

Surface scattering: Made simple

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Appendix: surface scattering in a quantum well

Here we consider surface roughness scattering in the quantum well with confinement along the z axis, transport direction x and the unconfined transverse dimension y.

We start with the semi-classical expression for the rate of surface roughness scattering¹.

The square of the Hamiltonian for scattering normalized per area with sizes L_x and L_y is

$$|H_{k,k'}|^2 = M^2 Y(k'-k) / (L_x L_y) \quad (1)$$

is expressed via the square of the matrix element (with the units of $(\text{J}\cdot\text{m})^2$), which is for small² and large³ quantum well thickness L_w , respectively,

$$M^2 = \pi\Delta^2\Lambda^2 \frac{\pi^4\hbar^4}{m^{*2}L_w^6} \quad \text{and} \quad M^2 = \pi\Delta^2\Lambda^2 e^2 F_s^2, \quad (2)$$

where the correlation length is Λ , the roughness r.m.s. is Δ , and the effective normal field at interface is F_s , and the carrier confinement mass is m^* . And the dimensionless factor in the Fourier transform of the roughness correlation function can have, for example, of Gaussian form

$$Y(q) = \exp\left(-\frac{\Lambda^2 q^2}{4}\right). \quad (3)$$

Then the total rate of scattering of the of electrons with in-plane momentum k to all possible final momenta k' is then given by the Fermi's golden rule

$$\frac{1}{\tau(k)} = \frac{2\pi}{\hbar} \sum_{k'} |H_{k,k'}|^2 \delta(E_{k'} - E_k). \quad (4)$$

Now we can substitute the Hamiltonian and use the representation of the sum over the momentum states as an integral

$$\sum_{k'} = \frac{L_x L_y}{(2\pi)^2} \int d^2 k'. \quad (5)$$

Then the scattering rate becomes

$$\frac{1}{\tau(k)} = \frac{M^2}{2\pi\hbar} \int Y(q) \delta(E_{k'} - E_k) d^2 k'. \quad (6)$$

This rate should be distinguished from the momentum relaxation rate.

$$\frac{1}{\tau_m(k)} = \frac{M^2}{2\pi\hbar} \int Y(q) \delta(E_{k'} - E_k) (1 - \cos\theta) d^2k' . \quad (7)$$

Here the exchange of in-plane momentum is $q = k' - k$, and θ is the angle between the momenta k', k . By expressing the differential of energy via the momentum magnitude

$$dE = \frac{\hbar^2 k' dk'}{m_d} , \quad (8)$$

where m_d is the density-of-states mass. Performing the integral over energies which results in a unity factor

$$\frac{1}{\tau_m(k)} = \frac{m_d M^2}{\hbar^3} \cdot \frac{1}{2\pi} \int_0^{2\pi} d\theta (1 - \cos\theta) Y(q) . \quad (9)$$

Note that for small correlation length $Y(q) = 1$ (isotropic scattering), the last factor in the above equation turns to unity, and the total scattering rate becomes equal to the momentum relaxation rate.

This limit is valid when most of electrons have momentum such that $k\Lambda \ll 1$. For non-degenerate carriers, the momentum is given by the thermal velocity

$$v_t = \sqrt{\frac{2k_B T}{\pi m_c}} \approx 120 \text{ km/s} . \quad (10)$$

and thus the momentum is

$$k = \frac{m_d v_t}{\hbar} \approx 0.2 \text{ nm}^{-1}. \quad (11)$$

Therefore the approximation valid to a correlation length of a couple of nanometers.

The part of mobility limited by surface roughness scattering contains the averaged scattering time and the conduction mass m_c

$$\mu_{srs} = \frac{e \langle \tau_m \rangle}{m_c}. \quad (12)$$

For sufficiently wide quantum wells, one retrieves the well-known ‘universal mobility’ dependence

$$\mu_{srs} \propto \frac{1}{F_s^2}. \quad (13)$$

In the isotropic limit the scattering rate is

$$\frac{1}{\tau} = \frac{m_d M^2}{\hbar^3}. \quad (14)$$

And the mobility becomes

$$\mu_{iso} = \frac{e \hbar^3}{m_c m_d M^2}. \quad (15)$$

We see that mobility decreases with correlation length in the isotropic limit

$$\mu_{iso} \propto \Lambda^{-2} . \quad (16)$$

In the opposite limit of long correlation length, the angle-dependent factor

$$\int_0^{2\pi} d\theta (1 - \cos \theta) Y(q) \approx \frac{2\sqrt{\pi}}{(k\Lambda)^3} . \quad (17)$$

And therefore mobility increases with correlation length.

$$\mu \propto \Lambda . \quad (18)$$

The intuitive explanation for this is that when the correlation length is longer than the wavelength of electrons, they are able to adiabatically adjust to the changes in the waveguide width and not to experience scattering.

When fitting the experimental data, the r.m.s. roughness and the correlation length are not well known. Therefore it is necessary to fit the value of mobility, which is easier to obtain.

For example, for electrons in silicon, $\Delta = 0.5nm$, $\Lambda = 2nm$, and $F_s = 1MV/cm$ would produce scattering rate of $\tau^{-1} = 2.0 \cdot 10^{14} / s$ and mobility $\mu_{iso} = 44 \frac{cm^2}{V \cdot s}$.

