

Two-Dimensional Scattering Rates

David K. Ferry and Dragica Vasileska

Arizona State University
Tempe, AZ 85287-5706



Nanostructures Research Group

CENTER FOR SOLID STATE ELECTRONICS RESEARCH

Scattering rate calculation for Confined carriers

There are numerous examples of quantum confinement. The most commonly observed ones are Quantum wells (Modulation Doped Heterostructures) and Triangular wells (in MOS capacitors and MOSFETS).

Brief Review of Quantum Confinement:

Quantum wells : For simplicity we consider only the infinite quantum well. The stationary solutions to the 1D TISE in the one electron time approximation are of the form.

$$\psi(z) = \sqrt{\frac{2}{L}} \sin(k_n z)$$

The carriers are free to move in the xy plane and for that direction the 2D DOS function is given by where E_i is the energy level due to the quantization of k_z .

$$\rho_{2D}(E) = \frac{m^*}{\pi \hbar^2} \theta(E - E_i)$$

The Quantization along the z direction modifies the carrier dispersion relation

$$E_n(k_{\parallel}) = \frac{\hbar^2 k_{\parallel}^2}{2m^*} + \frac{\hbar^2 k_n^2}{2m^*} = \frac{\hbar^2 k_{\parallel}^2}{2m^*} + E_n$$

Kinetic + Potential

Here K_{\parallel} is the crystal momentum in the xy plane and, E_n is the sub-band energy due to the quantization in the z direction

Even when we have intravalley scattering, there are 2 cases : Intrasubband and Intersubband scattering.

Using Fermi Dirac statistics, the sheet electron density is calculated as the # of carriers (electrons) per unit area.

$$N_n = \int_0^{\infty} \rho_{2D}(E) f(E) dE = \frac{m^*}{\pi \hbar^2} K_B T \ln\left(1 + e^{\left(\frac{E_f - E_n}{K_B T}\right)}\right)$$

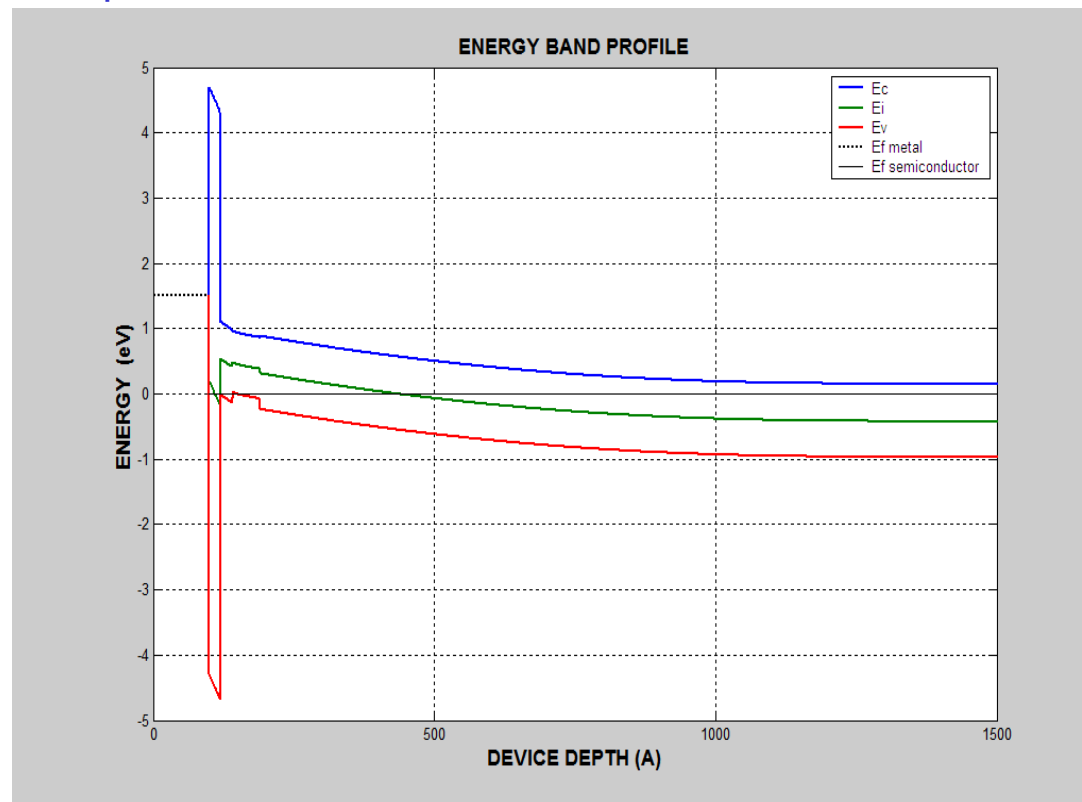


The z variation of the electron density is calculated using
 Because of the particle's confinement, the uncertainty
 in the particle's momentum increases.

