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# ENERGY OF THE SCREENED COULOMB INTERACTION IN MOS STRUCTURE WITH THE DIELECTRIC ENVIRONMENT OF FINITE THICKNESS

In the inversion channel of the MOS device structure the properties of the screened Coulomb interaction potential considering the finite thickness of the dielectric layer and the dielectric inhomogeneity of the environment are comprehensively discussed. The explicit dependences of the screened Coulomb potential on the dielectric constants of the semiconductor and oxide layer, as well as the oxide layer thickness are obtained. The analytical features of the received interaction potential are provided.

***Keywords:*** inversion channel, screening, screened interaction potential.

Nowadays, silicon-based electronics has reached possible physical limits and the continued optimization trend has insisted on the decisive importance of the semiconductor quasi-two-dimensional (Q2D) channels with the highly mobile electron gas (Q2D EG) on the dielectric gate layers with sub-nanometer equivalent thickness in metal–oxide semiconductor (MOS) devices. Various materials such as III-V group semiconductors, few-layer graphene and metal dichalcogenides are promising candidates for low- power consumption and high switching speed of MOS device requirements whereas dielectric gate layers with a high (relative to $SiO_2$) dielectric constant value (high – κ dielectric) are of key interest [1]. In turn, the downscale technology goes also in an alternative way, and the gate dielectric layers with a low dielectric constant value relative to $SiO_2$ (low – κ dielectric) of the same thickness are demanded as well. The latter may reduce particularly the parasitic capacitance of the MOS device, enabling to make the switching speeds faster as well as lowering the heat dissipation performances [2].

Successful scaling of MOS structures towards shorter channel lengths requires higher doping levels to achieve high drive currents and minimized short-channel effects. The high levels of substrate doping needed in nanodevices to prevent the punch-through effect, leading to the Q2D nature of the carrier transport, were found responsible for the increased threshold voltage and decreased channel mobility.

Every MOS device, regardless of the component materials combination choice, its for own operation exhibits joint features requiring one or several strongly finite thickness dielectric layer media, demonstrating dielectric polarization effects due to the difference between the dielectric constants of the semiconductor channel and dielectric barriers' regions. As a result, the spatial nearness of the metal gate and finite thickness dielectric environment would reasonably modify the Coulomb interaction properties in the inversion channel region in comparison with the host semiconductor itself.

The MOS device structure inversion channel region related real-space screened by 2D EG Coulomb interaction potential calculations taking into account the inhomogeneous and finite dielectric environment is provided in the presented paper for the first time. Let us have a four-layer heterogeneous MOS structure in which the region $z \leq -(L+D)$ is occupied by a gate metal, the region $-(L+D) < z \leq -L$ by a dielectric oxide layer with dielectric constant $\varepsilon_D$ of thickness $D$, region $-L < z \leq 0$ by an intermediate dielectric layer with dielectric constant $\varepsilon_L$ of thickness $L$ and the region $0 < z \leq \infty$ by a semiconductor substrate with dielectric constant $\varepsilon_S$ as shown in Fig. 1. Here the z axis is perpendicular to the dielectric layer interfaces. The point charge $e$ at the site with coordinates $\rho = 0$, $z = z_0 > 0$ ( $\rho$ - is two-dimensional (2D) plane coordinate) is placed in the oxide/semiconductor junction region with 2D inversion layer containing 2D EG.

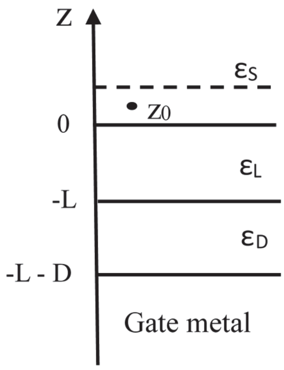

*Fig. 1. Four layer MOSFET system*

The screened Coulomb interaction potential $\varphi(\rho, z)$ of the point charge is related to Poisson's equation as

$$\varepsilon(z)\nabla_{\vec{r}}^{2}\varphi(\vec{r},\vec{r}_0) = -4\pi[e\delta(z-z_0)\delta(\vec{\rho}) + \rho_{ind}(\vec{r},\vec{r}_0)], \quad (1)$$

where $\delta$ is the Dirac-delta function, $\vec{r} = \vec{r}(\vec{\rho}, z)$. In Exp (1), $\rho_{ind}$ is the induced charge density, which, in accordance with the Tomas – Fermi method, has the form:

