Chapter 5 Multi Valley Effective Mass Approximation

Chapter 5 .1 Motivation

There are several disadvantages to the tight binding simulation. Self-consistent tight binding simulation run times are at least 20 times longer than simple effective mass based simulations because there must be a node at each atomic site in the crystal each with five bands in the sp^3s^* hybridization. This restricts the size of devices that can be modeled. It would be advantageous to develop coupling parameters for use with the effective mass approximation to duplicate band mixing results observed in tight binding simulations discussed in the previous chapter, both for carrier concentration and current.

A parametric study has been done to determine Γ-X valley mixing parameters which produce simulations similar to those obtained with tight binding. In simulations internal concentrations and potentials may be compared. If comparisons are made only to laboratory measurements only terminal current and potential may be used. Internal comparisons constrain the chosen coupling parameters beyond work done previously [52].

Chapter 5 .2 Multi-valley

The effective mass simulations will be modeled by a method similar to that presented by Sun[52] who claimed the first self-consistent Schrödinger Poisson device simulations with Γ-X mixing. In this process coupling between Γ, X and L valleys may be done using a constant coupling factor applied at or around the interface and band offset values. This is done in an *ad hoc* fashion. Here we will

show similar simulations compared to tight binding approximations. The envelope equation containing the coupling parameters between Γ and X is given by

$$\begin{bmatrix} -\frac{\hbar^2}{2}\frac{\partial}{\partial x}\frac{1}{m_\Gamma}\frac{\partial}{\partial x} & 0 \\ 0 & -\frac{\hbar^2}{2}\frac{\partial}{\partial x}\frac{1}{m_X}\frac{\partial}{\partial x} \end{bmatrix} \cdot \begin{bmatrix} \psi_\Gamma \\ \psi_X \end{bmatrix} + \begin{bmatrix} V_\Gamma - E + \frac{\hbar^2 k||^2}{2m_\Gamma} & 0 \\ 0 & V_X - E + \frac{\hbar^2 k||^2}{2m_X} \end{bmatrix} \cdot \begin{bmatrix} \psi_\Gamma \\ \psi_X \end{bmatrix} + \begin{bmatrix} 0 & S_{\Gamma,X} f(x) \\ S_{X,\Gamma} f(x) & 0 \end{bmatrix} \cdot \begin{bmatrix} \psi_\Gamma \\ \psi_X \end{bmatrix} = 0$$

,

(Chapter 5 .1)

where m_v is the effective masses, ψ_v is the wave equation solution, $S_{v,v'}$ is the coupling parameter which is assumed to be reciprocal, and V_v is the potential function with band offset for valley v = Γ or X. These coupling parameters may be accurately approximated by constants because offsets are taken into account in the potential functions, and the Fermi Dirac distribution functions reduce any effects that might be observed at high energy. For many problems a constant coupling coefficient might be thought to be a good first order approximation. For comparison single barrier devices in the GaAs/AlAs materials system with AlAs barriers of different widths are used.

Parameters are determined in two steps. In step one the coupling parameters are selected to provide simulation of the carrier concentration in the

barrier region. The coupling coefficients are then varied until the self-consistent potential matches that determined by tight binding. At this point the concentration profiles should be similar. In the second step the coupling parameters may be determined to accurately simulate current through the device. This is convoluted because the current is dependent on the potential profile as well as the transmission spectrum. A quicker and clearer approach is to match the transmission spectrum for the same potential profile. Hopefully the coupling parameters determined in these two steps are compatible.

The coupling parameters will be chosen to match carrier concentration and potential profiles on simple structures. Then those parameters will be applied to more complex structures containing a superposition of the simple structures, as a test. The basic structure is a single barrier diode of varying AlAs barrier widths. In addition to the parameters describing function f(x) in (Chapter 5 **.1)** the effective mass in the AlAs barrier must be chosen. For very thin barriers the effective mass of the surrounding GaAs layers is used.

Simulations for varying coupling parameters are shown for a single 100 Å barrier diode in Figure Chapter 5 .1 and Figure Chapter 5 .2. The concentration and potential profiles are very similar for a coupling parameter of $S_{\Gamma,X} = 0.42$. This is a very high value compared to the value of 0.15 from the literature [52].

