

MATERIAL SELECTION FOR THREE LEVEL TRANSITION USING QUANTUM WELL STRUCTURE

K. Ghosh, S.P. Bremner, C.B. Honsberg
Department of Electrical and Computer engineering
University Of Delaware
Newark, DE 19711

ABSTRACT

Nanostructured devices (Quantum dot and Quantum well) have been proposed as a way to overcome the Shockley-Quiesser limit of a single junction solar cell as they have the potential to show three quasi Fermi levels. In this paper the material combinations that can be used in a Quantum Well solar cell to realize a multiple quasi-Fermi level device will be discussed. The calculations were done on different possible combinations of direct band gap III-V semiconductors, with the effect of strain being taken into account by applying 6 band K.p model. A detailed balance calculation was done on the materials selected to determine their maximum efficiency under 1 sun AM0. The material combination of $\text{Al}_{0.63}\text{In}_{0.37}\text{As}$ as the barrier and $\text{InAs}_{0.16}\text{P}_{0.84}$ as the well with InP as the substrate is found to be the best material combination giving a theoretical efficiency of 43% under 1 sun AM0, compared to the maximum three-level efficiency of 47% under the same conditions.

INTRODUCTION

The three level transition in nanostructured devices has been proposed as a means to overcome the efficiency limit of Shockley and Quiesser [i] in a solar cell [ii]. A three level transition system is one which shows three sets of complementary radiative absorption-emission processes (two interband and one intraband) due to the simultaneous spatial existence of three quasi Fermi levels. Both quantum dot (QD) solar cells, particularly the intermediate band solar cell, and quantum well (QW) based devices are candidate structures that can be used to realize the above mentioned effect [iii,iv]. Much of the previous work in this field has concentrated on QDs [v,vi]. Preference has been given to QDs over QWs [vii] because of the discrete energy level in QDs compared to continuous energy level in QWs resulting in an increased loss of carriers by phonon scattering, thereby decreasing the probability of having a radiative intraband transition. However, quantum well infrared photodetector [viii] shows that the intraband transition from well to the continuum of states in the conduction band is possible for QWs with high escape rate from the well under reverse bias. Moreover, the collection

efficiency in QW solar cells can be high in forward bias if the electrical field is maintained above a critical value [ix]. Provided that carriers can be collected as indicated by such experimental results, QW devices have the advantage of increased absorption volume and more straight forward fabrication. Consequently, the optimum material systems for QW three level solar cells are important in analyzing advanced concept solar cells. In this paper, the optimum material combination with negligible valence band offset that can be used to realize three level transition system for QW solar cells are calculated, taking strain into account while calculating the band structure. A schematic diagram of a three level transition system after ref [iii] is shown in Fig 1.

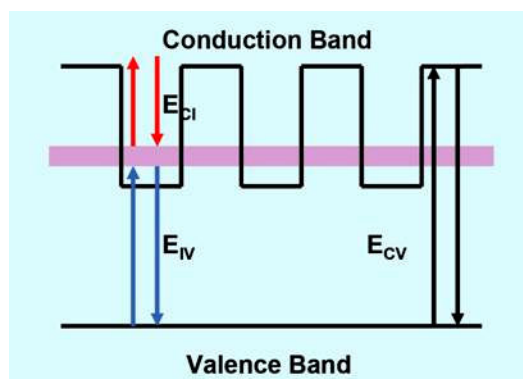


Figure 1: A schematic diagram of a three level Transition system.

MATERIAL SELECTION CRITERIA

A critical factor in growing multiple layer QW structure is that the layers should be lattice matched to each other and also to the substrate. Further, the conduction band offset and valence band offset are also important parameters to be considered for the above mentioned device. The criteria for ideal QW solar cell materials are:

- i) The lattice mismatch between the barrier material and any one of the common substrates (GaAs, InP, GaSb, InAs) to be within $\pm 2\%$
- ii) The lattice mismatch between the well and the barrier or the common substrates to be within $\pm 2\%$.

- iii) The conduction band confinement in the well to be as close to 0.9 eV, the CBO value giving the maximum efficiency under 1 sun AM0 [x].
- iv) The confinement in the valence band of the well to be negligible (to be less than 3KT/2).

CALCULATIONS

For an alloy most of the parameters is given by the relationship

$$P(A_{1-x}B_x) = (1-x).P(A) + x.P(B) - C(A-B).x.(1-x) \quad (1)$$

where, $P(A_{1-x}B_x)$ denotes the parameter for the alloy of A and B with the fractional composition of A being (1-x) and that of B being x

$P(A)$ and $P(B)$ are the parameters for the individual compounds, A and B

$C(A-B)$ is the bowing parameter for the alloy of A and B. The individual values of these parameters for III-V materials (9 diads and 18 triads) were obtained from Vurgaftaman *et. al.* [xi].

For the band structure calculations strain was taken into account and k.p method of band structure calculation. To determine the effect of strain on the band structure neglecting the spin orbit interaction, the relationship given below is used:

a) Conduction band

For the conduction band the band edge as per ref [xii] shifts according to the relationship:

$$\Delta E_c = a_c (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) \quad (2)$$

where, ΔE_c is the shift in the conduction band edge
 a_c is the deformation potential.

