MICRO-435

Exercises W10: MT fabrication, Circuits and Transport Numerical Simulation

Question 1: array circuits with MT

Refer to figure 1 where the sketch of an Inverter based on MT organized as in an ARRAY of NanoGAPs, and to the general structure in figure 2

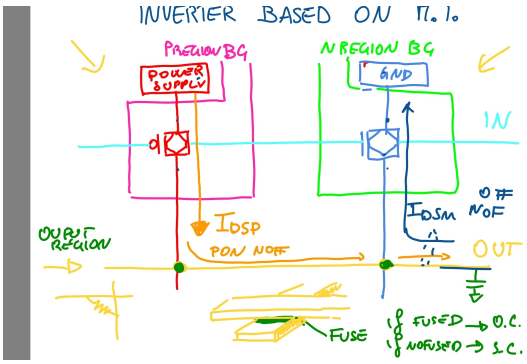

Figure 1: Inverter based on MT in a MATRIX of NANOGAPS

Design the following circuits:

- a) NAND, AND
- b) NOR, OR
- c) XOR, XNOR
- d) Half-Adder

In all the cases clarify: the position of backgates, the input and output, and explain the current flow depending on the input conditions. Verify the whole truth's table. Discuss where problems could arise.

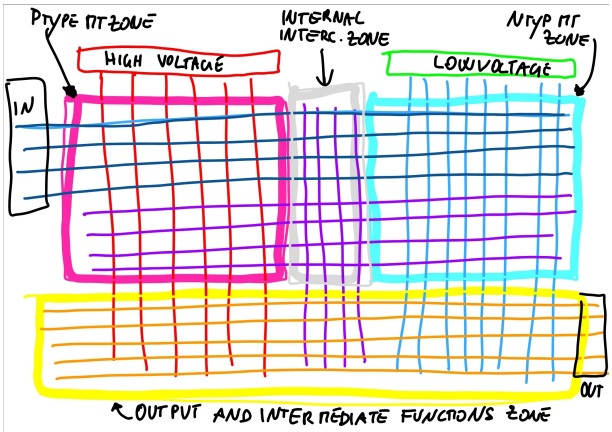

Figure 2: General MATRIX of NANOGAPS for MT

Question 2: fabrication of MT and molecule selection

It is necessary to estimate for a CDBJ process the lenght L_{bridge} of the bridge wire to be fabricated. L_{bridge} must be chosen depending on the optimal number of rings N rings of a molecule derived by oligothiophene maximizing the I_o/I_{off} ratio of a MT.

- (a) Formulate the lenght L_{bridge} dependency on the number of rings N rings knowing that the average elastic strain ϵ for TiN is 0.0053 and that the crack in the brige wire d_{wire} depends linearly on the crack in TiN w_{TiN} by a constant k = 0.2. Consider that a single ring length is approximately l_{ring} = 2nm
- (b) Analyze and sketch approximately the Transmission spectrum $T(E)$ and the Current $I(T(E))$ of the molecules with the increasing number of rings. Name the molecules M-1R, M-2R, and so on, the Transmission spectrum to be identified $T(E)_{1R}$, $T(E)_{2R}$ and so on, and the current I_{1R} , I_{2R} and so on. Explore up to a maximum of 5 rings. Consider a maximum BW of 5eV. Use the following simplified model:
  - in the simple case of 1 ring (M-1R) the HLG is 3.5eV , E F = 0eV, HOMO and LUMO peaks are symmetrical w.r.t. E F , and, considering broadening, the area A Lz90 associated to 90% of the Lorentian distribution corresponds approximately to a "Lorenzian base" LzB = 1eV . Only the HOMO peaks and LUMO are included in the BW.
  - when the number of rings increases $HLG(N_{rings}) = \frac{3.5-(1-N_{rings})^2}{6}$
  - for each new ring introduced, a new peak (both in HOMO and LUMO sides) is introduced in the BW
  - when a new ring is considered the A Lz90 for each peak in the BW corresponds to a halved base LzB w.r.t. the case with the previous nr. of rings. For simplicity keep the same peak height as in the initial 1 ring situation.
  - when new peaks are added they are consecutive but not superposed (e.g. the HOMO and HOMO+1 peaks have two consecutive "Lorenzian bases")
- (c) Identify and discuss the optimum number of rings N_{rings} in order to Maximize the I_o/I_{off} ratio of a MT based on these possible molecules. Select the useful BW $<$ 5eV
- (d) Identify and discuss the lenght L bridge derived by the optimum N rings calculated above

Question 3 - Working with the EEBESD numerical model

From now on, you will be guided with a few exercises using EEBESD (e.g. EEBESD-focus1, EEBESD-focus2,...) and a few questions to help you focus on essential notions. Please use the same notation in your report by explicitly reporting the question code near the answer. The MATLAB code of the EE-BESD algorithm is given on moodle. Please download the whole zipped kit W10-EEBESD-EX3-files.zip and unzip it in a directory of your system.

he code is organized as follow:

- The *EEBESD_MAIN.m* is the main file. It is heavily commented so it should be easy to modify.
- The file *SetParameters.m* defines the physical constants and main physical functions and, depending on the molecule chosen in the main file, imports molecule parameters.
- The file *SetVoltages.m* sets the voltages applied to the molecules.

