Chapter 3

Quantum Mechanical Aspects of Capacitance-Voltage Measurements of Low Dimensional Structures
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3.1 Introduction

The formulas, used for the construction of the carrier profiles from the measured $C-V$ data, were developed for the bulk structures and no modification has been made to include the quantum mechanical properties of the low dimensional structures and their temperature dependence. So, for quantum structures, different type of errors and ambiguities are encountered in the carrier profile obtained from $C-V$ measurements [1-6].

The QW structure for $C-V$ measurements has been discussed in chapter 1. After growing such quantum structures by MBE or MOCVD we have often found that the structures have not been properly grown due to the improper estimation of the parameters like position of the QW, doping level etc. Thus the sample is rejected and it calls for a second growth.

For proper and accurate measurements on a QW, the depth of the QW from the Schottky is of utmost importance. This, in turn, depends on the doping of the structure and on the temperature at which the measurements are carried out. The design of the QW structure should be done following the two extremely necessary conditions. On one end the QW should have a minimum distance from the Schottky so that, initially, without any reverse bias the built-in field of the Schottky junction does not alter the carrier accumulation in the QW. On the other end the QW should
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not be too far from the Schottky so that field break down occurs at the surface before the field crosses the QW to deplete it.

In the $C-V$ profiling of a QW structure there are certain important observations which call for proper explanations. Usually the ACD, obtained from experimental $C-V$ measurements, is matched with the ACD obtained from theoretical simulations. Both of these, are widely different from the calculated actual carrier profile of the QW [1,2]. At room temperature the ACD peaks, obtained from both experimental observations and theoretical simulations, are much smaller than the peak of the actual carrier distribution whereas at low temperatures those are very sharp and higher [1]. Moreover in experimental measurements the ACD peak shifts away from the Schottky as the temperature decreases [1,6] but in the simulated ACD the peak moves in the opposite direction [3,6]. These observations are not well explained.

In this chapter we point out the ambiguities in the $C-V$ profiling of QW structures due to the non-inclusion of quantum mechanical aspects in the measurement technique through the self-consistent solutions of the Schrödinger and Poisson equations. We have discussed the guidelines for suitable design of quantum structures for proper $C-V$ measurements, considering different doping levels and different band offsets at different temperatures. We have explained the mechanism of the ambiguous temperature dependence of the $C-V$ profiles of a single QW structure. It emerges from these studies that the series resistance has a significant role in the temperature dependence of the carrier profiles.

3.2 Theoretical and Experimental Considerations

The model QW structures considered in our studies are single QWs sandwiched in n-doped bulk semiconductors. The structure consists of an Au Schottky at the top and
an ohmic contact at the bottom of the substrate. The actual carrier profiles are computed using the self-consistent simulation as described in chapter 2. In the Newton-Raphson iteration the boundary condition for \( \phi \) is at the surface \( \phi \) is equal to the Schottky barrier height corresponding to Au [7] and in the neutral region, far away from the Schottky, \( \phi \) is equal to the potential corresponding to the energy at the bottom of the conduction band. The latter boundary condition is computed taking into account the splitting of the Fermi level due to the applied bias, the conduction band offset and the carrier concentration.

To construct the \( C-V \) profile the total capacitance per unit area is calculated as

\[
C = \frac{\Delta Q}{\Delta V_a},
\]

where \( \Delta Q \) is the change in the sheet charge due to the small change in the applied bias \( V_a \), \( \Delta V_a \). \( \Delta Q \) is computed by the change of the electric field across the surface according to the Gauss theorem [2]. The ACD is determined using the conventional formulas of the \( C-V \) technique [8,9],

\[
n_{c-v} (w) = \frac{2}{q \varepsilon \frac{d}{dV_a} \left( \frac{1}{C^2} \right)}, \tag{3.2}
\]

and

\[
w = \frac{\varepsilon}{C}, \tag{3.3}
\]

where \( w \) is the depletion width.

The experimental data, used in this chapter, was obtained by \( C-V \) measurements on an In\(_{0.24}\)Ga\(_{0.76}\)As/GaAs single QW structure at different temperatures. The sample was grown by metalorganic vapour phase epitaxy
(MOVPE). The details of the growth condition, structure and measurements are discussed in Ref. 7.

