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# Influence of barrier height on interface roughness scattering and coherent transport in AlGaAs quantum cascade lasers

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Quantum cascade lasers (QCLs) are promising sources of terahertz (THz) radiation that have applications such as security and medical screening. While optical output power has recently exceeded 1 W [1], their highest operating temperature is currently limited to  $\sim 200$  K [2] due to mechanisms such as thermal back filling and non-radiative phonon emission between lasing states. Another possible cause of performance degradation is parasitic leakage currents over barriers into continuum states as subband electron temperatures increase with lattice temperature. Novel designs with new injection schemes remain an intensive research area and new efforts are being made assuming that barrier heights no longer need to be constant [3,4]. A possible advantage of this is using tall barriers to reduce the leakage current, and in this work we present a theoretical study of the effects of increased barrier heights on transport between states in the structure. Similar to previous efforts, we initially restrict the modification of barrier height to the injection barrier; these are typically the thickest in THz QCLs and allow the reduced barrier widths necessary for AIAs barriers to remain above 1 ML. Figure 1 shows the band structure for the reference structure [2] and structure with modified injection barrier.

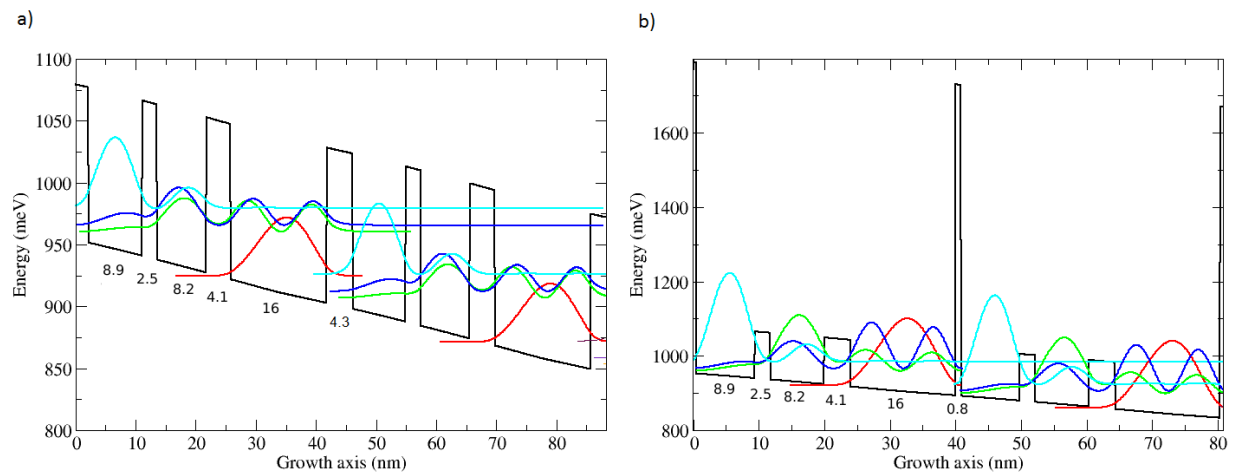


Figure 1: (a) Band diagram of the relevant wavefunctions for the current  $T = 200$  K record design [2] at  $12.2$  kV/cm (b) structure with AIAs injection barrier width modified to obtain similar injection coupling of  $\sim 2.9$  meV at  $18$  kV/cm.

The difference in barrier size needed to obtain the same coupling strength  $\hbar\Omega \sim 2.9$  meV for the reference  $200$  K structure [2] is shown in Figure 2a. From Fermi's golden rule, interface roughness (IFR) scattering scales with the conduction band discontinuity squared and the calculations also assume a typical correlation length  $\Lambda$  and root mean roughness value  $\Delta$  which are related to growth quality of the individual sample. We take typical values of  $\Lambda=60$  Å and  $\Delta=3$  Å for these parameters. Gain and current output characteristics are calculated using an extended density matrix solver which models transport through the injection barrier coherently. Changing the barrier height will have a direct influence on the alignment of energy levels as well as dephasing times which significantly alter the I-V behavior. These dephasing terms are calculated as in ref. 5 and include both intra- and inter- subband transitions from IFR, ionized impurities, alloy disorder and phonon scattering.

