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"Theory of conduction subband dispersion in GaAs/AlGaAs quantum wells calculated using a virtual two-band model"

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These are preliminary lecture notes, intended only for distribution to participants.

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Theory of conduction subband dispersion in GaAs/AlGaAs quantum wells calculated using a virtual two-band model

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Motivations of this work

For the conduction band, eigenvalue problem needs to diagonalize the 14x14 Luttinger Hamiltonian?

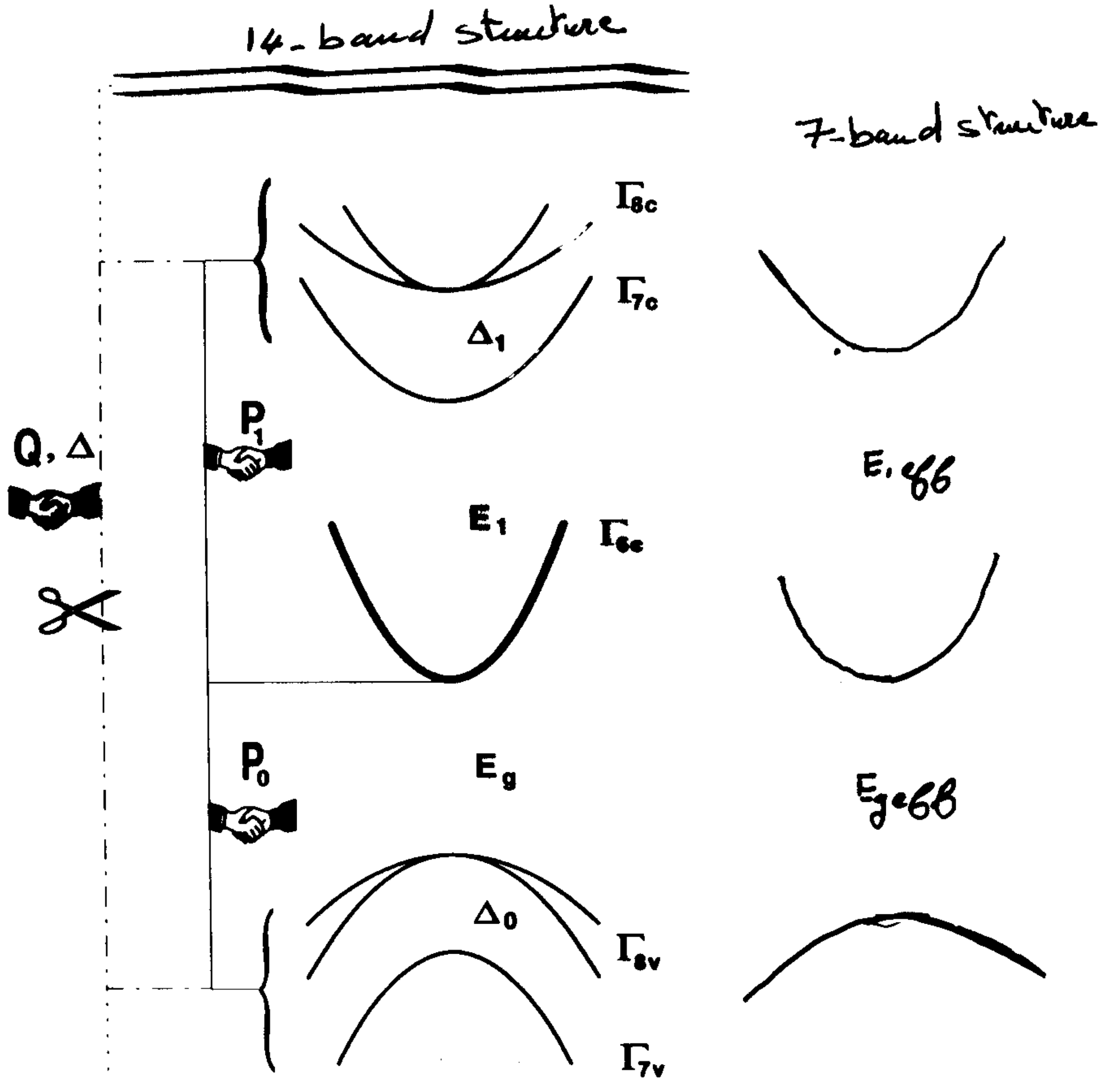
Or there is an alternative solution?

In the quantum well case, what is the influence of the boundary conditions at the interfaces barrier/well??

How Can we use the k.p theory in the quantum well case?

What can this work bring compared to the other works existing in the literature?

Band structure near the Γ centre of the Brillouin Zone

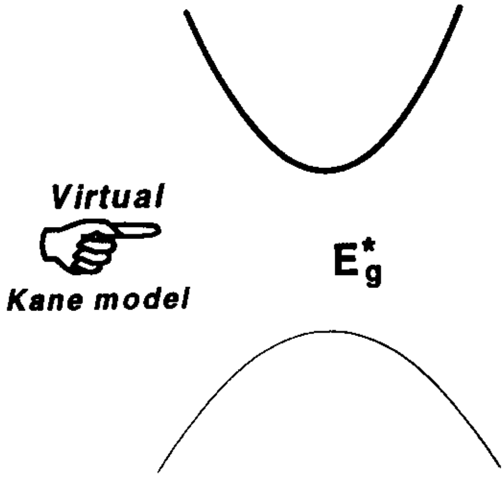


Dispersion in 7-band model with Q≠0

$$E-\left(1+\frac{E_{P_0}}{E_{geff}+E}-\frac{E_{P_1}}{E_{1eff}-E}+CC\right)\frac{\hbar^2k^2}{2m_0}-\frac{4E_QE}{\left(E_{geff}+E\right)\left(E_{1eff}-E\right)}\frac{\hbar^2}{2m_0}\left(\frac{k_x^{\,2}k_y^{\,2}+k_x^{\,2}k_z^{\,2}+k_y^{\,2}k_z^{\,2}}{k^2}\right)=0$$

$$E_{P_i(Q)}=\frac{2m_0}{\hbar^2}P_i^2(Q)$$

$CC \rightarrow$ remote bands contribution.