$$n(z) = \sum_n N_n \psi_n^2(z)$$

Triangular wells

In some types of devices, electric fields or material properties are used to restrict the motion of carriers, so that they are confined to a narrow channel, unable to move in the perpendicular direction. One such example are quantum wells that were discussed previously and the second example are MOS structures.



The Energy band diagram of a n MOS capacitor is shown below. If the band bending is sufficient as in this case, holes will accumulate near the surface. The carriers are now confined in the z direction and are free to move in a plane perpendicular to it. Due to quantum confinement, a set of discrete energy levels arise. Since the Kinetic energy term in the 1D TISE depends inversely upon the mass, the Lowest levels will correspond to the heavy hole sub-bands.

p MOS Si / SiGe Quantum well at $V_G = -1.5$ V

The TISE is given by

$$\left[-\frac{\hbar^2}{2m_x^*} \frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_y^*} \frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_z^*} \frac{\partial^2}{\partial z^2} + V(z) \right] \Psi(x, y, z) = E \Psi(x, y, z)$$

Since carriers are free in the xy plane, they can be represented as plane waves in the xy plane

$$\left[-\frac{\hbar^2}{2m_z^*} \frac{\partial^2}{\partial z^2} + V(z) \right] \psi(z) = \left[E - \frac{\hbar^2 k_x^2}{2m_x^*} - \frac{\hbar^2 k_y^2}{2m_y^*} \right] \psi(z)$$

E_n $\psi_n(z)$

$$\Psi(x, y, z) = \frac{1}{\sqrt{A}} e^{i(xk_x + yk_y)} \psi(z)$$

Substituting this in the SWE, we get

To solve this equation, we need to know the potential energy of the system. Here we can consider 2 cases.

1. Airy function approximation (Low N_s)
2. Full blown Self consistent solution.

Scattering rates for a Quasi 2DEG

Calculation of scattering rates is similar to 3D but instead of a plane wave in 3D for the wavefunction, we will use a plane wave in 2D and a z component as the wavefunction. As an application we will derive the scattering rate for acoustic phonons and for surface roughness scattering which is the dominant mechanism in MOSFETS with high substrate doping or in strong inversion layers.

Once again we use the Fermi Golden rule to get the expression for the transition rate from state k to state k', but in this case we will have to take into account for sub-bands as well.

$$S_{nm}(k_{||}, k'_{||}) = \frac{2\pi}{\hbar} |M_{nm}(k_{||}, k'_{||})|^2 \delta(E - E' \pm \hbar\omega)$$

Assuming plane wave basis for the electronic wave functions, the total wave functions of the initial and final states are of the form:

$$\psi_n(k_{||}) = \frac{1}{\sqrt{A}} e^{ik_{||} \cdot r} \psi_n(z) \quad (\text{initial}) \quad \psi_m(k'_{||}) = \frac{1}{\sqrt{A}} e^{ik'_{||} \cdot r} \psi_m(z) \quad (\text{final})$$

A = Area of sample
 $k_{||}, k'_{||}$ = wave vectors in xy plane

The matrix element between the initial and final states in sub-bands n and m is given by

$$M_{nm}(k_{\parallel}, k'_{\parallel}) = \frac{1}{A} \int e^{i(k_{\parallel} - k'_{\parallel}) \cdot r} d^2 r \int dz \psi_m^*(z) H_{qv}(R) \psi_n(z)$$

ACOUSTIC DEFORMATION POTENTIAL SCATTERING: In the discussion for deformation potential scattering for bulk materials, the interaction potential is $H_{ep,dp} = C \nabla_r \hat{U} = \Xi_{ac} \nabla_r \hat{U}$

where,
$$\hat{U} = \sum_{qv} \sqrt{\frac{\hbar}{2MN\omega_{qv}}} \vec{e}_{qv} \left[\hat{a}_{qv} e^{i\vec{q} \cdot \vec{R}} + \hat{a}_{qv}^{\dagger} e^{-i\vec{q} \cdot \vec{R}} \right]$$

