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Indjin, D., Ikonic, Z., Harrison, P. et al. (1 more author) (2003) Surface plasmon waveguides with gradually doped or NiAl intermetallic compound buried contact for terahertz quantum cascade lasers. Journal of Applied Physics, 94 (5). pp. 3249-3252. ISSN 1089-7550

https://doi.org/10.1063/1.1599630

Citation for the published paper
Indjin, D. and Ikonic, Z. and Harrison, P. and Kelsall, R.W. (2003) *Surface plasmon waveguides with gradually doped or NiAl intermetallic compound buried contact for terahertz quantum cascade lasers.* Journal of Applied Physics, 94 (5). pp. 3249-3252.

Surface plasmon waveguides with gradually doped or NiAl intermetallic compound buried contact for terahertz quantum cascade lasers

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Abstract

Improved designs of surface plasmon waveguides for use in GaAs/AlGaAs terahertz quantum cascade lasers are presented. Modal losses and confinement factors are calculated for TM modes in novel metal– variably doped multilayer semiconductor and metal – intermetallic compound layer clad structures and compared with those obtained in recently realized metal – highly doped semiconductor clad layer structures. Considerable improvements of the mode confinement factors are predicted, and guidelines for choosing the confinement layer parameters are given.

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The active medium of quantum cascade lasers (QCLs)[1,2] comprises a stack of cascade unit cells, each having a number of quantum well/barrier layers which must be carefully designed[3] and analysed[4], particularly in the terahertz range, in order to provide population inversion. Among the most important difficulties in achieving terahertz lasing are the high intrinsic optical losses induced by the free electrons in the material, and the large size of the optical mode - imposed by the emission wavelength. Even with ~100 periods of the cascade, the structure is very thin ($\sim 10\mu$m), and one requires a waveguide configuration, in order to circumvent diffraction losses and confine, as much as possible, the optical field to the active medium. The fact that the active medium is immersed in just a part of the optical mode[5], implies that the actual gain is proportionally smaller than the nominal (local) gain, which the active medium could provide under full confinement conditions. At shorter, near infrared (IR) wavelengths reasonably large confinement may be achieved in conventional dielectric waveguides via the refractive index contrast, as is the case in bipolar semiconductor lasers. This approach becomes increasingly difficult in, the mid- and particularly, the far-IR range. Therefore, another concept has been introduced in this range, that of waveguides based on surface plasmons at interfaces between materials with opposite signs of dielectric permittivity, where the negative permittivity material is either a metal or a highly doped semiconductor. These materials are lossy, leading to waveguide mode losses. The quality of the QCL waveguide structure may be roughly estimated from the ratio of the mode propagation loss and the model overlap factor, $\alpha_{\mathrm{w}}/\Gamma$, provided the mirror losses (which include the outcoupling) are significantly smaller than the waveguide losses. This value has to be exceeded by the local gain for laser oscillation to be possible.

A single metal-semiconductor interface supports a TM surface plasmon mode, which typically has very small losses (a few cm^{-1} or less). This type of waveguide was the first plasmon based waveguide to be used in QCLs[6]. The field decays strongly inside the metal layer, but relatively slowly inside the semiconductor. This leads to a small mode confinement factor for typical active layer widths of a few microns, especially at longer wavelengths. Therefore, more complex waveguide structures, comprising two confining layers for the optical field, are necessary to achieve a better figure of merit.

The double metal clad (double plasmon) waveguide[7] provides almost total optical confinement, but has much larger losses than the single plasmon waveguide. Furthermore, double metal clad waveguides present serious fabrication difficulties, requiring special processing technology to etch away the substrate and stop at the active layer, before the reverse side metal layer is deposited. Another approach is to employ a (thick) highly doped semiconductor instead of the metal on one side, such that the free carrier contribution to the dielectric permittivity dominates and it has a negative (i.e. metallic) overall permittivity[8]. This is much easier to realize in a single growth procedure, and also gives almost as good confinement as the double metal waveguide, but unfortunately larger losses. Better results have been obtained with a thin, leaky but much less lossy, highly doped bottom contact layer as was implemented in the recently reported terahertz QCLs[8–10]. The optcmal mode was broader, hence Γ was reduced, but the losses α_{w} decreased even more, and optimal figure of merit was achieved by adjusment of the bottom confinement layer parameters. In this letter we propose improvements in this type of waveguide, based on profiled doping of the bottom contact/confinement layer. Furthermore, we propose and analyse an alternative configuration of THz QCL waveguide based on a buried intermetallic compound layer which can substitute the highly doped semiconductor while simultaneously offering the possibility of growth by means of molecular beam epitaxy (MBE).

