Effect of dielectric mismatch on transport in Nanostructures

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It is theoretically proved that mobility in semiconductor nanostructures can be modified by dielectric environment. We will use Fermi's Golden rule to calculate the Coulombic scattering rate in GaAs nanomembrane by considering the electron wave function in a finite quantum well. The mobility can be calculated by Mathessian rule incorporating other scattering mechanisms thereafter.

Performances of the modern solid state devices are often dictated by mobility of charge carriers. The mobility in bulk materials is mainly governed by impurity and phonon scattering [1]. For bulk materials the unscreened Coulombic potential at distance z from an ionized impurity has the form of V(z) $\sim e^2/4\pi\epsilon_s$z. When semiconductor is confined to nanometer range, such as thin semiconductor films and 1-D nano crystals, the Coulombic scattering potential will be modified by both envoronmental dielectric constant ϵ_e and semiconductor dielectric constant ϵ_s [2],[6],[9]. The mobility of semiconductor nanaostructures is determined by phonon scattering, surface roughness scattering[7] and Coulombic scattering. Here in our work, we mainly focus on Coulombic scattering, which captures the role of dielectric mismatch.

2D semiconductor nanomembranes can be grown by MBE or LPE and can be further coated with materials of different dielectric constants. The charge carriers are assumed to be inside an infinite quantum well representing semiconducting membrane. Using Fermi's golden rule, the Coulombic scattering matrix of a charged impurity is theoretically calculated as[3]:

$$\widetilde{V}^{Coul}_{unsc}(q) = \frac{e^2}{2\epsilon_0\epsilon_s q}\cdot F_{n_z m_z}(aq)\cdot[\frac{e^{qa}+\gamma}{eqa-\gamma}], \tag{1}$$

where $q =\mid \mathbf{k_i} \mid - \mid \mathbf{k_f} \mid$, $F_{n_z m_z}(aq)$ is a form factor arising from quasi-2D nature of the electron gas and $\gamma = (\epsilon_s-\epsilon_e)/(\epsilon_s+\epsilon_e)$

With consideration of screening effects by applying Thomas Fermi theory, the dielectric-modfied momentum scattering rate is given by

$$\frac{1}{\tau_i(E_k)} = \frac{2\pi}{\hbar}\int\frac{d^2k'}{(2\pi)^2}\mid \widetilde{V}^i_{scr}\mid^2(1-\cos\theta)\delta(E_k-E_{k'}), \tag{2}$$

where $\cos\theta = \mathbf{k_i}\cdot\mathbf{k_f}/\mid\mathbf{k_i}\mid\cdot\mid\mathbf{k_f}\mid, k=\mid\mathbf{k_i}\mid, k'=\mid\mathbf{k_f}\mid$ and scattering rate is evaluated over the final density of state.

Such theoretical calculation proves that Coulombic scattering rate in an ideal membrane below a critical thickness can be changed by environmental dielectrics to one order of magnitude. However, in reality, quantum well depth of thin semiconductor membranes is always finite. Thus the envelope function of the 2-D electron gas(2DEG) will not be completely confined inside the well.

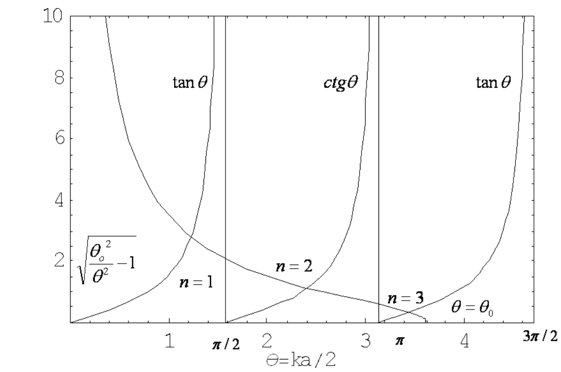

FIG. 1: Numerical solution of wave function in a finite quantum well. $\theta_o = \sqrt{\frac{mV_o a^2}{2\hbar^2}}$.