$$\rho_{ind} = -\frac{2\pi e^2}{\varepsilon_w}\frac{\partial n_s}{\partial \mu_0} g(z)\overline{\varphi}(\vec{\rho}) \;, \quad (2)$$

where $n_S$ is the surface density at temperature $T$, $\mu_0$ – the chemical potential in the absence of the Coulomb perturbing field, $g(z) = |\psi(z)|^2$ is the normalized charge distribution. In Exp.(2), $\overline{\varphi}(\vec{\rho})$ is the averaged screened potential acting on the electron:

$$\overline{\varphi}(\vec{\rho}) = \int_0^{\infty} \overline{\varphi}(\vec{\rho}, z)\, g(z)\, dz \quad (3)$$

and gives no change in the normalized eigenfunction $\psi(z)$ of the electrons' self-consistent effective mass equation but gives a change in the latter's eigenvalue.

Exp. $(\partial n_s / \partial \mu_0)$ in (2), on the condition of the size quantum limit, i.e. when the one-particle ground quantum level in the active chanel is occupied only, is determined from the Debye model as:

$$\frac{\partial n_s}{\partial \mu_0} = \frac{m_e}{\pi \hbar^2}[1 - \exp(-\pi n_s \hbar^2 / m_e k_B T)] \;, \quad (4)$$

where $m_e$ is the electron effective mass, $k_B$ is the Boltzmann parameter.

Poisson's equation (1) with Exps. (2) and (4) then gets the well-known form [3]:

$$\nabla^2 \varphi(\vec{\rho}, z) - 2q_s\, g(z)\overline{\varphi}(\vec{\rho}) = \begin{cases} -\dfrac{4\pi e}{\varepsilon_s}\delta(\vec{\rho})\delta(z - z_0) & z \geq 0 \\ 0 & z < 0 \end{cases} , \quad (5)$$

where $q_s$ is the 2D screening parameter defined as:

$$q_s = \frac{2\pi e^2}{\varepsilon_s}\frac{\partial n_s}{\partial \mu_0}. \quad (6)$$

Exp. (6) in particular for the non-degenerate ($\pi\ n_s\ \hbar^2\ /\ m_e\ k_B\ T<<1$) and degenerate ($\pi\ n_s\ \hbar^2 / m_e k_B T >>1$) Q2D EG statistic has the forms:

$$q_S = \frac{2}{a_0} \text{ and } q_S = \frac{2}{a_0}\frac{\pi n_s \hbar^2}{m_e k_B T} \quad (7)$$

where $a_0 = \varepsilon_w \hbar^2 / m_e e^2$ is the electron Bohr radius.

To solve Eq.(1), here we utilize the cylindrical coordinate system expressing the interaction potential in Fourier components $\varphi(k,z)$ with respect to the coordinate $\rho$ as:

$$\varphi(\vec{r}) = \varphi(\vec{\rho}, z) = \frac{1}{(2\pi)^2}\int_0^{\infty} e^{i\vec{k}\vec{\rho}}\varphi_k(z)\, d^2\vec{k} = \int_0^{\infty} J_0(k\rho)\,\varphi_k(z)\, kdk \;, \quad (8)$$

where $\vec{k}$ is the electron 2D plane vector, and $J_0$ is the 0-th order Bessel function.

The Poisson's equation (1) with Exp. (8) for the discussed system gets the form:

$$\begin{cases} \nabla_z^2 \varphi_k(z) - k^2 \varphi_k(z) - 2q_s g(z)\varphi_k(z) = -\dfrac{2e}{\varepsilon_s}\delta(z - z_0) & z \geq 0 \\ \nabla_z^2 \varphi_k(z) - k^2 \varphi_k(z) = 0 & z < 0 \end{cases}, \qquad (9)$$

which would be solved applying appropriate electrostatic boundary conditions:

$$\begin{cases} \varphi_k(z)\big|_{-(L+D)} = 0 \\ \begin{cases} \varphi_k(z)\big|_{z_i^-} = \varphi_k(z)\big|_{z_i^-} \\ \varepsilon_{i^+} \dfrac{\partial \varphi_k(z)}{\partial z}\bigg|_{z_i^+} = \varepsilon_{i^-} \dfrac{\partial \varphi_k(z)}{\partial z}\bigg|_{z_i^-} \\ z_i = -L;\ 0 \end{cases} \end{cases}. \qquad (10)$$

