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ELECTRON SCATTERING IN SCREENED IMPURITY-DOPED $HfO_2/InSb/HfO_2$ HETEROSTRUCTURES

The effect of screened ionized background impurities on electron scattering in **$HfO_2/InSb/HfO_2$** two-dimensional (2D) nanostructure is considered. The expression of differential scattering cross-section depending on the 2D screened Coulomb potential analytical features is calculated analytically. A numerical analysis of the scattering relaxation time in the presence of electronic screening and quantum well/high-κ dielectric heterojunction effects is carried out. Taking these effects into account, a substantial suppression of electron scattering is obtained.

Keywords: Quantum well, high-κ dielectric, screening, impurity scattering.

Currently, an intensive study is carried out in quantum nanostructures related to electronic, optical and transport phenomena on the base of narrow band gap III–V group semiconductors combined with high-κ dielectric materials (HfO_2, ZrO_2,) correspondingly as the quantum well (QW) and barrier media ([1] and Refs. therein). Such systems can provide high carrier mobility in nanosamples (~ $10^4 \div 10^5$ cm^2 V^{-1} s^{-1}) responsible mainly for high-speed power switching, low dissipation and other benefits of electronic nanodevices.

In [1] the screened impurity scattering relaxation time both analytical and numerical analysis for the realistic $InSb/HfO_2$ interface is performed by using the two-dimensional (2D) Debye-Hückel type potential as an integral result of quantum confinement (QC), QW/high-κ dielectric mismatch and impurity electronic screening effects balanced influence. In the present paper, a problem is considered where the larger values of 2D distances are used for consideration.

Consider a semiconductor single QW (SQW) with the dielectric constant ε_w and thickness d surrounded by the barrier medium, for which a symmetrical outline of dielectric mismatch on both sides is adopted, characterized by the condition $\varepsilon_b = \varepsilon_{b_1} = \varepsilon_{b_2}$ for the dielectric constant values. In the discussed model, only the n-type 2D charged channel with the average surface density n_S contributes to the impurity center screening. For such QW heterostructure QC and high κ-dielectric barrier effects are characterized by conditions $a_0 >> d$ and $\varepsilon_r = \varepsilon_w / \varepsilon_b < 1$, respectively, where the Bohr radius is $a_0 = \varepsilon_w \hbar^2 / m_e e^2$, m_e – the electron effective mass. As a gas of carriers is confined to move in the x-y plane, i.e., their motion in

the z direction is taken as the direction perpendicular to the plane of the charged channel is confined. Necessarily, we also assume that the QW thickness d is small compared with the Debye radius for bulk samples as $r_D >> d$.

In these circumstances for the suitable range of effectively large 2D distances as:

$$\begin{cases} \rho > \varrho(\rho_s, \varepsilon_r) \\ \rho > \frac{d}{2\varepsilon_r} \end{cases} \tag{1}$$

where $\varrho(\rho_s, \varepsilon_r) = \frac{\rho_s}{\varepsilon_r}\left[\left(\frac{e^3+1}{e^3-1}\right)^2 - \varepsilon_r^2\right]^{1/2}$, $e = 2.71.$, the screened background impurity interaction potential $V_S(\rho)$ takes the following 2D form [2]:

$$V_s(\rho) = -\frac{e^2}{\varepsilon_b}\left\{\frac{1}{\rho} + \pi\varepsilon_r q_s[H_0(2\varepsilon_r q_s\rho) - N_0(2\varepsilon_r q_s\rho)]\right\}, \tag{2}$$

which for the asymptotic distances $\rho \gg (\varepsilon_r q_s)^{-1}$ takes the form:

$$V_s(\rho) = -\frac{e^2}{\varepsilon_b}\left(\frac{1}{\varepsilon_r q_s\rho}\right)^2\frac{1}{\rho}. \tag{3}$$

Note that the calculations in [1] are concerned to the appropriate range of moderately large 2D distances ρ such as $d \ll \rho \leq \varrho(\rho_s, \varepsilon_r)$.

