Finite difference k.p modeling of type II MQWs

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***Abstract*—In this talk, we will show some of the limitations of the finite difference technique when applied to k.p modeling of type II MQW structures. Improvements to the commercial APSYS software were made to overcome these limitations and provide sturdy rejection of spurious QW solutions. Dispersion relations and dipole moments for a sample GaAsSb/InGaAs structure will also be discussed.**

I. Introduction

The use of artificial periodicity to affect material properties has long been known and has many applications in semiconductor technology such as Bragg mirrors and photonic crystals. Likewise, multi-quantum well superlattices (SL) offer many opportunities for bandgap engineering by offering control over the position of the confined energy levels. In particular, superlattices with type II band alignment may be used to create materials with very small transition bandgaps and have therefore attracted a great deal of interest for use in mid and long-wavelength infrared detectors[1].

One particular material system which has been considered for this application is InAs/GaSb due its "broken-gap" (type IIb) configuration. However, it is known that material interfaces without a shared common atom may create an overall superlattice structure without the full zincblende symmetry[2]. The inclusion of this crucial interface effect requires the use of full-band $k \cdot p$ models (at least 6x6 or 8x8).

Previous work on the subject has relied on detailed tight-binding methods and Fourier expansion analysis or used an extension of Pikus-Bir $k \cdot p$ Hamiltonian with a plane wave expansion and periodic boundary conditions[2]. Such a periodicity assumption matches the composition but it does have its limitations: for example, if a superlattice is used in a real device, it may be subject to an applied field and the confining potential's periodicity will be affected. It is for this reason that we have chosen to use a finite difference method to approach the problem.

In this talk, we report on improvements made to the $k \cdot p$ solver in the commercial APSYS software developed here at Crosslight. We show that in type II structures, the spurious solutions induced by the finite difference model presents a far more serious challenge than for type I quantum wells (QW) but that these may be overcome by new eigenvalue picking algorithms. For the purposes of this talk, we limit ourselves to a simple $Ga_{0.51}As_{0.49}Sb$/InGaAs W-type MQW region[3] lattice-matched to InP. This will serve a first step towards a full model of a InAs/GaSb SL with non-common atom interface effects (IF).

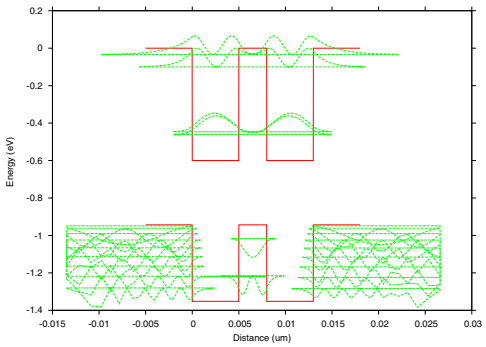

Fig. 1. Type II band profile and 1-band wavefunctions.

II. Implementation

We solve the Pikus-Bir Hamiltonian following the work of S.L. Chuang[4] and others with a potential discretized over a 1D finite difference mesh. The $k \cdot p$ solution is obtained using a sparse matrix restarted Arnoldi method[5]; an initial 1-band solution based on an iterative eigensolver is used to provide an estimate of the number of roots. We have chosen in this talk to work with an 8x8 solver and neglect the block-diagonalization simplifications of Chuang since these are not compatible with the IF correction terms.

Unlike periodic boundary conditions which assume that the wave extends unchanged to $\pm\infty$, the finite difference method enforces that the wave decays to zero at some finite point outside the confinement region; that is, the QW region being studied is always encased in a larger infinite potential well. When the finite difference method is used for SLs, the periodic solutions being sought may be approximated by solving for a sufficiently large subset of the SL.

For type I QWs, the infinite well approximation is often reasonable provided the boundary is sufficiently far away from the region of interest: there is little perturbation of the confined levels and any spurious levels from the larger infinite well are located above the barriers so they may be easily dismissed. For type II structures however, the electron barrier is the hole well (and vice versa) so that it is unavoidable that the infinite potential wall will serve to confine levels using the same well bottom as the QW region of interest. Therefore, the spurious solutions will have energies comparable to those of the "good" solutions we seek as can be seen in Fig.1.

While it is rather straightforward to eliminate these spurious solutions from the 1-band model, it is considerably less so for

the full $k \cdot p$ model. First, many of the spurious solutions have a lower energy than the first "good" confined level: the more we seek to distance the infinite potential wall from the QW region, the less confined the spurious solutions in the outer barriers become. A simple sort on the eigenvalue is therefore insufficient.

Second, automated rejection algorithms based on the position of the peaks or any other ab-initio aspect of the wavefunction's shape cannot reliably handle the distortions that occur when computing the dispersion relation at $k_t > 0$: with more kinetic energy, carriers have a higher probability of being outside their confinement region and even a "good" level may become rejected unjustly.

