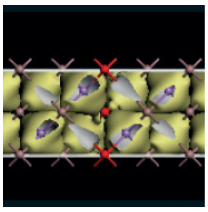

Image charge models for accurate construction of the electrostatic self-energy of 3D layered nanostructure devices

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Efficient analytical image charge models are derived for the full spatial variation of the electrostatic self-energy [1] of electrons in semiconductor nanostructures arising from dielectric confinement using semi-classical analysis. The effect of the electrostatic self-energy on the I_D-V_G characteristics of gate-all-around nanowire silicon transistors for different oxide thickness is subsequently studied numerically using the non-equilibrium Green's function formalism.

The semi-classical electrostatic self-energy due to a charge Q at location $\mathbf{x}$ within a region with dielectric constant ε that is embedded in a dielectric heterostructure is:

$$\Sigma(\mathbf{x};\varepsilon) = \lim_{\mathbf{x}\to\mathbf{x}_1} \frac{Q^2}{8\pi\varepsilon}\left(g[\mathbf{x},\mathbf{x}_1]-g_0[\mathbf{x},\mathbf{x}_1]\right)$$

Here, $g_0[\mathbf{x},\mathbf{x}']$ is the classical Green function of the Laplace equation for a homogeneous *bulk* region with dielectric constant ε; $g[\mathbf{x},\mathbf{x}']$ is the corresponding Green function for the dielectric heterostructure. Although the electrostatic self-energy may be pre-computed along with a tight-binding evaluation of nanostructure energy band structure [2] there are considerable advantages in deploying accurate compact analytical models for the self-energy: it aids understanding of the key physical processes and the scope of effective device design is considerably strengthened without complex NIC.

Our approach utilises rigorous analytical solutions [3] for the electrostatic self-energy in cylindrical and rectangular 3D geometries for wrap-round gate nanowire FETs (Figures 1, 2) in semiconductor dielectric structures (with obvious extensions to carbon based structures). The exact formulations involve infinite sums and integrations over the relevant special function combinations appropriate to the geometry (assumed to have a high degree of symmetry about the channel direction). These rigorous results are used to extract and validate very much simpler compact models based on image charge concepts (both point charge and line charge) for long channels and finite channels plus source-drain extensions. The summation over image charges is well known [4] to have convergence problems because the resultant series are *asymptotic*. However, provided a position independent contribution to the self-energy is correctly identified, we have determined that low-order truncation in image charge sequences can deliver very accurate approximations for the self-energy. This result follows from taking the local limit of the classical Green function and the subtraction of the Coulomb divergence. It should be noted that our methodology does not use an *ad hoc* construction (such as an Ewald sum) of the image sequences but uses a convergent deconstruction based on exact convergent integral representations of the Green function.

The strategy may be exemplified by considering the electrostatic self-energy for a charge Q embedded in the channel of an infinite planar double gate structure sketched in Figure 3. In Figure 4, curve A is numerically computed from the exact formulation; curve B is computed using just two image charges. More complex structures require of the order of kN images where N is the number of interfaces and k is related to the number of vertices. For cylindrical geometries we encounter *line image charges* that often take *limaçon* forms (Figure 5). Figure 6 shows schematically the location of leading image charges required to model the self-energy near an extension between source and drain. With heterostructures, the resultant image charges are re-normalised via parameters depending on the dielectric mismatches.

Finally, the formalism is applied to the Non-Equilibrium Green Function modelling [5] of wrap-round gate nanowire FETs based on silicon technology. Generally, the effect is to modulate the channel confinement potential [3] and to lower the barrier potential.

