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Atomistic study of Urbach tail energies in (Al,Ga)N quantum well systems

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***Abstract*—Aluminium gallium nitride is a system of interest for developing ultraviolet (UV) optoelectronic devices. Here Urbach tails induced by carrier localization effects play a key role in determining device behaviour. We study the electronic structure of $Al_xGa_{1-x}N/Al_yGa_{1-y}N$ single quantum wells using an atomistic framework. Results show that the density of states exhibits a tail at low energies due to disorder in the alloy microstructure. Our analysis allows for insight into the orbital character of the states forming the Urbach tails, which can affect light polarization characteristics, and important quantity for deep UV light emitters.**

I. Introduction

Optoelectronic devices operating in the ultraviolet (UV) part of the spectrum have myriad applications in areas such as water purification and sterilization [1]. A system currently attracting attention to realise these devices is III-nitride heterostructures, namely (Al,Ga)N quantum well (QW) structures, which can emit at wavelengths within the UV-A, -B and -C windows. Other III-N systems (such as (In,Ga)N for emission in the visible spectrum) have been studied extensively, however electronic, optical and transport properties of (Al,Ga)N systems are not well understood.

In light emitting diodes (LEDs) and lasers, carriers distribute across a range of energies which will depend on conditions such as the temperature and bias of a device. It is not necessarily sufficient to have a description of energy states near to the band edge; information about states over a broad energy range is required. Therefore the density of states (DOS) plays an important role in device simulations. Experimental [2] and theoretical [3] studies have indicated that (Al,Ga)N exhibits carrier localization attributed to alloy disorder. This will impact the DOS and introduce Urbach tails [4].

One approach to calculating the DOS of a QW is to treat the system in 1-D, using $\mathbf{k}\cdot\mathbf{p}$ theory to calculate subbands associated with the in-plane dispersion of each level. Assuming parabolic bands results in a step-like DOS, however it neglects the impact that localization has on the electronic structure – This calls for a 3-D treatment of the problem, which accounts for alloy disorder.

Localization effects have previously been considered in full device simulations using either expensive 3-D simulations [5] or via an ad-hoc broadening of the DOS [6]. Here we start from an atomistic electronic structure theory, and use this to determine the DOS and Urbach tails. This can be used in the future to establish new, numerically efficient, methods to include alloy induced localization in device simulations.

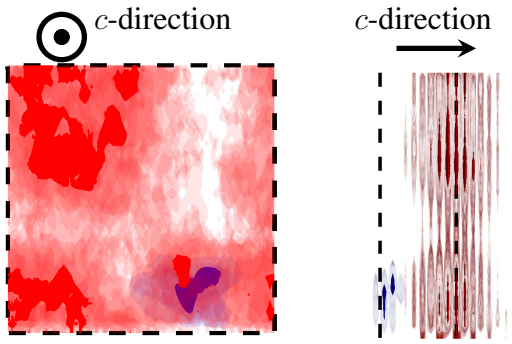

Fig. 1. Electron (red) and hole (blue) ground states in a 2.3 nm $Al_{0.48}Ga_{0.52}N/Al_{0.63}Ga_{0.37}N$ quantum well. The carriers are shown from (left) the top, looking parallel to the c-axis, and (right) the side, looking perpendicular to the c-axis. Dark (light) surfaces indicate 50% (10%) of the maximum charge density. Black dashed lines indicate well boundaries.

II. Theoretical Framework

The framework starts with an sp^3 nearest-neighbour tight-binding model. This allows for an atomistic description of an alloy, while also permitting the simulation of relatively large supercells. Local strain and polarization effects are calculated with a valence force field model [7] and local polarization theory [8] respectively.

The supercells have dimensions of $\approx 10 \times 9 \times 10$ nm^3 which corresponds to a total of $81,920$ atoms. The electron and hole ground state charge densities in an $Al_{0.48}Ga_{0.52}N/Al_{0.63}Ga_{0.37}N$ QW is shown in Fig. 1. Here the strong alloy-induced localization is evident for the hole, while the electron is mainly confined by the well geometry and built-in polarization field. As the alloy microstructre is less important for electrons, we shall focus only on holes while analyzing the impact of carrier localization on the DOS.

