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Anomalous capacitance–voltage profiles in quantum wells explained by a quantum mechanical model

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We have developed a quantum mechanical model for understanding and explaining the capacitance–voltage (C–V) carrier profiles observed in quantum wells (QW). The external field imposed on the QW during C–V profiling changes the carrier distribution of the system. This model considers the effects of field and quantum confinement of the carriers in the well. The results obtained by iterative solutions of Schrodinger's and Poisson's equations give a better understanding of the experiments than the previous models where quantum confinement is ignored. © *1997 American Institute of Physics.* [S0021-8979(97)03304-5]

Capacitance–voltage (C–V) measurements are widely used for carrier profiling of semiconductors and to estimate interface states.[1,2] We have recently shown that C–V measurements with time in the form of deep level transient spectroscopy (DLTS) can be used to determine the conduction and valence band offsets of quantum wells accurately.[3,4]

When an external field is imposed on a single quantum well for C–V profiling, a number of changes take place. The bands bend (Fig. 1), as carriers get depleted from the barrier on the Schottky side, and collect in the quantum well to increase the two-dimensional (2D) carrier concentration. Inside the quantum well the motion of the carriers is quantized along the well width. The carriers are free to move in planes parallel to the interface, making their motion 2D. Due to this quantum confinement, the entire carrier distribution changes[5,6] so that the estimation of the carrier profile becomes quite involved.

Our model accounts for this quantum effect and the field dependent phenomena inside the quantum well along with the band offset. The carrier distribution and the peak shifts with temperature are computed here when this quantum mechanical model is applied to a p-type Si/SiGe/Si quantum well. Self-consistent, iterative solutions of the Schrodinger's and Poisson's equations are adopted.

The cosine wave function representing the two-dimensional hole gas (2DHG) present in the quantum well is changed in the presence of an external field as given by Bastard. In our model, the wave function is modified to suit the requirements of a 2DHG.

The quantum confinement of the carriers leads to splitting of the degenerate heavy and light hole bands of the bulk semiconductor. Due to valence band anisotropy, the effective masses of the 2D holes are modified from their bulk values. From a knowledge of the measured effective masses of heavy and light holes in the subbands of the quantum well,[7,8] it is evident that for low doping and moderate temperatures almost 90% of the holes populate the first heavy-hole subband.

The wave function representing the first heavy-hole subband is given by

$$\varphi_\omega = N(\beta)|\cos(\pi z/L+\delta)\exp\,[\beta(Z/xL-1/2x)] \tag{1a}$$

$$\varphi_b = N(\beta)|\cos(\pi/2+\delta)\exp\left[-q_0\left(\frac{Z}{L}-\frac{1}{2}\right)\right] \tag{1b}$$

in the well and barrier, respectively.

$N(\beta)$ is a normalization constant and β is a variational parameter obtained by a process of minimization of the energy term

$$E(\beta)=E_0[1+\beta^2/4\pi^2+\phi\{-1/\beta-2\beta/(4\pi^2+\beta^2) - \tfrac{1}{2}\coth(-\beta/2)\}] \tag{2}$$

$$\delta=\tan^{-1}(q_0+\beta/x)/\pi-\pi/2 \tag{3}$$

is a phase factor

$$q_0^2 = 2_m^* L^2(E_0-\Delta E_v)/\hbar. \tag{4}$$

Here x is a fraction and L is the total well width so that xL represents the fractional well width over which the carriers are piled up due to the imposed field F. E_0 is the ground state, ΔE_v is the difference in the valence-band offset between the quantum well and the barrier layer

$$\text{and}\quad \phi=qFxL/E_0. \tag{5}$$

Without any field, Eq. (1a) reduces to the cosine function.

The carrier concentration is obtained by integrating the product of the 2D density-of-states (2D-DOS) function, Fermi function, and the probability density obtained from the carrier distribution in the quantum well. The concentration of holes within the quantum well and those split into the barrier away from the Schottky side are given respectively by

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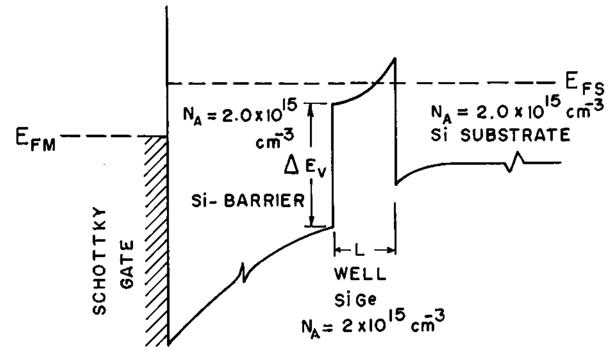

