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Transport in Quantum Well Wires

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ABSTRACT. Quantum theoretical results on dc transport in quantum well wires (QWW) indicate the suppression of ionized impurity scattering under stronger quantum confinement conditions, with enhancement of acoustic-phonons or point-defect or alloy scattering. The quantum size resonance linewidth, when radiations are polarized perpendicular to the wire, is shown to be proportional to $\lambda_D^2/A\tau_b$ where λ_D is the de Broglie wavelength, A is the confinement area, and τ_b is the bulk relaxation time. A quantum freeze-out of confined carriers is expected to induce a semimetal-semiconductor transition in semimetallic thin wires.

In recent years, there has been an intense interest in quantum transport involving carriers confined to geometries limited by their size. This has been possible due to the advent of molecular beam epitaxy, lithographic techniques, and other sophisticated semiconductor technology. In these small microstructures, the de Broglie wavelength (λ_D) of the carriers may become larger than or comparable to the size of sample in one or more directions. Then, the laws of classical physics become invalid and the system should be described by the prescription involving fundamental principles of quantum and statistical mechanics. An example of this confinement effect is that of electrons confined by a magnetic field, which has been extensively reviewed by Beer (1963) who has stressed the importance of quantum effects under strong confinement conditions. In the quantum limit, when most of the electrons populate the lowest quantum level, the system exhibits essentially a quasi-one-dimensional behavior (Arora and Prasad 1983). The electrons confined to quantum well wires (QWW) exhibit essentially the same behavior. An interesting anomaly in the temperature dependence of resistivity in thin-wire samples of bismuth has been reported (Gurvitch 1980), which is probably due to the existence of quantum size effect. In another development (Sakaki 1980), the high mobility effect of electrons in fields induced in ultrafine semiconductor wire structures has been demonstrated. In a more recent letter Petroff *et al.* (1982) have reported fabrication and optical properties of QWW.

In the light of these experimental developments, a systematic theoretical approach is needed to understand QWW. In an earlier work (Arora 1981), quantum transport in rectangular thin wires was studied for electron scattering predominantly by acoustic phonons and point defects. In a later work (Arora and Prasad 1983), we included alloy scattering which is important in thin wires made up of alloys. The importance of Coulomb scattering in thin wires by remote and background impurities has recently been reported (Lee and Spector 1983). The relative importance of these scattering mechanisms in dc transport is discussed in the following section for both the rectangular and cylindrical QWW. A comparison with electron confinement in a magnetic field may be useful in preparation and characterization of QWW and hence is included in this section. Then, we continue on to include the optical properties of QWW. Hassan and Spector (1983) have discussed the interband optical absorption in thin semiconducting QWW. Here, we study the quantum size resonance (Arora 1982a) in the inter-subband absorption in QWW, where the resonance linewidth and lineshift are calculated. This can give useful information about the scattering interactions in QWW. In semiconducting thin wires made up of an intrinsic material, the conductivity may be affected by the change in the bandgap due to quantization (quantum freeze-out) and hence this phenomenon is discussed in the next section.

Thin Wire dc Transport

In a rectangular thin-wire, the energy levels are given by (Arora 1981)

$$\varepsilon_{\ell pk} = \ell^2\varepsilon_{ox} + p^2\varepsilon_{oy} + \hbar^2k_z^2/2m^*, \ \ell(p) = 1, 2, 3, \ldots \quad (1)$$

with

$$\varepsilon_{ox} = \pi^2\hbar^2/2m^*L_x^2, \ \varepsilon_{oy} = \pi^2\hbar^2/2m^*L_y^2. \quad (2)$$