The appropriate general solutions of corresponding inhomogeneous andhomogeneous equations of Exp. (9) are respectively:

$$\varphi_k(z)\big|_{z>0} = \frac{2e}{\varepsilon_s}\frac{e^{-k|z-z_0|}}{2k} + C_1 e^{-kz} - 2q_s \overline{\varphi}_k \int_0^\infty g(z')G(z,z')dz' \qquad (11)$$

and

$$\varphi_k(z)\big|_{z<0} = \begin{cases} C_{2a}e^{-kz} + C_{2b}e^{kz} & 0 \geq z \geq -L \\ C_{3a}e^{-kz} + C_{3b}e^{kz} & -L \geq z > -(L+D) \\ 0 & z \leq -(L+D) \end{cases}, \qquad (12)$$

where $C_{3b} = C_{3a}e^{k(D+L)}\left(e^{k(2D+L)} - e^{-kL}\right)$, $G(z,z') = \dfrac{1}{2k}e^{-k|z-z'|} + C_1 e^{-kz}$ and $C_i = const$ ($i=1,\ 2,\ 3$) are the coefficients to be determined by the Exp.(10). In Exp.(12), the screening by the gate metal on the induced potential is taken into account by imposing the condition $\varphi_k(z)=0$ , while among the coefficients $C_i$ , in accordance with Exp.(11), just $C_1$ corresponds to the channel region and has to be calculated. Applying the boundary conditions after Exp.(10) at *i*-th interface, we have for $C_1$ :

$$C_1 = \frac{2e}{\varepsilon_s}\frac{1}{2k}e^{-kz_0}\frac{\varepsilon_S^* - \varepsilon_D^*}{\varepsilon_S^* + \varepsilon_D^*}, \qquad (13)$$

where $\begin{cases} \varepsilon_S^* = \varepsilon_S \varepsilon_L \sinh kD \cosh kL + \varepsilon_S \varepsilon_D \cosh kD \sinh kL \\ \varepsilon_D^* = \varepsilon_L^2 \sinh kD \sinh kL + \varepsilon_L \varepsilon_D \cosh kD \cosh kL \end{cases}$.

As a result, the general solution of Eq.(11) is given by :

$$\varphi_k(z)\big|_{z>0} = \frac{e}{\varepsilon_s}\left[\frac{e^{-k|z-z_0|}}{k} + \frac{\varepsilon_S^* - \varepsilon_D^*}{\varepsilon_S^* + \varepsilon_D^*}\frac{e^{-k(z+z_0)}}{k}\right] - 2q_s\overline{\varphi}_k\int_0^\infty g(z')G(z,z')dz' \; , \quad (14)$$

where $G(z,z') = \frac{1}{2k}\left[e^{-k|z-z'|} + \frac{\varepsilon_S^* - \varepsilon_D^*}{\varepsilon_S^* + \varepsilon_D^*}e^{-k(z+z')}\right]$

and

$$\overline{\varphi_k} = \int_0^\infty \varphi_k(z)\big|_{z>0}\, g(z)dz =$$

$$= \frac{e}{\varepsilon_s}\frac{\left[\int_0^\infty e^{-k(z+z_0)}g(z)dz + \frac{\varepsilon_S^* - \varepsilon_D^*}{\varepsilon_S^* + \varepsilon_D^*}\int_0^\infty e^{-k(z+z_0)}g(z)dz\right]}{k + q_s\left[\int_0^\infty g(z)dz\int_0^\infty e^{-k|z-z'|}g(z')dz' + \frac{\varepsilon_S^* - \varepsilon_D^*}{\varepsilon_S^* + \varepsilon_D^*}\left(\int_0^\infty e^{-kz}g(z)dz\right)^2\right]} \; . \quad (15)$$

Exps.(14) and (15) present the screened Coulomb interaction potential related to the inversion layer region for the discussed four-layer structure.

Let us now discuss the analytical features of the obtained interaction potential.

