Influence of strain on the radiative mass in optoelectronic devices

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***Abstract*—We investigate the strain dependent optical spectra of an $In_xGa_{1-x}As$ Quantum Well LED structure. It is common to calculate spectrum for emission and absorption with effective mass independent strain, on the other hand our model describes the effects of strain on the radiative mass of the holes. We use the 6-band k.p model to calculate the bandstructure of the device. This model is integrated in the $XienceSim$ software package.**

I. Introduction

There is a constant effort in designing better optical devices, and calculate their characteristics with higher precision. Most of the precise models deal with a drawback, that due their complexity the calculation takes long too.
Density functional theory incorporates each atom in the system, thus making it hard to use for full device structures. However, the continuum models can handle real devices, with acceptable precision. Approximations have to be applied, for example envelope function calculation, with **k.p** method. Even this continuity model can be time consuming in order to calculate a real 3D structure. We need to find reasonable approximation methods, that can be faster and remain accurate. In this paper we use the 6-band **k.p** method to calculate the band edges of the valence bands in the structure, and we propose a method how to calculate the deformed mass tensor due to strain. We developed a semiconductor device simulator with a drift diffusion solver to calculate the optical characteristics of the device.

II. Theoretical model

We use the 6-band Luttinger Kohn Hamiltonian [1], in order to calculate the valence band states. For known strain field it gives us 6 eigenvalues E_i with 6 eigenvectors φ_i corresponding to the heavy hole (HH), light hole (LH), and spin-orbit split-off (SO) bands with spin degeneracy at the Γ point ($k = 0$). From spectral dynamics of matrices the second derivative of the eigenvalue can be expressed with the following formula,

$$\frac{\partial^2 E_i}{\partial \vec{k}^2} = \varphi_i^T \frac{\partial^2 H}{\partial \vec{k}^2} \varphi_i + 2 \cdot \sum_{i \neq j} \frac{|\varphi_j^T \frac{\partial H}{\partial \vec{k}} \varphi_i|^2}{E_i - E_j} \tag{1}$$

The second term vanishes[1] at the vicinity $k = 0$, and the second derivative of the Hamiltonian matrix in $\vec{k}$ are the Luttinger parameters. From this the effective carrier mass of the valence bands is obtained,

$$\mathbf{m}_i^{-1} = \frac{1}{\hbar^2} \varphi_i^T \frac{\partial^2 H}{\partial \vec{k}^2} \varphi_i \tag{2}$$

The determinant of the effective mass tensor reflects the change of the Density of States (DOS) in the structure.

[1]If shear strain is applied, then it breaks the degeneracy of the HH valleys, if not than it can be simplified near $k = 0$ to a three band coupling Hamiltonian.

A. Spectrum Calculation

After the course of band edges, and of the quasi-Fermi levels are known we perform a spectrum calculation for inter-band transitions.
Emission spectrum:

$$\alpha(\omega)_{\text{sp}} = C \left(\frac{q}{m_0}\right)^2 \frac{\pi}{\epsilon_0 n \omega c} \frac{m_0 E_{\text{P}}}{6} \frac{1}{2\pi^2} \left(\frac{2m_{\text{r}}}{\hbar^2}\right)^{3/2} \sqrt{\hbar\omega - E_{\text{g}}} \cdot f_{\text{c}}\left(E_{\text{v}} + (\hbar\omega - E_{\text{g}})\frac{m_{\text{r}}}{m_{\text{e}}}\right) \cdot \left[1 - f_{\text{v}}\left(E_{\text{v}} - (\hbar\omega - E_{\text{g}})\frac{m_{\text{r}}}{m_{\text{h}}}\right)\right] \tag{3}$$

$$C = \left(\frac{\omega n}{\pi c}\right)^2$$

Absorption spectrum:

$$\alpha(\omega)_{\text{abs}} = \left(\frac{q}{m_0}\right)^2 \frac{\pi}{\epsilon_0 n \omega c} \frac{m_0 E_{\text{P}}}{6} \frac{1}{2\pi^2} \left(\frac{2m_{\text{r}}}{\hbar^2}\right)^{3/2} \sqrt{\hbar\omega - E_{\text{g}}} \cdot \left[f_{\text{v}}\left(E_{\text{v}} - (\hbar\omega - E_{\text{g}})\frac{m_{\text{r}}}{m_{\text{h}}}\right) - f_{\text{c}}\left(E_{\text{v}} + (\hbar\omega - E_{\text{g}})\frac{m_{\text{r}}}{m_{\text{e}}}\right)\right] \tag{4}$$

Here the radiative mass tensor is defined in the following:

$$m_{i,\text{rad}}^{-1} = m_i^{-1} + m_{\text{e}}^{-1} \tag{5}$$

Where $i = \text{HH}, \text{LH}, \text{SO}$. We have performed the spectrum calculation for each valence band, and summed up the intensity values. The determinant of the mass tensor contributes to the calculation.

B. Simulation Workflow

First program calculates the strain in the structure, and for each volume element it calculates the band edges and the effective mass tensor. It solves the Poisson equation and the drift diffusion equation self consistently. The spectrum was calculated as mentioned in II-A.

III. Model Structure

In order to test our model, we used a $In_xGa_{1-x}As/GaAs$ Quantum Well LED structure. The unstrained band profile is plotted in figure 1.

