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# **Transport Phenomena in Semiconductor Quantum wells**

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# Abstract

The problem of heat transport in quantum well structures is investigated with the help of newer concept of equivalence of relaxation times and phonon line width (i.e., a phonon life time). The various contribution of scattering mechanism in nanostructure has been described by taking the electron-phonon, disorder and anharmonicity effects as a central problem. This has been dealt with the help of double time thermodynamic Green's function theory for phonon via a newly formulated Hamiltonian which consists of the contribution from i. unperturbed electrons, ii. unperturbed phonons, iii. isotopic impurities and iv. anharmonicities and v. electron-phonon. In the present work the phonon frequency line width is observed as a very sensitive quantity to study the transport phenomena in quantum well structure.

Keywords: Quantum well, Phonon Confinement, Anharmonicity, Thermal Transport.

### Introduction

Quantum well heterostructures are key components of many optoelectronic devices, because they effectively increase the strength of electro-optical interactions by confining the carriers to small regions<sup>1</sup>. The transport properties in these low dimensional systems are an emerging field of research for experimentalists as well as for theoreticians<sup>2</sup> due to its potential applications in electronic devices<sup>3</sup>. A quantum well or superlattice is an anisotropic structure, with a different thermal conductivity along the layers and in the cross-plane direction, i.e., in plane conduction and that perpendicular to the plane. It has been reported by various authors that the electron transport is determined by scattering of electrons from phonons, impurities, and interface roughness, while the conduction perpendicular to the plane transport are dominated by the resonant tunneling effect in addition to the in plane scattering<sup>4</sup>. The experiments and the theories for these two are very different which has been well reviewed in literature <sup>2,5</sup>. The calculation of thermal conductivity including interference was first carried out by Hyldgaard and Mahan<sup>6</sup> for a Si/ Ge superlattice, and for a variety of superlattices by some other authors<sup>7</sup>. It is observed that the thermal conductivity in the cross-plane direction is typically a factor of 10 smaller than it is in either of the layer materials. The study of thermal conductivity of superlattice for Ge- type structure was made by several authors using Boltzmann transport equation<sup>8, 9</sup>. Even in superlattice one can develop the concept of internal boundary, these internal boundaries even at the interface considerably reduce the phonon mean path which can be well explained on the basis of combined boundary scattering<sup>10,11</sup>. Callaway presented a phenomenological model<sup>12</sup> which successfully explained the large amount of experimental data on thermal

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conductivity, but still there were some objections inaccessible from this model namely; i. the absence of phonon dispersion, ii. exclusion of phonon polarization indices due to isotropicity considerations and iii. additivity of inverse relaxation times for different scattering events (violation of Matthiessen's rule which applies only to the independent scattering processes). Heat carriers either phonons or electrons in solids undergo through a large number of collision events (interactions) such as phonon-phonon interactions, defect (impurity) interactions, electron-phonon interactions, etc. These interactions give rise to anharmonic modes, impurity (gap-, local-, and/or resonance-) modes and impurity- anharmonicity interaction modes. As a result, these interactions offer sufficient thermal resistance and the conductivity of any specimen is greatly affected. In the present work, all the inadequacies pointed out above in the Callaway model have been removed by replacing the relaxation time by electron (phonon) line widths<sup>13,14</sup> for quantum well structures.

**Formulation of Problem:** The thermal conductivity of quantum well along with the role of various scattering mechanisms in the relaxation time approximation with a new view point can be investigated by using modified Callaway expression<sup>12</sup>

$$k = \frac{k_{\mathcal{B}}\beta^2\hbar^2}{2\pi^2v} \int_0^{\omega_D} \frac{\omega^4 e^{\beta\hbar\omega}}{\Gamma_k(\omega,T) \left(e^{\beta\hbar\omega} - 1\right)^2} \tag{1}$$

where  $= (K_{\mathbb{B}}T)^{-1}$ ,  $v_{\text{gh}}$  and  $\Gamma_{\mathbb{R}}(\omega, T)$  are phonon velocity and phonon line width, respectively. Some provocative results show that under quite natural conditions the concept of additivity of inverse relaxation times (Matthiessen's rule) loses its meaning and is only approximately valid. Without any loss of generality, to avoid this inadequacy one can use the concept of equivalence