In a symmetrical finite quantum well without external applied bias, the wave function can be expressed as $\Psi(\mathbf{r},z) = \frac{1}{\sqrt{A}}e^{i\rho\cdot\mathbf{r}}\psi(z)$, where A is the surface area of the nanomembrane, ρ is wave vector in xy plane. The z component is given by

$$\psi(z) = \begin{cases} C_1 e^{-kz} & \text{for } z > a/2 \\ D_1 cos(\kappa z) + D_2 sin(\kappa z) & \text{for } -a/2 < z < a/2 \\ C_2 e^{kz} & \text{for } z < -a/2 \end{cases}$$

The coefficient constant C_1,C_2, D_1 and D_2 can be solved numerically from the transcendental equation, shown in Fig 1, and the normalization condition. The partially confined electron wave function, shown in Fig 2, leads to different scattering matrix than the one with complete quantum confinement. We consider the electric quantum limit, i.e. for intra-subband scattering within the frist subband ($n_z = m_z = 1$). We first calculate the form factor$F_{11}(aq)$, which summarize the change of unscreened scattering potential matrix due to incomplete confinement of electron wave function.

$F_{11}(aq) = \int_{-\infty}^{-a/2}(C_1 e^{\kappa z})^2 e^{qz}dz + \int_{-a/2}^{0}(D_1 cos(kz))^2 e^{qz}dz + \int_0^{a/2}(D_1 cos(kz))^2 e^{-qz}dz + \int_{a/2}^{\infty}(C_1 e^{-\kappa z})^2 e^{-qz}dz$

Considering screening effect, the screening function for a general (q,a) is still $\epsilon_{2d}^{eff} = 1 + q_{TF}^{eff}/q$, where q_{TF}^{eff} is

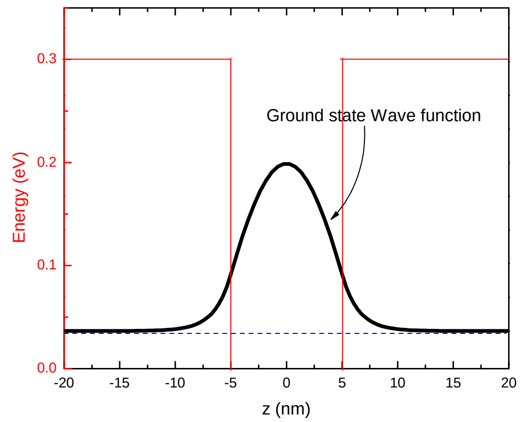

FIG. 2: Electron wave function in a finite quantum well with height of 0.3eV. All simulations are based on a GaAs thin film($m^* = 0.067m_0, \epsilon_s = 12.5$).

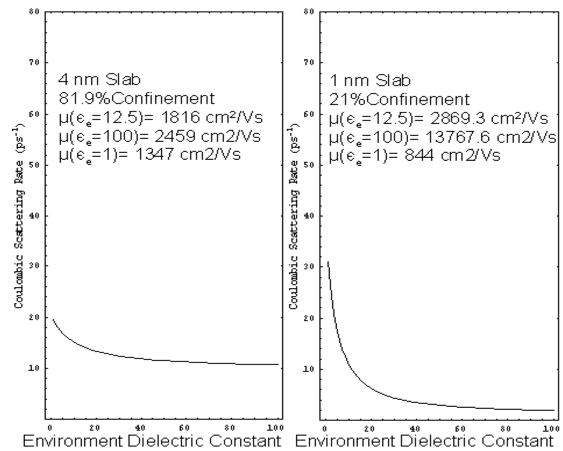

FIG. 4: Coulombic Scattering rate as a function of environmental dielectric constant.