$$E\left(1+\frac{E}{E_g^*}\right)=\frac{\hbar^2k^2}{2m^*}$$

with

$$\frac{1}{E_g^*}=\frac{1}{E_{g,sph}^*}+\alpha_0\left(\frac{\sin^2(2\varphi)\sin^4(\theta)+\sin^2(2\theta)}{4}\right)$$

and

$$\frac{1}{E_{g,sph}^*}=\frac{m^*}{3m_0}\left(2\left(\frac{E_{P_0}}{E_g^{\,2}}+\frac{E_{P_1}}{(E_1+\Delta_1)^2}\right)+\left(\frac{E_{P_0}}{(E_g+\Delta_0)^2}+\frac{E_{P_1}}{E_1^{\,2}}\right)\right)$$

E^*_g depends on wave vector direction

m^* is the effective mass in the bottom of the conduction band

Dispersion in 7-band model with (Q=0)

$$E - \left(1 + \frac{E_{P_0}}{E_{geff} + E} - \frac{E_{P_1}}{E_{1eff} - E} + CC\right)\frac{\hbar^2 k^2}{2m_0} = 0$$

$$\Downarrow \qquad\qquad \Downarrow$$

V-B **U-C-B**

With

$$\frac{1}{E_{geff}} = \frac{1}{3}\left(\frac{2}{E_g} + \frac{1}{E_g + \Delta_0}\right)$$

and

$$\frac{1}{E_{1eff}} = \frac{1}{3}\left(\frac{2}{E_1} + \frac{1}{E_1 + \Delta_1}\right)$$

Virtual 2-band model

$$E\left(1+\frac{E}{E_g^*}\right)=\frac{\hbar^2k^2}{2m^*}$$

where

$$\frac{m_0}{m^*}=1+\frac{E_{P_0}}{E_{g,eff}}-\frac{E_{P_1}}{E_{1,eff}}+CC$$

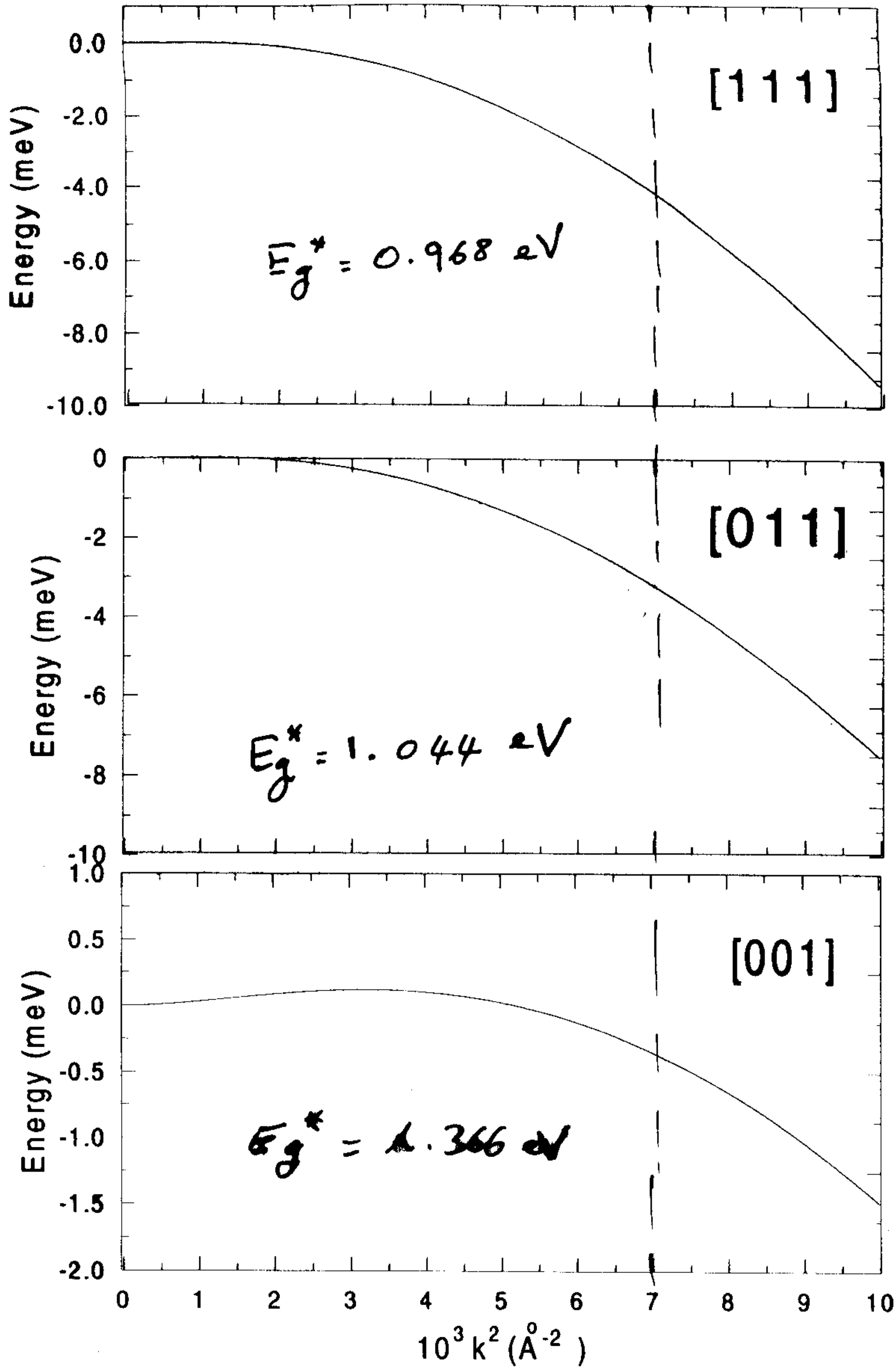
$$\frac{1}{E_g^*}=\frac{1}{E^*_{g_{sph}}}+\frac{1}{E_{an}}$$