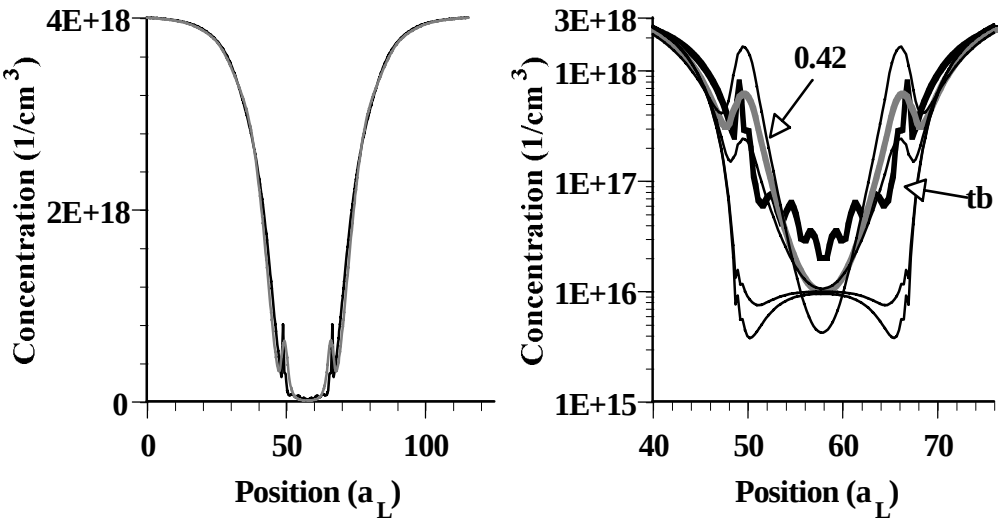

Figure Chapter 5 .1: This is a concentration profile comparison between tight binding and coupled effective mass simulations. On the left the tight binding and coupled effective mass simulation with $S_{\Gamma,X}$ = 0.42 are shown. On the right a logarithmic blow up of the concentration in the barrier region calculated by these two methods is shown. Coupled effective mass approximation based concentrations with $S_{\Gamma,X}$ ranging from 0.1 to 0.5 are compared to concentration calculations using the tight binding approximation.

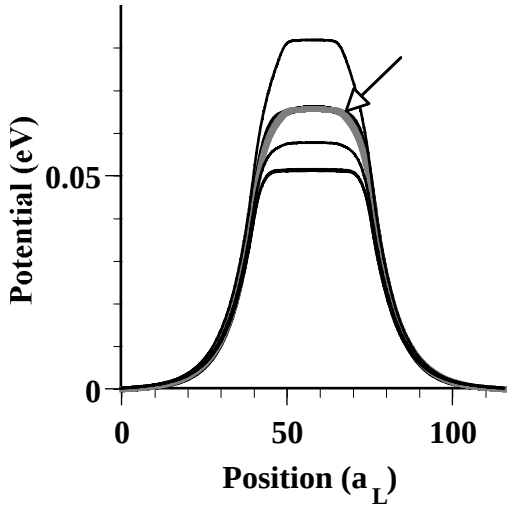

Figure Chapter 5 .2: This is the potential profile of the coupled and tight binding simulations. The arrow shows the two best matches where the dark curve is the

tight binding simulation and the light curve is the coupled effective mass simulation with $S_{\Gamma,X} = 0.42$.

For a thin AlAs barrier using a coupling parameter $S_{\Gamma,X} = 0.35$ the potential profile matches. The resulting concentration comparison is shown in Figure Chapter 5 .3. These parameters are then used in a DBRTD containing these AlAs barriers. For the case where the effective mass in the thin barrier AlAs is assumed to be the same as in the GaAs and $S_{\Gamma,X} = 0.30$, the resulting profiles are very similar. Note in Figure Chapter 5 .4 the concentration from this coupling method is inappropriately low in the heterostructure. The carrier concentration in the quantum well resonance is compromised by the coupling technique. The potential profile is between the single valley effective mass simulation and the tight binding value, as shown in Figure Chapter 5 .5.