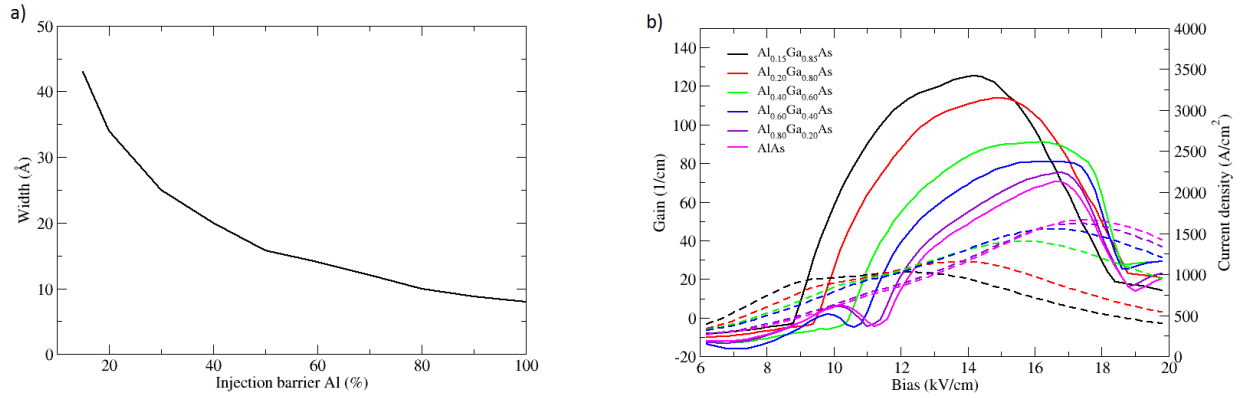


Figure 2: (a) Barrier width dependence on height to obtain injection coupling strength of  $\sim 2.9$  meV. (b) Gain (solid) and current (dashed) versus applied bias for varying injection barrier alloy content at 4.2 K lattice temperature.

Figure 2b illustrates that changing the injection barrier only will result in degraded unsaturated gain as well as an increase in current density. This is due to broadening caused by IFR scattering as well as decreased injection efficiency into the downstream period. However, it is noted that these are not equivalent structures due to the shift of energy separations and associated carrier transport paths. Recent experimental work [3] which attempted to change other barrier/well layer widths to make an equivalent structure when changing barrier heights demonstrated evidence of current density suppression with a taller injection barrier. Our results in Figure 3 are consistent with their findings that carrier injection dephasing does not reduce current transport significantly. We obtain similar current and gain values at resonance for both structures labelled ‘NRC-V775A’ and ‘NRC-V775C’ in ref. 3 indicating that the experimentally observed reduction in current density could be accredited to the reduction of parasitic current leakage.

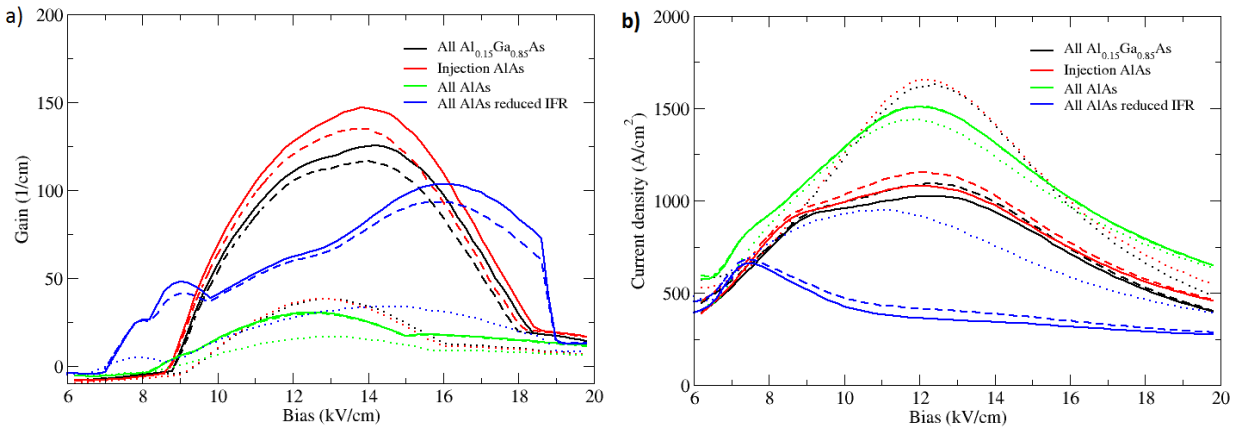


Figure 3: Gain (a) and current (b) versus applied bias for the reference structure [2], reference with AIAs injection barrier and all AIAs barrier structures [3] at 4.2 K (solid), 77 K (dashed) and 200 K (dotted) lattice temperatures.

Additionally, this work [3] attempted a similar design with all AIAs barriers which did not lase and it was conjectured that this was due to excessive IFR scattering as well as increased susceptibility to monolayer fluctuations with thinner layers. Our model, which accounts for the lifetime broadening in the gain calculation, confirms that modifying the IFR parameters to  $\Lambda=100$  Å and  $\Delta=1$  Å (i.e. unrealistically sharp interfaces) leads to a significant improvement in performance as shown in Figure 3. We extend this work by proposing designs which aim to balance leakage current reduction and excessive scattering to achieve higher operating temperatures.

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