Here k_z is the momentum of a carrier parallel to the wire, m^* is the carrier effective mass, $L_{x(y)}$ is the length of the wire in $x(y)$-direction. $\varepsilon_{ox(y)}$ is of the order of 56 meV for GaAs ($m^* = 0.067$) and for $Lx = Ly = 10$ *nm*, a typical dimension of wire size grown experimentally. $\varepsilon_{ox(y)}$ is, therefore, much larger than the thermal energy $k_BT \sim 25$ meV at room temperature. Under these conditions, most of the carriers are in the lowest quantum state ($\ell = p = 1$) and the relative resistivity ratio ϱ_{zz}/ϱ_b as compared to bulk restitity ϱ_b is given by Arora (1981), Arora and Prasad (1983) and Lee and Spector (1983),

$$\varrho_{zz}/\varrho_b = 4\pi\lambda_D^2/3A, \quad (3)$$

with

$$\lambda_D = \hbar/(2m^* k_B T)^{1/2}, \tag{4}$$

$$A = L_x L_y. \tag{5}$$

Similar result is obtained for cylindrical thin wires if $A = \pi R_0^2$ *in Eq.(3), where* R_0 is the radius of the wire. λ_D in Eq.(4) is defined corresponding to average electron energy $\langle \varepsilon_k \rangle = k_B T$ in order to make comparison with bulk cases possible, although the average energy of quasi-one-dimensional system is $\langle \varepsilon_k \rangle = \frac{1}{2} k_B T$.

The Coulomb scattering is suppressed (Lee and Spector 1983) and isotropic scattering by acoustic phonons, or point defects or alloys is enhanced (Arora and Prasad 1983) with respect to those in bulk materials under strong carrier confinement conditions. Because of this enhancement, the latter scattering mechanisms can become important even in a temperature range at which isotropic scattering is neglected in the bluk material. For example, in most bulk materials at sufficiently low temperatures, the ionized-impurity scattering is the dominant mechanism of scattering. In a QWW made of the same material, this scattering can give way to acoustic phonon scattering or to point defect scattering if the number of defects are known to be very large as is normally the case with fabrication of thin samples. Similar conclusions hold good for cylindrical QWW which are more difficult to fabricate in the present state of technology. An effect analogus to Hall effect appears in the calculation of conductivity in QWW because of the presence of nonzero σ_{xy} component of conductivity. This could be confirmed only when it is possible to fabricate cylindrical QWW and the transverse conductivity can be measured in dc or ac field. In rectangular thin wires σ_{xy} vanishes as x- and y- directions are independent.

The behavior of electrons in cylindrical thin wires is, in many ways, similar to that in a magnetic field in spite of the different nature of wavefunctions. In both cases, the resistivities are inversely proportional to the area of confinement (Arora 1975, Arora and Peterson 1975, Arora *et al.* 1977, Arora and Prasad, 1983). The electrons in QWW of radius R_0 are found to behave similarly as if they were confined in a equivalent magnetic field B_{eq} given by (Arora and Prasad 1983).

$$\mathrm{B}_{eq} = hc\alpha_{01}^2 \alpha_{11}^2 (\alpha_{11}^2 - \alpha_{01}^2)^{-2} / 2e\mathrm{R}_0^2, \tag{6}$$

where α_{nm} is the m^{th} zero of the Bessel function of order n. In particular

$$\alpha_{01} = 2.405 \quad , \quad \alpha_{11} = 3.832. \tag{7}$$

If $\mathrm{R}_o = 10$ nm, the equivalent magnetic field $\mathrm{B}_{eq} \approx 35$ Kg, an easily obtainable value in the laboratory these days. Only future experiments could conclusively establish such similarity.

Quantum Size Resonance

An appropriate way to study the subband structure, as given by Eq.(1), is to observe intersubband optical transitions (Arora 1982b) and associated resonances. These resonances are extensively studied in silicon inversion layers (Ando *et al.* 1982) and other heterostructures (Price 1981). Similarly, with the levels suitably occupied, the electronic properties of QWW could include the polarization phenomena in the direction of confinement, the low dimensional ac conduction and non-reciprocal cross-effects between them.

