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Computational modelling of the reflectivity of AlGaAs/GaAs and SiGe/Si quantum well solar cells

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Abstract

In this paper the modelling of the reflectivity of two quantum well solar cells (QWSC) are theoretically developed and computationally analysed. The *new* reflectivity model is based on the Modified Single Effective Oscillator model combined with Fresnel's equation. The model takes into consideration the effects of the design parameters including concentration levels, structural properties of the device (well length, etc.), operating temperature and electric field effects. The results generated are for a bare AlGaAs/GaAs cell and the same cell with a ZnS antireflection coating (ARC). Further investigations include a bare SiGe/Si cell and the same cell with a Ta_2O_5 ARC. The results generated are accurate and match with experimental data for similar cells. The analysis is performed for AM 1.5 spectrum. The model is intended to be an aid to QWSC designers.

Keywords: Computational modelling; Quantum well solar cell; Reflectivity; AlGaAs/GaAs; SiGe/Si

1. Introduction

In the past few years, development of quantum well solar cells (QWSCs) have generated great interest. These cells originally developed by Prof. Keith Barnham (Imperial College, UK) have shown great promise in achieving high efficiency [1]. A key problem common to all solar cells is the optical losses due to reflection. In the

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case of the QWSC, it is not immune from this loss. Depending on the material a considerable amount of photon energy is wasted.

In this paper, the author has theoretically developed and computationally investigated the reflective losses of two hypothetical QWSCs. In order to do this, the author puts forth a *new approach* to modelling the reflectivity of the QWSC. The model presented here is based on a theoretical model of the refractive index of the QWSC established elsewhere [2–5] combined with the Fresnel formula [6].

The model of the QWSC's refractive index is based on the Modified Single Effective Oscillator (MSEO) model for semiconductor alloys [2]. The MSEO model allows the calculation of the refractive index of a semiconductor layer. In the previous works [3–5] investigations into the three major areas essential to design and determining the QWSC's refractive index are performed. These major areas are:

1. Concentration levels and barrier length effects on the refractive index of quantum wells and the additional semiconductor layers such as p/n regions.
2. Operating/environmental temperature effects on the refractive index of quantum wells and the additional layers.
3. Electric field effect on the refractive index of quantum wells.

Using these approaches and combining with Fresnel's formula a *new* reflectivity model was achieved. The reflectivity model is dependent upon the design parameters of the QWSC. The reflectivity analysis presented here will be for two hypothetical QWSCs, with their dimension defined below. The first cell was based on the commonly used AlGaAs/GaAs semiconductor alloy. The analysis was performed for a bare cell and the same cell coated with an antireflection coating (ARC) of ZnS ($n = 2.3$). This material has been the foundation of QWSC research. Having established the model's foundation, with the AlGaAs/GaAs material, the author investigated the potential and capability of the *new* model by considering a *new* material alloy. The author generated the reflectivity curves for a hypothetical Silicon–Germanium alloy. Like previously, the analysis was performed for a bare cell and the same cell with an ARC of Ta_2O_5 ($n = 2.1$). To show the effectiveness of the model's results, a comparison with existing experimental data for similar cell structures was performed. The choice of a SiGe/Si QWSCs was based on the recent research interest into this material alloy and it seems to be one of the new avenues to pursue[1] in photovoltaics.

Furthermore, it is intended that the model presented here is to be an aid to QWSC designers. It is hoped that it can be used to optimise designs and forged with other models achieve higher efficiency designs.

The calculation and simulation of the QWSCs' reflectivity were performed for the operating solar spectrum on the earth's surface (0.3–1.11 μm) (AM1.5).

[1] Private communication with Prof. Martin A. Green UNSW.

2. A complete model of the reflectivity of QWSC

In order to determine the reflectivity of the QWSC one must first determine the cell's refractive index. This can be done through the models documented in Refs. [2–5]. In all the individual alloy layers to make up the QWSC; the effects of molar concentration and operating temperature on the refractive index of these alloy layers can be determined using the equations and techniques established in Refs. [3,4]. This is simply done by representing the band gap (E_g) parameter equation for each respective layer of the cell with a function of molar concentration and temperature.