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of total relaxation time  $\tau(\omega, T)$  (used in original Callaway model) with electron and phonon frequency line widths  $\Gamma_k(\omega, T)$ (i.e. quantum excitations directly related to the electron and phonon life time of a particular scattering event), i.e.,  $\tau^{-1}(\omega, T) \approx \Gamma_k(\omega, T)$  (2)

Induction of this concept eradicates the deficiencies introduced due to violation of Matthiessen's rule and exclusion of dispersion relations. The concept of separate heat transport channels, i.e., electronic thermal conductivity  $k_{z}$  or phonon conductivity  $k_{y}$  is not insisted here, instead above expression is taken up as representative equation to describe the thermal conductivity and the decency of phenomena is centered in the configuration of  $\Gamma_{k}(\omega, T)$ .

**Hamiltonian:** In order to investigate the quantum dynamics of the low dimensional system and to explore the various scattering mechanism underlying the microscopic mechanism of quantum well structure we have consider the Hamiltonian of the second quantized form as

$$H = H_e + H_p + H_{ep} + H_A + H_D$$
(3) with

$$H_e = \sum_q \varepsilon_q b_q^* b_q$$
 (Electron Hamiltonian) (3a)

$$H_p = \sum_{k} \left( \frac{\varepsilon_k}{4} \right) \left( A_k^* A_k + B_k^* B_k \right)$$
(Harmonic phonon Hamiltonian) (3b)

$$H_{ep} = \sum_{q,k} g_k b_Q^* b_q B_k \quad \text{(electron-phonon Hamiltonian)} \tag{3c}$$

$$H_A = \sum_{s \ge 3} \sum_{k_1, k_2 \cdots k_s} V_s(k_1, k_2 \cdots k_s) A_{k_1} A_{k_2} \cdots A_{k_s} \text{ (anharmonic Hamiltonian) (3d)}$$

$$H_D = \sum_{k_1, k_2} \left[ D(k_1, k_2) A_{k_1} A_{k_2} - C(k_1, k_2) B_{k_1} B_{k_2} \right]$$
(defect Hamiltonian) (3e)

In above equations  $A_k = a_k + a_{-k}^* = -A_{-k}^*$  and  $B_k = a_k - a_{-k}^* = -B_{-k}^*$  represent the phonon field and momentum operators, respectively. Also,  $g_k$  stands for the electron-phonon coupling constant and  $a_k(a_k^*)$  and  $b_q(b_q^*)$  are the phonon and electron Annihilation (creation) operators with wave vectors k (for phonons) and q (for electrons), respectively. The coefficients  $C(k_1,k_2)$  and  $D(k_1,k_2)$  depend upon change in mass and force constants due to substitutional point impurities, respectively and are given by Indu B. D.<sup>13</sup> and Sharma P. K. et al<sup>14</sup>

$$C(k_{1},k_{2}) = \left(\frac{M_{0}}{4N\mu}\right) \left(\omega_{k_{1}}\omega_{k_{2}}\right)^{1/2} \left[e(k_{1})e(k_{2})\right] \left[\sum_{i}^{N} c e^{i(k_{1}+k_{2})R_{i}} - \sum_{i}^{n} e^{i(k_{1}+k_{2})R_{i}}\right]$$
(4a)  
$$D(k_{1},k_{2}) = (4N)^{-1} \left(\omega_{k_{1}}\omega_{k_{2}}\right)^{-1/2} \sum_{i,i'} \left(\frac{\phi_{i,i'}}{M_{0}}\right) \left[e(k_{1})e(k_{2})\right] e^{i(k_{1}.R_{i}+k_{2}.R_{i'})}$$
(4b)