Layers in a multilayer structure are characterized by their complex dielectric permittivity $\tilde{\epsilon} = \epsilon_r + i\epsilon_i$, or complex refractive index $\tilde{n} = n - ik$, where $\tilde{n}^2 = \tilde{\epsilon}$. These parameters are wavelength dependent, and are usually parametrized via the Drude model. In its simplest form, good enough in the THz range, it requires two constants – the plasma frequency $\hbar\omega_p$ and the damping parameter $\hbar\gamma$, to describe a material[11]. Their values for metals may be found e.g. in Refs. 12–15. In semiconductors the plasma frequency depends on the free carrier density (i.e. doping N), $\omega_p^2 = Ne^2/(m^*\epsilon_0\epsilon_\infty)$, where m^* is the electron effective mass and ϵ_∞ is lattice permittivity. The damping coefficient γ may be related to resistivity ρ (or mobility μ) as $\gamma = e/(m^*\mu) = \rho e^2 N/m^*$. The n-GaAs parameters have been measured for a wide range of electron densities, from lightly to very highly doped[16,17], and the damping parameter γ (usually deduced from mobility measurements) depends on the doping density. For the higher doping densities of practical interest, experimental results[16,17] for GaAs suggests values of the damping parameter $\hbar\gamma$ ranging from 2 meV to 6.3 meV as the doping density changes from 0.5×10^{18} cm^{-3} to 5×10^{18} cm^{-3}. In contrast to the case of light doping, the carrier mobility in heavily doped GaAs is mostly limited by ionized impurity scattering and the damping parameter is very weakly dependent on the temperature[18].

To find the mode intensity pattern and the propagation losses we used a numerical calculation based on the transfer matrix method[19–23]. The results for a recently reported THz QCL lasing at $\lambda \approx 70\mu$m[9] are presented in Fig. 1. From the experimental data for gold (the top metal layer) the Drude model parameters are: $\hbar\omega_p = 9.03$ eV and $\hbar\gamma = 0.053$ eV. Two types of the bottom contact layer were considered: (i) a single layer with a doping density of $n = 2 \times 10^{18}$ cm^{-3} (originally used as optimal in experiment[9]); (ii) a graded (multi-layered) region comprising four thin layers with thicknesses 35%, 30%, 20% and 15% of the total layer thickness, and doped with 5×10^{18} cm^{-3}, 2×10^{18} cm^{-3}, 1×10^{18} cm^{-3} and 0.5×10^{18} cm^{-3}, respectively. Whilst the calculated mode propagation losses, with the same total bottom contact thickness of $d = 1\mu$m, remain almost unchanged (~ 25 cm^{-1}), the modal overlap is around 30% higher in the graded structure. We should point out that the graded layer is better than the homogeneously doped one only if the doping decreases in the "outwards" direction, as in Fig. 1, in the opposite case it would be worse. Furthermore, Fig. 2 clearly shows that a thicker bottom contact layers will lead to larger values of the mode overlap factor (particularly in the multi-layer case) at the cost of a larger loss, with an overall decrease of $\Gamma/\alpha_{\rm w}$. The mode overlap for the single layer contact shows a slower increase with the total layer thickness than is the case in the multi-layer structure. An improvement of 20–30% in the waveguide figure of merit in the proposed multi-layer structure is present over a wide range of d. It is not clear how thin the highly doped contact layer may be, for either fabrication and further processing reasons; i.e., precise etching, or before size quantization effects come into play, in spite of the strong carrier scattering therein (the TM mode electric field is mostly perpendicular to the layers, and the simple Drude model would fail in this limit). However, a recent experiment[8] has suggested that reduction of the total bottom contact thickness down to 0.3μm is possible.