Since the design parameters of the QWSC are known, with the knowledge of the doping concentration levels of the p/n regions and the length of the intrinsic region, one can determine the electric field across the quantum well (intrinsic) region. We assumed the cell to replicate an electric dipole with the p/n regions to be the respective positive/negative charged particles and the intrinsic region containing the quantum wells placed in between these two respective charges. The calculation of this electric field generated by the p/n regions is simply performed using standard electrostatic equations [7]. Having calculated the total electric field (E), the equations and techniques established in Ref. [5] are used to determine the effects of electric field on the parametric equation E_d and hence on the refractive index of the layer. The effects of electric field on refractive index of the quantum well region can be determined and incorporated.

We have obtained the refractive indices for each respective layer as a function of design parameters (see the appendix for in depth calculation). Using the refractive index summation equations [8]:

$$n_{TE}^2 = \frac{\sum_j n_j^2 d_j}{\sum_j d_j} \quad \text{for transverse electric TE,} \tag{1}$$

$$\frac{1}{n_{TM}^2} = \frac{\sum_j \frac{1}{n_j^2} d_j}{\sum_j d_j} \quad \text{for traverse magnetic TM,} \tag{2}$$

where n_j is the refractive index of the jth layer, and d_j the thickness of the jth layer.

One can incorporate each respective layer of certain length and index and determine the overall average refractive index of the cell. The refractive index of the complete solar cell can be determined for transverse electric (TE) or transverse magnetic (TM). For normal incidence these would be equal.

Having obtained a model of the refractive index of the QWSC, it is possible to determine the reflectivity of the cell. The reflectivity of the solar cell can be calculated using the Fresnel formula combined with the previous work. According to the Fresnel equation the reflectivity is given as [6]

$$R = \frac{r_1^2 + r_2^2 + 2r_1 r_2 \cos 2\theta}{1 + r_1^2 r_2^2 + 2r_1 r_2 \cos 2\theta} \tag{3}$$

with

$$r_1 = \frac{n_0 - n_1}{n_0 + n_1}, \tag{4}$$

$$r_2 = \frac{n_1 - n_2}{n_1 + n_2}, \tag{5}$$

$$\theta = \frac{2\pi n_1 d_1}{\lambda}, \tag{6}$$

where n_0 is the refractive index of the incident medium (air) = 1.00, n_1 the refractive index of the ARC, n_2 is the refractive index of the substrate; in this case the QWSC, d_1 the thickness of the antireflection layer (= 0.00 for no coating).

It is the incorporation of the refractive index into the Fresnel formula that gives the reflectivity as a function of design parameters.

The thickness of the ARC can be determined by minimising Eq. (5). It is common practice to have the minimum trough located at approximately 0.6 μm since this produces the lowest total reflection.

3. Hypothetical QWSC

3.1. $Al_{1-x}Ga_xAs/GaAs$ QWSC

P-type region doping is $2 \times 10^{16}\,cm^{-3}$ ($x = 0.33$) and length 140 nm. Six (6) quantum wells are $x = 0.33$ with length 5.5 nm and barrier length 17.0 nm. N-type region doping is $2 \times 10^{16}\,cm^{-3}$ ($x = 0.33$) and length 140 nm.

3.2. $Si_{1-x}Ge_x/Si$ QWSC

P-type region doping is $2 \times 10^{16}\,cm^{-3}$ ($x = 0.4$) and length 100 nm. Nine (9) quantum wells are $x = 0.4$ with length 2.0 nm and barrier length 8.0 nm. N-type region doping is $2 \times 10^{16}\,cm^{-3}$ ($x = 0.4$) and length 100 nm.

Cell area was assumed to be $0.09\,cm^2$ (Fig. 1).

Fig. 1. Cross-sectional area of a hypothetical QWSC.

4. Computer-generated results

4.1. $Al_{1-x}Ga_xAs/GaAs$ QWSC

Computer generated results for $Al_{1-x}Ga_xAs/GaAs$ are shown in Figs. 2–4.

