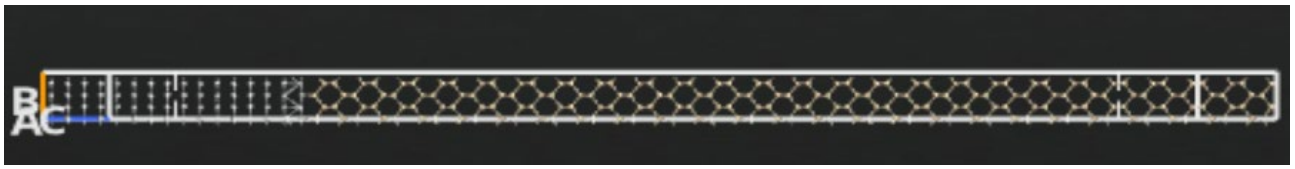

Figure 3 - Metal-Semiconductor Device

The configuration of the final device is therefore as follows:

- Left Electrode: Ag
- Right Electrode: Si
- Central Region: Ag–Si junction

The device was constructed along the z-axis, with an overall length of 140 Å, which is sufficiently large for the study of electron transport.

2 CALCULATION SETTING

Compared to typical numerical calculation models, the semi-empirical Slater-Koster method, available in QuantumATK, was chosen for the simulations due to its ability to correctly reproduce qualitative phenomena in nanoscopic devices. This enabled the desired results to be obtained with a reduced computational demand. The model was assigned to the entire device using the Set DeviceSemiEmpiricalCalculator block, which also allows the electrical potential conditions at the electrodes to be defined.

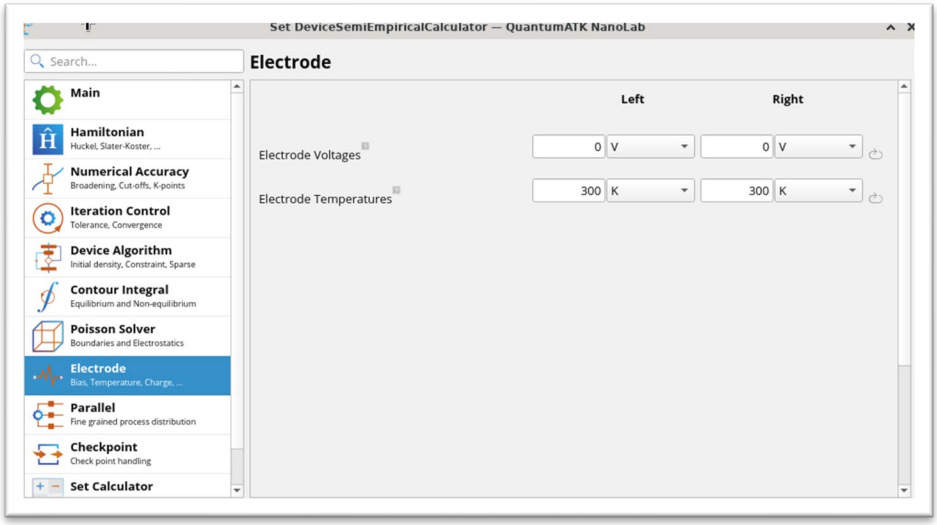

Figure 4 - Electrical Potential Conditions

Separate simulations were performed:

1. Null bias (0 V): voltage equal to 0 V on both left (Ag) and right (Si)
2. Positive bias (1-2-3 V): voltage of 1-2-3 V applied to the left electrode (Ag), keeping the right electrode (Si) at 0 V

This potential difference simulates the application of an electric field across the device, a prerequisite for studying its electronic behaviour.

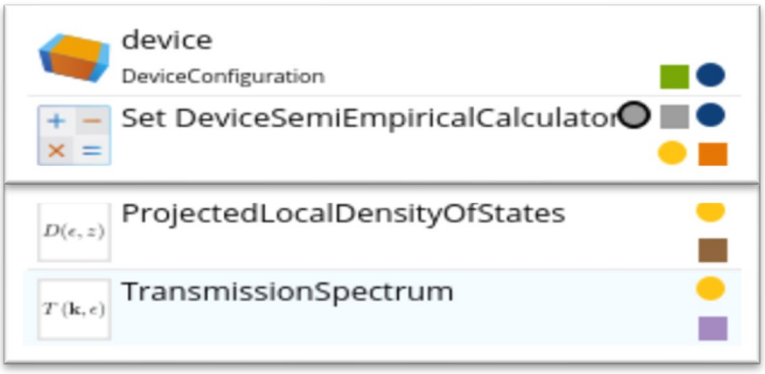

Figure 5 - Project Workflow

The workflow also presents the two blocks necessary for the simulations in which we are interested to study the electronic operation of our device: the ProjectedLocalDensityOfStates and the TransmissionSpectrum.

