Investigation of intersubband transitions in wide bandgap oxide quantum well structures for optoelectronic device applications

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MOTIVATION

- There is a growing interest in wide bandgap oxides like ZnO, MgO, Ga_2O_3, etc. [1], [2].
- These materials possess unique properties suitable for high-performance optoelectronic devices in sensing, communications, and imaging applications.
- Ga_2O_3 has a wide bandgap energy of about 4.8 to 4.9 eV, making it transparent to UV radiation and opaque to visible light [3].
- ZnO exhibits exceptional optical and electrical properties, including a high exciton binding energy and substantial oscillator strength [4].
- Intersubband transitions in multiple quantum well (MQW) structures hold promise for efficient light absorption and emission in the mid-infrared to terahertz spectral range.
- The study aims to numerically simulate the absorption spectra of wide bandgap oxide MQW structures, focusing on the light-matter interaction where the dominant many-body contribution is the depolarization field.

THEORETICAL MODEL

- 1D effective mass Schrödinger equation:

$$-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d\psi_i(z)}{dz}+U_{eff}(z)\psi_i(z)=E_i\psi_i(z)\,,$$

$$U_{eff}(z)=\;U_c(z)-e\varphi(z)+U_{xc}(z)-eF_ez$$

- U_{xc} is the local exchange correlation potential:

$$U_{xc}(z)=-\frac{e^4}{32\pi^2\hbar^2}\frac{m^*(z)}{\varepsilon^*(z)^2}\left(\frac{9\pi}{4}\right)^{\frac{1}{3}}\frac{2}{\pi r_s{}^*}\left[1+0.0545r_s{}^*\log\left(1+\frac{11.4}{r_s{}^*}\right)\right]$$

- For the electrostatic potential, the Poisson equation reads:

$$\frac{d^2\varphi(z)}{dz^2}=\frac{e}{\varepsilon^*(z)}\big(n(z)-N_d(z)\big),\qquad n(z)=\sum_i N_{s,i}|\psi_i(z)|^2\,,$$

$$N_{s,i}=\frac{m_{ti}k_BT}{\pi\hbar^2}\ln\left(1+e^{\frac{E_F-E_i(0)}{k_BT}}\right)$$

- The single particle absorption coefficient is [5]:

$$\alpha_{2D,s}(\omega)=C_s\sum_\alpha f_\alpha\Delta N_\alpha G(\omega-\omega_\alpha)$$

- The Hamiltonian describing the intersubband plasmon:

$$H_{plasmon}=\sum_\alpha\hbar\widetilde{\omega}_\alpha p_\alpha^\dagger p_\alpha+\frac{\hbar}{2}\sum_{\alpha\neq\beta}\Xi_{\alpha,\beta}(p_\alpha+p_\alpha^\dagger)(p_\beta+p_\beta^\dagger)$$

- The coupling due to dipole-dipole Coulomb interaction is described by the coupling strength:

$$\Xi_{\alpha,\beta}=\frac{\omega_{P\alpha}\omega_{P\beta}}{2\sqrt{\widetilde{\omega}_{P\alpha}\widetilde{\omega}_{P\beta}}}\frac{S_{\alpha\beta}}{\sqrt{S_{\alpha\alpha}S_{\beta\beta}}},\qquad S_{\alpha\beta}=\frac{1}{\hbar\omega_\alpha}\frac{1}{\hbar\omega_\beta}\left(\frac{\hbar^2}{2m^*}\right)^2\int_{-\infty}^{+\infty}dz\xi_\alpha(z)\xi_\beta(z)\,,$$

$$\xi_\alpha(z)\equiv\xi_{ij}(z)=\;\psi_i(z)\frac{\partial\psi_j(z)}{\partial z}-\psi_j(z)\frac{\partial\psi_i(z)}{\partial z}.$$

- The new *N* frequency W_N can be calculated by diagonalizing the following $2N\times 2N$ matrix:

$$M=\begin{bmatrix}I_1 & C_{12} & \dots & C_{1N}\\ C_{12} & I_2 & \dots & C_{2N}\\ \vdots & \vdots & \ddots & \vdots\\ C_{1N} & C_{2N} & \dots & I_N\end{bmatrix},\qquad I_\alpha=\begin{bmatrix}\widetilde{\omega_\alpha} & 0\\ 0 & -\widetilde{\omega_\alpha}\end{bmatrix},$$

$$C_{\alpha,\beta}=\begin{bmatrix}\Xi_{\alpha,\beta} & -\Xi_{\alpha,\beta}\\ \Xi_{\alpha,\beta} & -\Xi_{\alpha,\beta}\end{bmatrix}$$

- Current density for n-th multisubband plasmon:

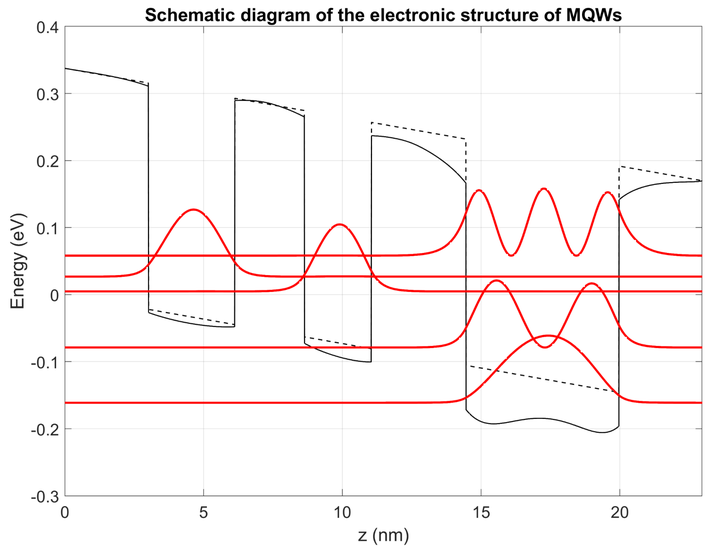
$$J_n(z)=\frac{e\hbar}{2m^*\sqrt{S}}W_n\sum_\alpha\frac{\xi_\alpha(z)\sqrt{\Delta N_\alpha}}{\sqrt{\omega_\alpha\widetilde{\omega}_\alpha}}(a_{n\alpha}+b_{n\alpha})^{-1}$$

- Absorption can be calculated by integrating all the current densities associated with different multisubband plasmons:

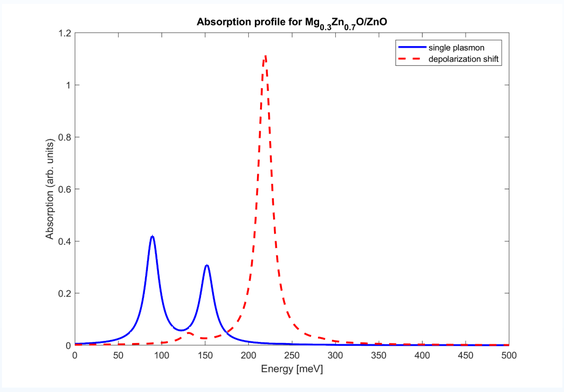
$$\alpha_{2D,m}(\omega)=C_m\sum_n\frac{1}{W_n}\left|\int_{-\infty}^{+\infty}J_n(z)dz\right|^2G(\omega-W_n)=\;C_m\sum_n W_nF_n\,G(\omega-W_n)$$

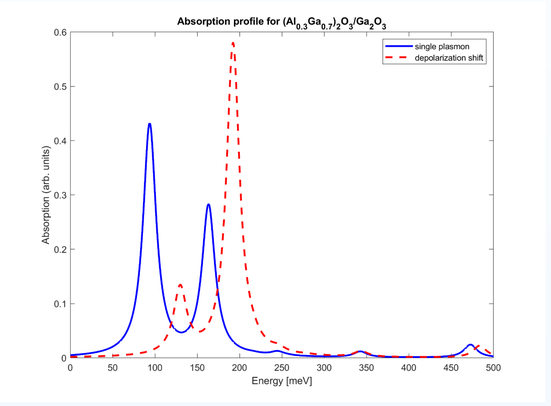
SIMULATION RESULTS

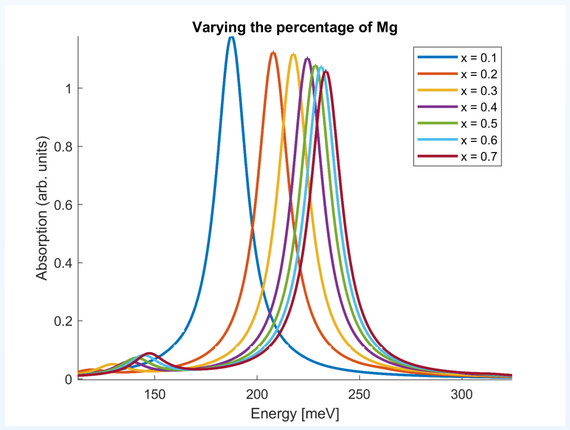
- We study a multiple quantum well design, focusing on $Mg_xZn_{1-x}O$ /ZnO and $(Al_xGa_{1-x})_2O$/ Ga_2O_3 materials. The results of our numerical simulations are absorption profiles for these material systems.

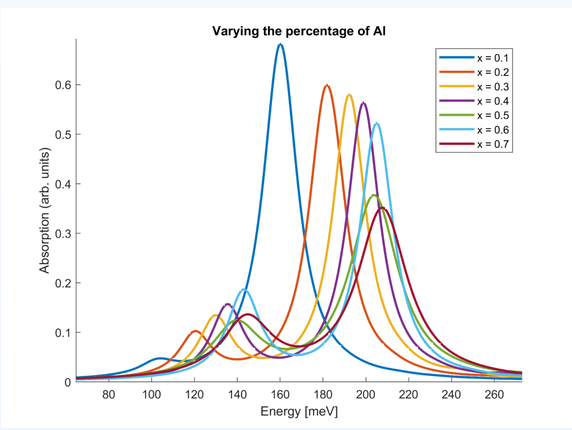


- The structure shown is for the $Mg_{0.3}Zn_{0.7}O$ /ZnO material system. The same layer thickness is further used for simulating the $(Al_xGa_{1-x})_2O$/ Ga_2O_3 material system.









- The layer sequence in nm, starting from the left barrier reads: **3**/3.1/**2.5**/2.4/**3.4**/5.5/**3.** The widest well is uniformly dopped with $n=30\times10^{18}cm^{-3}$
- The electronic structure is calculated at applied field of $F=7.3\times10^6\frac{V}{m}$

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