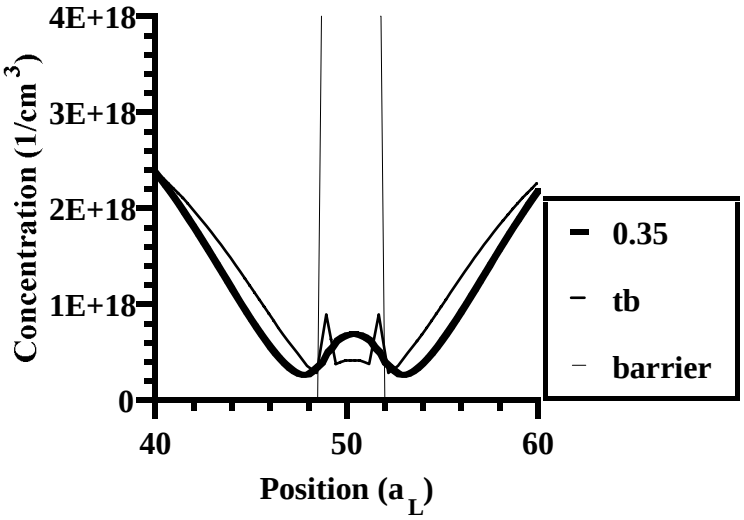

Figure Chapter 5 .3: This is a comparison between the tight binding and coupled effective mass simulations for an AlAs barrier of 17Å.

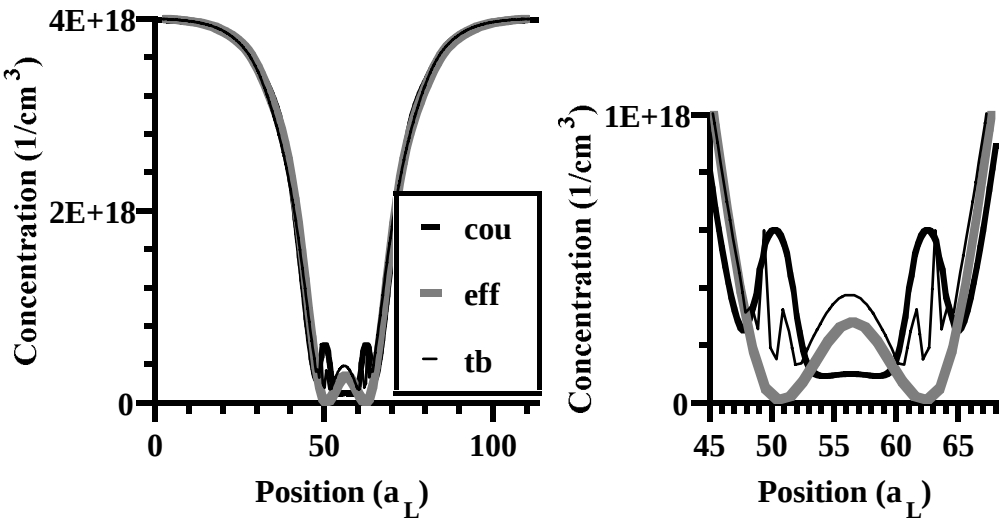

Figure Chapter 5 .4: Using the coupling parameter $S_{\Gamma,X}$ = 0.35 the concentration in the barrier region is a fairly good match. In the heterostructure itself the concentration is flat.

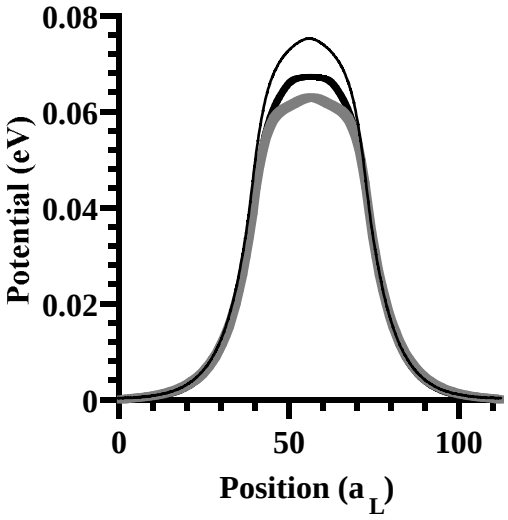

Figure Chapter 5 .5: The potential profile using coupling is between the single valley effective mass and tight binding curves.

