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COULOMB INTERACTION ENERGY IN THIN OXID-BASED MOSFEET SYSTEMS

Inclusive analysis of the MOSFET structure inversion channel region-related real-space in the Coulomb interaction potential properties, considering the inhomogeneous and finite dielectric oxide background, is provided. In particular, the explicit dependence of the Coulomb potential on the thickness of the oxide layer is established. It is shown that the efficiency of the Coulomb interaction on a number of existing structures is the highest in the **InSb/SiO_2** MOSFET system.

Keywords: inversion channel, interaction potential, low (high) – k dielectric contrast.

The MOSFET (metal–oxide–semiconductor field-effect transistors) systems have been traditionally scaled on silicon (Si) for more than four decades. As nowadays MOSFETs scaling is reaching its physical and best possible limits, both the use of semiconductors with higher carrier mobility and the scaling down into the sub-nanometer equivalent oxide thickness range by dielectric layer with a high (relative to SiO_2) dielectric constant value (high – κ dielectric) are of decisive significance [1]. Materials such as III-V key semiconductors (InAs, InSb, InGaAs), few-layer graphene and metal dichalcogenides are promising candidates for ultra-low power, high-speed MOSFET application [2]. At the same time, the downscale technology is expanding in alternative direction as well, i.e. using the gate dielectric layer with a low dielectric constant value relative to SiO_2 (low – κ dielectric) of the same thickness.

All MOSFET systems for their functioning demonstrate a common feature that is, it requires one or several strongly finite thickness dielectric layer media, exhibiting important polarization effects due to the difference between the dielectric constants of the channel and the barrier regions. As a result, the spatial proximity of the metal gate and the finite thickness dielectric environment would reasonably modify the interaction potential in the inversion channel region in comparison with the host semiconductor environment itself.

Calculation of the MOSFET structure inversion channel region related real-space Coulomb interaction potential in account of inhomogeneous and finite dielectric background is the main aim of the presented paper.

Let us have a three-layer heterogeneous MOSFET structure in which region $z \le -D$ is occupied by a gate metal, region $-D < z \le -0$ by a dielectric oxide layer with dielectric constant ε_D of thickness D and region $0 < z \le \infty$ by a semiconductor

substrate with dielectric constant ε_S . The z axis is perpendicular to the interfaces. The point charge e at the site with coordinates $\rho = 0$, $z = z_0$ (ρ - is two-dimensional (2D) plane coordinate) placed in the oxide/semiconductor junction region with 2D inversion layer. Under these conditions, the expression of the e and $-e$ point charge real–space, the Coulomb interaction potential $V(\rho) = -e\ \varphi(\rho)$ in a three-layer MOSFET structure is

$$V(\rho) = -\frac{e^2}{\varepsilon_S/2}\left\{\frac{1}{\rho} - \frac{\pi}{2}\frac{1}{\varepsilon_r D}\left[H_0\left(\frac{\rho}{\varepsilon_r D}\right) - N_0\left(\frac{\rho}{\varepsilon_r D}\right)\right]\right\} \qquad (1)$$

where $H(x)$ and $N(x)$ are Struve and Neumann functions.

As obtained, the Coulomb interaction potential in the discussed case holds both the same k - and ρ - dependences as a corresponding potential in semiconductor / dielectric two- [3] and three- [4] layer dielectrically homogeneous systems in the presence of two-dimensional electron gas (2DEG). As it follows, the metal gate here modifies the Coulomb interaction in the same manner as the 2DEG by means of the statically screening effect in the aforementioned systems. Thereby, the metal gate in this case effectively shields the interaction of charges in the inversion channel towards weakening, which is to be expected. The quantity $\rho_D = \varepsilon_S D / \varepsilon_D$, analogous to the screening parameter in the noted homogeneous systems, here depends on both the dielectric oxide layer thickness and the neighboring media dielectric constant ratio. In turn, due to the factor $\varepsilon_S/2$ in the denominator, $V(\rho)$ is enhanced twice which is the characteristic feature of the discussed structure. The noted factor appears just in the two-layer system inversion channel with the strong low-k environment case [5] and in the strong "one-side" low-k environment three-layer case [6].