with

$$\frac{1}{E^*_{g_{sph}}}=\frac{m^*}{m_0}\left(\frac{E_{P_0}}{E_{g,eff}{}^2}+\frac{E_{P_1}}{E_{1,eff}{}^2}\right)$$

and

$$\frac{1}{E_{an}}=\frac{m^*}{m_0}\frac{E_Q}{E_{g,eff}E_{1,eff}}\left(\sin^2(2\varphi)\sin^4(\theta)+\sin^2(2\theta)\right)$$


[111]
$E_g^* = 0.968$ eV
[011]
$E_g^* = 1.044$ eV
[001]
$E_g^* = 1.366$ eV
Energy (meV)
$10^3 k^2$ (Å^{-2})

Spherical approximation

$$\frac{1}{E_g^*} = \left\langle \frac{1}{E_g^*(\theta,\varphi)} \right\rangle$$

$$= \frac{1}{E_{g\,sph}^{*}} + \frac{11}{16}\,\frac{m^*}{m_0}\,\frac{E_a}{E_{g\,eff}\,E_{1\,eff}}$$

For GaAs $E_g^* \approx 1.1$ eV

Quantum well case

with $k_x = k_y = 0$

$$\frac{\hbar^2}{2m^*_{w(b)}} k_z^2 = \left(E - V_{w(b)}\right)\left[1 + \frac{E - V_{w(b)}}{E^*_{g\,w(b)}}\right]$$

$$\equiv$$

$$H_{w(b)} = \begin{bmatrix} V_{w(b)} & P_{w(b)} k_z \\ P_{w(b)} k_z & V_{w(b)} - E^*_{g\,w(b)} \end{bmatrix}$$

$$P^2_{w(b)} = \frac{\hbar^2 E^*_{g,w(b)}}{2 m^*_{w(b)}}$$

Tl

Boundary conditions

The boundary conditions requires the continuity of the envelope wave function $f(z)$ and the conservation of probability current at the interface

Before 1980:

$f(z)$ and $\frac{d}{dz}f(z)$ Continuous at the interface

Bastard 1981-82 :