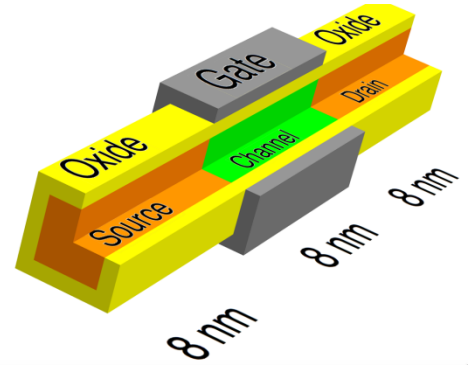


Figure 1: schematics of a wrap round gate nanowire FET: rectangular geometry

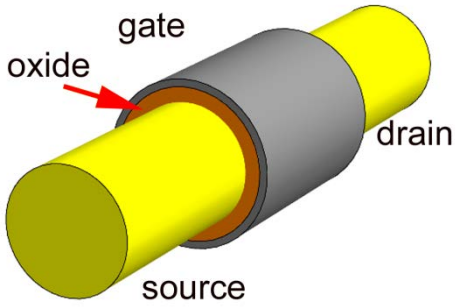
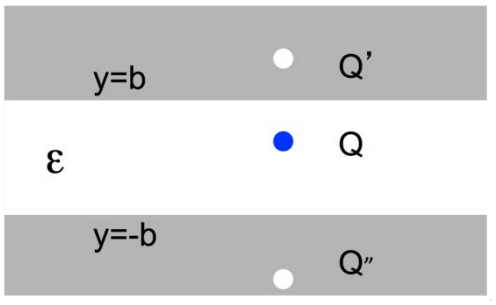


Figure 2: schematics of a wrap round gate nanowire FET: cylindrical geometry



$$\Sigma(\mathbf{x},\varepsilon) = \frac{-Q^2}{16\pi\varepsilon}\left(\frac{1}{b-y} - \frac{1}{2b} + \frac{1}{b+y}\right)$$

Figure 3: a planar double gate structure showing point charge Q, and leading image charges Q', Q''

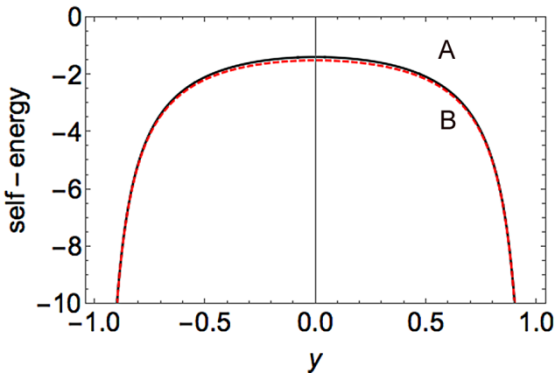


Figure 4: exact electrostatic self-energy (A) compared with (B) a two image model for the structure in Fig. 3. Interfaces at $y = b = \pm 1.0$.

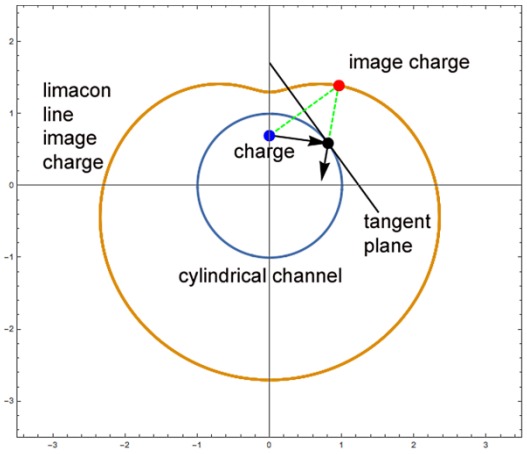


Figure 5: A limaçon line image charge for a cylindrical channel.

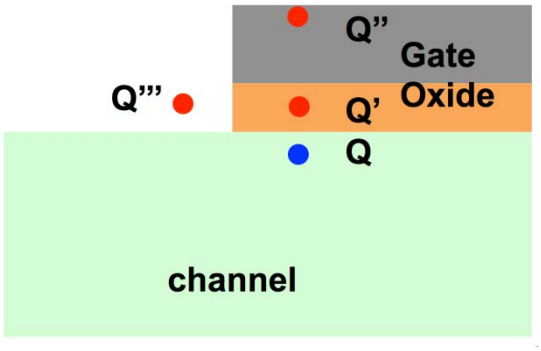


Figure 6 Leading image charges required to model the self-energy near an extension between source and drain.

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