1. The low – k dielectric contrast case with $\varepsilon_r = \varepsilon_S/\varepsilon_D >> 1$.

There are distinct 2D distance ρ ranges, such as $\rho_D = \varepsilon_r D >> \rho \geq D$ and $\rho >> \rho_D = \varepsilon_r D$ that $V(\rho)$ possesses the following analytical features.

(i) For the moderate small wave vectors with $k\ D \leq 1$ and 2D distances $\rho_D = \varepsilon_r D >> \rho \geq D$ in the first approximation, we get:

$$V(\rho) = -\frac{e^2}{(\varepsilon_S/2)}\frac{1}{\rho}\left[1 + \left(\frac{\rho}{\varepsilon_r D}\right)\ln\left(\frac{\rho}{\varepsilon_r D}\right)\right]. \qquad (2)$$

(ii) For the small enough wave vectors with $k\ D << 1$ and large 2D distances $\rho >> \rho_D = \varepsilon_r D$ we obtain :

$$V(\rho) = -\frac{e^2}{\varepsilon_S/2}(\varepsilon_r D)^2\frac{1}{\rho^3}. \qquad (3)$$

As it follows, at large 2D distances, the interaction potential falls off as ρ^{-3} and, at the same, time strongly depends on the oxide layer parameters such as ε_D and D.

2. The high – k dielectric contrast case with $\varepsilon_r = \varepsilon_S / \varepsilon_D < 1$**.**

For the long wave related $k \leq 1 / D$ vectors, there are 2D distance ρ ranges such as $\rho \geq D$ that the variable $\rho / \varepsilon_r D$ in $V(\rho)$ by condition $\varepsilon_r = \varepsilon_S / \varepsilon_D < 1$ is always greater than unity. For the moderate small wave vector case $V(\rho)$ is preserved but for the wave vectors case small enough Exp.(3) would be consistent as well.

We carried out the numerical analysis of the $V(\rho$ interaction potential in two cases of oxide layer thickness $D = 2.5nm$ and $5nm$.

At first, we demonstrate the Coulomb interaction energy properties with **Si/SiO$_2$** *low–k dielectric contrast case* where the following material parameters are adopted: $\varepsilon_S = 11.7$, $\varepsilon_D = 3.9$ and the Bohr radius in the bulk Si sample $a_0 = 6.27$ nm.

In Fig.1, we outline the interaction potential $V(\rho)$ (scaled by meV) as a function of the intercharge planar distance ρ (scaled by bulk sample Bohr radius a_0). The bold and thin solid curves are relating to the $D = 2.5$nm and $D = 5$nm cases correspondingly. For comparison, the graphical curve (dashed line) relating to the two-layer (for that $D \to \infty$ and, thus, metal gate is absent) low–k dielectric contrast case $\varepsilon_S / \varepsilon_D > 1$ described by expression $V(\rho) = 2e^2 / (\varepsilon_S + \varepsilon_D)\rho$ [3] is demonstrated as well. The latter, as expected, holds the highest position since screening by metal gate is excluded. By decreasing D, the influence of the metal gate enhances and $V(\rho)$ weakens.