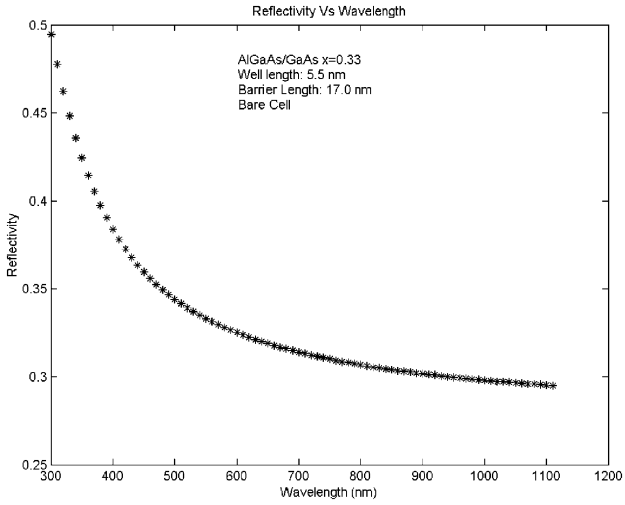

Fig. 2. Reflectivity of a bare AlGaAs/GaAs QWSC.

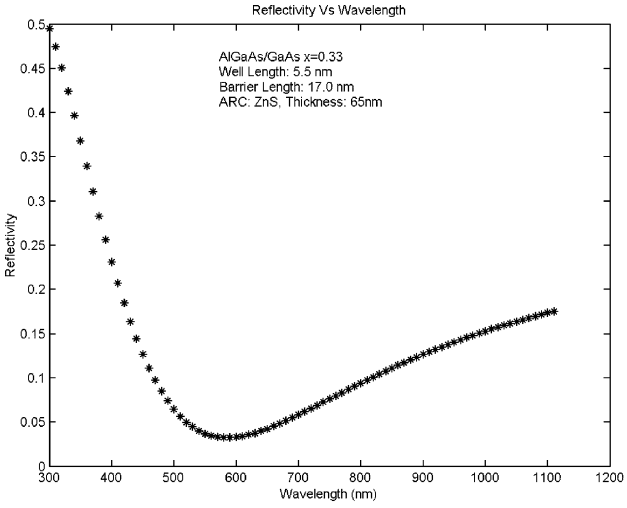

Fig. 3. Reflectivity of the AlGaAs/GaAs QWSC with ZnS ARC.

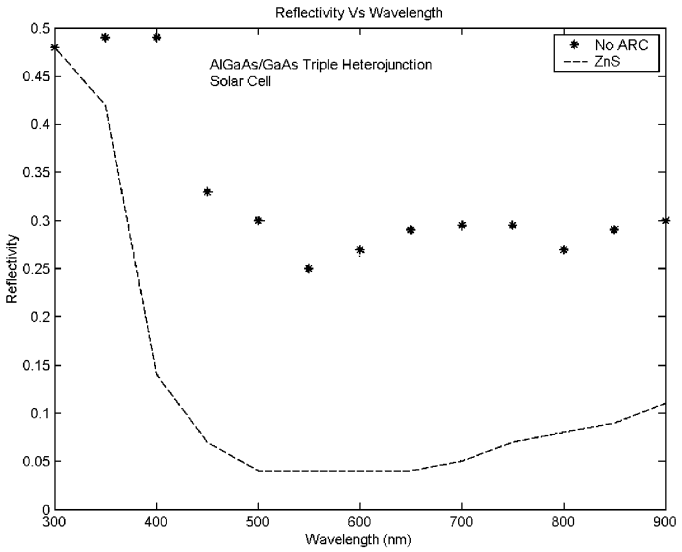

Fig. 4. Experimental reflectivity of triple heterojunction AlGaAs/GaAs cell bare and with ZnS ARC.

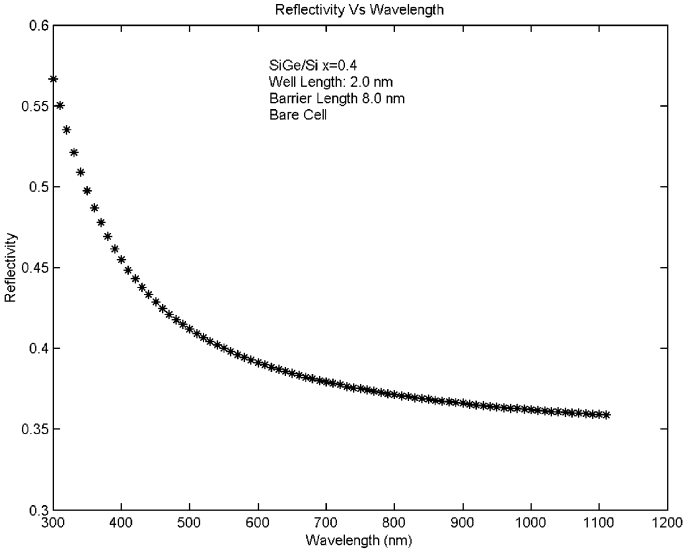

Fig. 5. Reflectivity of a bare SiGe/Si QWSC.

