The Einstein Relation in Strained Quantum Wire Superlattices of Non-Parabolic Semiconductors With Graded Structures

9.1. Introduction:

In this chapter an attempt is made to investigate the DMR in strained quantum wire SLs of non-parabolic semiconductors having graded interfaces by formulating the appropriate dispersion law incorporating the influence of the finite thickness of the interface. This we have formulated in section 9.2.1. The results for the corresponding electronic concentration and DMR in stressed constituent semiconductors are given in section 9.2.2. from which the simplified well-known limiting cases of stress free ID electronic materials having parabolic energy bands are written in section 9.2.3. In section 9.2.4. we shall suggest an experimental method of determining the DMR in degenerate materials having arbitrary dispersion laws. We shall study the influence of doping and thickness of the DMR.

9.2. Theoretical Background:

9.2.1. Formulation of the DMR in strained quantum wire SLs of non-parabolic semiconductors with graded structures

The dispersion relation of the conduction electrons in bulk specimens of strained non-parabolic semiconductors for a stress along <110> direction can be expressed in the absence of any quantization, by equation (5.24). Therefore the dispersion law in strained quantum wire SLs of non-parabolic semiconductors with graded structures can be written, extending the methods as given in [9.1] and [9.2], as
\( k_i^2 = \Psi(E, n, L) - \left( \frac{n\pi}{d_x} \right)^2 - \left( \frac{L\pi}{d_y} \right)^2 \)  

(9.1a)

where \( \Psi(E, n, L) = \left[ \cos^{-1} \left( \frac{e(E, n, L)}{2} \right) \right]^2 \cdot \frac{1}{(d_x + d_y)^2} \)

\( e(E, n, L) = [2 \cosh(\beta(E, n, L)) \cos(\gamma(E, n, L))] + T(E, n, L) \sinh(\beta(E, n, L)) \sin(\gamma(E, n, L)) + \Delta_o \left[ \frac{p_2^2(E, n, L)}{p_1(E, n, L)} - 3p_1(E, n, L) \right] \cosh(\beta(E, n, L)) \sin(\gamma(E, n, L)) + \left[ 3p_2(E, n, L) - \frac{p_1^2(E, n, L)}{p_1(E, n, L)} \right] \sinh(\beta(E, n, L)) \cos(\gamma(E, n, L)) \]

\( \Delta_o \left[ \frac{5p_2^2(E, n, L)}{p_1(E, n, L)} + \frac{5p_1^2(E, n, L)}{p_2(E, n, L)} - 34p_1(E, n, L)p_2(E, n, L) \right] \]

\( \sinh(p_1(E, n, L)) \sin(\gamma(E, n, L)) \)

\( T(E, n, L) = \left[ \frac{p_1(E, n, L)}{p_1(E, n, L)} + \frac{p_2(E, n, L)}{p_1(E, n, L)} \right] \)

\( \beta(E, n, L) = p_1(E, n, L)(d_x - \Delta_o) \)

\( \gamma(E, n, L) = p_2(E, n, L)(d_y - \Delta_o) \)

\( p_1(E, n, L) = \frac{(V_0 - E - H_z)}{(E + G_z^2)} \left( 3E_i^2 + E_iq_2 - R_2 \right) + \frac{1}{(E_i + G_z^2)} + \frac{1}{(E_i + G_z^2)} \left( \frac{n\pi}{d_x} \right)^2 + \frac{1}{(E_i + G_z^2)} \left( \frac{n\pi}{d_y} \right)^2 \)

