

Phonon-limited Electron Mobility In a Semiconductor Nanowire

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The electron mobility for one dimensional semiconductor nanowire is studied for scattering due to acoustic phonons via deformation potential and polar-optical phonons. Instead of assuming constant envelope wave function for electron inside the cylindrical nanowire, we implemented the full cylindrical wave function to obtain analytical expression for mobility for above two cases. Confinement effect on the phonon band-structure and its effect on electron mobility has also been investigated.

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Recent advances in semiconductor technology, such as Molecular Beam epitaxy (MBE), metal oxide chemical vapor deposition (MOCVD) have made possible to fabricate semiconductor structure of wire-like region of narrow-band gap material surrounded completely by high-band gap material hence enables us to grow free-standing 1D quantum wires. In these low-dimensional structures the smallest length scale (for example radius of a cylindrical nanowire) is comparable to electron's de Broglie wavelength. This quantum effect strongly controls the transport properties hence the electron mobility. In 3D semiconductors the mobility is mainly dominated by impurity scattering and at low temperature the phonon scattering can be completely neglected. On the contrary, in a 2D semiconductor where electrons are constrained to move in a plane, for a pure sample (minimum impurity) scattering due to acoustic phonon can be observed[1, 2]. This shows that as in 3D semiconductor case, phonon scattering cannot be neglected at low temperature in the modulation-doped samples where ionized impurity scattering is strongly suppressed.

The problem is similar in a one-dimensional semiconductor nanowire and has gained much attention to both theorist and experimentalists in past few years[3, 4]. Lee and Vassel[5] have first proposed an analytical model for phonon scattering in 2D rectangular quantum well based on Froehlich Hamiltonian and confinement effect on phonon dispersion relation. Later Fishman[6] showed mobility calculation in 1D nanowire by taking a constant envelope wave function of electrons and keeping three-dimensional behavior of phonons.

Reduction of spatial dimension effects carrier band structure and phonon modes. Indeed, recent models and measurement have shown striking evidence of confinement of phonon modes in low dimensional structure[7]. In this work we have investigated the phonon-limited scattering using exact cylindrical electron wave function and also has exploited the confined phonon modes on the mobility.

For 1D semiconductor we took axis of the nanowire is along z direction. For the electron, $\rho=(x,y)$ and $r=(\rho,z)$; k_z is the electron wave vector, and for the phonon

$Q=(q_x, q_y)$, and $q=(Q, q_z)$; phonons retain their 3D behavior. The electron energies are

$$E_{mnk_z} = \frac{\hbar^2 z_{mn}^2}{2m_{\perp}^* R^2} + \frac{\hbar^2 k_z^2}{2m_z} \quad (1)$$

and the electron wave function is given by

$$\Psi(\rho, \theta, z) = \frac{1}{\sqrt{\pi R^2 L_z}} J_m(z_{mn} \frac{\rho}{R}) e^{in\theta} e^{ik_z z} \quad (2)$$

Here envelope function is a Bessel function rather than a constant reported in previous work by Fishman[6]. We are only interested in intraband scattering so we will take 1st subband of electron. Longitudinal acoustic phonon can be regarded as a sound wave for long wavelength and corresponding phonon field can be written as[8]

$$H(r, t) = i \sqrt{\frac{\hbar q}{2\rho v_s}} E_{ac} (e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)} - h.c.) \quad (3)$$

Where E_{ac} is the deformation potential and v_s is the sound velocity. Relaxation time due to the interaction of Fermionic field (electrons) with the Bossonic field (phonon) is given by Fermi-Golden rule as

$$\frac{1}{\tau^{\pm}(k_z)} = \frac{2\pi}{\hbar} \sum_{k_z} \sum_{q_z} |\langle k_z | H | k_z \rangle|^2 \delta(\dot{E} - (E \pm \hbar\omega)) (1 - \cos\theta) \quad (4)$$

The momentum conservation rule is embedded in the matrix element and \pm sign is for emission and absorption of phonon, with the matrix element

$$|\langle k_z | H | k_z \rangle| = C \frac{\delta_{k_z, k_z \pm q_z}}{\pi R^2} \int_0^R \rho d\rho J_0^2(2.41 \frac{\rho}{R}) \int_0^{2\pi} d\phi e^{iQ\rho \cos\phi} \quad (5)$$