4.2. $Si_{1-x}Ge_x/Si$ QWSC

Computer generated results for $Si_{1-x}Ge_x/Si$ are shown in Figs. 5–8.

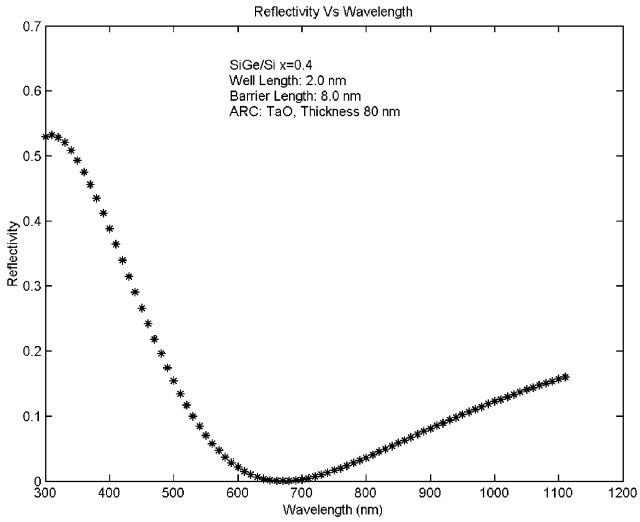

Fig. 6. Reflectivity of the SiGe/Si QWSC with Ta_2O_5 ARC.

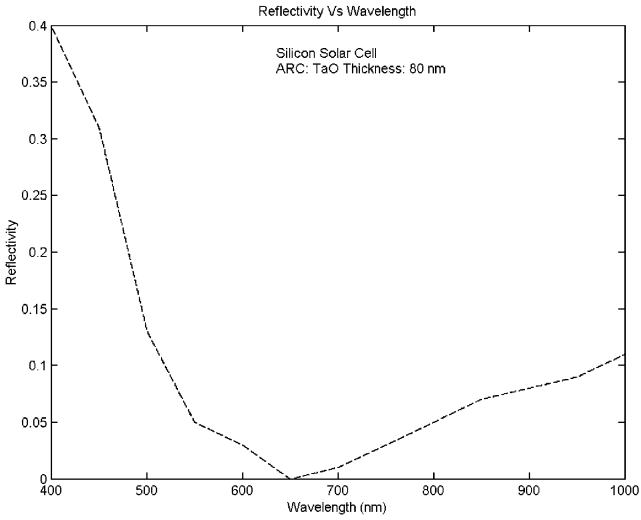

Fig. 7. Experimental reflectivity data for Silicon solar cell with Ta_2O_5 ARC.

5. Discussion and post analysis

The development of a *new* theoretical model of the reflectivity of a QWSC is proposed. The analysis of the reflectivity of the hypothetical QWSCs was performed

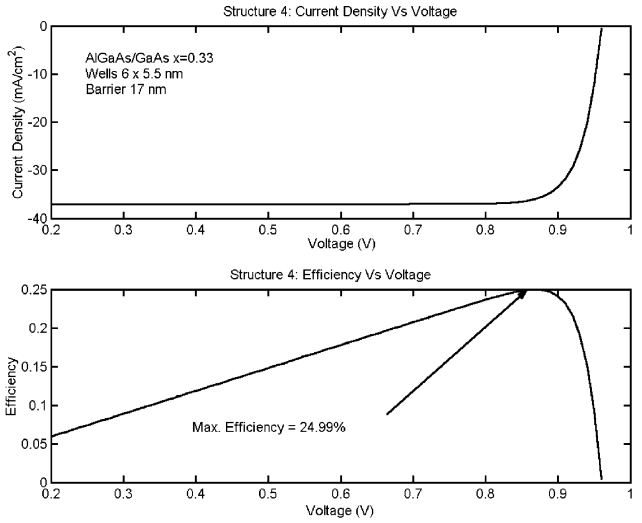

Fig. 8. Cell performance of AlGaAs/GaAs QWSC described above. Efficiency of approximately 25% is achieved.

for the operating wavelength 0.3–1.11 μm (AM1.5). The simulation was performed for laboratory conditions (temperature 298 K).