Hassan and Spector (1983) have studied the interband resonance effects when an electron jumps from the valence band to conduction band by absorbing an optical photon whose energy is equal to the bandgap which varies with the size of QWW because of quantum confinement of electrons and holes. Quantum size resonance in QWW refers to intersubband resonance when an electron jumps from lowest quantized subband to the higher subbands by absorbing a photon. By following the complicated but straightforward density matrix formalism developed earlier (Arora *et al.* 1981), we find that the dynamic conductivity $\sigma_+ = \sigma_{xx} + i\sigma_{yx}$, whose real part is proportional to the power absorbed, is given by

$$\sigma_+ = \frac{e^2}{m^*\Omega} \sum_{nmks} \alpha^2_{(n+1)m}\alpha^2_{nm}(\alpha^2_{(n+1)m} - \alpha^2_{nm})^{-3}(f_{nmk} - f_{(n+1)mk})$$

$$[\tau^{-1}_{nmk,(n+1)mk} + i\omega - i(\alpha^2_{(n+1)m} - \alpha^2_{nm})\varepsilon_o/h], \tag{8}$$

where f_{nmk} is the Fermi-Dirac distribution function corresponding to the quantized energy ε_{nmk} in cylindrical thin wires which is given by

$$\varepsilon_{nmk} = \alpha^2_{nm}\varepsilon_o + \hbar^2 k_z^2/2m^*, \tag{9}$$

with

$$\varepsilon_o = \pi^2\hbar^2/2m^* R_o^2. \tag{10}$$

$\tau^{-1}_{nmk,(n+1)mk}$ is average of relaxation rates τ^{-1}_{nmk} and $\tau^{-1}_{(n+1)mk}$ which can be calculated from Fermi golden rule for given scattering interactions. Equation (8) shows a resonant character at photon frequenties $\omega = \omega^*$ given by

$$\omega^* = (\alpha^2_{(n+1)m} - \alpha^2_{nm})\varepsilon_o/\hbar, \tag{11}$$

when σ^+ is entirely real and the current and electric field are oscillating in phase.

In the quantum limit limit ($\varepsilon_o \gg k_B T$), only the lowest quantized state ε_{01k} is appreciably populated. Then the most prominent resonance line is at frequency $\omega^* = (\alpha^2_{11} - \alpha^2_{01})\varepsilon_0/\hbar$. If acoustic-phonon scattering is considered to be the dominant mechanism of scattering, then near the resonance σ_+ is approximated as

$$\sigma^+ = \sigma^{+\max}\delta E_1(\delta)\exp(\delta), \tag{12}$$

with

$$\sigma_{+\max} = 3n_e e^2\alpha_{11}^2\alpha_{01}^2(\alpha_{11}^2 - \alpha_{01}^2)^{-3}\tau_b A/8\beta_o\pi\lambda_D^2 m^*, \tag{13}$$

$$\tau_b = 4\ell_d u^2\pi h^4/3m^*(2\pi m^* k_B T)^{1/2}E_1^2 k_B T, \tag{14}$$

$$\delta = [(8\beta_o\pi^{1/2}\lambda_D^2/3A)\tau_b^{-1}/(\omega - \omega^*)]^2. \tag{15}$$

Here $E_1(\delta)$ is the exponential integral, n_e is the electronic concentration per unit volume, $\beta_o = 2.37$, ϱ_d is the crystal density, u is the speed of sound, and E_1 is the deformation potential constant. σ^+ of Eq. (10) reduces to half of its maximum value $\sigma^{+\max}$ at $\delta = 0.61$ at frequency $\omega = \omega_{1/2}$. The full-width Γ at half of maximum is, therefore, given by

$$\Gamma \equiv 2(\omega_{1/2} - \omega^*) = [2/(0.61)^{1/2}](8\beta_o\pi^{1/2}\lambda_D^2/3A)\tau_b^{-1}. \tag{16}$$

The resonance line width is therefore proportional to $\lambda_D^2/A\tau_b$, where τ_b is the bulk relaxation time.

The linewidth is enhanced by stronger carrier confinement for an isotropic scattering mechanism considered. If ionized-impurity scattering is also included, a minimum similar to that predicted for cyclotron resonance (Arora *et al.* 1981) and observed experimentally (McCombe *et al.* 1976) should become observable as the wire size is reduced. The resonance frequency given by Eq.(11) may shift if inelastic nature of the scattering is also included in Eq.(18). Therefore, the lineshift and linewidth can give useful information about dominant scattering interactions in QWW. These studies can be supplemented with dc transport studies to make a powerful tool for the study of QWW.