This leads to,
$$H_{ep,dp} = \Xi_{ac} \sum_{qv} \sqrt{\frac{\hbar}{2MN\omega_{qv}}} i\vec{q} \cdot \vec{e}_{qv} \left[\hat{a}_{qv} e^{i\vec{q} \cdot \vec{R}} - \hat{a}_{qv}^{\dagger} e^{-i\vec{q} \cdot \vec{R}} \right]; \quad \vec{q} \cdot \vec{R} = \vec{q}_{\parallel} \cdot \vec{r} + q_z z$$

$$M_{nm}(k_{\parallel}, k'_{\parallel}) = \Xi_{ac} \sum_{qv} \sqrt{\frac{\hbar}{2MN\omega_{qv}}} q \left(Nq + \frac{1}{2} \mp \frac{1}{2} \right)^{1/2} \underbrace{\frac{1}{A} \int e^{i(k_{\parallel} - k'_{\parallel} \pm q_{\parallel}) \cdot r} d^2 r}_{2\pi \delta(k_{\parallel} - k'_{\parallel} \pm q_{\parallel})} \underbrace{\int dz \psi_m^*(z) e^{\pm i q_z z} \psi_n(z)}_{I_{nm}(q_z)}$$

Therefore the transition rate is

$$S_{nm}(k_{\parallel}, k'_{\parallel}) = \frac{2\pi}{\hbar} \Xi_{ac}^2 \frac{\hbar}{2\rho V \omega_{qv}} q^2 \left(Nq + \frac{1}{2} \mp \frac{1}{2} \right) I_{nm}^2(q_z) \delta(k_{\parallel} - k'_{\parallel} \pm q_{\parallel}) \delta(E_n + E_{k_{\parallel}} - E_m - E_{k'_{\parallel}} \pm \hbar \omega_{qv})$$

This rate is very different from the rate obtained in the 3D case.

1. Momentum conservation applies only to the xy plane
2. There is an overlap factor, $I_{nm}(q_z)$ which depends upon the magnitude of q_z and whether we have intra or inter band transitions
3. In the energy conservation, the sub-band energy appears.

To get the scattering rate, we have to integrate over all possible final states and final sub-bands.

$$\frac{1}{\tau_n(k_{\parallel})} = \frac{2\pi\Xi_{ac}^2 K_B T}{\hbar\rho v_s^2} \frac{1}{A} \sum_{q_{\parallel}} \underbrace{\delta(k_{\parallel} - k'_{\parallel} \pm q_{\parallel})}_{\frac{1}{2} g_{2D}(E_n - E_m + E_{k_{\parallel}})} \underbrace{\delta(E - E') \int_{-\infty}^{\infty} \frac{dq_z}{2\pi} I_{nm}^2(q_z)}_{D_{nm} = \int dz |\psi_m^*(z)|^2 |\psi_n(z)|^2}$$

From the above result we may conclude that

- The scattering rate is proportional to the 2D DOS
- For intra sub-band scattering to occur, the electric field must accelerate the carriers to energies exceeding the final sub-band energy.
- For infinite well it is straightforward to show that $D_{nm} = \frac{2 + \delta_{nm}}{L}$

Surface Roughness Scattering: Confined carriers at the Si/SiO₂ interface are subject to all the mechanisms that affect the 3D carriers as well as some additional ones. The most important one is that the carriers can scatter off the boundaries of the confining potential. Since the gate is at fixed potential, any fluctuations in the oxide thickness will produce variations in the confining potential and therefore, on the energy spectrum in the triangular potential well. The effect increases when the applied voltage on the gate increases, as carriers are more closely confined to the interface.

- At Low Gate biases, Coulomb scattering due to ionized acceptors or donors dominates.
- At Higher biases, Coulomb scattering is less important due to screening effect. Surface Roughness now dominates.

