The Electrical Field Distribution in Molecular Electronics Devices

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Abstract:

The purpose of this paper is to study the gate field penetration and modulation of molecular channels by presenting field analysis results for different nanoscale geometry structure of SAMFETs. This kind of structure was originally studied by Hendrick Schön[1)] and Damle[2)]. We have performed numerical simulations in three terminals atomic scale device geometry field effect transistors (FETs), with L_{ch} of the order of 2 or 4nm. Our electrostatic analyses characterize the electric field distribution inside the device structure when the ratio of dielectric thickness T_{ox} to L_{ch} (T_{ox} /L_{ch}) ranges from 0.2 to 50.The molecular channel contains self-assembled monolayer (SAM). These molecules are modeled as rigid dielectric material with relative permittivity of 2 (ref. 2) or 6.3 (ref. 3). We use a Schrödinger solver coupled with the Poisson equation to examine the electric field distribution in the region of interest. The TCAD tools were used to perform the simulations. The tool flow starts with the editor MDRAW (mesh generator/device). DESSIS performs the device simulation. The results to be presented in the final paper, 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 K (>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)].

We discuss and compare our previous[5)] and present findings with previously published theoretical results[2)]. The relation between β, the gate control parameter and T_{ox}/L_{ch} was extracted from figure 8 (ref. 2) to allow comparing our respective results. This relation is only approximate, since Damle *et al.*'s calculations are based on a Hamiltonian with rigorous electrostatic modeling [2)], whereas our calculations are based on a simple electrostatic model. This approximation could change the limits of separate lines boundaries between good, average and bad gate modulation regions.

Based on our results, for a value of T_{ox}/L_{ch} as low as 0.1, very strong gate effect is expected, while Damle *et al.* predicted good gate control. Moreover, we found that there is strong gate effect on the channel electric field for values of T_{ox}/L_{ch} as high as 0.6. From our results, such gate effect decreases, but remains significant when the value of T_{ox}/L_{ch} reaches 1.5, where Damle *et al.* reported that some gate modulation is present.

Our results approximately correspond to Damle *et al.*'s work[2)]. It seems that some gate modulation may still be present, even for larger value of T_{ox}/L_{ch} such as 1.5. This quantitative agreement is rather encouraging.

Our results are based on a conventional electric field analysis, which has not included quantum mechanical effects. It can provide useful guidelines for the design of future nanoscaled FETs. Moreover, it also gives useful information for detailed calculations of I-V characteristics.

References

[1] Jan Hendrick Schön, Nature/Vol.413/18 Oct. 2001/pp.713-715
[2] Prashant Damle, Titash Rakshit, Magnus Paulsson, Suppriyo Datta, IEEE Transactions on Nanotechnology, Vol. 1, No. 3, 3002, pp. 145-152.
[3]C. Zhou et al., Appl. Phys. Lett., 71, 1997, pp 611-613.
[4] David J. Frank et al., Proceedings of the IEEE, vol.87, No4, April 1999, pp.537-570
[5] Aissa Boudjella, Zhongfang Jin Yvon Savari, 2003 International Microprocess and Nanotechnology Conf. (MNC2003), pp.240-241 Tokyo, 2003.