An alternative approach to GaAs/AlGaAs THz QCLs waveguide design is to use a buried metallic layer. A decade ago, intermetallic compound systems such as CoAl or NiAl were successfully grown on GaAs and AlAs substrate via MBE[24,25]. Very thin NiAl buried layers in GaAs/AlGaAs were subsequently fabricated[26,27], and were studied for possible use as metal–base ballistic transistors or resonant tunneling devices. Such systems are potential candidates for applications in novel optoelectronics devices. The important property of NiAl is that its lattice constant closely matchs that of GaAs, yielding low defect density interfaces between the two, and consequently a high–quality multiple quantum well GaAs/AlGaAs structure can be grown on top of a NiAl layer which may serve as buried contact/confinement layer. Fig. 3 shows the calculated results of the propagation losses $\alpha_{\rm w}$ and the mode confinement factor Γ for a waveguide configuration with an Au top layer and a NiAl intermetallic compound bottom layer, in a 70μm THz QCL. The Drude parameters for NiAl used in calculations are[28] $\hbar\omega_p = 4.83$ eV and $\hbar\gamma = 0.233$ eV. The waveguide losses increase and the confinement decreases when going from a very thin NiAl layer up to a critical value of $d_{\rm mc} \sim 0.07\mu$m, when the lowest-loss optical mode becomes unbound. For

$d_{\rm m} > d_{\rm mc}$ the previously first higher-loss optical mode takes over as the lowest-loss guided mode, and losses decrease significantly to the minimum value $\sim$ 38 cm^{-1} for $d \sim 0.3\mu$m. The mode overlap simultaneously increases and saturates to almost full confinement for $d_{\rm m} \sim 0.4\mu$m. In the full range of $d_{\rm m}$, the calculated mode intensity changes the pattern from single plasmon mode behavior to a double plasmon profile, as clearly indicated in the inset of Fig 3.

It is also important to note that above results were calculated with the 'worst case' set of Drude parameters for NiAl. For the more 'optimistic' values[28] of $\hbar\omega_p = 5.54$ eV and $\hbar\gamma = 0.096$ eV, and for a bottom layer width of $d_{\rm m} = 0.3\mu$m, the calculated losses decrease from 38 cm^{-1} to 30 cm^{-1} while the mode overlap increases from 93% to 98%. Therefore, an improvement of the figure of merit $\Gamma/\alpha_{\rm w}$ from 2.4×10^{-2} cm to 3.3×10^{-2} cm (up to 35%) is obtained. Furthermore, in the same example, replacing[6] the top gold layer with palladium (characterized with the almost same plasma frequency but with a significantly lower damping factor i.e. $\hbar\omega_p = 9.72$ eV and $\hbar\gamma = 0.008$ eV) yields an additional reduction of the losses to 24 cm^{-1}, with $\Gamma/\alpha_{\rm W} = 4.2 \times 10^{-2}$ cm (an increase of 70%).

In summary, design considerations have been described for improved types of waveguides for GaAs/AlGaAs QCLs. Calculations of losses and confinement factors indicate that waveguides based on graded doping of the semiconductor contact/confinement layer are likely to be very good candidates for QCLs operated in the terahertz range. The novel metal – intermetallic-compound based waveguide could produce an even better overall performance with carefully designed layer thicknesses. Such improvements will be very important for lowering the threshold current and increasing the maximum operating temperature of THz QCLs[4].

The authors would like to thank A. Tredicucci from NEST-INFM and Scuola Normale Superiore in Pisa, Italy, and M. Beck from University of Neuchâtel, Switzerland, for very useful discussions related to THz QCL fabrication. This work is supported by EPSRC grant No. GR/R04485.