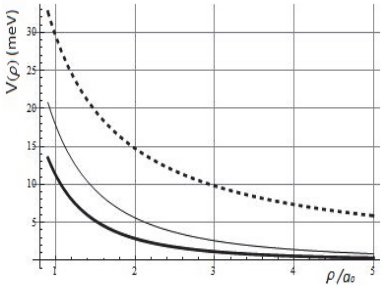

Fig. 1. V(ρ) (scaled by meV) as a function of planar distance ρ (scaled by a_0) for the ***Si/SiO$_2$*** *MOSFET structure. The bold and thin solid curves are related to the D = 2.5nm and D = 5nm cases respectively. The dashed curve is related to the two-layer (D→∞) metal absent case*

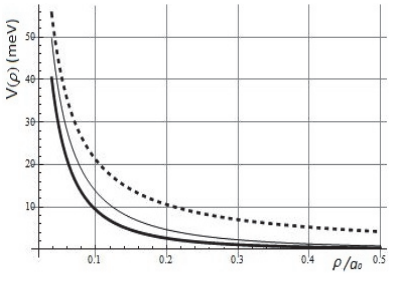

Fig. 2. V(ρ) (scaled by meV) as a function of planar distance ρ (scaled by a_0) for the ***InSb/SiO$_2$*** *MOSFET structure. The bold and thin solid curves are related to the D = 2.5nm and D = 5nm cases respectively. The dashed curve is related to the two-layer (D→∞) metal absent case*

In Fig.2, we draw the Coulomb interaction energy properties with **InSb/SiO_2** *low–k dielectric contrast case* where the following material parameters are adopted $\varepsilon_S = 16.8$, $\varepsilon_D = 3.9$, the Bohr radius in the bulk InSb sample $a_0 = 65.8$ *nm*. The details here are the same as in Fig. 1. As it follows, the Coulomb interaction energy here is more enhanced than in the Si/SiO_2 based MOSFET case. At the same time, the graphical lines particularly in the region with $\rho > (D \div 3D)$ are closer to each other which means that for this case, with decreasing the oxide layer thickness, the influence of the metal gate grows slowly. The latter is a consequence of dielectric enhancement of the Coulomb interaction (dielectric confinement effect) which for the noted planar distances balances the metal gate -induced interaction energy weakening tendency.

Finally let us numerically discuss the *high–k dielectric contrast case*. In Fig.3 and 4 the Coulomb interaction energy properties both with **Si/HfO_2 and InSb/HfO_2** MOSFET structures respectively is demonstrated where the oxide layer dielectric constant value is taken as $\varepsilon_D = 25$ (the details are the same as in Figs. 1, 2). As we can see, two graphical lines relating to the oxide layer width D =2.5*nm* and 5nm cases in both graphs are located far below the two-layer metal gate absent ($D \to \infty$) related line. This is because the metal gate-induced screening and already dielectric de-confinement ($\varepsilon_S < \varepsilon_D$) effects act together and significantly weaken the Coulomb interaction in the MOSFET channel region. At the same time, since the dielectric de- confinement effect for the InSb based structure is manifested relatively less than in the Si-based counterpart thus in the region with $\rho > (D \div 3D)$, the Coulomb interaction efficiency is more obvious.

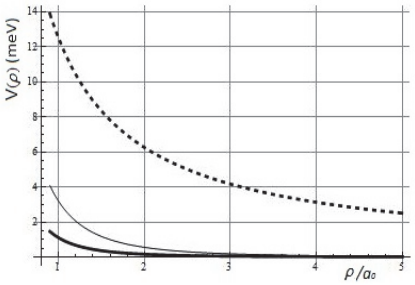

Fig. 3. V(ρ) (scaled by meV) as a function of planar distance ρ (scaled by a_0) for the Si/HfO_2 MOSFET structure. The bold and thin solid curves are related to the D = 2.5nm and D = 5nm cases respectively. The dashed curve is related to the two-layer (D→∞) metal absent case

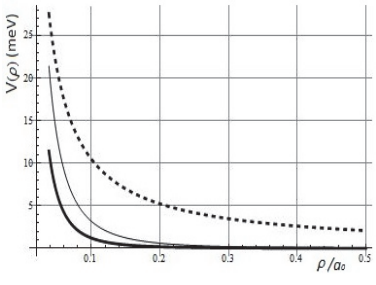

Fig. 4. V(ρ) (scaled by meV) as a function of planar distance ρ (scaled by a_0) for the InSb/HfO_2 MOSFET structure. The bold and thin solid curves are related to the D = 2.5nm and D = 5nm cases respectively. The dashed curve related to the two-layer (D→∞) metal absent case

From the foregoing, it can be concluded that the efficiency of the Coulomb interaction intensity in the aforementioned MOSFET structures except the **Si/HfO_2** case is quite effective, which would be a sufficient ground to discuss the prospective problems related to the Coulomb binding states in these structures.