$f(z)$ and $\frac{1}{m^*}\frac{d}{dz}f(z)$ Continuous at the interface

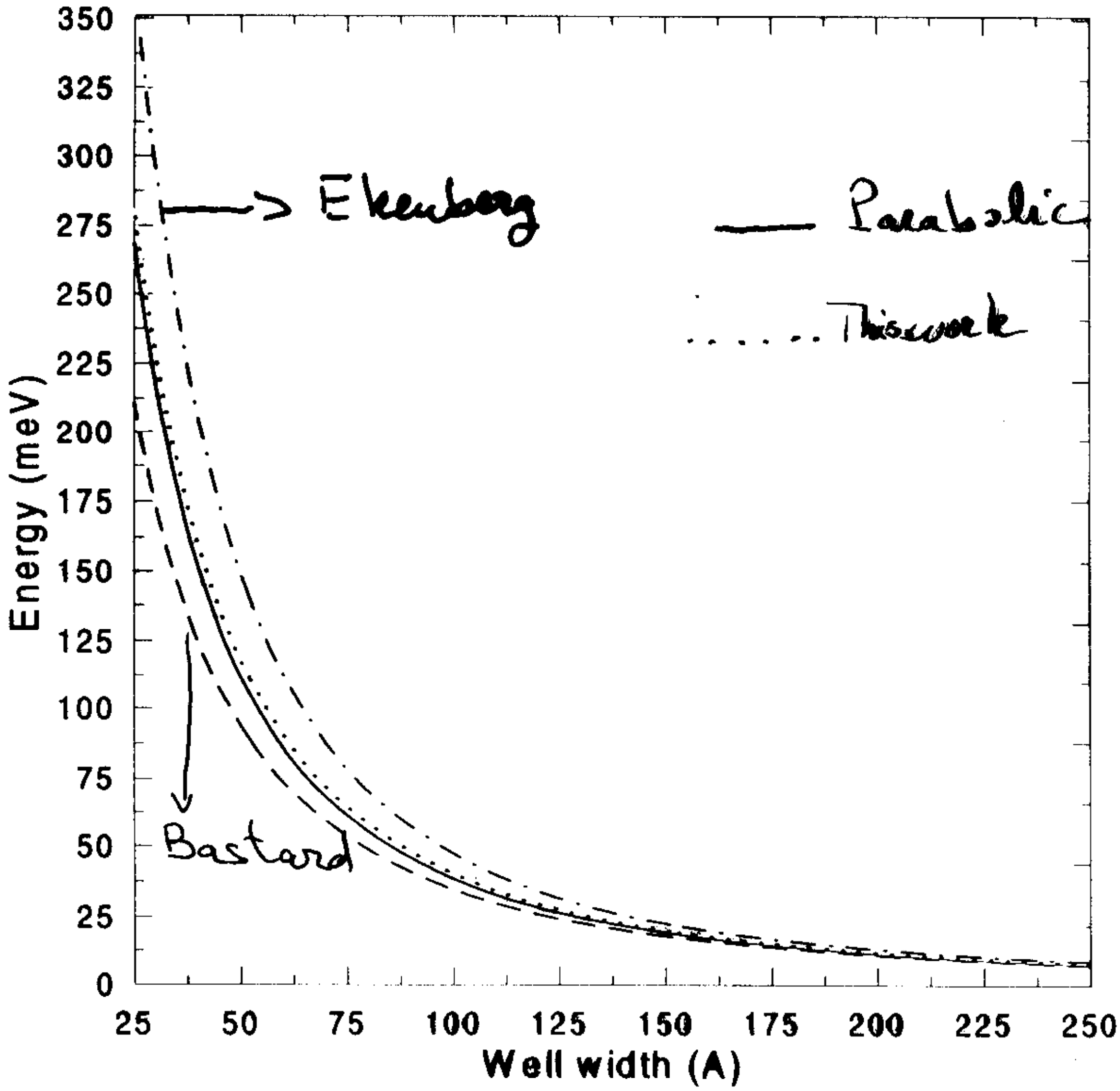
Ekenberg 1989 :

$$f(z) \text{ and } \frac{1}{m^*\left(1+2\frac{E-V}{E_g^*}\right)}\frac{d}{dz}f(z) \text{ continuous} \equiv Tan(bk_w) = \frac{\frac{\hbar^2 k_B}{2m_B^*} - 2\alpha_B k_B^3}{\frac{\hbar^2 k_w}{2m_w^*} + 2\alpha_w k_w^3}$$

