Scaling of Molecular Electronics Devices

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1 characterization procedure

Here, we use Poisson equation[1] to examine the electric field distribution in the simplified device structure shown schematically in figure 1. We study different oxide thickness and present all results for both thin (T_{ox}=*1 nm*) and thick dielectric (T_{ox}=*100 nm*). The gap distance between the drain and source is *1* or *4 nm*, and contains 4-thioacethylbiphenil or PDT material. These molecules are modeled as rigid dielectric material with suitable relative permittivity 2 [ref. 2] or 6.3 [ref. 3]. We performed simulations using TCAD tools[1]. The set of simulations were run under GENESISe. The tool flow starts with the two dimensional editor MDRAW (mesh generator/device). DESSIS was used to perform the device simulation. The results, e.g. the electric field distributions inside the device structure are visualized with the plotting and extraction tool Tecplot. Since TCAD tools do not normally allow device dimensions as small as those considered in this research, a possible approach is to scale voltages and dimensions. For example, a classical method to maintain the short channel MOSFETs behavior is to reduce all dimensions and voltages of larger device by a scaling factor κ (>*1*), so that the internal electric fields are the same as those of a long channel FET. This widely used approach is called constant field scaling [4]. Based on the fundamental limits, it may be possible to scale the FETs down to very small dimensions such as *10nm* of channel length or smaller [5]. We use the scaling relations at constant field to determine all dimensions and voltages of nanoscale FETs [4, 6]. Nanoscaled SAMFET circuit parameters are scaled up by a factor κ=1000 to produce larger FET with similar internal electric fields behavior.

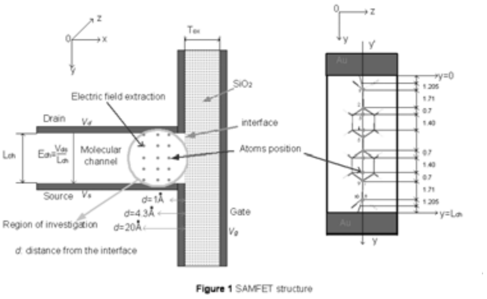
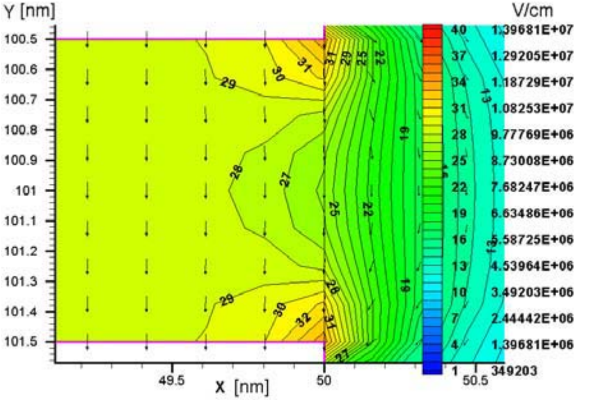


Figure 1 *cross section view of molecular field effect*

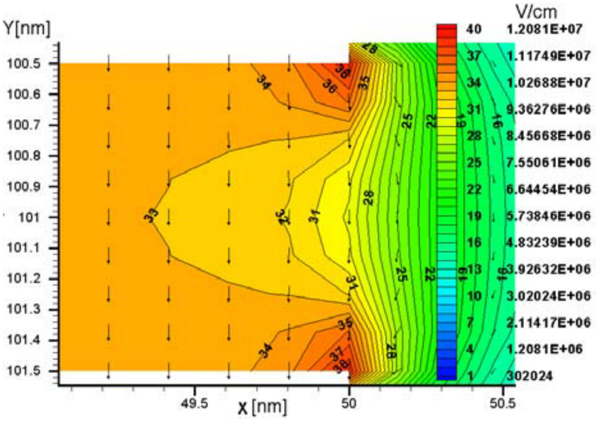
2 Simulation Results

Fig. 2 and 3 show the fields distribution for T_{ox}/L_{ch} *=5* and *15* respectively with the dielectric constant ε=2 and 6.3. Near the drain or source electrode, from the interface, the non-uniform field region penetrates the molecular channel for *4Å* (fig.2) and *3Å* (fig.3). At mid distance between drain and source, the electric field penetration from the interface is about *3Å* for fig. 2 and *6Å* for fig. 3. By comparison with the results in fig.2 and 3, a typical representative of the region where T_{ox}/L_{ch} is increased from *15* to *50* (not shown in here), the gate field seems to have little effect on the fields inside the molecular structure.

In order to compare the electric field distribution inside the active region along the molecular channel at atoms position, fig. 4 and 5 show the variation of channel electric field versus the gap distance at different distances *d* from the interface 1, 2, 2, 4 or 5 Å. The drain electrode is located at *y=0* and the source at $y=L_{ch}$. Certain points in the y-axis correspond to the atoms positions. The details are reported by the author in ref.7. The electric field distribution is completely symmetrical with respect to a horizontal line at mid-distance between drain and source. High field are near the source or drain electrode. The field becomes larger when *d* decreases. Low fields are observed in the middle of the drain and source electrode. The same symmetry (not shown in this paper) was observed for ε=*6.3*.



(a) ε =2.

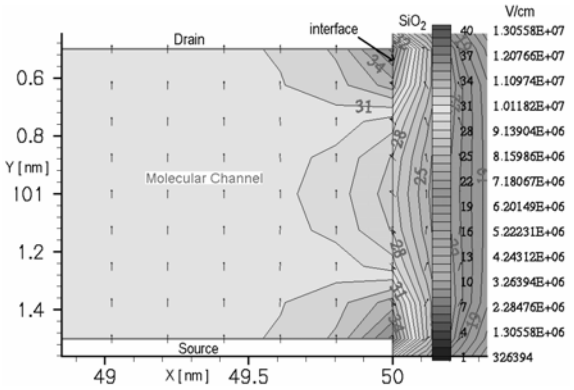


(b) ε =6.3.