To evaluate the scattering rate due to Surface Roughness, we need to identify the scattering potential. Let $V(z')$ be the confining potential along the growth direction, where $z' = z + \Delta(r)$

$$V(z + \Delta(\vec{r})) = V(z) + \frac{\partial V}{\partial z} \Delta(\vec{r}) = V(z) + q\varepsilon_z(z)\Delta(\vec{r})$$

$$H_{SR} = q\varepsilon_z(z)\Delta(\vec{r})$$

The matrix element between the initial and final states in sub-bands n and m is given by

$$M_{nm}(k_{\parallel}, k'_{\parallel}) = \underbrace{q \int dz \psi_m^*(z) \varepsilon_z(z) \psi_n(z)}_{F_{nm}} \frac{1}{A} \int \Delta(\vec{r}_1) e^{i(k_{\parallel} - k'_{\parallel}) \cdot r} d^2 r$$

$$|M_{nm}(k_{\parallel}, k'_{\parallel})|^2 = q^2 \frac{1}{A} \int \Delta(\vec{r}_1) e^{i(k_{\parallel} - k'_{\parallel}) \cdot \vec{r}_1} d^2 \vec{r}_1 \frac{1}{A} \int \Delta^*(\vec{r}_2) e^{-i(k_{\parallel} - k'_{\parallel}) \cdot \vec{r}_2} d^2 \vec{r}_2$$

$$q^2 |F_{nm}|^2 \frac{1}{A^2} \int d^2 \vec{r}_1 \int d^2 \vec{r}_2 e^{i(k_{\parallel} - k'_{\parallel}) \cdot (\vec{r}_1 - \vec{r}_2)} \Delta^*(\vec{r}_2) \Delta(\vec{r}_1)$$

$$\langle |M_{nm}(k_{\parallel}, k'_{\parallel})|^2 \rangle = q^2 |F_{nm}|^2 \frac{1}{A^2} \int d^2 \vec{r}_1 \int d^2 \vec{r}_2 e^{i(k_{\parallel} - k'_{\parallel}) \cdot (\vec{r}_1 - \vec{r}_2)} \langle \Delta^*(\vec{r}_2) \Delta(\vec{r}_1) \rangle$$

$$R(\vec{r}_1, \vec{r}_2) = \int d^2 \vec{r}_1 \int d^2 \vec{r}_2 \Delta^*(\vec{r}_2) \Delta(\vec{r}_1) P[\Delta(\vec{r}_2), \Delta(\vec{r}_1)]$$

When the process is stationary, the auto correlation function depends only on the difference in the random variables.

$$R(\vec{r}_1, \vec{r}_2) = \langle \Delta^*(\vec{r}_2) \Delta(\vec{r}_1) \rangle = R(\vec{r}_1 - \vec{r}_2)$$

Position of the point without roughness

Random function that describes deviations from the atomically flat interface

$$\begin{aligned}
\langle |M_{nm}(k_{\parallel}, k'_{\parallel})|^2 \rangle &= q^2 |F_{nm}|^2 \frac{1}{A^2} \int d^2 \vec{r}_1 \int d^2 \vec{r}_2 e^{i(k_{\parallel} - k'_{\parallel})(\vec{r}_1 - \vec{r}_2)} R(\vec{r}_1 - \vec{r}_2) \\
&= q^2 |F_{nm}|^2 \frac{1}{A^2} \int d^2 \vec{r}_1 \int d^2 \vec{r}_2 e^{i(k_{\parallel} - k'_{\parallel})\vec{r}} R(\vec{r}) = q^2 |F_{nm}|^2 \frac{1}{A^2} \int d^2 \vec{r}_1 S(q_{\parallel}) \\
&= q^2 |F_{nm}|^2 \frac{1}{A} S(q_{\parallel})
\end{aligned}$$

The auto correlation function is usually assumed to be exponential as experimental data fits this form more accurately

$$R(r) = \Delta^2 e^{-r/L}$$

$$S(q_{\parallel}) = \pi \Delta^2 L^2 \frac{1}{1 + \frac{1}{2} L^2 q_{\parallel}^2}$$

$$S_{nm}(k_{\parallel}, k'_{\parallel}) = \frac{2\pi}{\hbar} q^2 |F_{nm}|^2 \frac{1}{A} S(q_{\parallel}) \delta(E - E')$$

Note on the strength of the scattering process:

Surface roughness is affected by both delta and F_{nm} . Delta is the measure of the roughness of the interface and F_{nm} is a measure of how close (on an average) the carriers are from the oxide – semiconductor interface.