Where C is a constant containing strength of the phonon potential. As $\hbar\omega \ll E$ or \dot{E} , we will take scattering is elastic and no of phonon taking part in absorption or emission are equal, then $\tau_{DP}^- = \tau_{DP}^+$. Then total scattering time for a single scattering can be written in a compact form as

$$\frac{1}{\tau_{DP}(k_z)} = \frac{2m^* E_{ac}^2 k_B T I(R)}{\hbar^3 v_s \pi^2 R^4 |k_z|} \quad (6)$$

Where $I(R)$ is a complicated integral which is still to be evaluated, defined as

$$I(R) = \int Q dQ \int_0^\infty \rho d\rho J_0^2(2.41 \frac{\rho}{R}) J_0(Q\rho) \quad (7)$$

As different phonon scattering have no correlation among them, then statistical average scattering time at a temperature T is evaluated using following relation

$$\langle \tau(T, R) \rangle = \frac{\int_0^\infty dE g(E) (-\frac{\partial F_0}{\partial E}) \tau_j(E, R)}{\int_0^\infty dE g(E) (-\frac{\partial F_0}{\partial E})} \quad (8)$$

Where $g(E)$ is the DOS for 1D nanowire and $F_0(E)$ is the FD distribution function. At very low temperature (degenerate) derivative of FD function will give $\delta(E - E_f)$, hence only change in eq.(6) is, k_z should be replaced by Fermi wave vector k_f . Mobility due to acoustic phonon scattering is then can be calculated using standard Drude formula $\mu = \frac{e\tau}{m^*}$.

For optical phonons which also have 3D behavior, the scattering time can be calculated following procedure discussed in the previous sections but with a different integral as

$$I(R) = \int \frac{Q dQ}{Q^2 + k_z^2} \int_0^\infty \rho d\rho J_0^2(2.41 \frac{\rho}{R}) J_0(Q\rho) \quad (9)$$

and with a different constant factor defined as

$$C = N_{LO} \frac{e}{\epsilon} \hbar \omega_{LO} [\frac{1}{\epsilon(\infty)} - \frac{1}{\epsilon(0)}] \quad (10)$$

. Detailed calculation for optical phonon with no confinement effect will be given in the next report.

As we are dealing with 1D nanowire it is well expected that phonons can not retain their 3D behavior, spatial confinement should effect the phonon potential also like electron's band structure. As nanowire is translationally invariant along z direction and other two direction is confined, the potential describing optical phonon modes may be taken as

$$\Phi(\mathbf{r}) = \sum_{m, q_z} e^{im\phi} e^{iq_z z} \phi(\rho) \quad (11)$$

As optical phonon field is related to the displacement vector and electric field, in the absence of free charge this field should obey Laplace equation[9, 10] as

$$[\frac{1}{\rho} \frac{\partial}{\partial \rho} (\rho \frac{\partial}{\partial \rho}) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \theta^2} - k_z^2] \phi(\rho) = 0 \quad (12)$$

Solving Laplace equation the potential can be written as

$$\Phi(\mathbf{r}) = \sum_{m, k_z} e^{im\phi} e^{ik_z z} \times AK_m(k_z R) I_m(k_z \rho), \rho < R, \\ BI_m(k_z R) K_m(k_z \rho), \rho > R \quad (13)$$

Where A and B are unknown constant yet to be calculated. Now this phonon potential will also satisfy the same boundary as electrostatics[11]. So the Froehlich type Hamiltonian for electron-phonon interaction for 1D nanowire can be modeled as

$$H_{e-ph}^{1D} = \sum_{k_z, m} (-e) e^{i(m\phi + k_z z)} \phi(\rho) (\frac{\hbar}{2\omega_{LO}})^{\frac{1}{2}} \\ \times [a_m(k_z) + a_m^\dagger(-k_z)] \quad (14)$$

Where $a_m(k_z)$ and $a_m^\dagger(k_z)$ are phonon creation and annihilation operators having commutation relation as

$$[a_m(k_z), a_{m'}^\dagger(-k_z)] = \delta_{m, m'} \delta_{k_z, k_z} \quad (15)$$

With this modified Hamiltonian and using Fermi-Golden rule phonon limited electron mobility can be calculated. In the next report we will try to evaluate $I(R)$ integrals to have complete analytical result of electron mobility for 3D phonon scattering. With the help of new Froehlich type Hamiltonian we will try to calculate the scattering matrix element. During the evaluation of constants A and B in confined phonon potential environmental dielectric constant will enter in the potential. We will also try to investigate the effect of environmental dielectric constant on the phonon-limited electron mobility.

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