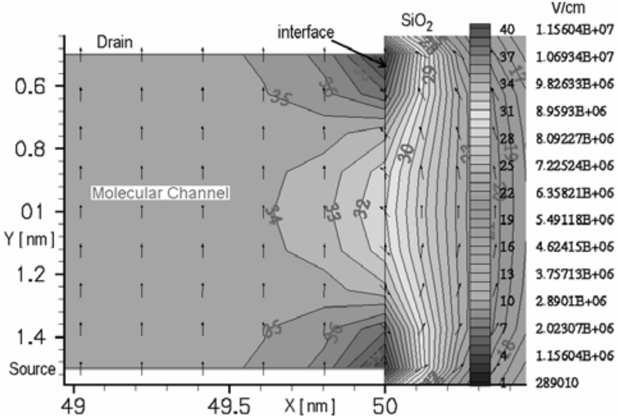
Figure 2 *Electric field distribution for T_{ox}/L_{ch} =5 with V_d=1 V, V_g=1 V, T_{ox}=5nm, L_{ch}=1 nm, V_d/L_{ch}= 0.1 Kv/A.*

3 Conclusion

Calculations of electric field distribution on FETs molecular channel is carried out on the range of T_{ox}/L_{ch} =[0.2-50] under different dielectric constant of the molecular environment. Based on numerical simulations, to evaluate the voltage gate effect on the molecular channel, three regions can coarsely be defined as follows:1) strong gate effect, T_{ox}/L_{ch} =[0.2-0.66], 2)significant gate effect, T_{ox}/L_{ch} =[0.66-5] and 3)limited gate effect, T_{ox}/L_{ch} >5. For T_{ox}/L_{ch} of the order of 5, V_g has a limited impact on the channel field. A high T_{ox}/L_{ch} limits this effect. When T_{ox}/L_{ch} is too large, V_g does not have much effect on the channel field distribution. The difference of the dielectric constant seems has no effect on modifying the channel field distribution.



(a) ε =2.



(b) ε =6.3

Figure 3 *Electric field distribution for* T_{ox}/L_{ch}*=15 with* V_d*=-1V,*V_g*=-05V,*T_{ox}*=15nm,*L_{ch}*=1nm,*V_d/L_{ch}*=0.1Kv./A*

Reference

[1] Integrated Systems Engineering (ISE)of Technology Computed Aided Design (TCAD)software. Simulation structure in our paper is 2D dimensional.
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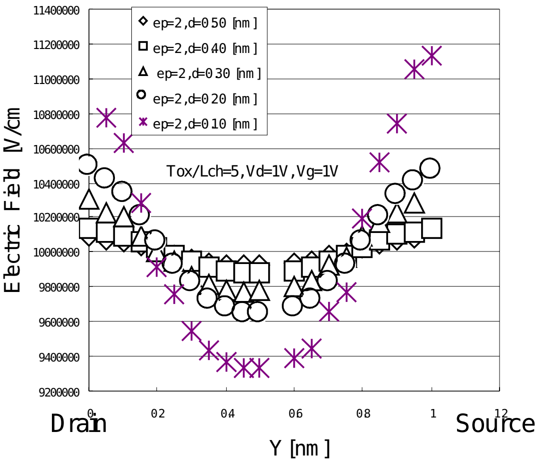
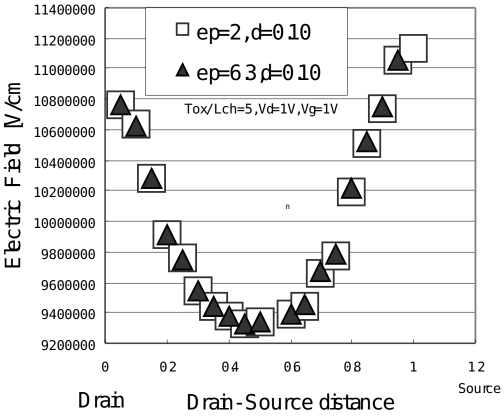
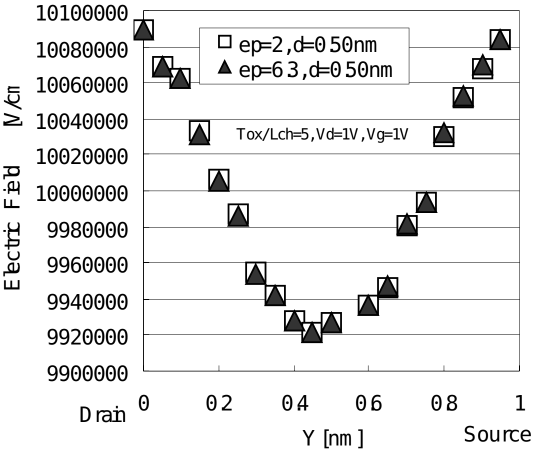


Figure 4 *Electric field versus gap distance. d=1, 2, 3, 4 and 5Å..* L_{ch} *=10Å ,* T_{ox}/L_{ch}*= 5,* V_d*=1V,* V_g*=1V and ε=ep=2*



(a)



(b)

Figure 5 *Electric field versus gap distance.* L_{ch} *=10Å ,* T_{ox}/L_{ch}*= 5 with* V_d*=1V,* V_g*=1V ε=ep=2 and 6.3.*