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# Implementation of a Spurious Solution Free 8-band k.p Model for the Identification of Absorption Spectra of InAs Quantum Dots grown on GaAs

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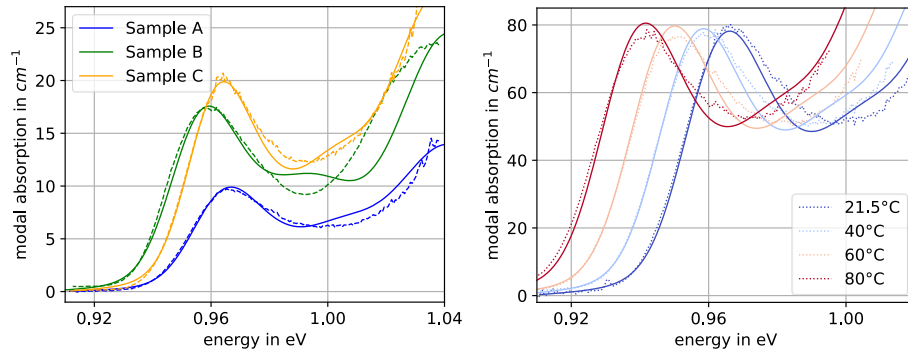
Despite QD devices presenting a reduced threshold current density, improved device lifetime, and their insensitivity to defects, which enables monolithic growth on silicon [1], they have yet to have a commercial impact. A potential reason for this delay is the lack of a reliable model that can be used to simulate the functionality of QD based devices, prior to fabrication. Such models exist for structures based on e.g. QWs and have significantly facilitated the fabrication of state-of-the-art photonic devices. The final aim of this research is to implement a similar easy-to-use model for QD based photonic devices.

To achieve this, the optical and electrical properties of individual dots are investigated using the 8-band k.p Burt-Foreman Hamiltonian description [2]. Allowing the identification of the energy levels and wavefunctions of individual charge carriers within InAs QDs grown on GaAs. These results can then be used to simulate the absorption through the following equation [3],

$$A(h\nu) = \frac{\gamma_t \sigma_0 E N_d}{w_m} \int L(E_i, h\nu) P(E_i) dE_i,$$

where  $\gamma_t$  is the degeneracy factor,  $N_d$  is the dot density,  $w_m$  is the width of the optical mode in the growth direction,  $L(E_i)$  is the Lorentzian distribution function, used to describe the homogeneous broadening,  $P(E_i)$  is the inhomogeneous broadening, and  $\sigma_{E0}$  is the optical cross-section. The inhomogeneous broadening is caused by the distribution of dot sizes; to this end simulations were repeated over a range of dot sizes. The optical cross section depends on the overlap of wavefunctions of carriers located at the initial and final state of the transition.

The simulated absorptions are directly compared to measurements, which have been obtained using the segmented contact method (SCM) [4]. A match between simulations and measurements are only possible if commonly labelled forbidden transitions are included, selected by significant (>30%) wavefunction overlap, and by calibrating the dot dimensions and the extent of material mixing. Under these conditions the modal absorption has been simulated for three dot structures, grown at different times or by a different organisation and an excellent match with experiments has been achieved as depicted in Figure 1. Additionally, temperature effects can be accounted for by using empirically identified Varshni parameters [5] as depicted in Figure 1.



**Fig. 1** (LHS) Depiction of the simulated (solid) and measured (dashed) modal absorption of sample A, B, and C. (RHS) Simulated (solid) and measured (dashed) temperature variations of sample A.

The absorption is an intermediary step towards the simulation of forward bias effects of QD structures. Which, additionally, requires the identification of the occupation probability of the energy levels of the confined carriers within the dot as well as the effects of Coulomb interactions.

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