- The file *AtkResults.m* allows generating the transmission spectrum and current-voltage curve obtained from ATK.
- The file *EeBesdStandard.m* executes the EE-BESD algorithm.

For the moment, have a quick look at the mentioned files. Later on, you will have to answer questions requiring you to understand the code better.

EEBESD_focus1: An initial analysis of 3TT molecule

Let us start with the 3TT molecule. If you don't remember the structure have a look at the description in the theoretical section. Let us observe in figure 3 the Transmission Spectrum (named TS from now on) at the equilibrium (V_{ds} = 0 V) calculated using an atomistic calculation. The figure shows two clear peaks in the LUMO side and a few peaks in the HOMO side. However, the main current contribution is generated by the peaks close to the Fermi level (0 eV); therefore, the HOMO and LUMO peaks. Also, second-order HOMO-1 and LUMO+1 peaks play a relevant role in the conduction.

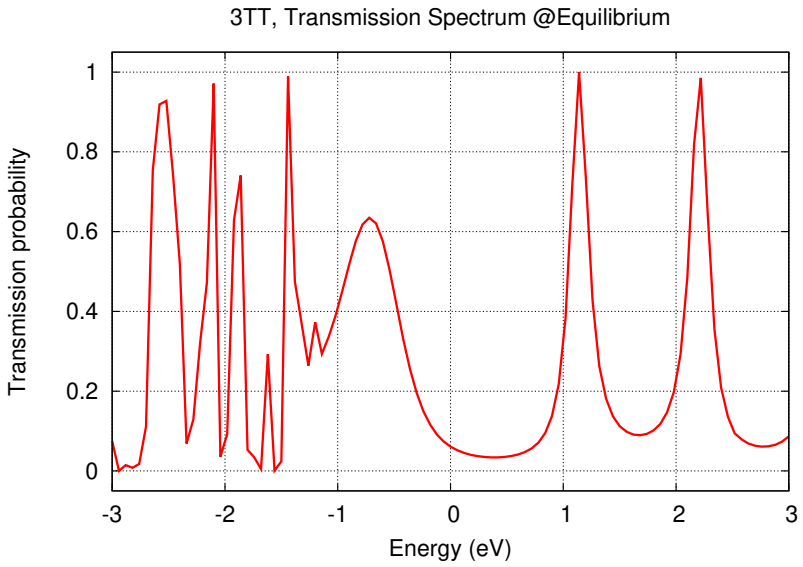

Figure 3: TS of 3-rings thiophene molecule at equilibrium

Let us consider to apply to the molecular transistor a drain-source voltage V_{ds} in the range comprised between -3 V and 3 V. Let's assume that the Transmission Spectrum (TS) remains the same of figure 3 when the V_{ds} is varied.

EEBESD_focus1_Q1: In the considered V_{ds} voltage range [-3 V, +3 V], which is the maximum width of the Bias Window (named BW from now on) you may have? Does the BW **width** changes if you consider $V_{ds} = -3$ V or $V_{ds} = +3$ V?

EEBESD_focus1_Q2: *Qualitatively* sketch the behavior of the current I_{ds} as a function of the applied voltage V_{ds} by hand.

By removing the fixed TS assumption, we let the transmission spectrum free to change when the bias voltage is varied. To do this, we need to know how the TS evolves, since for each different applied V_{ds} the molecular system reaches a new energy level due to the charge effect. Figure 4 shows a few spectra obtained with different V_{ds}s, the spectra are superposed and vertically shifted for the sake of clarity. The V_{ds} varies from -1.5 V (bottom graph) to 0 V (top graph). Other spectra for larger V_{ds} (in absolute values, not shown for the sake of clarity) behave similarly to the trend shown here.

IMPORTANT: notice that each curve of the TS, figure 4, is shifted by a quantity equal to V_{ds}. That means, the TS in the bottom of the figure, which seems to have a transmission probability in the range [-1.5, -0.5], is actually shifted by a quantity $V_{ds} = -1.5$ V. Therefore, the transmission probability is actually in the range [0.0, 1].

EEBESD_focus1_Q3: What do you observe in the trend of the represented spectra?

EEBESD_focus1_Q4: Try to sketch the behavior of the current Ids as a function of the applied voltage V_{ds}.