The model is based on the MSEO model [2] combined with the work on the refractive index of quantum wells [3–5] and Frensel's formula [6]. The model generates the reflectivity of a QWSC for a given concentration level, configuration, electric field and operating temperature. It is to be used as a designer's aid in optimising QWSC designs. Preliminary simulations (discussed later) show the model is effective in producing QWSC design with respectable efficiency.

The MSEO model was intended to be used for wavelengths up to the absorption edge of a semiconductor material (GaAs $\lambda \geqslant 0.86\,\mu m$) [2]. Furthermore, the MSEO model's accuracy degrades at higher photon energies. Given these reasons, it seems a poor choice to model QWSCs, but regardless of the results generated by this model when compared to experimental data of a similar cell fall within reasonable accuracy of one another (see below for comparison). Further justification for the use of the MSEO model can be seen in the original work of Barnham et al. [9]. The purpose of the introduction of quantum wells into a standard p–i–n junction is to extend the long-wavelength ($\lambda \geqslant 0.8\,\mu m$) absorption of a conventional p–i–n solar cell. Given these points the use of the MSEO model to generate the model presented here seems reasonable.

The reflectivity of two hypothetical QWSCs is discussed next. In both cases the author has performed a comparison of computer-generated results compared with experimental data in order to establish the effectiveness of the model presented here. Initially, we consider the AlGaAs/GaAs QWSC.

Referring to Figs. 2 and 5: As can be seen, the reflectivity of the uncoated AlGaAs/GaAs QWSC varies with wavelength. The reflectivity for the QWSC varies from 49% to 29% across the AM 1.5 spectrum. Comparing this to the results for the AlGaAs/GaAs triple junction (TJ) cell [10]. The TJ cell's reflectivity varies from 48% to 25% for the same spectrum. Although, there are slight discrepancies in the values, the values correspond well with one another, to a degree of accuracy. The slight discrepancies can be attributed to the use of different solar cells for the comparison and the MSEO inaccuracy at higher photon energies.

Referring to Figs. 3 and 5: The introduction of an ARC to the AlGaAs/GaAs cell has an impact straight away. For the QWSC the reflective loss is approximately 49% at short wavelengths reducing to approximately 3% at the optimum wavelength of 0.6 μm and rising up again to approximately 12% at the longer wavelengths. Again the generated values of the reflectivity are similar to the TJ solar cell with similar ARC [10]. For the TJ cell the reflective losses with the presence of an ARC is 48% at short wavelengths, reaching a minimum of 4% at 0.6 μm and rising to 10% at longer wavelengths. Again the results fall within a degree of accuracy with one another and the discrepancy can be attributed to the reason given above.

We have established the model's foundation with the AlGaAs/GaAs alloy. The real test of the model would be its performance in generating results for a cell of another material. In order to do this the author considered a SiGe/Si QWSC.

Referring to Figs. 5 and 6: In the case of the bare QWSC cell the reflectivity is approximately 57–37% across the AM 1.5 spectrum. The introduction of ARCs has an immediate impact. As can be seen the computational model results compared to the experimental results documented in Ref. [11] for the Ta_2O_5 ARC are in good agreement with one another. At the short wavelengths the results of 41% (computational) compared to 40% (experimental) are observed. At the 0.6 μm wavelength both models generate a reflectivity value of 0% and as we move to the longer wavelengths results of approximately 11% (computational) and 10% (experimental) are observed. These values are very accurate and show the models capability. The slight discrepancies can be attributed to those reasons given above.

A comparison of theoretical and experimental results of identical QWSCs would be better. Unfortunately, the author was unable to obtain experimental reflectivity data for the QWSC;[2] therefore, the results of a similar structure of the same material and antireflection coating was used for the comparison. Nonetheless, it is clear that the model produces values which are within reason when compared to a cell of similar structure.

Having established the AlGaAs/GaAs design above, further justification that the optical model presented here is worthy and effective at producing high efficiency QWSCs, is to simply determine the efficiency of the design above. Using the Rimada/Hernandez model [12], the $J-V$ curve and efficiency versus voltage curve showing

[2] Due to a lack of financial resources.

the maximum efficiency point was computed (Fig. 8). According to the Rimada model the AlGaAs/GaAs cell design documented above has an efficiency of approximately 25%. The control p–i–n structure was simulated to have an efficiency of approximately 18%. This is clearly an improvement in cell efficiency by approximately 7%. These results show the model to be very effective in designing and optimising ideal QWSCs. The author is currently pursuing the SiGe/Si QWSC design and hopes to publish results in a later publication.