Where c = n / N and  $\mu = MM / (M - M)$ . Here  $M_0^{-1} = c / M + (1 - c) / M$  is the effective atomic mass as seen by the phonon in the crystal,  $R_l$  label the equilibrium position of the  $l^{th}$  atom in the crystal,

the symbol *i* designates the position of impurity atom, e(k) is the polarization vector and  $\phi_{l,l'}$  represents the change in the harmonic force constant due to defects. For brevity, we have used index *k* to denote kj, where *j* labels the branch of the frequency spectrum. The anharmonicity coefficients  $V_s(k_1, k_2 \cdots k_s)$  are the Fourier transform of  $s^{th}$  order anharmonic force constant and are symmetric with respect to the pair of lattice vibration indices  $k_s$ :

$$V_{3}(k_{1},k_{2},k_{3}) = \frac{1}{3} \left(\frac{\hbar}{8N}\right)^{1/2} \frac{\Delta(k_{1}+k_{2}+k_{3})}{(\omega_{k_{1}}\omega_{k_{2}}\omega_{k_{3}})^{1/2}} \phi_{3}(k_{1},k_{2},k_{3})$$
(5a)

$$V_4(k_1, k_2, k_3, k_4) = \frac{\hbar}{4!(4N)} \frac{\Delta(k_1 + k_2 + k_3 + k_4)}{(\omega_{k_1} \omega_{k_2} \omega_{k_3} \omega_{k_4})^{1/2}} \phi_4(k_1, k_2, k_3, k_4)$$
(5b)

with

$$\phi_{3}(k_{1}, k_{2}, k_{3}) = \frac{1}{M^{3/2}} \sum_{l,l'} \sum_{x_{1}, x_{2}, x_{3}} \phi_{x_{1}, x_{2}, x_{3}}^{(3)}$$

$$(l, l')e(k_{1})e(k_{2})e(k_{3})e^{2\pi i(k_{1}, k_{2}, k_{3}).r_{0}(l, l')}$$
(5c)

$$\phi_{4}(k_{1},k_{2},k_{3},k_{4}) = \frac{1}{M^{2}} \sum_{l,l'} \sum_{x_{1},x_{2},x_{3},x_{4}} \phi_{x_{1},x_{2},x_{3},x_{4}}^{(4)}$$

$$(l,l')e(k_{1})e(k_{2})e(k_{3})e(k_{4})e^{2\pi i(k_{1},k_{2},k_{3},k_{4}).r_{0}(l,l')}$$
(5d)

In the above expressions the prime over summation stands for the exclusion of the terms with l = l' and  $\phi_{x_1, x_2, \dots, x_s}^{(s)}(l, l')$  are the expansion coefficients<sup>13,14,15</sup>.

**Phonon Green's Functions:** In order to obtained the line shape of phonon spectrum let us consider the evaluation of the double time temperature dependent retarded Green's function

$$\begin{aligned} G_{k,k'}(t-t') &= \langle A_k(t); A_{k'}(t') \rangle \\ &= -i\theta(t-t') < \left[ A_k(t), A_{k'}^*(t') \right] > \end{aligned}$$
(6)

via Hamiltonian (2) with the help of quantum dynamical equation of motion technique and Dyson's equation approach. This results in the following form<sup>13</sup>

$$G_{k,k}(\omega) = \frac{\omega_k \eta_{k,k}}{\pi [\omega^2 - \omega_k^2 - 2\omega_k F(k,k;\omega)]}$$
(7)

Where  $\tilde{\omega}_k$  is the renormalized phonon frequency and  $\tilde{P}(k, k', \omega)$  is the self energy operator or response function.

$$P(k,k',\omega) = \lim_{\varepsilon \to 0^+} \Delta_k(\omega) - i\Gamma_k(\omega)$$
(8)