Now we draw the connection between the semi-classical scattering rate and the full quantum description via NEGF. In the NEGF formalism, the surface scattering has the form of the broadening function for elastic process with transfer of momentum expressed via the spectral function, that is

$$\Gamma(k_x, k_x', k_y, k_y', E) = \frac{1}{N_x N_y} \sum_q K_s Y(q) A(k_x + q_x, k_x' + q_x, k_y + q_y, k_y' + q_y, E)$$

(19)

Here we separated the scattering prefactor [which is determined by Eq. (77) of Ref.⁴] into a constant K_s (with units of J^2) and the dimensionless factor of the correlation function $Y(q)$.

For 2-dimensional systems, the spectral function A

$$A(E_{k'}) = g_{2D}(E_{k'}) \pi a_x a_y. \quad (20)$$

Is related to the local density of states (LDOS)

$$g_{2D} = \frac{m_d}{\pi \hbar^2}. \quad (21)$$

Taking the special case of isotropic scattering, we can obtain the relation between the constants which is valid for the general case. In this case the scattering broadening

$$\Gamma = \frac{1}{N_x N_y} \sum_q K_s A = K_s A = \frac{K_s m_d a_x a_y}{\hbar^2}. \quad (22)$$

On the other hand the broadening is related to the scattering rate

$$\Gamma = \frac{\hbar}{\tau} = \frac{m_d M^2}{\hbar^2}. \quad (23)$$

A comparison of these expressions demands that

$$K_s = \frac{M^2}{a_x a_y}. \quad (24)$$

Now we need to transform the broadening function and the spectral function to real coordinates along the transport direction x according to Eqs. (63) and (64) of Ref. 4

$$\Gamma(x_1, x_2) = \frac{1}{N_x} \sum_{k_x, k_x'} \Gamma(k_x, k_x') \exp(ik_x x_1 - ik_x' x_2) \quad (25)$$

$$A(k_x, k_x') = \frac{1}{N_x} \sum_{x_3, x_4} A(x_3, x_4) \exp(ik_x' x_4 - ik_x x_3) \quad (26)$$

Upon substitution of these equations to (19), performing summation over momenta according to the identity

$$N_x \delta(x_1, x_3) = \sum_{k_x} \exp(ik_x x_1 - ik_x x_3), \quad (27)$$

and performing summation with Kronecker delta symbols under the sums, we obtain

$$\Gamma(x_1, x_2, k_y, k_y', E) = \frac{K_s}{N_x N_y} \sum_q Y(q) A(x_1, x_2, k_y + q_y, k_y' + q_y, E) \exp(iq_x x_2 - iq_x x_1), \quad (28)$$

At this point we neglect correlations between the transverse momenta, and treat them as a set of independent modes by dropping the second momentum variable in all functions as follows $\Gamma(x_1, x_2, k_y, E)$. Taking advantage of the fact that this particular form of the roughness correlation admits splitting into a product $Y(q) = Y(q_x)Y(q_y)$, we can perform summation over the transferred x -momentum

$$I_{trx} = \sum_{q_x} \exp\left(-\frac{\Lambda^2 q_x^2}{4}\right) \exp(iq_x \Delta x) = \frac{L_x}{\Lambda\sqrt{\pi}} \exp\left(-\frac{\Delta x^2}{\Lambda^2}\right). \quad (29)$$

Now we would like to perform summation over the transverse momenta and will limit ourselves to cases where the Green's function is approximately independent of the transverse momentum (and thus can be taken out of the summation). Then the summation over transferred y-momentum is performed similarly, to yield

$$\Gamma(x_1, x_2, E) = \frac{K_s}{N_x N_y} \frac{L_x L_y}{\pi \Lambda^2} \exp\left(-\frac{(x_2 - x_1)^2}{\Lambda^2}\right) A(x_1, x_2, E). \quad (30)$$

Not surprisingly, the broadening function contains the spatial correlation function of roughness. However with this dependence the broadening, self-energy matrices, as well as the whole NEGF equations become strongly non-diagonal. Instead of the desired one sub-diagonal and one super-diagonal, their number is equal to the ratio of the correlation length and the spatial grid size Λ / a_x , which can be >30 . That would drastically increase the computational burden of solving these equations. In order to approximate the reality by diagonal equations, we make a not-well-justified by useful assumption that the off-diagonal terms are close to diagonal

$$A(x_1, x_2, E) \approx A(x_1, x_1, E). \quad (31)$$

Here we sum off-diagonal terms

$$\sum_j \exp\left(-\frac{(x_j - x_1)^2}{\Lambda^2}\right) = \frac{\Lambda\sqrt{\pi}}{a_x} . \quad (32)$$

and place all the contributions into the the diagonal one:

$$\boxed{\Gamma(x_1, x_1, E) = \tilde{K}_s A(x_1, x_1, E)} . \quad (33)$$

Where the factor used in the nanoMOS simulator is

$$\tilde{K}_s = \frac{M^2}{a_x \Lambda \sqrt{\pi}} . \quad (34)$$

This results in a convenient expression for surface scattering which can be tested against other simulation methods. For the above roughness parameters and $a_x = 0.4nm$ one obtains the constant $\tilde{K}_s = 0.022(eV)^2$. Note that in the case when one of the transverse dimensions is confined, the rates of scattering between various subbands must contain the formfactors, as described in Ref. 4.

References

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