FIG. 1. Bending of the valence band of the Si–SiGe–Si QW under reverse bias.

$$p_w = \int_{L(1-2x)/2}^{L/2} p_{2\mathrm{D}} N^2(\beta)\ \cos^2\left(\frac{\pi z}{L} + \delta\right) \times \exp 2\beta\left(\frac{z}{xL} - \frac{1}{2x}\right) \ln \left| \frac{1+\exp\dfrac{(E_0 - E_F)}{KT}}{1+\exp\dfrac{(\Delta E_v - E_F)}{KT}} \right| dz \tag{6a}$$

$$p_B = \int_{L/2}^{\alpha} p'_{2\mathrm{D}} N^2(\beta) \cos^2\left(\frac{\pi}{2} + \delta\right) \exp^{-2q_0}\left(\frac{z}{L} - \frac{1}{2}\right) \times \ln \left| 1 + \exp\frac{(\Delta E_v - E_F)}{KT} \right| dz. \tag{6b}$$

Starting with a trial value F, the fractional well-width xL and a trial hole concentration within the well, the 2D-hole concentration is obtained by iterating. Repeated iterations give a unique set of values for F and x.

Our main objective is to explain the anomaly between the carrier profile obtained experimentally by C–V measurement and the theoretical interpretations offered by Tittelbach–Helmrich.[9] Our model is applied to a p-type Si/SiGe/Si quantum well shown in Fig. 1. The calculations are done at different temperatures and repeated for different valence-band offsets in the expected ranges of 25–40 meV.

Figure 2 shows the carrier distribution inside the quantum well with the reverse field. As the field increases, more carriers are depleted from the barrier and are pushed into the quantum well where they pile up, raise the peak height, and cause the peak position to shift away from the Schottky end. The peak carrier concentration changes from $\simeq 4.0 \times 10^{15}$ cm^{-3} at equilibrium to nearly 8.0×10^{16} cm^{-3} at a field required to bring the depletion edge into the well. It is interesting to note that without any field the peak concentration is very close to the theoretical result of T-H.[9]

The variations of the peak height and the peak position with temperature are shown in Fig. 3, for a valence band offset of 25 meV and at a field required to completely deplete the cap layer. The peak position shifts towards the Schottky end with a rise in temperature as in that obtained experimentally. The shift in peak position with temperature in the 3D model is in the opposite direction and remains

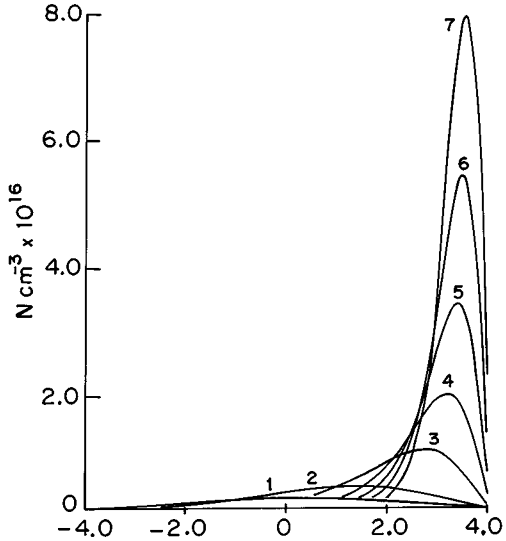

FIG. 2. Hole concentration inside the quantum well on application of reverse bias. Field increases in steps of 12 kV/m.

unexplained. The carrier peak height also decreases with rise in temperature because the carrier confinement diminishes with an increase in temperature. Such decrease in peak heights is more pronounced when measured experimentally. This seems to arise from the fact that the error between the actual peak and the measured peak increases at a considerable rate due to an increase in Debye length with temperature. Figure 4 plots the variation of the peak heights with temperature for both the theoretical model as well as the experimental data of T-H. The nature of variation of Debye length is also shown in Fig. 4. It is apparent that at low temperatures the measurement error diminishes with the decreasing Debye length. In fact, it has been shown by Wu *et al.*[10] and Johnson *et al.*[11] that the effect of Debye length

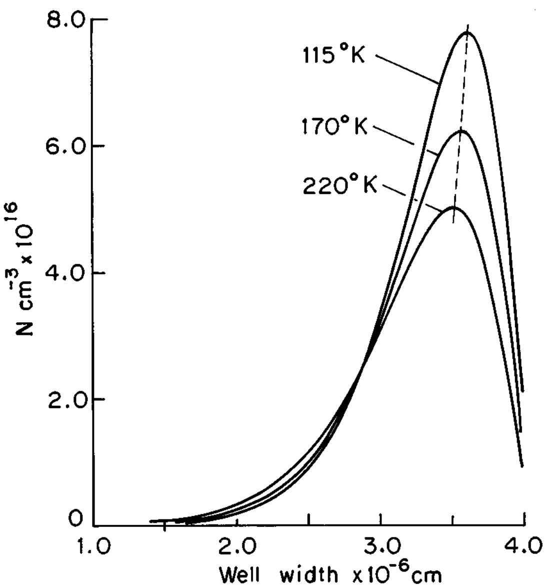

FIG. 3. Variation of peak height and peak position inside the QW with temperature. Left hand half of the well is shown.