In Exps. (1) - (3) ρ_s and q_s are the 2D screening radius and 2D screening parameter, respectively, which according to Tomas – Fermi method model are given as [2]:

$$\rho_s = \sqrt{\frac{d}{2q_s}}, \tag{4}$$

$$q_s = \frac{2\pi e^2}{\varepsilon_w}\frac{\partial n_S}{\partial \mu_0}, \tag{5}$$

where $\mu_0 >> k_BT$ is the chemical potential in the absence of the Coulomb perturbing field, k_BT is the energy scale factor, $\partial n_S / \partial \mu_0$ on the condition of the SQL is determined from the Debye model as:

$$\frac{\partial n_S}{\partial \mu_0} = \frac{m_w}{\pi\hbar^2}\left[1 - \exp\left(-\frac{\pi n_S\hbar^2}{m_w k_B T}\right)\right]. \tag{6}$$

In particular, for the degenerate and non-degenerate 2DEG statistics, the screening parameter q_s takes, correspondingly, the forms:

$$q_s = \frac{2}{a_0}, x = \frac{\pi n_S\hbar^2}{m_{ew}k_B T} >> 1 \tag{7}$$

and

$$q_s = \frac{2}{a_0}\frac{\pi n_S \hbar^2}{m_w k_B T},\ x = \frac{\pi n_S \hbar^2}{m_w k_B T} << 1. \quad (8)$$

Note that both the screened potential after Exp.(2) and the Debye-Hückel type screened potential used in [1] are received in the leading order of parameter $d / \square_0$ which permits to get a solution for any arbitrary normalized charge distribution function in z direction normal to the QW plain.

The scattering rate due to the scattering of carriers by impurities in the relaxation time approximation is given by [3]:

$$\frac{1}{\tau} = N_s v_k \int_0^{2\pi} \sigma(\varphi)\,(1 - cos\varphi) d\varphi \quad (9)$$

In Exp. (9) $N_s = N_V d$, where N_V is the 3D density of background impurities, $v_k = \hbar k / m_w$ is the electron velocity, φ is the electron scattering angle expressed by the initial $\vec{k}$ and final $\vec{k}'$ 2D wave vectors of a scattered electron in the QW plane as $cos\varphi = \frac{\vec{k}\vec{k}'}{|\vec{k}||\vec{k}'|}$. Here $\sigma(\varphi)$, determining a 2D flux of particles scattered at the angle φ is

$$\sigma(\varphi) = \frac{S^2 W_{kk'}}{(2\pi)^2 v_k}\, d^2k, \quad (10)$$

where S is the normalizing area in the QW plain, $W_{kk'}$ - the rate of transition probability between the initial and final states of the scattered electron. Under such circumstances, we will deal with the electron momentum relaxation time τ calculations by the 2D screened impurity potential after Exp.(2) which in accordance with the validity criterion (2.4) related to the moderately long wave region as [2]:

$$k < \frac{1}{\varrho(\rho_s, \varepsilon_r)} \quad (11)$$

Since, for the potential form after Exp. (2), an exact analytical solution of the Schrödinger equation is clearly im possible, we make use of a cut-off Coulomb potential method successfully implemented before in calculating the Q2D Somerfield exciton factor [4]. In accordance with that method, we studu the potential form as:

$$V_s(\rho) = \begin{cases} \frac{e^2}{\varepsilon_b \rho}\ \rho \le \rho_0 \\ 0\ \rho > \rho_0 \end{cases}, \quad (12)$$

where $\rho_0 = max\{\rho_1, \rho_2\}$ and $\rho_0 = \frac{\rho_s}{\varepsilon_r}\left[\left(\frac{e^3+1}{e^3-1}\right)^2 - \varepsilon_r^2\right]^{1/2}$, $\rho_2 = \frac{d}{2\varepsilon_r}$.

Subsequently, the wave function $\psi(\rho)$ can be a solution of 2D Schrödinger equation corresponding to the potential after Exp. (12) describing a scattering.

At $\rho \leq \rho_0$, $\psi(\rho)$ can be defined as the exact solution in the continuous spectrum for the 2D Coulomb potential [3]:

$$\psi(\rho)|_{\rho\leq\rho_0} = \frac{1}{\sqrt{\pi}} exp\left(\frac{\pi}{2\varepsilon_r a_0 k}\right) \Gamma\left(\frac{1}{2} - \frac{i}{\varepsilon_r a_o k}\right) e^{ik\rho}\ {}_1F_1\left(\frac{i}{\varepsilon_r a_o k}, \frac{1}{2}, ik\rho(1 - cos\varphi)\right), \quad (13)$$

where ${}_1F_1(x)$ is the confluent hypergeometric function, $\Gamma(x)$ - the gamma function. Here, a normalization constant in $\psi(\rho)$ provides a unit amplitude in the incident plane wave.