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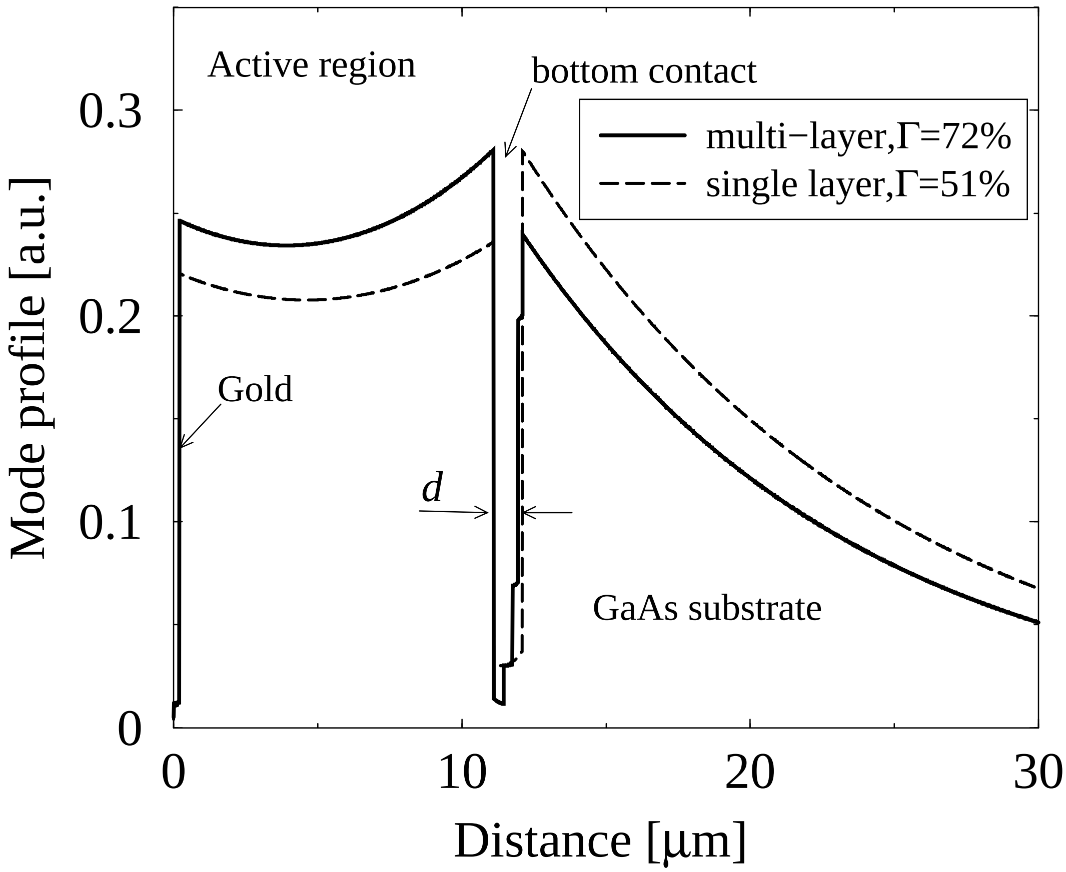

Fig. 1. A mode intensity profiles in the direction perpendicular to the layers in the waveguides analysed. The thin bottom confinement layer (of total thickness d) is either a single highly doped layer or of a graded multi–layer type with varying doping density.