There have been a number of publications by various authors regarding QWSC. The majority of authors have concentrated on modelling/simulating the electrical aspect of the QWSC [12–16]. In doing so they have obtained current and voltage models of the cell based mostly on Fermi–Dirac statistics. In these cases, it was common to simulate the optical properties (determine refractive index, etc.) using the absorption coefficient (defined as (α) in the above references) or taking an average value of the refractive index. For the AlGaAs/GaAs case this is commonly 3.5. Using these parameters the reflectivity was generated.

The model presented here has a number of features that are advantageous when compared to the absorption coefficient technique. First, the same model can be used to determine the refractive index and hence reflectivity of each respective layer of the QWSC. This is simply done by limiting the unwanted layers to length equalling zero. In doing so they are not considered in the calculation. This is very convenient as only one program is written and reduces computation time and resources. Secondly, the model is very design orientated. It encapsulates a number of design parameters (mention above) in one simulation. The effects of concentration, dimension, temperature and electric field effects on the semiconductor alloys are easily incorporated. The author is unaware of any attempt of using this absorption coefficient technique. This will clearly be an aid to designers attempting to optimise their designs.

A final advantage over the absorption coefficient technique is this model's simplicity. The absorption coefficient technique uses a complex step function, which is often approximated using a Lorentzian function [17,18]. This requires the oscillator strength (f_n) to have a compensating unit (per cubic Angstroms). Conventionally, the oscillator strength is a *unit-less* value ranging between 0 and 1 [19]. In the presented model, this convention is followed. This reduces confusion and follows standard practice.

Granted that there are more sophisticated modelling techniques compared to the one presented above; however, the use of a simple model, considering all the design aspects, that generates very accurate results would prove to be an advantage and aid to designers.

6. Conclusion

A *new approach* to theoretical and computational modelling of the reflectivity of QWSCs are presented and investigated. The model presented is based on previous work regarding the QWSC refractive index combined with the Fresnel formula. It is

to be used by QWSC designers as an aid to optimise designs. This model is capable of considering the major design parameters associated with the QWSC including concentration level, operating temperature and electric field. The results generated for an AlGaAs/GaAs and SiGe/Si QWSC show the model presented here is effective and generates accurate values within reason when compared to experimental results. Further justification of the model's capability is that existing models show the model presented here can be used to design and optimise an "ideal" QWSC of 25% efficiency. Finally, its simplicity to implement and its following of conventional terminology will reduce confusion. The model will prove to be an aid to QWSC designers.

Acknowledgements

The author would like to thank Professor Martin A. Green (University of New South Wales, Australia) for his thoughtful discussion on the subject.

Appendix

Using the hypothetical AlGaAs/GaAs QWSC defined above.

One must initially realise which layers are affected by what design parameters (molar concentration, temperature and electric field). Molar concentration and temperature will clearly affect each layer of the cell (p region, intrinsic region and n region). Therefore, using the techniques in Ref. [4] and substituting the energy gap parametric equation E_g for these layers with an equation dependent on both molar concentration and temperature; the effects of these two design parameters on the refractive index are observed and modelled. Since E_0 and E_g are related, the two parametric equations are obtained for each respective layer.

In the case of the electric field only the quantum well region's refractive index will be effected since they lie between the p/n regions and the incorporation of strained layers. Therefore, using the techniques in Ref. [5] for the electric field (in this case p/n induced and strain induced) determination of the parametric equation E_d for the quantum well layers (intrinsic region) is possible.

The p/n region's E_d parametric equations remain only molar concentration related as documented in Ref. [2]. They are assumed to be unaffected by the temperature and electric field parameters. The zero effect of electric field is assumed because the p/n regions are not surrounded by an electric field. They induce an electric field.

Each respective layer's refractive index as a function of wavelength, molar concentration and temperature can be determined using the MSEO model [2]:

$$n^2 = 1 + \frac{E_d}{E_0} + \frac{E_d}{E_0^3}E^2 + \frac{\eta}{\pi}E^4 \ln\left(\frac{2E_0^2 - E_g^2 - E^2}{E_g^2 - E^2}\right), \tag{A.1}$$

where

$$\eta = \frac{\pi E_d}{2E_0^3(E_0^2 - E_g^2)}.$$

E is the photon energy.[3]

The parametric equations E_0, E_d and E_g are related elsewhere [4,5].