At $\rho > \rho_0$ following the accepted scattering theory method, $\psi(\rho)$ should be expressed by the superposition of plane wave propagating in the positive *x* direction and diverging 2D scattered wave characterizing the scattering amplitude $f(\varphi)$. With this, the asymptotic expression of $\psi(\rho)$ takes the form:

$$\psi(\rho)|_{\rho>\rho_0} = exp(ik\rho cos\varphi) + \frac{f(\varphi)}{\sqrt{\rho}}\ exp(ik\rho). \quad (14)$$

From the continuity condition of the normalized functions $\psi(\rho)|_{\rho\leq\rho_0}$ and $\psi(\rho)|_{\rho>\rho_0}$ at $\rho = \rho_0$, the scattering amplitude $f(\varphi)$ can be obtained which leads to the 2D scattering cross section by impurities $\sigma(\varphi) = |f(\varphi)|^2$ as:

$$\sigma(\varphi) = \rho_0 \left|\frac{1}{\sqrt{\pi}} exp\left(\frac{\pi}{2\varepsilon_r a_o k}\right) \Gamma\left(\frac{1}{2} - \frac{i}{\varepsilon_r a_o k}\right).\ {}_1F_1\left(\frac{i}{\varepsilon_r a_o k}, \frac{1}{2}, ik\rho_0(1 - cos\varphi)\right) - 1\right|^2. \quad (15)$$

The latter, in accordance with Exp. (9), leads to the electron momentum relaxation time final expression with the integral form which cannot be reduced to an explicit analytic form and, therefore, should be investigated numerically. It should be noted that the 2D scattering cross section $\sigma(\varphi)$ in Exp. (15) directly depends on ε_r.

As an illustration of the propesed theoretical model, let us now carry out the impurity scattering time numerical calculations for the realistic InSb/HfO_2 interface [1]. For that the dielectric constants ratio $\varepsilon_r = \varepsilon_w / \varepsilon_b = \varepsilon_{InSb} / \varepsilon_{Hf\,O2} \approx 16.8 / 25 = 0.625$ value is taken. InSb bulk sample holds the smallest electron effective mass ($m^* \approx 0.014 m_0$, m_0 is the free electron mass)) and a macroscopically large impurity effective Bohr radius as $a_0 \approx 63.7$nm. In accordance with the strong QC condition $a_0 >> d$, we will display a numerical data for the QW width values $d < 10$ nm.

At the same time, the conduction band of ***InSb*** material is highly non-parabolic due to the narrow band gap ($\approx 0.17eV$ under $T=300^0K$), and so the

electron effective mass m^*_{ew} becomes energy-dependent. It is consequently required to take into account the *NP* effect on m^*_e in order to evaluate more precisely τ. Within the Kane model, the conduction energy band can be described by dispersion equation:

$$E\left(1+\frac{E}{E_g}\right)=\frac{\hbar^2 k_w^2}{2m^*_{ew}}, \tag{16}$$

where E is the electron energy. In Exp,(16) the electron wave vector k_w has the direction normal to the QW plain and might be defined from the secular equation:

$$tg\left(\frac{k_w d}{2}\right)=\frac{m_w(E)}{m^*_b}\frac{k_b}{k_w} \tag{17}$$

related to rectangular band QW/barrier system with the appropriate conduction (c) and valence (v) band offsets which for the ***HfO₂*/InSb/ *HfO₂*** SQW can be characterized by the energy scheme after Fig.1 in accordance with the data after [5]. Here, the wave vectors k_w and k_b in the QW and barrier regions with the conduction band offset Δ^c are defined as:

$$k_w^2=2\frac{m_w(E)\,E}{\hbar^2} \text{ and } k_b^2=2\frac{m_b(\Delta^c-E)}{\hbar^2}, \tag{18}$$

where m_b is the electron effective mass in the barrier region. In Exp (17), the energy-dependent effective mass $m_w(E)$ is related to the first derivative of the dispersion relation with respect to wave vector as:

$$m_w(E)=\hbar^2 k_w^2\frac{\partial k_w}{\partial E}. \tag{19}$$

From Exps.(16) - (19), bearing in mind that Δ^c is large related to *Egw,* we come to the *NP* corrected electron effective mass expression $m_w(E)= m^*_e m_{NP}$ with the characteristic *NP* parameter m_{NP} as:

$$m_{NP}=\sqrt{1+2\frac{\hbar^2 k_w^2}{m^*_e E_g^w}}. \tag{20}$$

On the basis of Fig.1, data and an electron effective mass value $m^*_b \approx 0.6\ m_0$ in the case of bulk cubic c-HfO_2 material [6]**,** the allowed values of the $k_w d$ and m_{NP} parameters are obtained as: $k_w d \approx 1.496$ *and* $m_{NP} \approx 3.03$. As follows, owing to finite conduction band offset Δ_c in discussing structure, the size quantized $k_w d$ and corresponding electron effective mass *NP* correction parameter m_{NP} are softly related to infinite potential barrier model with $k_w d = \pi$.

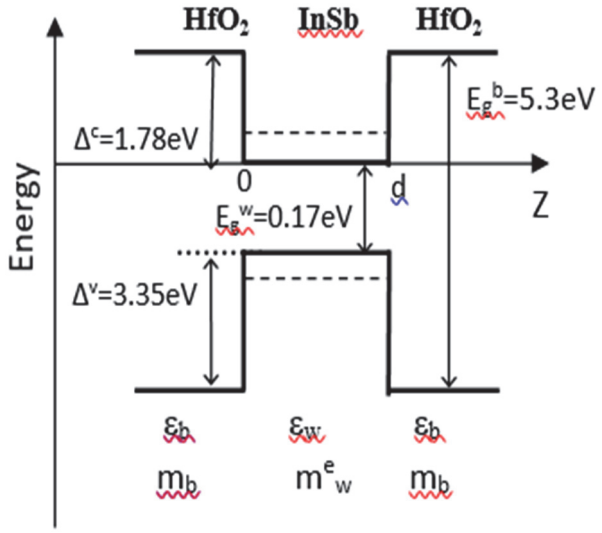

Fig. 1 The energy scheme of the HfO_2/InSb/ HfO_2SQW

In Fig. 2, $\tau(ka_0)$ dependence is displayed for the QW width value $d_1 = 2$ *nm* correlated with the $n_s /T |_2 = 6.8.10^8$ $cm^{-2}/^0K$ parameter corresponded to near degenerate type of 2DEG (2D density $n_s \approx 2.10^{11}$ cm^{-2} at $T \approx 300$ ^0K) at the density of ionized background impurities as $N_V \approx 6.10^{16} cm^{-3}$. The obtained graph is a result of contribution from the screened impurity potential after Exp. (2) and takes the complete range of ka_0 under discussion. Such a setting follows from the validity criteria after Exp. (11). As received, for values $ka_0 < 1$, with a decrease in 2D wave vector *k*, the graphic line starts to grow oscillating and finally reaches values $\tau \sim 10^{-11}$ s. Whereas in the interval $ka_0 > 1$ it falls smoothly and near the point $ka_0 \approx 2$ (marked with a vertical dashed line in Fig. 2) becomes saturated, taking the scattering time value $\tau|_{d_1} \approx 0.8.10^{-12}$s (marked with a horizontal dashed line in Fig.2). For the large ka_0, this saturating line, in turn, limits the graphics corresponding to the QW/high-κ dielectric mismatch and impurity electronic screening effects absent case in dielectrically homogenous ***InSb*** QW structure.