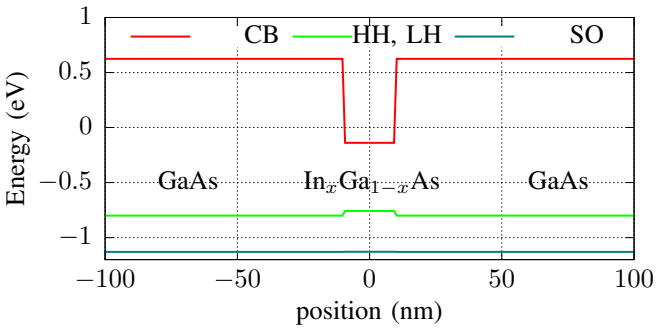

Fig. 1. Band structure profile of the simulated device. The alloy concentration was chosen to be $x = 0.8$

The material parameters were taken from [2]
We apply additional deformation over the strain due to lattice mismatch. One end of the device is fixed, and additional displacement is applied on the other end. With this method we could modulate the applied strain, for a constant alloy profile. The growth direction is chosen to be [001]. The GaAs regions is weakly doped with 10^{15} cm^{-3}, with 1 level dopants. The doping was p-type on the left side and n-type on the right side. We applied a voltage in forward bias $U = 0.1$ V. The mobility of all carriers in the full device is assumed to be constant with $\mu = 1\frac{m^2}{Vs}$. We do not include piezoelectricity because we focus in this work on the effect of the change of the mass tensor on the spectrum.

IV. Results

In the case when there is no external strain applied we plot the band diagram with Fermi levels for [001] growth direction, and the emission and absorption spectra.

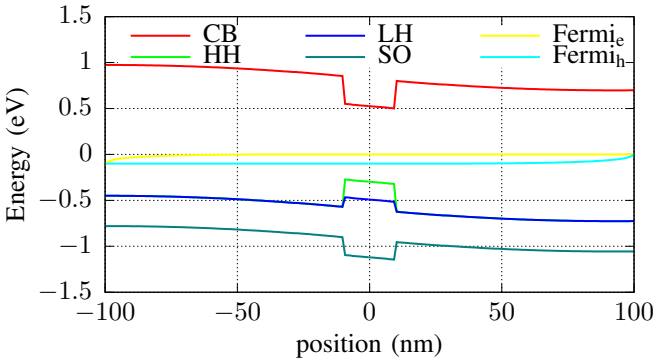

Fig. 2. Band structure profile of the lattice mismatch strained device grown in the [001] direction.

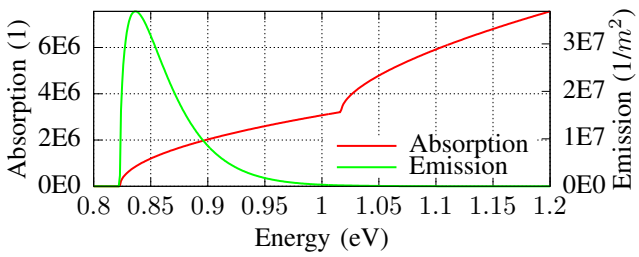

Fig. 3. Emission and absorption spectra of the $In_xGa_{1-x}As$ region

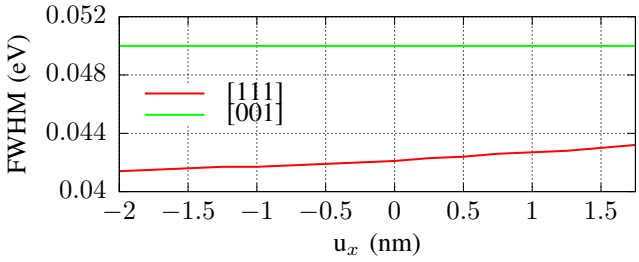

Fig. 4. The FWHM plots of the emission spectra of the $In_xGa_{1-x}As$ region, when the right edge of the structure was shifted by u_x

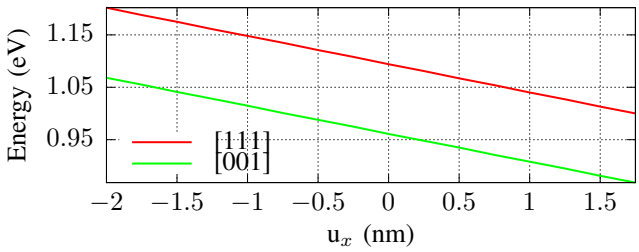

Fig. 5. The maximum emission energy of the $In_xGa_{1-x}As$ region, when the right edge of the structure was shifted by u_x

For two different growth directions [001], and [111] the FWHM values were plotted in figure 4. It reflects that the tension [001] direction does not change the mass of the HH states, which contributes the most to the light emission. The peak maximas are plotted in figure 5.

V. Summary

We use a semi-classical approximation to analyze the optical spectra of a LED structure. Also we have calculated the change of the spectra when external tension is applied to the device.

References

[1] Igor Ivashev. Theoretical investigations of zinc blende and wurtzite semiconductor quantum wells on the rotated substrates. 2016.
[2] I Vurgaftman, JR Meyer, and LR Ram-Mohan. Band parameters for iii–v compound semiconductors and their alloys. *Journal of Applied Physics*, 89(11):5815–5875, 2001.