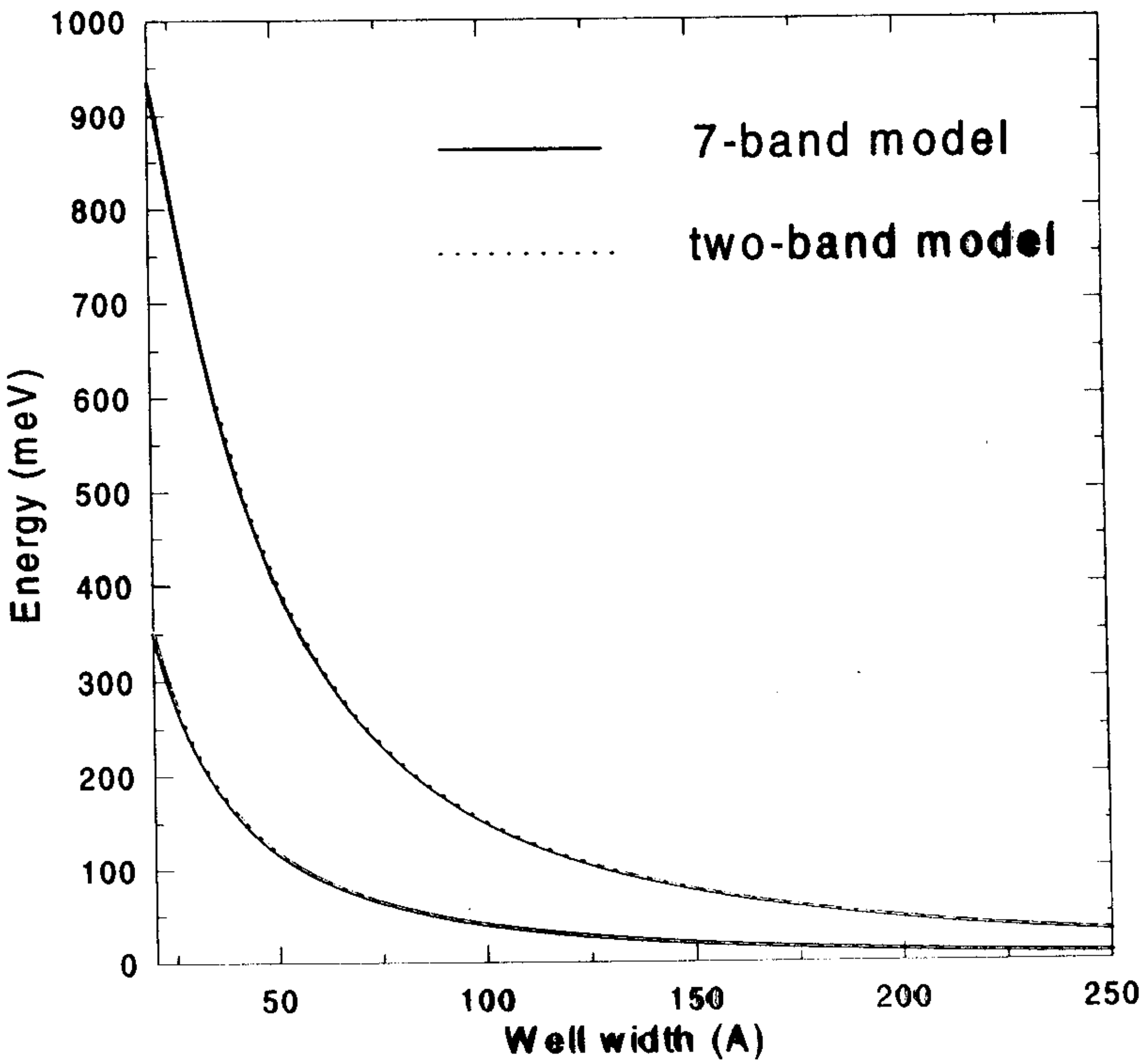
This work

$$f(z) \text{ and } \frac{1}{m^*\left(1+\frac{E-V}{E_g^*}\right)}\frac{d}{dz}f(z) \text{ continuous}$$

Ground subband energy us function of well width using different boundary conditions



First and second subband energy variation us function of well width



[redacted]

With the virtual two-band model the conduction band dispersion near the centre of the Brillouin zone takes the form,

$$\frac{\hbar^2}{2m^*_{w(b)}}k_z^2 = [E - V_{w(b)} - E^0_{//,w(b)}][1 + \frac{E + E^0_{//,w(b)} - V_{w(b)}}{E^*_{g,w(b)}}]$$

$$E^0_{//,w(b)} = -\frac{E^*_{g,w(b)}}{2} + \sqrt{\frac{E^{*2}_{g,w(b)}}{4} + \frac{E^*_{g,w(b)}\,\hbar^2 k^2_{//}}{2m^*_{w(b)}}}$$

$$\equiv$$

$$H_{w(b)} = \begin{pmatrix} V_{0,w(b)} & P_{w(b)}k_z \\ P_{w(b)}k_z & V_{0,w(b)} - E^*_g \end{pmatrix} + E^0_{//,w(b)}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$P^2_{w(b)} = \frac{\hbar^2 E^*_{g,w(b)}}{2m^*_{w(b)}}$$

In (k_x=0, k_y=0) basis

$$H = \begin{pmatrix} E_0 & 0 \\ 0 & -E_0 - E_g^* \end{pmatrix} + \begin{pmatrix} H_{11} & H_{12} \\ H_{12} & H_{22} \end{pmatrix}$$

$$H_{11} = -H_{22} = \Pr_w(1+\lambda_w)E^0_{//,w} + \Pr_b(1+\lambda_b)E^0_{//,b}$$

$$H_{12} = \left[\frac{(V_0 - E_0)}{P_b k_b^2}\frac{\cos^2(k_w b)}{N_1^2}\right]E^0_{//,b}$$

H_{12} does not depend on dispersion in the well

$H_{12} \ll H_{11}$

$$\Rightarrow \quad E(k_{//}) = H_{11} = \Pr_w(1+\lambda_w)E^0_{//w} + \Pr_b(1+\lambda_b)E^0_{//}b$$

$$\begin{cases} P_{rw} = \dfrac{b}{N_1^2}\left[\dfrac{2E_0 + E_{gw}^*}{E_0 + E_{gw}^*} + \dfrac{\sin(2k_w b)}{2k_w b} \, \dfrac{E_{g,w}^*}{E_0 + E_{g,w}^*} \right. \\[2ex] P_{rb} = 1 - P_{rw} \end{cases}$$

$$\begin{cases} 1 + \lambda w = 1 + \dfrac{2E_0}{E_0 + E_{gw}^*} \, \dfrac{\sin(k_w b) - k_w b}{\left(\sin(k_w b) + k_w b\right) - \left(\sin(k_w b) - k_w b\right)\dfrac{E_0}{E_0 + E_{gw}^*}} \\[3ex] 1 + \lambda b = 1 - \dfrac{2 E_0^2 \, tg^2\left(k_w b/2\right)}{E_0\left(E_0 + E_{gw}^*\right) + E_0^2 \, tg\left(\dfrac{k_w b}{2}\right)} \end{cases}$$

Perpendicular effective mass ($k_{//}=0$)

$$\frac{1}{m^*_\perp} = \frac{\Pr_w}{m^*_{\perp,w}} + \frac{\Pr_b}{m^*_{\perp,b}}$$