Where  $\Delta_k(\omega)$  is the shift in the phonon frequency of the perturbed mode and is the real part of  $P(k, k', \omega)$  (phonon self energy) and the imaginary part  $\Gamma_k(\omega)$  is the phonon frequency line width at the half maximum of the phonon frequency peak is given by

$$\Gamma_{k}(\boldsymbol{\omega}) = \Gamma_{k}^{D}(\boldsymbol{\omega}) + \Gamma_{k}^{A}(\boldsymbol{\omega}) + \Gamma_{k}^{AD}(\boldsymbol{\omega}) + \Gamma^{ep}(\boldsymbol{\omega})$$
(9)

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\_\_\_ISSN 2320–4796 Res. J. Physical Sci. The various terms in Eq.(9) can be calculated with some tedious algebra<sup>16</sup> in the form

$$\Gamma_k^D(\omega) = \Gamma_k^m(\omega) + \Gamma_k^F(\omega)$$
(10a)  
$$\Gamma_k^m(\omega) = 8\pi \varepsilon(\omega) \sum_{k=1}^{\infty} (k - k)^2 \omega^3 \omega^{-2} \delta(\omega^2 - \tilde{\omega}^2)$$
(10b)

$$\Gamma_{k}^{F}(\omega) = \Im \mathcal{L}(\omega) \sum_{k_{1}} |\mathcal{L}(k_{1}, -k_{1})|^{2} \omega_{k_{1}} \omega_{k_{2}} \partial_{k_{1}} \partial_{$$

$$\Gamma_{k}^{\prime}(\omega) = 8\pi\varepsilon(\omega)\sum_{k_{1}}|D(k_{1},-k)| \quad \omega_{k_{1}}\delta(\omega^{2}-\omega_{k_{1}}^{2})$$
(10c)

$$\Gamma_k^A(\boldsymbol{\omega}) = \Gamma_k^{3A}(\boldsymbol{\omega}) + \Gamma_k^{4A}(\boldsymbol{\omega}) \tag{10d}$$

$$\Gamma_k^{JA}(\boldsymbol{\omega}) = 18 \pi \varepsilon \left(\boldsymbol{\omega}\right) \sum_{k_1, k_2} [V_3(k_1, k_2, -k)]^{-} \boldsymbol{\eta}_1$$

$$\left[ g_1 \approx \varepsilon \left( x_1^2 - \alpha^2 \right) + g_2 \approx \varepsilon \left( x_2^2 - \alpha^2 \right) \right]$$
(10e)

$$[S_{+\alpha}\omega_{+\alpha}\delta(\omega - \omega_{+\alpha}) + S_{-\alpha}\omega_{-\alpha}\delta(\omega - \omega_{-\alpha})]$$
  

$$\Gamma_{k}^{4A} = 48 \pi \varepsilon (\omega) \sum_{k_{1},k_{2},k_{3}} |V_{4}(k_{1},k_{2},k_{3},-k)|^{2} \eta_{2}$$
(10f)

$$\begin{bmatrix} S_{+\beta}\widetilde{\omega}_{+\beta}\delta(\omega^2 - \widetilde{\omega}_{+\beta}^2) + 3S_{-\beta}\widetilde{\omega}_{-\beta}\delta(\omega^2 - \widetilde{\omega}_{-\beta}^2) \end{bmatrix}$$
  
$$\Gamma_k^{AD}(\omega) = \Gamma_k^{3D}(\omega) + \Gamma_k^{4D}(\omega)$$
(10g

$$\Gamma_{k}^{3D}(\omega) = 16 \sum_{k_{1}} |C(-k,k_{1})|^{2} \omega_{k}^{-2} \Gamma^{3A}(\omega)_{k_{1}}$$
(10h)

$$\Gamma_{k}^{4D}(\omega) = 16 \sum_{k_{1}} |C(-k,k_{1})|^{2} \omega_{k}^{-2} \Gamma^{4A}(\omega)_{k_{1}}$$
(10i)

$$\Gamma_k^{ep}(\omega) = 8\pi\varepsilon(\omega) \sum_q N_Q^2 g_k^2 \omega_Q^4 \delta(\omega^2 - 2\tilde{\omega}_Q^2)$$
(10j)

