Quantum cascade laser simulation using an sp^3s^* full Brillouin zone tight-binding model

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The quantum cascade laser (QCL) is an electrically pumped unipolar semiconductor laser based on intersubband transitions in quantum wells. It is capable of coherent light emission over a wavelength range of at least 3.5 µm to 88 µm, and its main application is as a light source for opti
The gain medium of a QCL is compo
25 to 35 identical stages, each contair
epitaxial layers. Given the resulting l
design parameters, a tool that can accur
properties of the gain medium is requi
the device performance and to tailo
wavelength.

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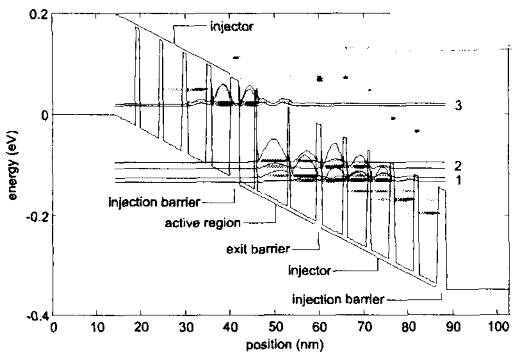

FIG. 1. The resonant states found for the AlAs/GaAs design of Becker *et al.* [2]. The moduli squared of the sums of the tight-binding expansion coefficients for each lattice plane are shown for all the resonant states using grey scale bars and in addition, for the pairs of states forming levels 1, 2 and 3, with curves. The bulk conduction band edge energy is also plotted: for the AlAs barriers, this is the bulk X-valley energy.

The first steps towards producing such a tool are reported here. The NanoElectronic MOdeling 3.0.2 software package [1], *NEMO*, has been used to calculate the electronic structure of a portion of various biased QCL gain media. The second nearest neighbour sp^3s^* tight-binding model used is capable of accurately modelling the conduction band non-parabolicity and the X-like nature of some of the resonances. The results of such a calculation for a particular AlAs/GaAs
um are shown in fig. 1.

structure of various other QCL gain
s have been simulated and the results
edictions of the photon energy at which
icient is maximized (E_{peak}). These
e been compared with experimental
e designs – see fig 2.

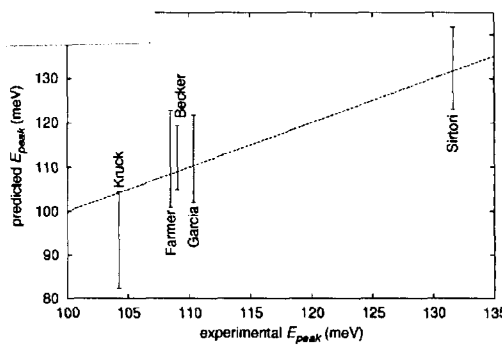

FIG. 2. Comparison of predicted and experimental photon energies that maximize the gain coefficient for various QCL gain medium designs. The straight line shows the ideal case of perfect agreement between the predictions and the experimental results.

The results from the tight-binding model calculations have also been compared to results from empirical two-band ***k·p*** model simulations. It has been shown that the tight-binding model is better able to predict E_{peak} and is able to model states with X-like character.

[1] http://www-hpc.jpl.nasa.gov/PEP/gekco/nemo
[2] Cyrille Becker, Carlo Sirtori, Hideaki Page, Geneviève Glastre, Valentin Ortiz, Xavier Marcadet, Max Stellmacher and Julien Nagle. AlAs/GaAs quantum cascade lasers based on large direct conduction band discontinuity. Appl. Phys. Lett. 77, 463 (2000).