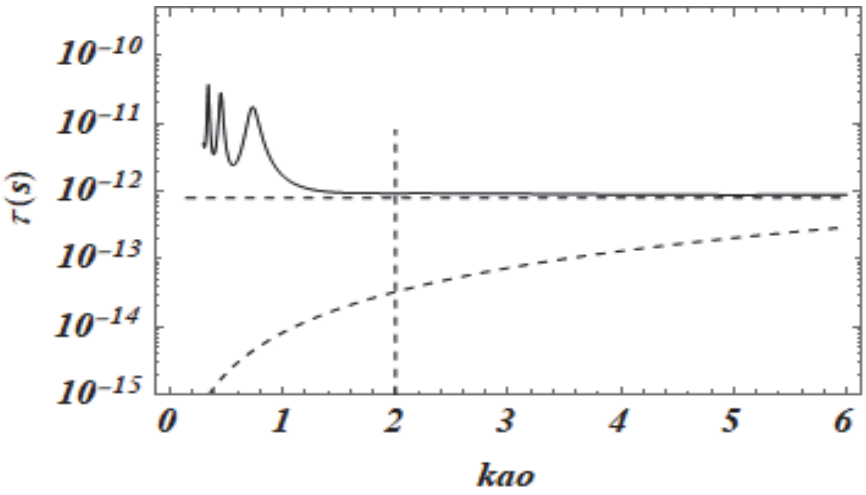

*Fig. 2. Electron momentum relaxation time $\tau(ka_0)$ dependence for the **$HfO_2/InSb/HfO_2$** high - κ type SQW structure in the case of d_1 = 2 nm (upper bold line) with the near degenerate 2D EG ($n_s/T=6.8.10^8$ $cm^{-2}/^0K$) at the density of ionized background impurities as $N_V \approx 6.10^{16}$ cm^{-3}. The lower dashed graphic line corresponds to QW/high-κ dielectric mismatch and impurity electronic screening effect absent case in **InSb** based SQW structure with d_1 = 2nm*

As we can see from the graphical data, a strong suppression of electron impurity scattering process is revealed when taking into account the electronic and quantum well/high-κ dielectric mismatch caused screening effects simultaneously. This suppression effect, expressed by increasing of τ, is more essential for a small d QW width values and it becomes more clearly starting from the region $ka_0 < 2.85$ corresponding to interval $\tau < 5.5.10^{-13}$ s. Such behavior, in accordance with Exps. (15), is due to the decline of cross section σ with the decrease of d. A suppression of ionized impurity scattering by decreasing the latter can be understood on the basis of the $\sigma(E)$ behavior. Indeed, scattering cross section is decreasing as the scattered electron energy E increases. In the SQL, as the QW width decreases, the electron energy increases in accordance with Exp. (18).

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ԷԼԵԿՏՐՈՆՆԵՐԻ ՑՐՈՒՄԸ ԷԿՐԱՆԱՎՈՐՎԱԾ ԽԱՌՆՈՒԿՆԵՐՈՎ ԼԵԳԻՐՎԱԾ HfO_2/InSb/HfO_2 ՀԵՏԵՐՈԿԱՌՈՒՑՎԱԾՔՆԵՐՈՒՄ

Դիտարկվել է իոնացված էկրանավորված հենքային խառնուկների ազդեցությունը էլեկտրոնների ցրման վրա **HfO_2/InSb/HfO_2** երկչափ նանոկառուցվածքում: Վերլուծականորեն հաշվարկվել է ցրման դիֆերենցիալ կտրվածքի արտահայտությունը՝ կախված երկչափ էկրանավորման դեպքում կուլոնյան պոտենցիալի առանձնահատկություններից: Կատարվել է ցրման վերականգնման ժամանակի թվային վերլուծություն՝ էլեկտրոնային էկրանավորման և քվանտային հոր / բարձր-κ դիէլեկտրիկ հետերոանցման երևույթների առկայությամբ: Այս երևույթների հաշվառմամբ՝ ստացվել է էլեկտրոնների ցրման էական ճնշվածություն:

Առանցքային բառեր. քվանտային հոր, բարձր-κ դիէլեկտրիկ, էկրանավորում, խառնուկային ցրում:

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РАССЕЯНИЕ ЭЛЕКТРОНОВ В ГЕТЕРОСТРУКТУРАХ HfO_2/InSb/HfO_2, ЛЕГИРОВАННЫХ ЭКРАНИРОВАННЫМИ ПРИМЕСЯМИ

Рассмотрено влияние ионизированных экранированных фоновых примесей на рассеяние электронов в двумерной наноструктуре HfO_2/InSb/HfO_2. Аналитически рассчитано выражение для дифференциального сечения рассеяния в зависимости от особенностей двумерного экранированного кулоновского потенциала. Проведен численный анализ времени релаксации рассеяния при наличии эффектов электронного экранирования и гетероперехода квантовая яма/высокий-к диэлектрик. С учетом этих эффектов получено существенное подавление эффекта рассеяния электронов.

Ключевые слова: квантовая яма, высокий-к диэлектрик, экранирование, примесное рассеяние.