To calculate an Urbach tail, a large number of microscopic configurations must be considered. In this case we calculate the electronic structure of 75 different alloy configurations. To evaluate the DOS the first 100 hole states are calculated, their energies are grouped into bins of 15 meV width, and the

derivative is taken with respect to energy. Below, we report initial results on a 2.3 nm $Al_{0.48}Ga_{0.52}N/Al_{0.63}Ga_{0.37}N$ QW.

III. Results

The DOS is shown in Fig. 2 – Energy is defined relative to the valence band edge such that the hole ground state has a lower energy than excited states. From the atomistic simulations, including alloy disorder, we observe an approximately constant DOS between ≈ 100 meV and 150 meV. The sharp increase in the DOS above these energies occurs when the bottom of the next hole sub-band is reached. This is in line with the step-like DOS seen in 1-D calculations.

At the low-energy side of the DOS (energies < 100 meV), instead of a step-like change we observe a decaying tail. This Urbach tail is attributed to the presence of localized states; similar results have been observed for (In,Ga)N QWs [4]. By fitting an exponential function to this tail, $\mathrm{DOS}(E) = A\exp(E/E_U)$, an Urbach energy, E_U, can be extracted. The resulting curve for QWs studied is shown in Fig. 2 (red). As mentioned above, this is important input for device simulations which will depend on the alloy composition, and may also be modified by the well width.

The DOS, together with TB wave functions, can in future be used to construct a *local* DOS. This is important input for, e.g., drift-diffusion simulations of optoelectronic devices.

Additionally, the orbital character of the wave functions will impact light polarization characteristics. If the wave function which takes part in a radiative process consists primarily of p_x and p_y orbitals, the emission will be transverse electric (TE) polarized. However, if the wave function is consisting mostly of p_z orbitals emission will be transverse magnetic (TM). This has consequences for light extraction efficiency of UV devices [1].

The probability of measuring a given state whose energy is in the bin centered at the energy E_j in a p_x orbital is

$$\mathrm{P}_x(E_j) = \frac{1}{N}\sum_i |\langle p_x|\Psi_i\rangle|^2$$

where $|\Psi_i\rangle$ is a wave function calculated from TB, and the sum runs over the N wave functions whose energy is within the 15 meV energy interval surrounding E_j. Similar expressions can be written for p_y and p_z orbitals.

We find that the tail states, and the first plateau, are largely dominated by a combination of p_x and p_y orbitals. At more excited hole states the p_z orbitals begin to contribute to the wave function composition, corresponding with the addition of the next sub-band in the DOS. Therefore, in the systems studied here light would be primarily TE polarized, although emission arising from recombination with highly excited states will exhibit more TM characteristics.

IV. Conclusions

In this work we have outlined a framework to calculate Urbach tails from an atomistic tight-binding theory, which can form input for device simulations. Our results show that the DOS exhibits an exponential tail due to the presence of disorder in the alloy microstructure. These tail states, and the first plateau in the DOS, are constructed predominantly of p_x and p_y orbitals, which indicates primarily TE polarized light emission. Higher energy states begin to include p_z orbitals, and thus increase the probability of TM emission.

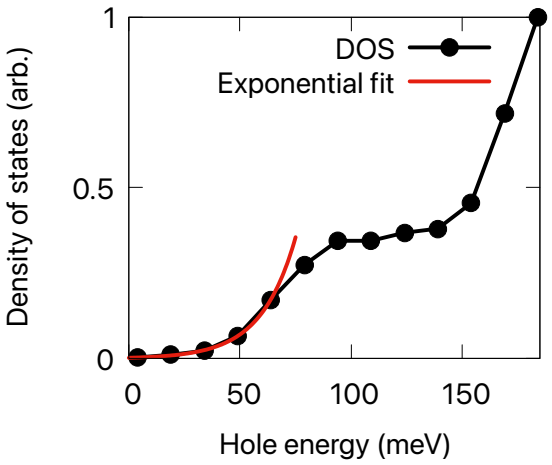

Fig. 2. Hole density of states (DOS, black) of a 2.3 nm $Al_{0.48}Ga_{0.52}N/Al_{0.63}Ga_{0.37}N$ quantum well calculated from atomistic tight binding. The tail of the DOS has been fitted with an exponential function, $\mathrm{DOS}(E) = A\exp(E/E_U)$, (red).

V. Acknowledgements

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