ϵ_{xx} , ϵ_{yy} , ϵ_{zz} are the strains as according to [xii] given by

$$\epsilon_{xx} = \epsilon_{yy} = (a_{\text{subs}} - a) / (a_{\text{subs}}) \quad (3)$$

$$\epsilon_{zz} = -(C_{12}/C_{11}) \epsilon_{xx} \quad (4)$$

where, a_{subs} , is the lattice parameter of the substrate
 a , is the lattice parameter of the epilayer perpendicular to the growth direction
 C_{12} , C_{11} are the elastic constants

b) Valence Band

Neglecting the spin orbit interaction the shift in the heavy hole and the light hole for the valence band as given by ref [xiii] is as follows:

$$E_{\text{HH}} = -P\epsilon - Q\epsilon \quad (5)$$

$$E_{\text{LH}} = -P\epsilon + Q\epsilon \quad (6)$$

where, $P\epsilon = -a_v (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) \quad (7)$

$$Q\epsilon = -b (\epsilon_{xx} + \epsilon_{yy} - 2\epsilon_{zz}) / 2 \quad (8)$$

Although the concept of a single valence band edge is not valid in the case of strained structure, we here define valence band edge in terms of the deepest energy level at a particular position and hence obtain the energy band diagram.

The material combinations that satisfy the conditions are given in table 1 along with the corresponding value of conduction band offset (CBO).

DETAILED BALANCE

To determine the performance of the materials as tabulated in table 1 when used as a solar cell, detailed balance calculation was done on each combination. The equations used for the calculations are according to ref [iii,xii,xiv]. The values of the maximum efficiency are tabulated in the last column of Table 1.

RESULTS

	Barrier	Well	Substrate	CBO (In meV)	Max. Eff. (1 sun)
1	Al _{0.63} In _{0.37} As	InAs _{0.16} P _{0.84}	InP	593	43.46
2	Al _{0.26} Ga _{0.74} Sb	GaP _{0.17} Sb _{0.83}	GaSb	553	22.59
3	Al _{0.30} In _{0.70} As	Ga _{0.11} In _{0.89} As	InAs	423	23.16
4	Al _{0.26} Ga _{0.74} Sb	GaP _{0.1} Sb _{0.9}	InAs	403	23.47
5	Al _{0.26} In _{0.74} As	InAs	InAs	408	21.14

Table 1

The results show that there are no III-V material combinations with direct band gap which has a CBO of 0.9 eV and which satisfies the above mentioned criteria. If the range of CBO is expanded to include values of approximately 0.6 eV, then there are a larger number of possible materials. The material combination with the highest theoretical efficiency is Al_{0.63}In_{0.37}As as the barrier and InAs_{0.16}P_{0.84} as the well with InP as the substrate. The efficiency of the material is 43% under 1 sun AM0 as compared to maximum value of 47%. This material system has been previously used and

demonstrated in optoelectronic devices, such as 1.3 μm lasers. The other material combinations have a very low theoretical efficiency as compared to the one mentioned. The mentioned material system also has the advantage of using InP as the substrate which is technologically more developed and studied as compared to the InAs and GaSb substrate growth.

CONCLUSION

The calculations of the material systems highlight several important features. First, material considerations play an important role in the realization of advanced concept approaches as well as conventional tandem approaches. Further, the material requirements highlight an additional advantage of QW approaches, in the feasibility of tertiary materials for the wells. This flexibility is important in realizing a relatively optimum material system. The material system as chosen by this study is $\text{Al}_{0.63}\text{In}_{0.37}\text{As}$ as the barrier and $\text{InAs}_{0.16}\text{P}_{0.84}$ as the well with InP as the substrate.

References:

- [i] W.Shockley, H.Queisser ,*Journal of Applied Physics* **32**,(1961), 510
- [ii] A. Luque and A. Marti, *Phys. Rev. Letters*, Vol 78, No. 26,pg. 5014-5017
- [iii] S.P.Bremner, R.Corkish, C.B Honsberg, *IEEE Transaction on electron devices*,**46**,(1999),1932
- [iv] A.Marti et.al, *Phys Rev. Letters*, **97**, 247701(2006)
- [v] L.Cuadra et.al.,*Physica E* **14**(2002) 162-165
- [vi] A.Marti et.al., *Thin Solid Films*, **511-512**(2006),638-644
- [vii] J. Nelson, "*The Physics of Solar cells*", Imperial college Press
- [viii] B.F.Levine ,'Quantum well Infrared Photodetectors", *Journal of Applied Physics*, **74** No.8, 1993
- [ix] I. Serdiukova et.al."Criticalbuilt-in electric field for an optimum carrier collection in multiquantum well p-i-n diodes," *Applied Physics Letters*, vol. **74**, no.19, p. 2812-14, (1999).
- [x] M.Y.Levy and C.B.Honsberg, Precise and Rapid Calculations of Energy and Particle flux for Detailed Balance Photovoltaic applications, 20th European Photovoltaic Energy conference,6-10 June,2005,Barcelona, Spain

[xi] I.Vurgaftaman,J.R.Meyer, L.R.Ram Mohan, *Jour.Appl.Phys*.Vol **89**,No.11, pg 5815-5875

[xii] S.L.Chuang, *Phys.Rev.B*, Vol 43(1991),pg 9649-9661

[xiii] S.L.Chuang, *Physics of Optoelectronic Devices*, John Wiley & Sons.,1995

[xiv] A.De Vos, " *Endoreversible thermodynamics of Solar Energy Conversion*, " Oxford University Press,1992,96,99