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 2 dimensional semiconductor nanostructures by considering the electron wave function in a finite quantum well. The mobility will be calculated by Mathessian rule incorporating other scattering mechanisms. A critical well height will be calculated in terms of sufficient electron confinement. Finally a list will be generated for mobility improvement by dielectric engineering in a set of important semiconductors and dielectrics.

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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].

We aspire to study the transport in thin 2D semiconductor membranes of nanoscale range.These types of structures can be grown by MBE or CVD 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 it is theoretically calculated that the Coulombic scattering matrix of a charged impurity can be express as[3]

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

where q is magnitude of initial and final wave vector, $F_{n_z m_z}(aq)$ 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

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

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 such 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 finite. Thus the envelope function of the 2-D electron gas(2DEG) will not be completely confined inside the well.

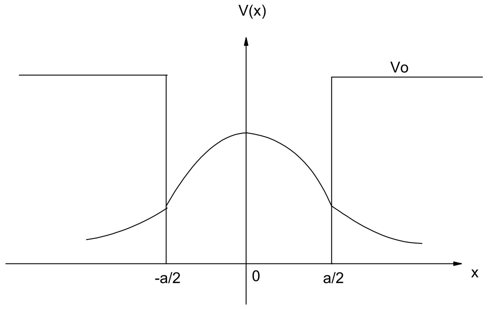

FIG. 1: electron wave function in a finite quantum well.

In a symmetrical finite quantum well(Fig1) without external applied bias, the electron wave function is given by

$$\psi(x) = \begin{cases} Ae^{-\alpha x} & \text{for } x > a/2 \\ Bcos(\kappa x) + Csin(\kappa x) & \text{for } -a/2 < x < a/2 \\ De^{\alpha x} & \text{for } x < -a/2 \end{cases}$$

This leads to different scattering matrix than the one with complete quantum confinement. This scattering matrix and scattering rates are calculated again by Fermi's Golden Rule. The electron waves leak into environmental dielectrics and encounter different scattering potentials than the electron waves inside the well irrespective of whether Coulombic Scattering potential or LO phonon scattering is seen. We plan to construct a evaluation criterion, in terms of the ratio of electron probability density, defined as the following:

$$g = \int \mid \psi(insidewell) \mid^2 dv, \qquad (3)$$

Our goal is to quantitatively evaluate the effects of incomplete confinement of electron waves on scattering mechanisms, and hence, on mobility. We will consider mainly Coulombic Scattering and surface roughness scattering. LO phonon scattering is comparatively weaker and negligible in this case. Based on our calculation, we plan to find the critical band offset for different material systems. Specifically, we plan to build up a list for quantum well systems, such as GaAs/AlGaAs system, GaN/AlGaN system, GaSb/AlGaSb system, Si/Ge etc.

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[1] R. F. Pierret, Advanced Semiconductor Fundamentals, (2003):Prentice Hall Inc, Page 179
[2] L. V. Keldysh, JLTP Lett. 92, 658 (1979)
[3] D. Jena, (2006)Communicated