\( E_i = E - V_o, \ V_o = Eg_z - Eg_2, \ d_x and d_y \) are the films widths along \( x \) and \( y \) directions respectively, \( n(= 1, 2, 3, \ldots) \) and \( L(= 1, 2, 3, \ldots) \) are the respective size quantum numbers and
The electron statistics can be expressed as

\[ n_0 = \frac{\pi}{2} \sum_{\nu} [A(E_F, n, L) + B(E_F, n, L)] \]  \tag{9.1b}

where

\[ A(E_F, n, L) = \left[ \frac{\Psi(E_F, n, L) - \left( \frac{n\pi}{d_x} \right)^2 - \left( \frac{nL}{d_y} \right)^2}{2} \right]^\frac{1}{2} \]

\[ B(E_F, n, L) = \sum_{r=1}^{S} \nabla_r [A(E_F, n, L)] , \ r \ \text{is the set of real of real positive integers whose upper limit is} \ S \]

and

\[ \nabla_r = 2(k_F^r)^{2r} \left( 1 - 2^{1-2r} \right) \zeta(2r) \frac{d^{2r}}{dE_F^{2r}} \]

Since the DMR can, in general, be expressed as

\[ \frac{D}{\mu} = \left( \frac{e}{\partial n_0} \right) \left( n_0 \right) \]  \tag{9.2}

\[ \frac{D}{\mu} = \frac{1}{e} \sum_{n, L} \left[ A(E_F, n, L) + B(E_F, n, L) \right] \]  \tag{9.3}

where the primes denote the differentiation with respect to \( E_F \).
9.2.2. **Formulation of the DMR in strained constituent materials**

The one dimensional electron energy spectrum can be written following equation (5.24) as

\[
k_s^2 = \omega(n, L, E)
\]  

where

\[
\omega(n, L, E) = \left[ L_s^1(E) \right]^2 \left[ 1 - \left( \frac{n \pi}{d_x} \right) \{a^*(E)\}^2 - \left( \frac{L \pi}{d_y} \right) \{b^*(E)\}^2 \right]
\]

The use of equation (9.4) leads to the expression of \( n_0 \) as

\[
n_0 = \frac{2}{\pi} \sum_{n, L} \left[ Y_0(n, L, E_F) + Z_0(n, L, E_F) \right]
\]

where \( Y_0(n, L, E_F) = \sqrt{\omega(n, L, E_F)} \) \( Z_0(n, L, E_F) = \sum_{r=1}^{s} \nabla_r [Y_0(n, L, E_F)] \)

The use of equations (9.2) and (9.5) lead to the expression of the DMR as

\[
\frac{D}{\mu} = \frac{1}{e} \left[ \sum_{n, L} \left[ Y_0(n, L, E_F) + Z_0(n, L, E_F) \right] \right]
\]

9.2.3. **Special Cases**

In the absence of stress and under the substitution \( e_r^2 = \frac{3h^2E_{r}^2}{4m_i^*} \), where \( m_i^* \) is the effective electron mass at the edge of the conduction band, equation (5.24) assumes the form
$E(1 + \alpha E) = \frac{\hbar^2 k^2}{2m_i^*}, \quad K = \frac{1}{E_{g'}}$  \hspace{1cm} (9.7)

Therefore, under the said conditions, equation (9.7) gets simplified as

$$E(1 + \alpha E) = \frac{\hbar^2 k^2}{2m_i^*} + \frac{\hbar^2}{2m_i^*} \left( \frac{n\pi}{d_x} \right) + \frac{\hbar^2}{2m_i^*} \left( \frac{L\pi}{d_y} \right)$$  \hspace{1cm} (9.8)

The electron concentration under the said conditions assumes the form

$$n_0 = \frac{2}{\pi} \sum \left[ T_1(n, L, E_p) + T_2(n, L, E_p) \right]$$  \hspace{1cm} (9.9)

where

$$T_1(n, L, E_p) = \sqrt{\frac{2m_i^*}{\hbar^2}} \left[ E_p (1 + \alpha E_p) - \left( \frac{n\pi}{d_x} \right)^2 - \left( \frac{L\pi}{d_y} \right)^2 \right]$$

and

$$T_2(n, L, E_p) = \sum_{r=1}^{\infty} \nabla_r \left[ T_1(n, L, E_p) \right]$$

Using equations (9.2) and (9.9) we get

$$\frac{D}{\mu} = \frac{1}{e^\frac{\sum_{r=1}^{\infty} \left[ T_1(n, L, E_p) + T_2(n, L, E_p) \right]}{\sum_{r=1}^{\infty} \left[ T_1'(n, L, E_p) + T_2'(n, L, E_p) \right]} \left[ 1 + \frac{3ab}{2} F_1(\eta^j) + \frac{3ak_BT}{4} F_2(\eta^j) \right]$$  \hspace{1cm} (9.10)