In above expressions various symbols are defined as follows:

$$S_{\pm\alpha} = n_{k_2} \pm n_{k_1}; \ S_{\pm\beta} = 1 \pm n_{k_1} n_{k_2} \pm n_{k_2} n_{k_3} \pm n_{k_3} n_{k_1}$$
(11)

$$\omega_{\pm\alpha} = \widetilde{\omega}_{k_1} \pm \widetilde{\omega}_{k_2} ; \quad \omega_{\pm\beta} = \widetilde{\omega}_{k_1} \pm \widetilde{\omega}_{k_2} \pm \widetilde{\omega}_{k_3}$$
(12)

$$\eta_{i-1} = \frac{\omega_{k_1} \omega_{k_2} \cdots \omega_{k_i}}{\widetilde{\omega}_{k_1} \widetilde{\omega}_{k_2} \cdots \widetilde{\omega}_{k_i}}; \ \widetilde{n}_k = \frac{\widetilde{\omega}_k}{\omega_k} \left\langle A_k^* A_k \right\rangle = \coth \frac{\beta \hbar \omega_k}{2};$$
$$\beta = (k_B T)^{-1} \tag{13}$$

#### **Results and Discussion**

Let us examine these Phonon (electron) line widths (life times) for the confinement in a quantum well structures. The phonon dispersion in quantum wells changes due to spatial phonon confinement in a quantum well induced by the miniboundaries developed inside it and reasonably affects the lifetimes. This results in  $\varepsilon = \varepsilon_n + \varepsilon_{\parallel}$ , where  $\varepsilon_n$  is the quantized phonon energy along z-axis and  $\varepsilon_{\parallel} = \varepsilon_x + \varepsilon_y$  with wave vector relation  $k_{\parallel}^2 = k_x^2 + k_y^2$ . The results given in earlier sections are for a bulk crystal and now can be extended to the quantum well structures using the appropriate confinement conditions in the following form:

$$\tau_e^{-1} = \Gamma_e(\omega) = \frac{\alpha\varsigma}{8\pi^2} \sum_n \int \left(\varepsilon_{\parallel} + \varepsilon_n\right)^2 \left[1 + \left(\varepsilon_{\parallel} + \varepsilon_n\right)^{-1}\right] d\varepsilon_{\parallel}$$
(14a)

$$\tau_p^{-1} = \Gamma_p(\omega) = \frac{4\zeta_1}{\pi} \sum_n \int \frac{\varepsilon(\varepsilon_{\parallel} + \varepsilon_n)}{(\varepsilon + \varepsilon_{\parallel} + \varepsilon_n)^2} d\varepsilon_{\parallel}$$
(14b)