### 3.3 Results and Discussion

#### 3.3.1 Design of Appropriate Structures

We first demonstrate what will happen, if the distance of the QW from the Schottky is too small or too large beyond a certain limit. Fig. 3.1 shows the variation of the two-dimensional electron concentration $n_{2D}$ with the external reverse bias $V_r$ in a 10 nm GaAs/In$_{0.2}$Ga$_{0.8}$As QW under C-V measurements for different depths of the well from the Schottky, considering $N^+D = 6 \times 10^{16}/\text{cm}^3$, $\Delta E_c = 0.16$ eV and $T = 300$ K. It is evident from the figure that without any applied reverse bias the QW situated at a distance of 100 nm from the Schottky is almost depleted. As the distance increases the depletion of the QW decreases and carriers in the QW remain unperturbed for a depth $\geq 300$ nm. So the C-V profile supplies wrong information about the position of the QW and the carrier profile of the structure if the QW is not situated at a sufficient distance from the Schottky. This may be seen clearly in the experimental C-V profile.

![Variation of the two dimensional electron concentration ($n_{2D}$) with the external reverse bias ($V_r$) in a 10 nm GaAs/InGaAs QW for the depths (a) 100 nm (b) 150 nm (c) 200 nm (d) 300 nm, considering $N^+D = 6 \times 10^{16} \text{ cm}^{-3}$, $\Delta E_c = 0.16$ eV and $T = 300$ K.](image-url)
on multiple QWs of Yamamoto et al [5]. The first three of the eight QWs are depleted and the adjacent QWs are partially depleted.

The field distribution in the QW and in the barrier for different depths of the QW is illustrated in Fig. 3.2. The vertical dotted lines indicate the positions of the centers of the QWs. As shown in the figure, when the depth is 150 nm (a) the QW is depleted by the built in field. The minimum necessary depth is 368 nm (b) for proper measurements below which the QW is partially depleted. At this depth, when the well is depleted the surface field is $3.7 \times 10^5$ V/cm. When the depth is 404 nm (d) the well can be depleted for measurements but the surface field is almost on the verge of breakdown ($\sim 4 \times 10^5$ V/cm) [10]. For a depth of 650 nm (e) the surface field crosses breakdown but the field does not reach the QW. So it is cleared that for proper $C-V$ measurements the depth of the QW for the parameters mentioned should lie in the range of 368 nm to 404 nm. So for a particular structure we can determine the

![Fig. 3.2. Field distribution in the GaAs/InGaAs QW structure for wells at different depths, (a) 150 nm, (b) and (c) 368 nm, (d) 404 nm and (e) 650 nm, considering $N^+ D = 6 \times 10^{16}$ cm$^{-3}$, $\Delta E_c = 0.16$ eV, $T = 300$ K and well width = 10 nm. Vertical dotted lines indicate the positions of the centers of the QWs.](image-url)
maximum and minimum depth of the QW by the quantum mechanical calculations depending on the different parameters.

Fig. 3.3 shows the variation of maximum and minimum depth with the ionized donor concentration for three different QW structures corresponding to different band offsets at $T = 300$ K (solid lines) and $T = 50$ K (dashed lines), considering well width 10 nm.

Fig. 3.3. Variation of maximum and minimum depth with the ionized donor concentration for three different QW structures corresponding to different band offsets at $T = 300$ K (solid lines) and $T = 50$ K (dashed lines), considering well width 10 nm.
donor concentration at $T = 300$ K and $T = 50$ K for three different QW structures, $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{GaAs}$, $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{Al}_{0.12}\text{Ga}_{0.88}\text{As}$ and $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ where $\Delta E_c$ gradually increases. The order of the breakdown field of Schottky barriers on GaAs and AlGaAs have been taken from standard references [10-12]. It is seen from Fig. 3.3 that, for a particular temperature, as the doping increases both the maximum and minimum distances decrease. But the maximum distance decreases more rapidly. So we obtain a critical value of doping concentration above which $C-V$ measurements lead to inaccuracies. This critical limit extends as the temperature decreases. So for the $C-V$ measurement of heavily doped structures, low temperature should be preferable. It should be noted that as the band offset increases this critical value of doping concentration decreases.