Under the conditions $\alpha E_p \ll 1$, equation (9.10) can be written as

$$n_0 = \frac{2}{h} \sqrt{2m_i^* \pi k_B T} \sum_{\alpha} \frac{1}{\sqrt{\alpha}} \left[ (1 + 3ab) F_1(\eta^j) + \frac{3ak_BT}{2} F_2(\eta^j) \right]$$  \hspace{1cm} (9.11)

where $a = (1 + \alpha \phi_{nL}), \quad \phi_{nL} = \frac{\hbar^2 \pi^2}{2m_i^*} \left[ \left( \frac{n}{d_x} \right)^2 + \left( \frac{L}{d_y} \right)^2 \right], \quad b = \frac{\phi_{nL}}{\alpha}, \quad \eta^j = \frac{E_F - b}{k_B T}$

and $F_j(\eta)$ is the one-parameter Fermi-Dirac integral of order j.

Under the conditions $\alpha E_p \ll 1$, equation (9.10) assumes the form
Under the conditions $\alpha \to 0$, as for wide-gap materials, equations (9.11) and (9.12) get simplified to the well-known forms [9.3] as

$$n_0 = \frac{2}{\hbar} \sqrt{2m^* \pi k_B T} \sum_{n,L} F_{\frac{1}{2}}(\eta)$$

(9.13)

and

$$D = \frac{k_B T}{\mu} \left[ \frac{1}{\sqrt{\alpha}} \left( \frac{1 + \frac{3\alpha \beta}{2}}{2} F_{\frac{1}{2}}(\eta) + \frac{3\alpha \beta k_B T}{4} F_{\frac{3}{2}}(\eta) \right) \right]$$

(9.12)

where

$$\eta = \frac{1}{k_B T} \left( E_F - \frac{\hbar^2 \pi^2}{2m^*} \left[ \left( \frac{n}{d_x} \right)^2 + \left( \frac{L}{d_y} \right)^2 \right] \right)$$

9.2.4. **Experimental suggestion for the determination of the DMR in degenerate materials having arbitrary dispersion laws**

It may be noted that the equation (5.30) is also valid in this case. Thus we can determine the DMR for any degenerate material having arbitrary dispersion law by knowing $G$.

The whole theoretical background can be summarized in the following way. In this chapter we first formulated the expressions of $n_0$ and DMR for strained quantum wire superlattices of non-parabolic semiconductors with graded structures as given by the equations (9.1a) and (9.3) on the basis of a new dispersion law (equation (9.1a)). We have also formulated the corresponding expressions for the constituent semiconductors as given by equations (9.10) and (9.11) for the purpose of relative comparison. Finally we have obtained the well-known
expressions for \( n_0 \) and DMR for the stress free quantum wires of parabolic semiconductors as
given by equations (9.13) and (9.14). It may be noted that such compatibility is the indirect
theoretical test of our analysis. In addition, we have suggested an experimental method of
determining the DMR in degenerate materials having arbitrary dispersion laws.