$$\begin{aligned} \tau_{3ep}^{-1} &= \Gamma_{3ep}(\omega) = \frac{18\xi_1}{\pi} \sum_{n} \sum_{k_1} |V_3(k_1, k, -k)|^2 \eta_1 \int \left[ \coth \frac{\beta(e - \varepsilon_{k_1})}{2} + \coth \frac{\beta(-(e + \varepsilon_{k_1}))}{2} + (14c) \right] \\ & \cosh \frac{\beta(-(e - \varepsilon_{k_1}))}{2} + \coth \frac{\beta(e + \varepsilon_{k_1})}{2} \right] \frac{d\varepsilon_{k_1}}{d\varepsilon_{k_1} + \varepsilon_{k_1}} \\ & \tau_{4ep}^{-1} &= \Gamma_{4ep}(\omega) = \frac{24}{\pi} \sum_{n} \sum_{k_1, k_2} |V_4(k_1, k_2, k, -k|)|^2 \eta_2 \\ & \int \left[ 8 - 4 \coth \frac{\beta e_{-k_1}}{2} \coth \frac{\beta e_{-k_2}}{2} + \coth \frac{\beta e_{-k_2}}{2} + \coth \frac{\beta(e - \varepsilon_{k_1} - \varepsilon_{k_2})}{2} \right] \\ & + \coth \frac{\beta(-e - \varepsilon_{k_1} - \varepsilon_{k_2})}{2} + 3 \coth \frac{\beta(-e + \varepsilon_{k_1} - \varepsilon_{k_2})}{2} + 3 \coth \frac{\beta(e - \varepsilon_{k_1} - \varepsilon_{k_2})}{2} \\ & + \coth \frac{\beta(-e - \varepsilon_{k_1} - \varepsilon_{k_2})}{2} - 3 \coth \frac{\beta(-e + \varepsilon_{k_1} - \varepsilon_{k_2})}{2} - \coth \frac{\beta(e - \varepsilon_{k_1} - \varepsilon_{k_2})}{2} \\ & + \cot \frac{\beta(-e - \varepsilon_{k_1} - \varepsilon_{k_2})}{2} - 3 \cosh \frac{\beta(-e + \varepsilon_{k_1} - \varepsilon_{k_2})}{2} \\ & + \cot \frac{\beta(-e - \varepsilon_{k_1} - \varepsilon_{k_2})}{2} \\ & = \frac{\beta^2 m^2 s}{\pi \hbar^2} ; \quad \xi_1 = \frac{N_0 g g^2 m^2 s}{\pi \hbar^2} \end{aligned}$$

Where  $m^*$  and S stand for the effective msass of electron and the surface area of well. In above results it is evident that the phonon occupancy depends on temperature and energies like  $\varepsilon_n$ and  $\varepsilon_{\parallel}$ . Above results for relaxation times thus obtained can be further examined for a modified dispersion relations

$$\varepsilon_{n} = v_{n} \hbar k_{n} = p_{n} \tag{15a}$$

$$\mathcal{E}_{k_{\parallel}} = v_{k_{\parallel}} \hbar k_{\parallel} = p_{\parallel} = v_{k_{\parallel}} \hbar (k_x^2 + k_y^2)^{\frac{1}{2}}$$
(15b)

where  $p_n$ ,  $p_{\parallel}$ ,  $v_n$  and  $v_{\parallel}$  are the phonon momentum and group velocities in  $k_n$  and  $k_{\parallel}$  directions, respectively. Further, a careful study of the terms like  $\operatorname{coth} \frac{\pm \beta \left( \varepsilon \pm \varepsilon_{k_1} \right)}{2}$  and  $\operatorname{coth} \frac{\pm \beta \left( \varepsilon \pm \varepsilon_{k_1} \pm \varepsilon_{k_2} \right)}{2}$ , which are some sort of distribution functions are not simple quantities in the present context but are heavily influenced by the dispersion relations (15) for every  $\varepsilon_{k_i} = \varepsilon_{k_{ni}} + \varepsilon_{k_{\mathbb{W}}}$ ;  $i = k_1, k_2$  and show highly anisotropic behavior in  $k_n$  and  $k_{\parallel}$  directions for the reason that  $\varepsilon_n$  and  $\varepsilon_{\parallel}$  exhibit quantized and continuous behavior thus changing the usual scenario of physics.

## Conclusion

Present work is based on general formulation of life times of phonons for quantum well structures and is very much different from the usual results for a bulk crystalline solid. It emerges from present study that the life times (relaxation times) can be successfully studied with the help of new formulation which can draw a clear demarcation line between the bulk and the low dimensional systems as quantum confinement. The importance of anharmonic effects cannot be ignored because they explore the inevitable dependences of life times on temperature, frequency, impurity concentration and electron phonon coupling. This work however presents general results but can be exploited for model calculations of some specific quantum well structures with the help of heavy computational work in future.

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