2.1 PLDOS (ProjectedLocalDensityOfStates)

PLDOS (*ProjectedLocalDensityOfStates*) is a spatial and energy representation of the density of states accessible to electrons along the device axis, which is particularly useful for studying the interfaces between two different materials. An electron cannot be everywhere: it needs a quantum state available at a certain energy. By 'accessible', therefore, we mean the available quantum states that an electron can occupy.

If,

- PLDOS is zero: There are no quantum states available at that position and energy, so there is no conduction.
- PLDOS greater than zero: There is a high probability that an electron can pass through that region, favouring conduction.

In summary, the density of electron-accessible states is a measure of where and with what energy an electron can pass through the material. The graphs show the energy level in eV along the length of the device. At the same time, the graph shows the LDOS value using a spectrum of colours, ranging from black to pink.

The window between ε_L and ε_R, visible within the transmission spectrum, is the so-called: Bias Window. This window represents the energies at which electrons can actually flow from one electrode to another:

- If there is transmission ≠ 0 inside this window → current flow.
- If the transmission is zero over the whole range → no current even if there is bias.

2.2 TRANSMISSION SPECTRUM

The Transmission Spectrum represents the probability of electrons transmission as a function of energy, in this case at the junction between silicon and silver.

The *TransmissionSpectrum* simulation in QuantumATK is a key tool for analysing quantum transport properties in nanoscale devices. It provides an accurate quantum-mechanical description of electron propagation, principally used when we have a junction between two different materials.

For the Ag–Si interface studied here, the *Transmission Spectrum* helps evaluate how efficiently electrons are transmitted from silver to silicon. Through this graph, it is possible to assess the probability of an electron with a given energy (given in eV) being transmitted and not reflected at the silicon-silver interface.

The *Transmission Spectrum* analysis also includes a 2D heatmap of the metal-semiconductor junction cross-section. Through this heatmap, it is possible to see graphically, with the aid of colours, in which areas of the junction cross-section electrons have more probability to cross from one material to another.

3 SIMULATIONS AND RESULTS

3.1 PLDOS RESULTS

Case 1 – Null Bias (0 V)

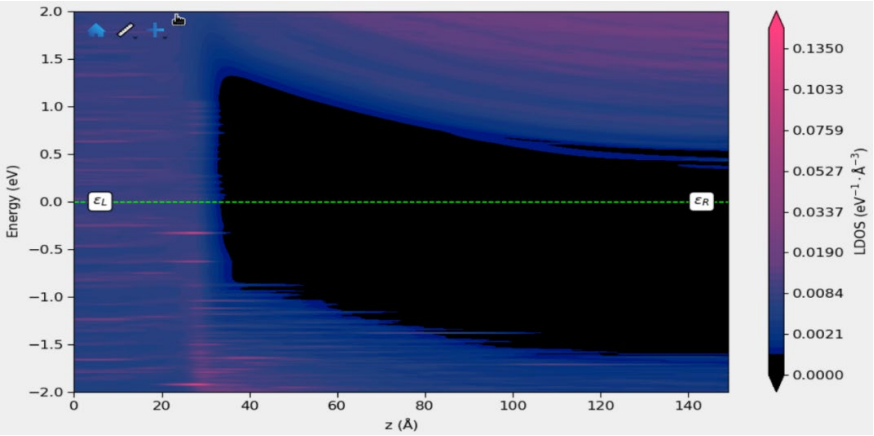

Figure 6 - PLDOS | Case Null Bias

The first simulation was carried out by applying a zero-voltage bias to the ends of the device. From the graph we can see that the 2 Fermi's levels are aligned, so there is no movement of electrons, i.e. there is no conduction.