The temperature dependence of the minimum and the maximum depth is presented in Fig. 3.4. At higher temperature the minimum depth becomes larger because of the spreading of the depletions over a wider region. On the other hand the change in the maximum depth with temperature is small. The material parameters, used in the computations of this section, are given in Table 3.1.

![Fig. 3.4.](image)

**Fig. 3.4.** Maximum and minimum depth as a function of temperature in a GaAs/InGaAs QW structure with $N^+_D = 5 \times 10^{16}$ cm$^{-3}$, $\Delta E_c = 0.16$ eV and well width =10 nm.
Table 3.1. Structures and parameters used for the simulation. \((m_0\) and \(\varepsilon_0\) are the rest mass of electron and permittivity of free space respectively.)

<table>
<thead>
<tr>
<th>QW structure</th>
<th>(\Delta E_c) (eV)</th>
<th>(m^*/m_0)</th>
<th>(\varepsilon/\varepsilon_0)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Well(^c)</td>
<td>Barrier(^d)</td>
</tr>
<tr>
<td>In(<em>{0.2})Ga(</em>{0.8})As/GaAs</td>
<td>0.16(^a)</td>
<td>0.055</td>
<td>0.067</td>
</tr>
<tr>
<td>In(<em>{0.2})Ga(</em>{0.8})As/Al(<em>{0.12})Ga(</em>{0.88})As</td>
<td>0.3(^b)</td>
<td>0.055</td>
<td>0.077</td>
</tr>
<tr>
<td>In(<em>{0.2})Ga(</em>{0.8})As/Al(<em>{0.35})Ga(</em>{0.65})As</td>
<td>0.5(^b)</td>
<td>0.055</td>
<td>0.096</td>
</tr>
</tbody>
</table>

\(^a\) From Ref. 2.
\(^b\) Calculated with the help of Refs. 13-15.
\(^c\) From Ref. 16.
\(^d\) From Ref. 13.
\(^e\) From Ref. 17.

### 3.3.2 Inconsistent Temperature Dependence

The experimental \(C-V\) characteristics and the corresponding apparent carrier profiles of the \(\text{In}_{0.24}\text{Ga}_{0.76}\)As/GaAs single QW structure for three different temperatures are shown in Fig. 3.5. The actual carrier profiles for these three temperatures are determined by the simulation as depicted in Fig. 3.6. It is seen from Fig. 3.5 and Fig. 3.6 that at 249 K the apparent peak height is smaller than the actual peak. With decrease of temperature the height of the experimental peak increases at a very high rate. At 49 K it is nearly 3 times larger than the actual peak height. It is also observed that the full width at half maximum (FWHM) of the experimental carrier peak decreases rapidly with temperature whereas the FWHM of the actual carrier peak has negligible change with temperature. To understand the basic difference between the apparent carrier profile and the actual carrier profile, the apparent profiles
Fig. 3.5. Experimental results: (a) $C-V$ characteristics of the structure at different temperatures and (b) apparent carrier profiles at different temperatures.

are evaluated theoretically as shown in Fig. 3.7. At 249 K the simulated apparent profile is almost similar to that derived experimentally but at lower temperature it has an opposite shift.

Fig. 3.6. Actual carrier profiles of the structure at different temperatures.
Fig. 3.7. Simulated apparent carrier profiles of the structure at different temperatures.

In the QW structure the distribution of the 2D carriers is determined by the normalized wave function. With the change in the applied reverse bias the change of this distribution is quite different from that of the bulk structure. For this reason the advancement of the depletion edge in and around the QW with increment of the reverse bias, as mentioned earlier, causes significant errors in the interpretation of the $C-V$ profile. To make it more clear, the change of $n_{2D}$ with the external reverse bias is illustrated in Fig. 3.8. It is seen that as the temperature decreases the slope of the $n_{2D}$ vs $V_r$ curves tends to become constant which corresponds to a plateau in the $C$ vs $V_r$ curve as well as an extremely large peak height in the carrier profile.