with

$$m^*_{0\perp,w(b)} = \frac{m^*_{w(b)}}{1+\lambda_{w(b)}}$$

quantum well virtual gap

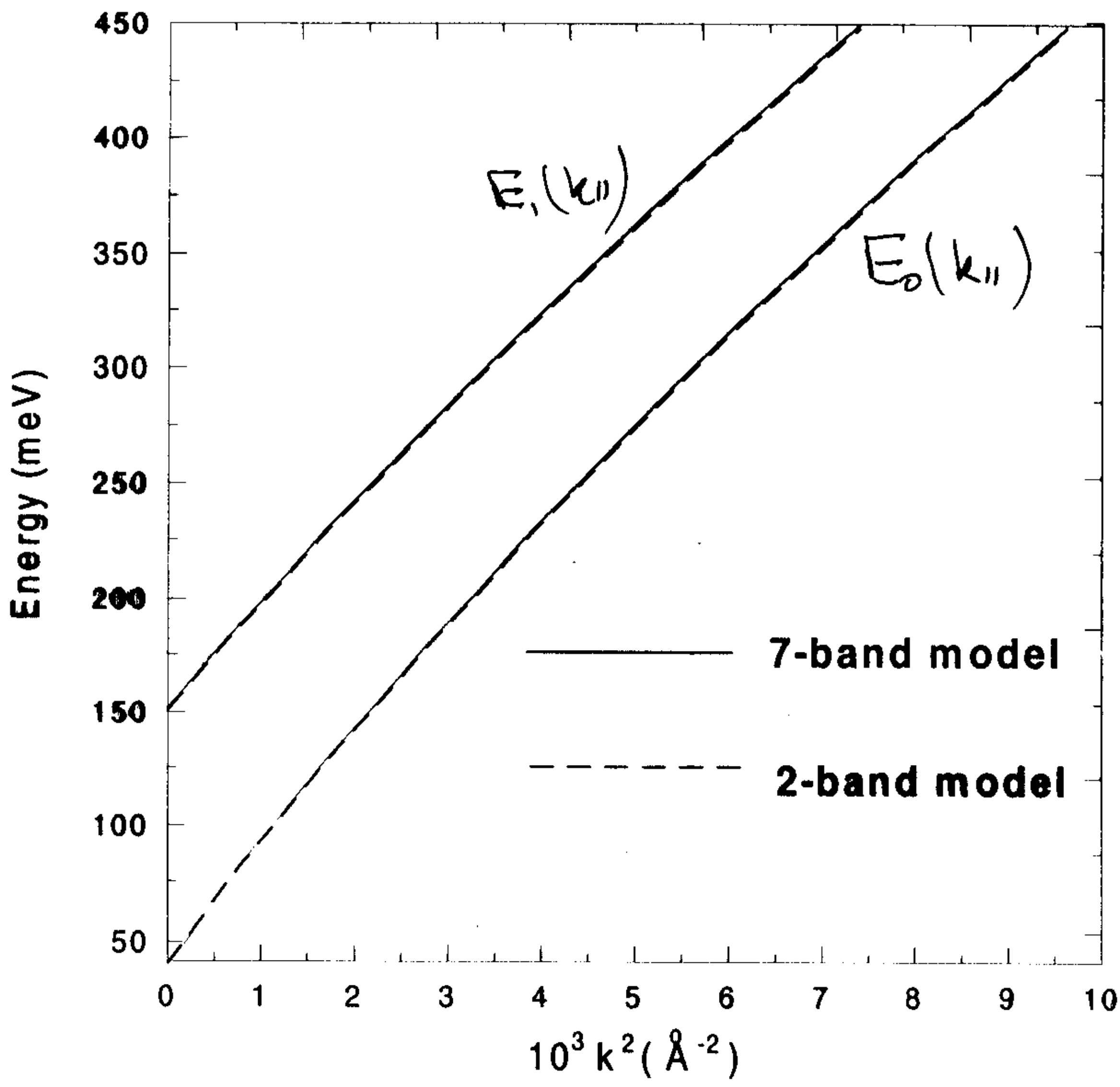
$$E^*_{g\perp} = \Pr_w\, E^*_{g\perp,w} + \Pr_b\, E^*_{g\perp,b}$$