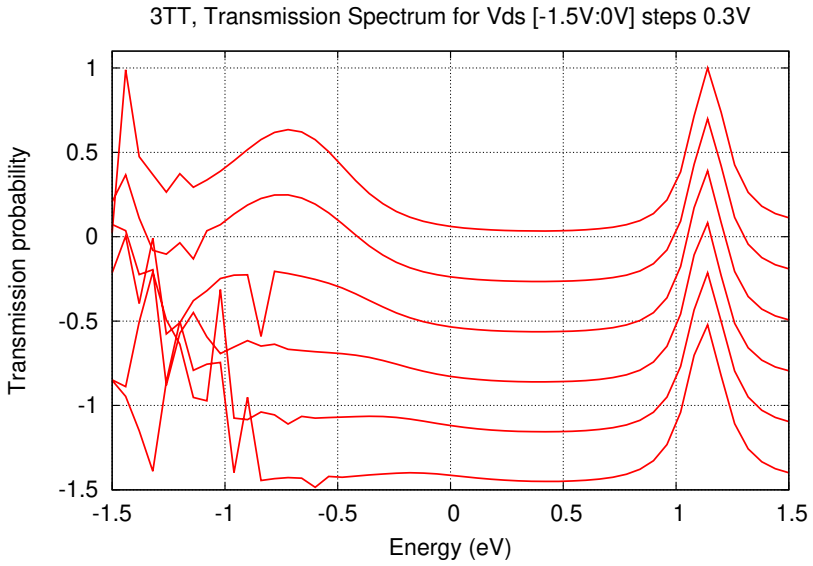

Figure 4: TS of 3-rings thiophene molecule for Vds changing from 0 (top graph) to -1.5V (bottom graph); variations are 0.3V from one graph to the next.

Let us start to use the algorithm. Open the file EEBESD_MAIN.m (you can use an editor, e.g. kwrite in the system for example, or the internal editor in matlab, as you prefer). As you notice, this module allows you to define which molecule you are working with, so make sure you select 3TT in this exercise by checking the variable "molec_name" has content '3TT'.

Moreover, this module also calls the other submodules. Open the *SetParameters* module. This file contains all the physical quantities needed by the EEBESD algorithm. The only parameter that can be changed and related to structural behavior is *vdf* (voltage division factor). The voltage division factor measures the two contact quality, i.e., how the molecule potential organizes concerning the source/drain potentials. If the drain and the source are identical, the default value 0.5

V is correct. Of course, source and drain contact are not perfectly equal in general in real systems; for this reason, the vdf value can be changed.

The *SetParameters* file automatically includes the file Molc_Inputs_3TT of the 3TT subdirectory (because the used molecule is the 3TT). Open this latter file and analyze the parameters which are written in the code. This set of parameters is extracted from ab initio simulations.

EEBESD_focus1_Q5: What do E0 array and all its values represent? HINT: Refer the values contained in E0 to the TS at the equilibrium shown in figure 3.

As you remember, the gamma parameters describe how "happy" the electron is to move between the electrode and the molecule. Of course, it includes the anchoring group characteristics.

EEBESD_focus1_Q6: Briefly describe the meaning of each parameter in the files *SetParameters.m* (lines 1-17, do not describe code after the comment 'Load molecule values') and *Molc_Inputs_3TT.m*. Make sure to understand the parameters as later you will be asked to change some of them.

Going back to the main module EEBESD_MAIN.m, after defining parameters, the script calls the function *SetVoltages* that defines the voltages applied to the transistor. This module is independent on the molecule.

The main module (in EEBESD_MAIN.m) calls the script *AtkResults* (open it), which loads and plots the TS at equilibrium and the final I/V curve obtained by ab initio simulation. These curves are used as a reference for these exercises. Finally, the main module calls the actual EE-BESD main function *EeBesdStandard*. For the moment, you are invited to take a look at the script, but you are not required to analyze this script line-to-line, just run it by pressing the green 'Run' button or writing *EEBESD_MAIN* in the MATLAB console.

After running the main code, you will see in the MATLAB figure 1 in a few seconds. MATLAB figure 1 reports the results obtained by atomistic ATK simulation.

EEBESD_focus1_Q7: Is the I/V curve similar to the one you have tried to sketch? If not, try to find the reason for your error.

Have a look at the remaining figures you obtained with the first execution. All the figures show the result of the EeBesdStandard module. Among these, there is also the current (MATLAB figure 2).

EEBESD_focus1_Q8: Do you observe substantial differences between the results obtained with the *ab initio* simulation and with the EE-BESD? It could be interesting to calculate the error between the two IV curves obtained.

EEBESD_focus1_Q9: Look at the figure showing the TS with the parametric curve (MATLAB figure 4). Do you observe a substantial difference with respect to the actual peak variations obtained by *ab initio* simulations reported in figure 4 of this document?

EEBESD_focus2: Analysis of molecule 4TT

Now, in the main module, change the molecule name from 3TT to 4TT and execute to plot the results for this molecule.

EEBESD_focus2_Q10: Observe the differences with respect to graphs obtained for molecule 3TT, what do you see? Did you expect these variations and how do you explain them?

We now focus on the effects introduced by the variation of gamma. In the file containing the parameters for molecule 4TT the gamma array is provided. You can see an attenuation factor 0.1 describing the "electronic compatibility" between the electrode and the molecule. Try to observe the effect when changing the gamma factor.

EEBESD_focus2_Q11: Before changing, what do you expect if you reduce the gamma factor? What if you increase it? Plot the results obtained by increasing and decreasing the gamma parameter, list and explain the main differences by relating the effects to the possible physical causes.