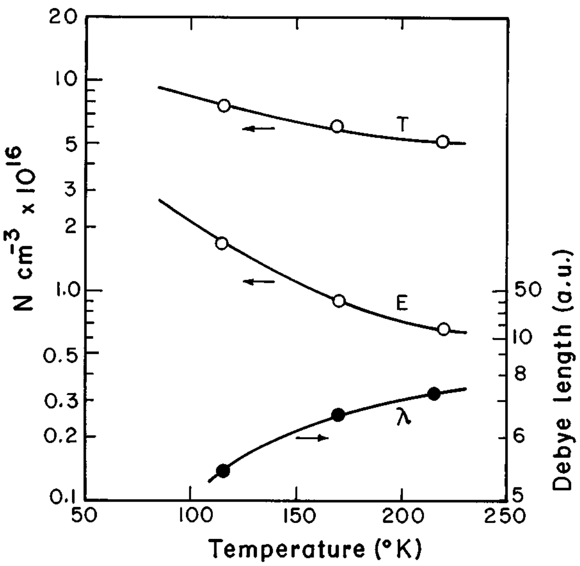

FIG. 4. The experimental (E) and theoretical (T) peak heights vs temperature. The Debye length variation with temperature is also shown.

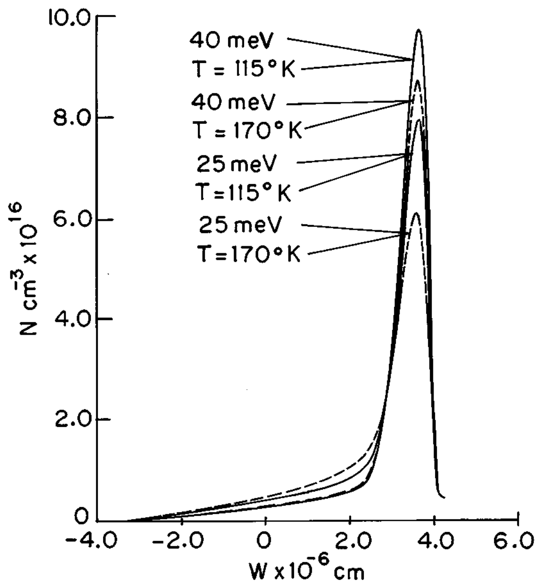

FIG. 5. The carrier distribution and peak heights for different valence-band offsets at different temperatures.

becomes very pronounced if the carrier distribution rises and falls very rapidly within a couple of Debye lengths as in a quantum well. So the higher the temperature and larger the Debye length the lower the measured carrier concentration compared to its actual value. The spatial resolution cannot be less than a couple of Debye lengths. The experimental data of Wu *et al.*[10] gives a clear picture of this underestimation. For a very sharp ion implanted profile, C–V measurement gives an experimental carrier concentration that is about 4–5 times less than the actual value. This effect is clearly indicated in our calculated value of the peak height which is roughly four times higher than the experimental data of T-H.[9] But the theoretical peak height of the model of T-H[9] is nearly 4 times less than the 3D measured value. Although the computation presented were done for the first heavy-hole subband, they were checked by including the light-hole subband as well. The difference in the two results was less than 3%. Inclusion of the first light-hole subband lengthens and complicates computational procedures without altering the results significantly. It seems logical not to include such unnecessary complexities, particularly, when the error between theory and experiment is so high.

There is still some ambiguity about the ratio of the band offsets. Results for different valence-band offsets in the expected range are shown in Fig. 5. It is seen that the carrier confinement and peaking are strongly dependent on the valence band offset. When the valence band offset is considered to be 40 meV, the peak carrier concentration rises to 1×10^{17} cm^{-3}.

We therefore conclude that our model outlines how the carrier distribution inside the quantum well changes with an imposed field and variations of temperature. These as well as the shift in the peak position with temperature obtained from our model support the nature of the experimental observation. But it should be noted that without precise knowledge of the valence band offset it is difficult to compute the exact value of the carrier peak concentration.

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