Case 2 - 1-2 V BIAS

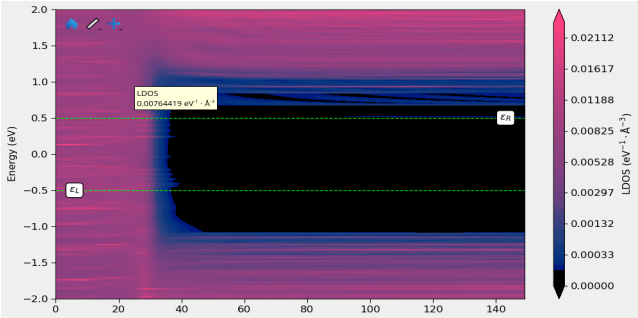

Figure 7 - PLDOS | Case 2 V bias

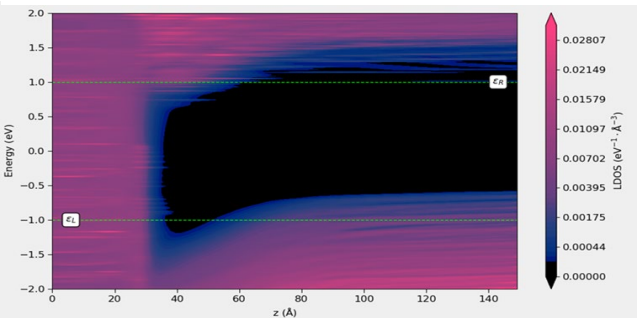

Figure 8 - PLDOS | Case 1 V bias

When a bias of 1 or 2 V is applied to the metal (Ag) contact the 2 Fermi's levels aren't aligned. However, in both cases, the Fermi's levels pass through forbidden regions (black bands) where no electrons are available. This indicates that the junction does not yet conductat this value of bias.

Case 3 – 3 V BIAS

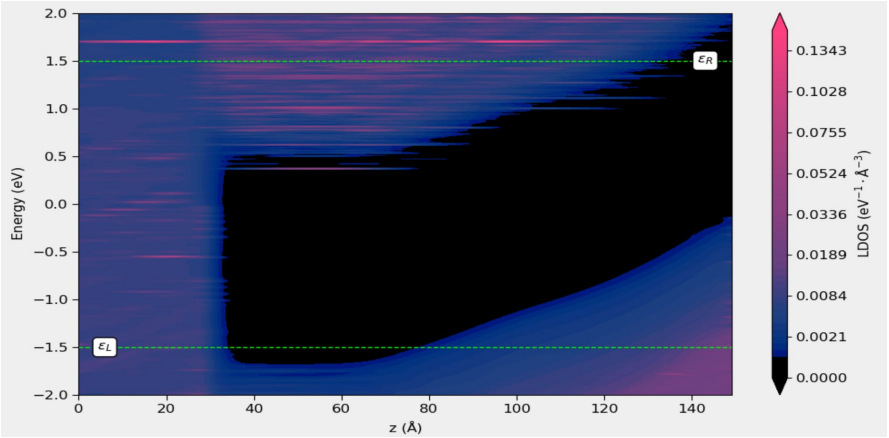

Figure 9 - PLDOS | Case 3 V bias

In this case, inside the Fermi's window there is a continuous pathway between the right and left electrodes that allows electrons to flow and avoid the forbidden regions.
This phenomenon is supported by the Transmission Spectrum.

3.2 TRANSMISSION SPECTRUM RESULTS

Case 1 – Null Bias (0 V)

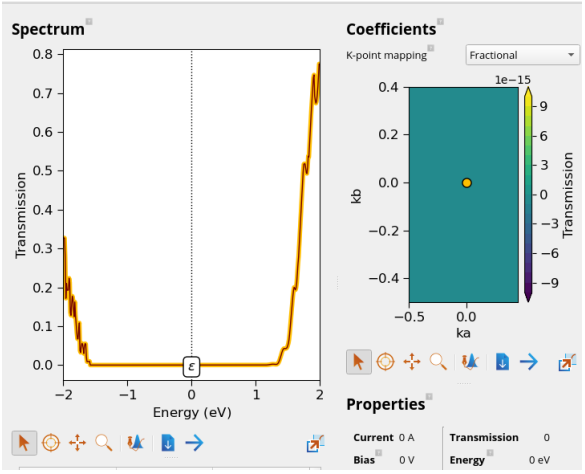

Figure 10 - Transmission Spectrum | Case Null Bias

In the first case, since the two Fermi levels are aligned, there can be no conduction and consequently no transmission of electrons through the junction.