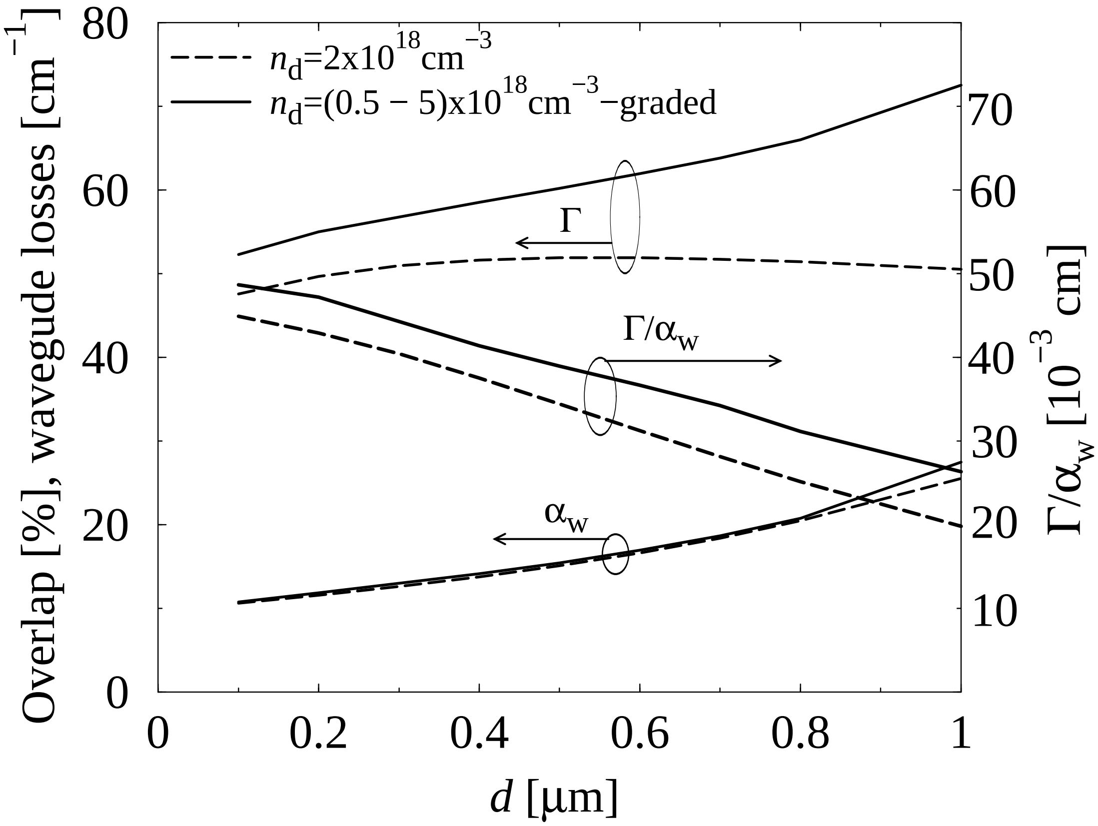

Fig. 2. The modal overlap factor, waveguide losses and figure of merit Γ/α_W as a function of total thickness of a single layer (dashed lines) and a multi-layer (solid lines) bottom contact.

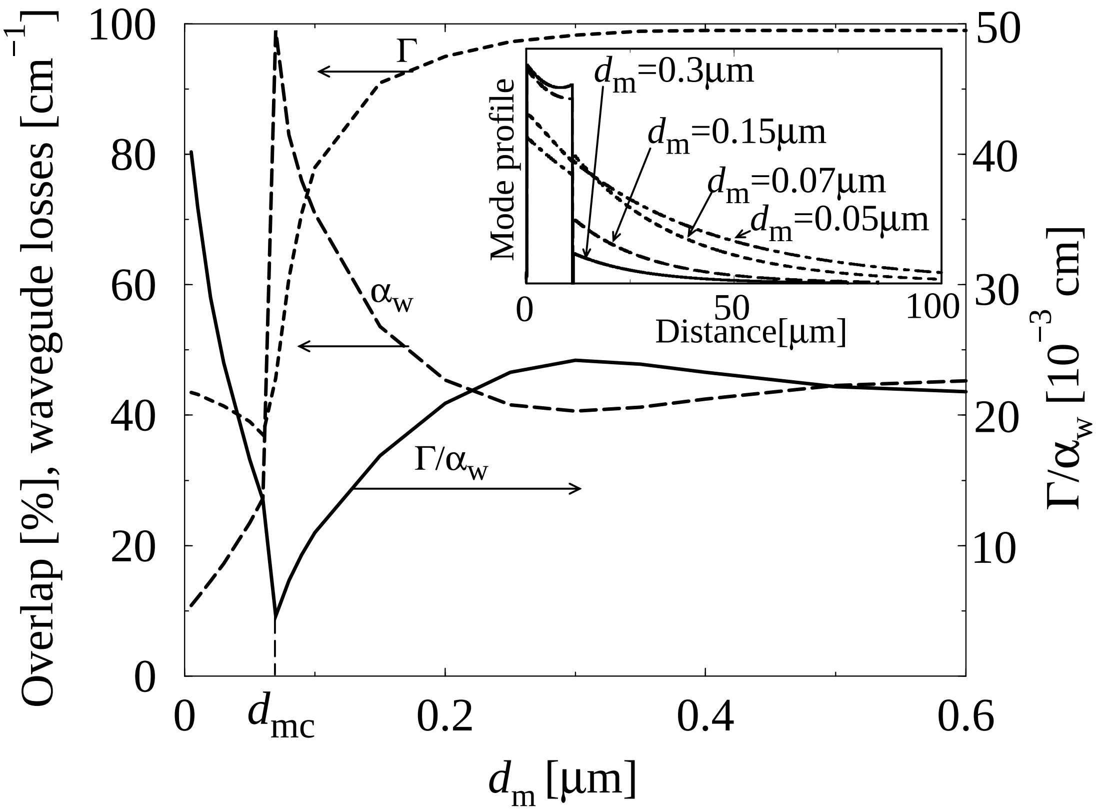

Fig. 3. The modal overlap factor, waveguide losses and figure of merit Γ/α_W versus total thickness of the NiAl bottom contact. The inset shows the mode intensity profiles in the direction perpendicular to the layers for a few different thicknesses of the bottom NiAl layer in the waveguide analysed.