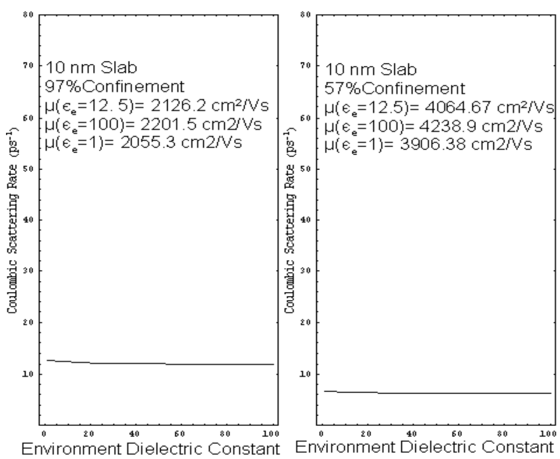

FIG. 3: Coulombic Scattering rate as a function of environmental dielectric constant.

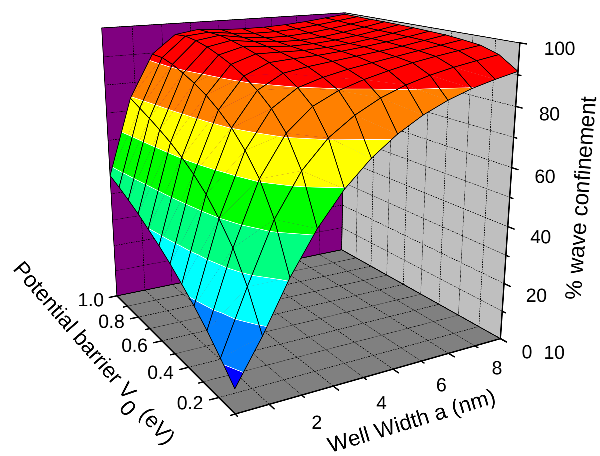

FIG. 5: The confinement of electron probability density as a funciton of quantum well barrier height and width.

Thomas-Fermi screening wave vector for the semi 2DEG with dielectric mismatch. Thus the scattering potential for each image charge is given by $\widetilde{V}^i_{scr} = \widetilde{V}^i_{unsc}/\epsilon^{eff}_{2d}$. And the momentum scattering rate for the i^{th} image charge is, again, given by Eqn 2 [4],[8],[5].

We simulated the Coulombic scattering rate for GaAs thin membrane of different barrier height V_o and width a, and calculated the mobility under the hypothesis that there is only coulombic scattering which limites the mobility, as shown in Fig 3 and Fig 4. The electron wave leakage into the enviroment dielectric was less effected by Coulombic scattering potential. The evaluation criterion of the confinement is electron probability density inside the well or $h = \int_{-a/2}^{a/2} \psi^* \psi dz$, which is a funciton of V_o and a. Fig 5 shows the confinement of quantum wells of varying width a and height V_o. It is theoretically demonstrated that for a semiconductor nanomembrane modeled as infinte quantum well, below a critical thickness (∼10nm for GaAs), the environmental dielectric can modulate the Coulombic scattering rate strongly. The higher the environmental dielectric constant, the stronger Coulombic scattering rate is damped. Our result shows that for an partially confined electron wave, the Coulombic scattering rate is even less for the same material system. The reason is the electron waves, which leak into the environment dielectric were scattered less by the charged impurity in side the well. Also, an imcomplete confinement can reduce the modulation effect of environmental dielectric constant on Coulombic scattering.

In conclusion, the mobility of semiconductor nanostructure can be modified by environmental dielectric constant, in terms of modulation of Coulombic scattering rate. A partially confined electron wave can reduce the modulation effect of environment dielectric constant. However, since the electron wave was less confined due to the finite barrier height, the electron wave outside the well was less effected by the charged impurity inside the well. So the total effect is improved mobility. Generally speaking, for mordern semiconductor devices such as HEMT, the mobility of 2DEG is a very critical parameter to improve. However, since the electron probability density inside the well is less, the current density under the same bias voltage is not necessarily improved due to the enhanced mobility. Based on the large variaty of diectric materials and modern MBE, LPE and other epitaxy technology, experimental work on dielectric engineering could be very promising.

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