With: $E^*_{g\perp,w(b)} = E^*_{g,w(b)}\left(1+\lambda_{w(b)}\right)$

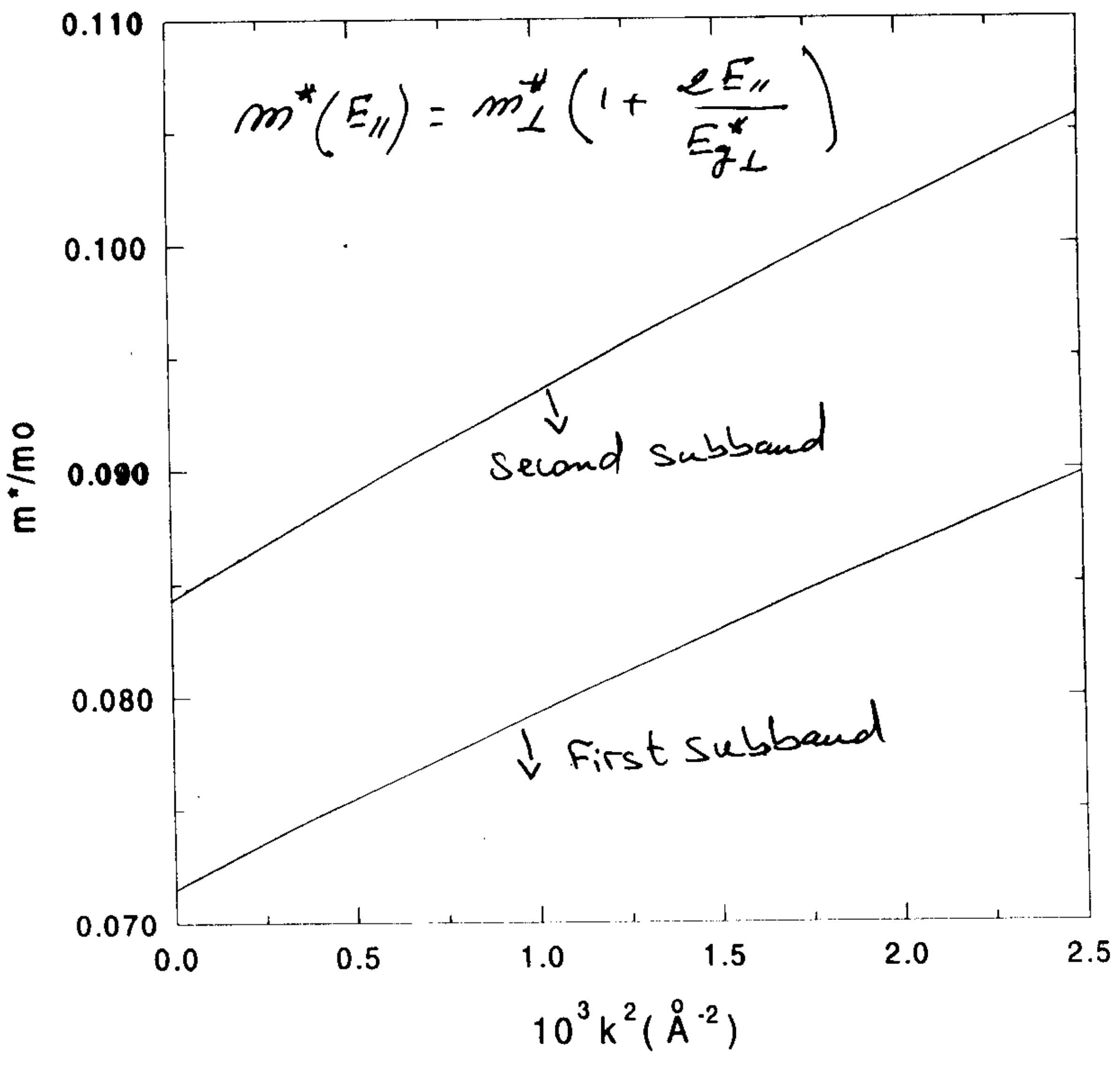
Dispersion is now described by:

$$E_{//}(k_{//})\left(1+\frac{E_{//}(k_{//})}{E^*_{g\perp}}\right) = \frac{\hbar^2 k_{//}^2}{2m^*_\perp}$$

First and second subband energy dispersion
in 100Å GaAs /Al Ga As quantum well



Parallel effective mass for the two first subbands in 100A GaAs/AlGaAs quantum wells using a virtual 2-band model



Density of states

$$\rho(E) = \frac{m^*_{//}(E)}{\pi \hbar^2}$$

Carrier density

$$N_S = \int_{-\infty}^{+\infty} \frac{\rho(E)}{1 + \exp\left(\frac{E - E_F}{KT}\right)} dE$$

$$\Downarrow$$

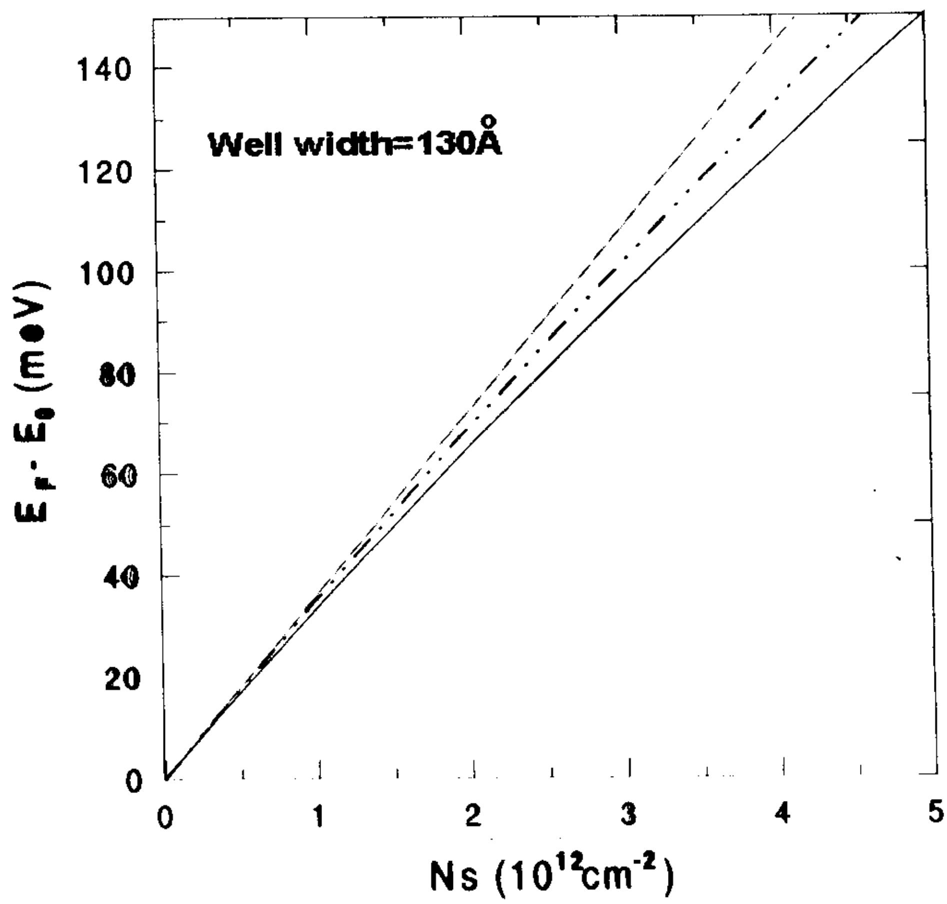
$$Ns = \frac{m^*_{0,\perp}}{\pi.\hbar^2} KT.Log\left(1 + \exp\left(\frac{E'_F}{KT}\right)\right) + 2\frac{m^*_{0\perp}}{\pi.\hbar^2 E^*_{g,\perp}} \int_0^{+\infty} \frac{EdE}{1 + \exp\left(\frac{E - E'_F}{KT}\right)}$$