Case 2 – 1-2 V Bias

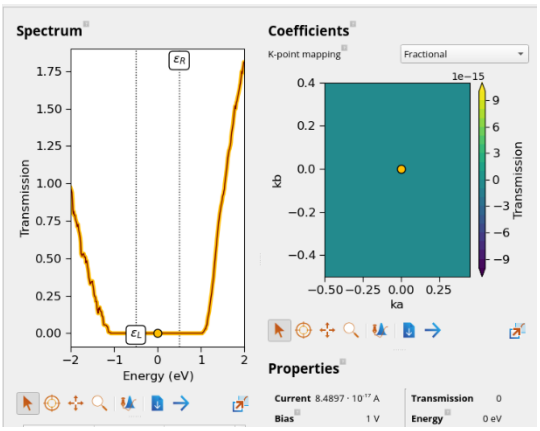

Figure 11 - Transmission Spectrum | Case 2 V bias

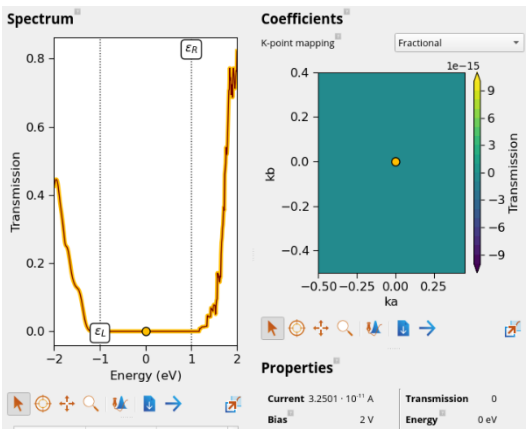

Figure 12 - Transmission Spectrum | Case 1 V bias

The results of the different simulations show that when the bias increases, the Fermi's window tends to be widened, so the range of energy values that an electron can assume in order to flow from one electrode to another increases.

However, to obtain electron transmission between silicon and silver, it is necessary that the transmission spectrum, within the Fermi's window, must assume non-zero values. Otherwise, the electrons arriving at the interface are reflected.

Case 4 – 3V Bias

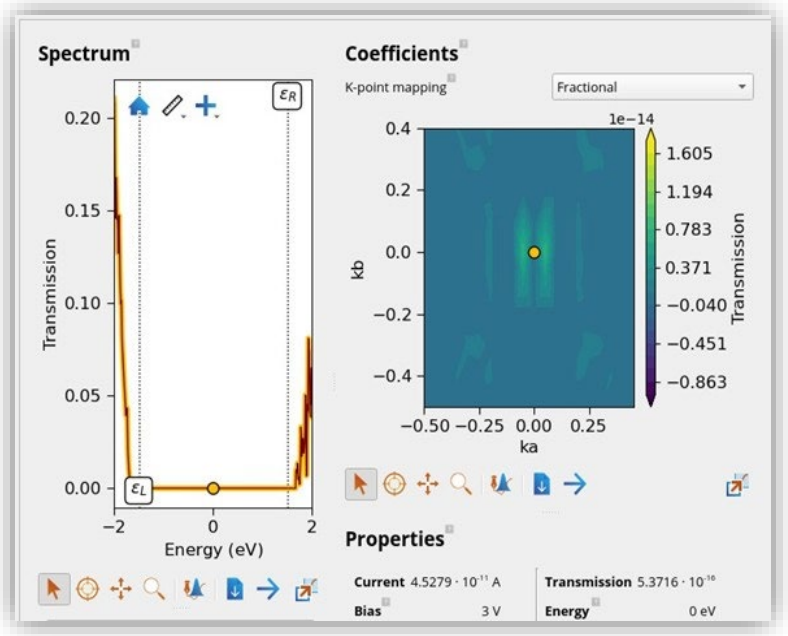

Figure 13 - - Transmission Spectrum | Case 3 V bias

An analysis of the various simulations carried out by varying the bias shows that there is a non-zero transmission only when the bias is 3V, although this value is extremely low. Consequently, the current that we can measure at the two electrodes will also be very low.

Regarding heatmaps on the right side, we can see that there are all dark, indicating that there is no transmission (0 V,1V and 2 V bias cases). The only exception is the heatmap referring to the 3 V bias where light areas can be seen. This means that there is beginning to be transmission between the 2 materials.

4 CONCLUSIONS

In conclusion, our study confirmed the expected behaviour of a Schottky junction between silver and silicon using QuantumATK.

The simulations, carried out by increasing different bias voltage, from 0 V to 3 V, and using a semi-empirical Slater-Koster method, clearly show that conduction only emerges above a bias threshold, in this case about 3 V. This highlights the presence of an effective potential barrier at the interface, typical of semiconductor-metal devices, and demonstrates the reliability of the model used to describe electronic transport at the nanoscale.

TECHNICAL APPENDIX

- Software: QuantumATK S-2025.06
- Computational Method: Extended Hückel (Semi-Empirical)
- Materials: Ag, Si
- Electrode Configuration: Ag (left), Si (right)
- Simulated Bias: 0 V, 1 V, 2 V, 3 V (left electrode)
- Used Modules: DeviceSemiEmpiricalCalculator, ProjectedLocalDensityOfStates, TransmissionSpectrum