For the case of AlGaAs/GaAs, the energy gap parametric equation $E_g = E_\Gamma$ is molar concentration and temperature dependent as follows [4]:

$$E_\Gamma = 1.519 + 1.247x - \frac{dT^2}{T + 204}$$

$(x \leqslant 0.45)$,

$$E_\Gamma = 1.519 + 1.247x + 1.147(1 - x)^2 - \frac{dT^2}{T + 204}$$

$(x > 0.45)$, (A.2)

where units are in eV, x is the molar concentration, T the temperature in Kelvin.

$$d = 5.4e - 4eV/K.$$

Substituting this equation in the E_g parametric equation (which leads to the E_0 parametric equation being determined, see Ref. [4]) for every layer of the cell allows the molar concentration and temperature effects to be incorporated and investigated.

(Note that we assume the cell to be quasi one-dimensional for the next section since doping level concentration is in units per cm^3.)

The electric field generated by the p/n region can be determined with the use of Coulomb's Law and assuming the cell to be an electric dipole with an intrinsic region between the two respective charge [7]. The electric field can be determined as follows.

The total P-type charge $q_p = 2 \times 10^{17} \times V_p$, where V_p is the volume of the p region and 2×10^{17} is the doping level in the AlGaAs/GaAs case. Similarly, it can be applied to determine the total N-type charge.

For an electric dipole the electric field is given as [7]

$$E = E_1 + E_2, \tag{A.3}$$

where E_1 is the positive charge's electric field and E_2 the negative charge's electric field. If we assume the charges are equal ($q_p = q_n$) we can simplify and obtain

$$E = \frac{1}{4\pi\varepsilon_0} \frac{2aq}{(a^2 + r^2)^{3/2}}, \tag{A.4}$$

where r is the distance perpendicular to the dipole plane. We assume this to be zero. $q = q_p$ is the p or n charge defined above (can be either since equal charges are assumed)

$$a = L_i + \frac{L_n}{2} + \frac{L_p}{2}, \tag{A.5}$$

[3] Please note E is not electric field in this equation.

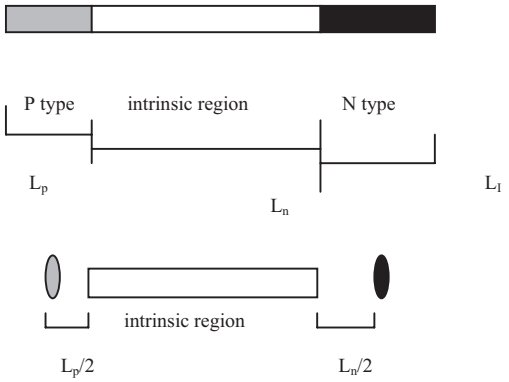

Fig. 9. Representation of QWSC as an electric dipole with intrinsic region within the dipole.

where L_i is the intrinsic region length, L_n is the length of the n-type layer and L_p is the length of the p-type layer. The half term above appears because it is assumed the total charge (point charge) of each p or n region to be at the centre of this region, therefore half the region's length away from the ends of the intrinsic region (Refer to Fig. 9).

The remaining parameters are those commonly encountered and their S.I. units can be found in any physics texts.

For the given hypothetical design the value of $E = 19\,\text{kV/cm}$ (AlGaAs/GaAs) is obtained.

As mentioned, using the technique established in Ref [5] to determine parametric equation E_d and substituting the value of E as the electric field, the effects of electric field across the quantum well region is determined.

Combining the temperature (parametric equations E_0 and E_g) and the electric field techniques (parametric equation E_d) into one program, the refractive index as a function of molar concentration, temperature and electric field of each respective layer can be determined. Using the summation Eqs. (3) and (4) above the complete refractive index of the cell can be determined. Having considered all the design parameters, a complete refractive index model is obtained.

In the case of $Si_{1-x}Ge_x/Si$ the lowest direct energy gap is shown to be a linear relationship with molar concentration (x) and is given as [20][4]

$$E_g = E_\Gamma = 2.615x + 0.805\ (\text{eV}). \tag{A.6}$$

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