with $E'_F = E_F - E_0$

Low temperatures or degenerate 2D electron gas case:

$$\frac{\hbar^2 k_F^2}{m^*_{0\perp}} = E'_F\left(1+\frac{E'_F}{E^*_{g,\perp}}\right)+\frac{\pi^2}{3}\frac{(KT)^2}{E^*_{g,\perp}}$$

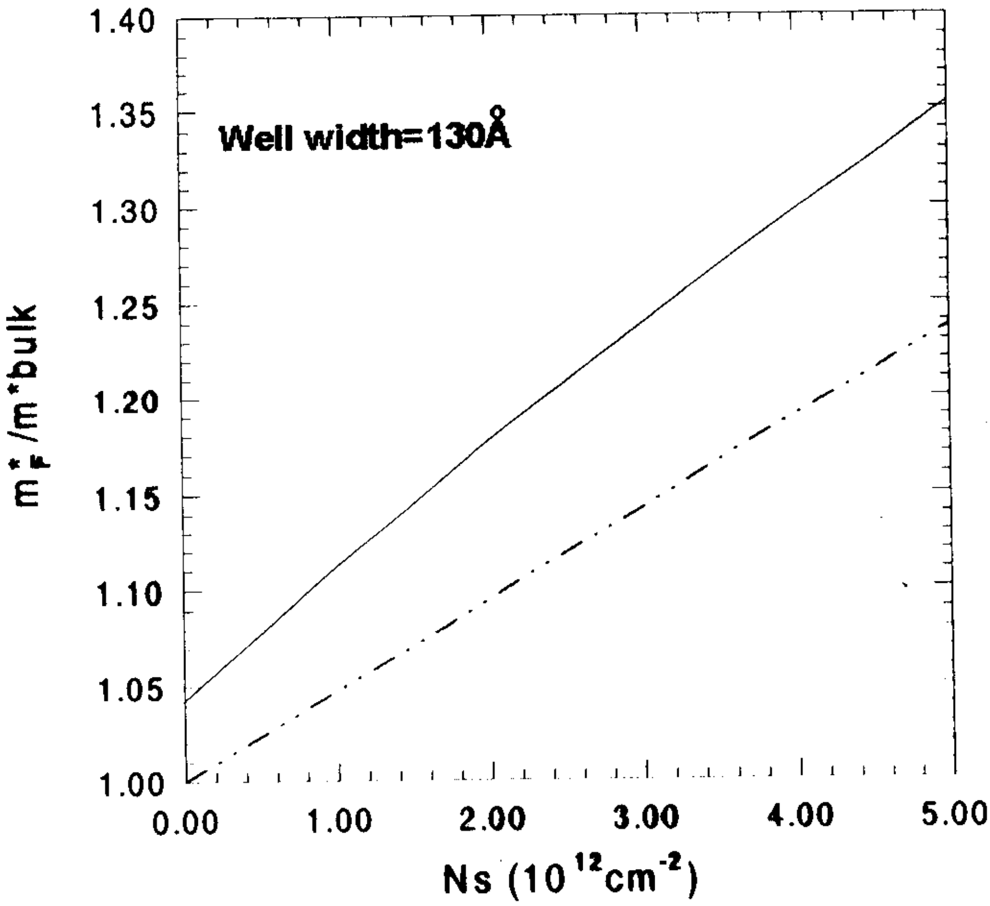
with $k_F = \sqrt{2\pi N_S}$ *and* $E'_F = E_F - E_0$



variation of the Fermi level position from the first electronic subband as fuction of first subband carrier density using modified Kane model (lower solid line); Kane model with experimental Eg and m* (dashed line) and the parabolic approximation (upper solid line)

Fermi level effective mass

$$m_F^*(E_F) = m_{0\perp}^*\left(1 + 2\frac{E_F - E_0}{E_{g,\perp}^*}\right)$$



variation of the Fermi level effective mass with first suband carrier density using modifief Kane model (solid line) and Kane model with experimental values of Eg and m* (dashed line)

Conclusion

The non-parabolicity effect depends on wave vector direction and the conduction ban dispersion can be represented by a virtual two-band model with an anisotropic band gap. Analytical expressions for the band-edge effective mass and the effective band gap are presented.

For a quantum well, we show that the virtual two-band model is still applicable, but requires the use of a modified effective band gap and effective mass and the model takes into account the wave function penetration in the barrier. The modification of the boundary conditions due to the non-parabolicity is analyzed.

This model is a convenient and simple approach to determine the confinement energies and the effective masses for motion parallel to the interface.

By considering this model, analytical expressions for the density of states, the electron effective mass relative to the first subband are given