1. In the absence of both any dielectric layer, i.e. $D = L = 0$ , and screening effect, Exp.(14) reduces to the well-know non-conductor/conductor junction expression:

$$\varphi(k,z,z_0) = \frac{2\pi e}{\varepsilon_S k}\left\{e^{-k|z-z_0|} - e^{-k(z+z_0)}\right\}; \qquad (16)$$

2. In the absence of both screening effect and metal with any dielectric layer, i.e. $L = 0$ $D\to\infty$ ($D = 0$ with $L\to\infty$)), the interaction potential (14) reduces to the semiconductor/bulk dielectric junction corresponding expression [3]:

$$\varphi(k,z,z_0) = \frac{2\pi e}{\varepsilon_S k}\left\{e^{-k|z-z_0|} + e^{-k(z+z_0)} \cdot \frac{\varepsilon_S - \varepsilon_{D(L)}}{\varepsilon_S + \varepsilon_{D(L)}}\right\}; \qquad (17)$$

3. In the presence of the screening effect, and in the absence of the metal with any dielectric layer, i.e. $L = 0$ with $D\to\infty$ ($D = 0$ with $L\to\infty$)), Exp.(14) reduces to the semiconductor/bulk dielectric junction corresponding expression (10 b) after Ref.[4];

4. In the absence of both screening effect and one dielectric layer, i.e. $L = 0$ , the interaction potential (14) goes to the expression:

$$\varphi(k,z,z_0) = \frac{2\pi e}{\varepsilon_S k}\left\{ e^{-k|z-z_0|} + e^{-k(z+z_0)} \cdot \frac{\varepsilon_S - \varepsilon_D cth(kD)}{\varepsilon_S + \varepsilon_D cth(kD)} \right\} \qquad (18)$$

for the semiconductor/dielectric layer/metal junctions case [5].

5. In the absence of the screening effect, Exp.(14) goes to the expression:

$$\varphi(k,z,z_0) = \frac{2\pi e}{\varepsilon_S k}\left\{ e^{-k|z-z_0|} + e^{-k(z+z_0)} \cdot \frac{\varepsilon_S - \varepsilon_D cth(kD) - \varepsilon_L th(kL) + \frac{\varepsilon_S\varepsilon_D}{\varepsilon_L} cth(kD)\, th(kL)}{\varepsilon_S + \varepsilon_D cth(kD) + \varepsilon_L th(kL) + \frac{\varepsilon_S\varepsilon_D}{\varepsilon_L} cth(kD)\, th(kL)} \right\}, \qquad (19)$$

which for the four-layer MOS structure case is discussed in Ref.[6].

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## ԷԿՐԱՆԱՎՈՐՎԱԾ ԿՈՒԼՈՆՅԱՆ ՓՈԽԱԶԴԵՑՈՒԹՅԱՆ ԷՆԵՐԳԻԱՆ ՎԵՐՋԱՎՈՐ ՀԱՍՏՈՒԹՅԱՄԲ ԴԻԷԼԵԿՏՐԻԿԱԿԱՆ ՄԻՋԱՎԱՅՐՈՎ ՄՕԿ ԿԱՌՈՒՑՎԱԾՔՈՒՄ

ՄՕԿ քառաշերտ կառուցվածքի ինվերսիոն շերտում համակողմանիորեն քննարկվել են էկրանավորված կուլոնյան փոխազդեցության պոտենցիալի հատկությունները՝ վերջավոր հաստությամբ և անհամասեռ դիէլեկտրիկական միջավայրի հաշվառմամբ: Ստացվել են կուլոնյան փոխազդեցության պոտենցիալի՝ կիսահաղորդչային և օքսիդային շերտերի դիէլեկտրիկական թափանցելիություններից, ինչպես նաև օքսիդային շերտի հաստությունից բացահայտ կախվածությունները: Քննարկվել են ստացված փոխազդեցության պոտենցիալի վերլուծական առանձնահատկությունները:

***Առանցքային բառեր.*** ինվերսիոն շերտ, էկրանավորում, փոխազդեցության պոտենցիալ:

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## ЭНЕРГИЯ ЭКРАНИРОВАННОГО КУЛОНОВСКОГО ВЗАИМОДЕЙСТВИЯ В МОП СТРУКТУРЕ С ДИЭЛЕКТРИЧЕСКОЙ СРЕДОЙ КОНЕЧНОЙ ТОЛЩИНЫ

В инверсионном слое МОП структуры всесторонне обсуждены свойства потенциала экранированного кулоновского взаимодействия с учетом конечности толщины диэлектрического слоя и диэлектрической неоднородности среды. Получены явные зависимости потенциала кулоновского взаимодействия от диэлектрических констант полупроводникового и оксидных слоев, а также от толщины оксидных слоев. Обсуждены аналитические особенности полученного потенциала взаимодействия.

***Ключевые слова:*** инверсионный канал, экранирование, потенциал взаимодействия.