Quantum Freeze-Out

In a two-band model of a semiconductor or a semimetal, the carrier confinement in QWW can produce quantum freeze-out of carriers, reminiscent of similar effects in a magnetic field reported earlier (Arora and Spector 1982). In a cylindrical thin wire of radius R_0, the ratio of the carrier concentration $n(T,R_0)$ to that in the bulk $n_b(T)$ is obtained as Arora and Spector (1984)

$$n(T, R_o)/n_b(T) = 4(a_e a_h)^{1/2}\exp(-\alpha_{01}^2\hbar^2/4MR_o^2 k_B T), \tag{17}$$

with

$$a_{e(h)} = \hbar^2/2m_{e(h)}^* R_o^2 k_B T, \tag{18}$$

$$M^{-1} = m^{*-1}_e + m^{*-1}_h. \tag{19}$$

Equation (17) shows that the number of carriers decrease as the wire radius is decreased because of increased bandgap (Hassan and Spector 1983).

An interesting manifestation of this quantum freeze-out of carriers is the semimetal-semiconductor transition as a result of the lift-out of the band overlap

Δ because of quantization. In cylindrical thin wires, the onset of semiconducting behavior is expected to take place at a critical radius R^*_0 given by

$$R_o^* = \alpha_{01}\hbar/(2M\Delta)^{1/2}. \tag{20}$$

For parameters appropriate to bismuth, $R_0 \sim 250$ Å, a value easily attainable in the current state of technology. This sort of semimetal-semiconductor transition for carrier confinement in a magnetic field which exhibits quasi-one-dimensional character similar to that in QWW has very recently been reported (Miura *et al* 1982). For wires of radii smaller than R_o^*, the electric conductivity of QWW will exponentially decrease with temperature because of the presence of an effective bandgap $\varepsilon_g^* = (\alpha_{01}^2\hbar^2/2MR_o^2) - \Delta > 0$ which is exhibited in Eq.(17).

As the technology of fabricating these micro-structures advances, semimetallic QWW may soon become a reality, where it will be possible to study semimetal-semiconductor transition. On the other hand, some QWW's may exhibit a semimetallic character because the valence band in the cladding surrounding QWW lies higher in energy than the conduction band in QWW.

In QWW of square cross-section made of bismuth, the critical dimensions for semimetal-semiconductor transition is 480Å, which is somewhat larger than that in cylindrical QWW.

Conclusion

We have presented above some interesting effects which are expected to occur in QWW for which technology of fabrication has advanced to a considerable stage. The above results are derived in the extended state model of an electron in a semiconductor. But, the experimental observation (Giordano 1980, Kimball 1981) in the localized regime indicate similar behavior creating scepticism regarding possible close relationship between the two regimes. The critical carrier concentration for the onset of degeneracy is enhanced with carrier confinement in QWW making samples less degenerate (Arora 1982). This is due to the depletion of low density states because of quantization, as no states exist below zero-point energy (lowest level). In the light of several of these new developments, we hope the results presented above will provide deeper insight in QWW and other quantum systems being fabricated with sophisticated semiconductor technology. These considerations could be quite important in the design and development of high speed devices, where this work is expected to be of great importance.

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النقل فى أسلاك البئر الكمية

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توضح الدراسات النظرية الكمية على النقل المباشر فى أسلاك البئر الكمية انخفاض التشتت الناتج عن الشوائب المتأينة تحت ظروف الحجز الكمى المتشدد، مع مضاعفة الفونونات الصوتية أو العيوب النقطية أو تشتت السبائك عرض خط الرنين الكمى بسبب الحجم. عندما تكون الإشعاعات مستقطبة عموديا على السلك تكون متناسبة مع $(\lambda_D^2/A\ \tau_b)$ حيث λ_Dهو طول دى بروجلى الموجى و A هو مساحة الحجز و τ_b هو زمن الاسترخاء فى المادة. يتوقع أن يجعل تجمُّد النواقل المحتجزة الانتقال من أشباه المعادن إلى اشباه الموصلات ممكنا فى الأسلاك الرفيعة.