Fig. 3.5 and Fig. 3.7 illustrate how the carrier peaks move with temperature. With the decrease of the temperature from 249 K to 49 K the position of the experimental peak shifts by 5 nm towards the substrate whereas the simulated peak moves 6 nm towards the Schottky. Since the shift of the carrier peaks at 249 K is negligible, the total shift of the peak at 49 K is about 11 nm. The reason behind the shift of the simulated peak seems to arise from the Debye smearing out between 2D and 3D electrons at higher temperatures [1]. This leads to a lower value of the capacitance at
Fig. 3.8. $n_{2D}$ and the simulated capacitance of the structure as a function of reverse bias $V_r$ at different temperatures. The selected portion of the capacitance plots is enlarged in the inset.

The peak position as shown in Fig. 3.8, because of the decrease in the 2D carrier confinement which in turn produces the higher depth of the peak.

The opposite shift of the carrier peak in the experimental profile can be explained by the existence of the temperature dependent series resistance $R_s$ across the structure [3,18]. At low temperature $R_s$ increases due to low current conduction across the heterojunction [19], the increase in the contact resistance, the decrease of ionization of carriers in the bulk or due to a front diffused back contact. In presence of $R_s$ the relationship between the actual capacitance $C$ and the measured capacitance $C_m$ is [3]

$$C_m = \frac{C}{1 + (2\pi f R_s C)^2},$$  \hspace{1cm} (3.4)

where $f$ is the frequency of the ac signal. With respect to the experimental capacitance at 249 K the variation of $C_m$ and the depth with $R_s$ at 1 MHz is shown in Fig. 3.9. It is
Fig. 3.9. The measured capacitance $C_m$ and the change in the depth as a function of the series resistance $R_s$. The variation is shown with respect to the experimental peak capacitance at 249 K.

It is evident from Fig. 3.9 why at low temperature the carrier peak in $C-V$ measurements recedes from the Schottky instead of moving to the Schottky as predicted theoretically. Material parameters, used in this section, are given in Table 3.2.

**Table 3.2.** Parameters used for the simulation on In$_{0.24}$Ga$_{0.76}$As/GaAs QW. ($m^*$, $m_0$ and $\varepsilon_0$ are the effective mass of electron, the rest mass of electron and the permittivity of free space respectively.)

<table>
<thead>
<tr>
<th>Well width (nm)</th>
<th>$\Delta E_c$ (eV)</th>
<th>$m^*/m_0$</th>
<th>$\varepsilon/\varepsilon_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Well$^b$</td>
<td>Barrier$^c$</td>
</tr>
<tr>
<td>8</td>
<td>0.175</td>
<td>0.054</td>
<td>0.067</td>
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<tr>
<td></td>
<td></td>
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<td>Barrier$^c$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>13.52</td>
<td>13.18</td>
</tr>
</tbody>
</table>

$^a$ From Ref. 2.
$^b$ From Ref. 16.
$^c$ From Ref. 13.
$^d$ From Ref. 17.
3.4 Summary

We have investigated different sources of errors and ambiguities, encountered in the \( C-V \) measurements of QW structures and have described some remedies to eliminate the errors in the measurements. Using quantum mechanical computations we have highlighted the limits of the distance of the QW from the Schottky, beyond which the QW is depleted by the Schottky built-in field or it is not completely depleted below the break down field at the surface, hence \( C-V \) measurements become erroneous. The limits widely depend on the band offsets, the doping concentration and the measurement temperature. It is observed that above a critical value of doping concentration, \( C-V \) measurements lead to inaccuracies. This critical limit depends on the temperature and the band offset. The study provides guidelines for suitable design of quantum structures for proper \( C-V \) measurements.

We have explained the wide difference between the actual carrier distribution, obtained from self-consistent simulations, and the experimental carrier distribution i.e. ACD, obtained from \( C-V \) measurements. The inconsistent temperature dependence of the ACD peak position and peak concentration have been explored with the help of simulated ACD. It emerges that the series resistance across the structure has a significant role in the shift of the experimental carrier peak at low temperature whereas the opposite shift of the simulated ACD is the contribution of Debye averaging process.

This work has been published in:

References