But the most important insight that must be gleaned from the existence of these spurious solutions is simply this: even though those states have no physical meaning, they are still valid numerical solutions to the sparse matrix eigensolver and must be included in the initial estimate of the number of roots. If they are rejected out of hand in the initial iterative search, then the full solver may miss the correct eigenvalues and a full k.p solution becomes impossible.

III. New algorithm and results

We have therefore implemented the following algorithm to pick the correct wavefunctions in the full $k \cdot p$ solver. First, the iterative eigensolver picks all the solutions in the expected confined energy range for $k_t = 0$ to get the number of search roots (n_1). A rejection algorithm based on the position of the wavefunction peak is then used to automatically select a few "good" roots amongst them ($n_2 < n_1$). In the example of Fig.1, we pick only and the HH1 and HH2 levels and a LH1 level which is not shown in the figure.

We then calculate the overlap

$$|< \Psi_1 | \Psi_2 >|^2$$

for every Ψ_1 wavefunction obtained from the sparse eigensolver and every Ψ_2 initialized from the 1-band solver. In this way, we pick not the eigenvalue with the lowest energy but the one which best matches the expected shape. For example, if the 1-band model predicts the existence of an HH1 state, then we pick the eigenvalue which has the highest overlap along the $\left|\frac{3}{2}, \pm\frac{3}{2}\right>$ bases.

For larger k_t values, the solution from the previous step is used to initialize Ψ_2 but the procedure is otherwise the same. In this way, the deformation of the wavefunction and increased band coupling is taken into account and we are assured to always pick the eigenstate which most closely resembles a previously known "good" solution.

Sample results of the algorithm are shown in Figures 2-3. Features of interest include the negative curvature of one of the conduction bands due to the strong coupling between the conduction and valence bands: even at $k_t = 0$, the $|< \Psi | iS >|^2$ overlap is approximately 50%. We also note the low dipole moment due to the physical separation between the electron and hole states.

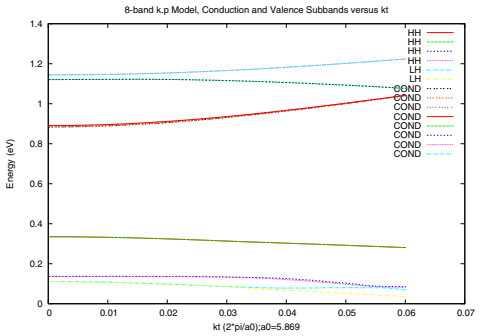

Fig. 2. 8x8 k.p dispersion plot.

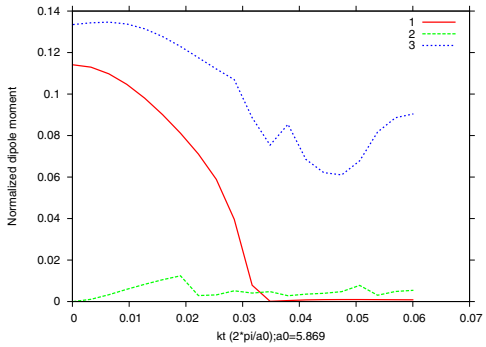

Fig. 3. Transistion dipole moments normalized to bulk dipole moment.

IV. Conclusion

In this talk, we have shown some of the limitations of the finite difference technique when applied to $k \cdot p$ modeling of type II MQW structures. Improvements to the commercial APSYS software were made to overcome these limitations and provide sturdy rejection of spurious QW solutions. Further research on the topic will focus on extending the model to include the effects of non-common atom interfaces in structures such as InAs/GaSb superlattices.

References

[1] N. Gautam *et al.*, "Performance improvement of longwave infrared photodetector based on type-ii inas/gasb superlattices using unipolar current blocking layers," *Appl. Phys. Lett.*, vol. 96, p. 231107, 2010.

[2] F. Szmulowicz *et al.*, "Effect of interfaces and the spin-orbit band on the band gaps of inas/gasb superlattices beyond the standard envelope-function approximation," *Phys. Rev. B*, vol. 69, p. 155321, 2004.

[3] R. Sidhu *et al.*, "A 2.3um cutoff wavelength photodiode on inp using lattice-matched gainas-gaassb type-ii quantum wells," in *2005 International Conference an Indium Phosphide and Related Materials*, 2005, p. 148.

[4] S. Chuang, "Efficient band-structure calculation of strained quantum-wells," *Phys. Rev. B*, vol. 43, no. 12, pp. 9649–9661, 1991.

[5] P. Mensz and Z. Li, "Comparison of k.p models for quantum well optoelectronic devices," in *Proceedings of the 5th International Conference on Numerical Simulation of Optoelectronic Devices. NUSOD '05*, 2005, pp. 75–76.