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ԿՈՒԼՈՆՅԱՆ ՓՈԽԱԶԴԵՑՈՒԹՅԱՆ ԷՆԵՐԳԻԱՆ ՕՔՍԻԴԻ ԲԱՐԱԿ ՇԵՐՏՈՎ ԿՄՕԿ ՀԱՄԱԿԱՐԳՈՒՄ

ԿՄՕԿ համակարգի ինվերսիոն շերտում քննարկված են կուլոնյան փոխազդեցության պոտենցիալի հատկությունները օքսիդային շերտի վերջավոր հաստության և միջավայրի դիէլեկտրիկական անհամասեռության հաշվառմամբ: Մասնավորապես, ստացված է կուլոնյան փոխազդեցության պոտենցիալի՝ օքսիդային շերտի հաստությունից բացահայտ կախվածության տեսքը: Ցույց է տրված, որ կուլոնյան փոխազդեցությունն իր ուժգնությամբ ավելի արդյունավետ է **InSb/SiO_2** ԿՄՕԿ համակարգում:

Առանցքային բառեր. ինվերսիոն շերտ, փոխազդեցության պոտենցիալ, մեծ (փոքր)-k դիէլեկտրիկական հակադրություն:

К.Г. АГАРОНЯН, Э.П. КОКАНЯН

ЭНЕРГИЯ КУЛОНОВСКОГО ВЗАИМОДЕЙСТВИЯ В МДП СТРУКТУРЕ С ТОНКИМ ОКСИДНЫМ СЛОЕМ

В инверсионном канале МДП структуры обсуждены свойства потенциала кулоновского взаимодействия с учетом конечности толщины диэлектрического слоя и диэлектрической неоднородности среды. В частности, получен явный вид зависимости кулоновского потенциала взаимодействия от толщины оксидного слоя. Показано, что кулоновское взаимодействие проявляется более эффективно в МДП структуре на базе **InSb/SiO₂**.

Ключевые слова: инверсионный канал, потенциал взаимодействия, высокий (низкий) - k диэлектрический контраст.

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CHARACTERIZING THE LATTICE PARAMETERS IN IRON-DOPED LITHIUM NIOBATE CRYSTALS WITH DIFFERENT STOICHIOMETRY

Lattice parameters a and c have been investigated for iron-doped lithium nioabate crystals with different stoichiometry by using powder X-ray diffraction. The results were compared with the ones obtained for pure lithium niobate crystals.

Keywords: X-ray diffraction, lithium niobate, lattice parameters.

1. Introduction

Lithium niobate crystal is one of the important synthetic crystals which is an attractive material for digital holographic memory storage due to its good photorefractive properties [1]. For the first time, light induced refractive index variation, the so-called photorefractive effect was investigated in 1966 by Ashkin et al. [2] utilized by Chen et al. [3] for the storage of volume phase holograms. The improvement of the photorefractive performance of lithium niobate is controlled by doping with transition metal ions, non photorefractive ions and by crystal composition as photorefractivity depends on the crystal structure and the content of intrinsic defects [4]. Among them, Fe-doped LN crystal is the most suitable material for data storage as it provides high capacity, rapidly transfer rate, good sensitivity and long data retention time.

The first investigation of the lithium niobate crystal structure was performed by Abrahams et al. [5]. Later studies of the lattice structure by X-ray and neutron