9.3. Results and Discussions:

Using the appropriate equations together with the parameters [9.4] \( m^*_1 = 0.023 m_e \),
\[ E_{g1} = 0.41 eV, \quad e_1 = 10 \times 10^{-11} eV m, \quad g_1 = 2 eV, \quad C_1^i = 20 eV, \quad (S_{11})_1 = 0.3 \times 10^{-3} K Bar^{-1}, \]
\( (S_{12})_1 = 0.48 \times 10^{-3} K Bar^{-1}, \quad \sigma (stress) = 4 K Bar \) for \( InAs \) and \( m^*_2 = 0.048 m_0 \),
\[ E_{g2} = 0.81 eV, \quad e_2 = 14 \times 10^{-11} eV m, \quad g_2 = 4 eV, \quad C_2^i = 30 eV, \quad (S_{14})_2 = 0.6 \times 10^{-3} K Bar^{-1}, \quad d_{a2} = -6 eV, \]
\[ (a_{a2} + C_2^i) = 10 eV, \quad \bar{b}_{a2} = -4 eV, \quad (S_{11})_2 = 0.71 \times 10^{-3} K Bar^{-1}, \quad (S_{12})_2 = 0.46 \times 10^{-3} K Bar^{-1}, \]
\( \Delta_0 = 5 nm, \quad n_0 = 10^{14} m^{-1}, \quad d_y = 40 nm \) and \( T = 2 K \) for \( GaSb \). We have plotted the
normalized DMR as a function of \( d_x \) as shown by curve a of figure 9.1 for \( InAs/GaSb \) quantum
wire SLs of non-parabolic semiconductors with graded interfaces where the plot b has been
computed for \( \Delta = 0 \) for the purpose of showing the influence of finite interface width on the
DMR. Plots c and d exhibit the same dependencies for \( InAs \) and \( GaSb \) respectively. In figure
9.2 we have plotted all the cases of figure 9.1 as functions on \( n_0 \).

The DMR is a function of the Fermi-energy, which increases with increasing electron
concentration in an oscillatory way. Therefore, the DMR will increase with increasing \( n_0 \) in
oscillatory manners. The basic dispersion relation in quantum wire SLs of non-parabolic
semiconductors with graded interfaces as given by equation (9.1a) is significantly complicated as
compared with that of the constituent materials equation (9.4) together with the fact that the
numerical values of DMR are greatest as for present SLs and the least for the constituent
semiconductors. In addition the influence of the finite interface width also enhances the values of
DMR for the whole range of the variables as considered here. It appears from figure 9.1 that the
Figure 9.1  Plots a and b indicate the variations of the normalized DMR as functions of $d_x$ for $\Delta = 0$ and $\Delta \neq 0$ respectively. Plots c and d exhibit the same variations for InAs and GaSb respectively.
Figure 9.2  Plots all the cases of figure 6.1 as functions of $n_0(d_x = 40\text{nm})$. 
DMR decreases with increasing $d_x$ in oscillatory manners. The oscillatory dependence is due to
the crossing over of the Fermi level by the subbands in steps. For each coincidence of a subband
with the Fermi level, there would be a discontinuity in the density-of-states function resulting in a
peak of oscillations and the origin of the oscillations in the DMR is the same as that of the
density-of-states function. The nature of oscillations in the DMR for SLs is different from that of
the constituent materials that is a characteristic feature of such semiconductor heterostructures. It
appears from the figure 9.1 that the DMR has become strongly dependent on the thickness of the
structure. Besides, the smaller the thickness the greater the magnitude of the DMR.

The appearance of the humps in the figure 9.2 is due to the redistribution of the electrons
among the quantized energy levels when the quantum numbers corresponding to the highest
occupied level changes from one fixed set to another.

It may be noted that the variations of the DMR are totally band structure dependent. With
different sets of energy band constants. We shall get the different numerical values of the DMR
though the nature of variations will be unaltered. The trends of the curves of the DMR versus
$n_0$ as shown here will be similar for all other types of non-parabolic materials. The basic aim of this
chapter is not solely to study the DMR on the basis of a newly formulated electron dispersion law
but also to suggest an experimental method of determining the DMR in degenerate materials
having arbitrary carrier energy spectra. It may be remarked that in recent years, the mobilities of
electrons have been extensively studied but the diffusion constants in such materials (a very
important device parameter whose exact experimental determination is rather difficult) have
relatively been less investigated. Thus the theoretical results of this chapter can be used to
determine the diffusion constants for the present SLs together with the constituents materials by
using the experimental values of the corresponding mobilities. Finally, we can write the
conclusions made here will be useful in view of the fact that the switching speed, the electronic
contribution to the elastic constants and the noise power can be connected with the DMR [9.3].