The second step is to match the transmission spectra. For clarity this is done on a 100Å single barrier structure. The coupling coefficient $S_{\Gamma,X}$ is varied

from 0.1 to 0.25 and the function governing its application is also varied. Transmission spectra from these simulations are compared to the transmission spectrum from a tight binding simulation for the same structure. The resulting spectra are shown in Figure Chapter 5 .6. The transmission spectra from simulations using the coupled effective mass approximation show much higher values than the single valley, uncoupled case, and much lower values than the tight binding simulations except above the approximate energy level of the Γ-X mixing. There should be significant differences in the simulated current but the coupled effective mass approximation current should be closer than a single valley assumption. Further, the $S_{\Gamma,X}$.value of 0.15 and the function with which it is applied in the literature [52] matches the transmission spectrum as well as any other value although it does not match the potential profile.

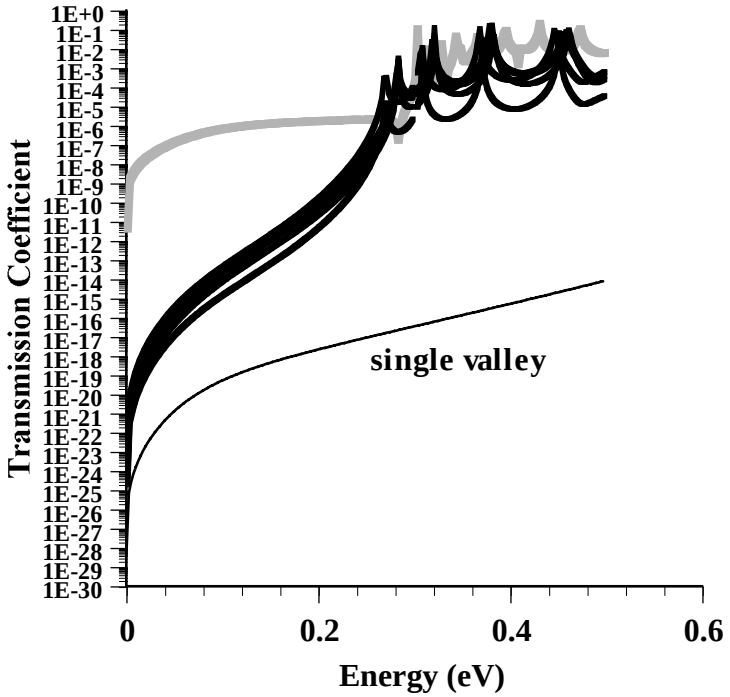

Figure Chapter 5 .6: This is a comparison between transmission spectrum from the tight binding and coupled valley effective mass approximations. The light curve is from the tight binding simulation and the dark curves are coupled effective mass simulations. Note compared to the single valley effective mass spectrum these coupled effective mass simulations show transmission peaks related to Γ-X mixing. The low energy transmission spectrum is much lower despite the coupling parameters ranging from $S_{\Gamma,X}$ = 0.1 to 0.25 tried. Note in addition that the transmission peaks are at a lower energy for the coupled effective mass case.

Chapter 5 .3 Summary

Concentration and potential profile comparisons show that coupled effective mass approximations cannot be generally fit to the values found in the tight binding approximations using the methods examined. This is a significant problem even with the very thin AlAs barriers in the devices shown. These effects should be considered in general heterostructure tunneling problems.

The transmission spectrum found using the single valley effective mass approximation is much lower than one based on the tight binding method for the thick AlAs barrier shown. The transmission spectrum based on a coupled effective mass based approximation is closer to the tight binding transmission spectrum below the X valley resonances. Above the first resonant peak the two spectra are similar. Based on the simulations shown these results are not very sensitive to the coupling parameter. Since current is most sensitive to transmission coefficients at resonance in cases with small space charge in the X valley these methods may give good results.