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On metal contacts of terahertz quantum cascade lasers with a metal–metal waveguide

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Abstract

This paper reports an experimental study of the effects of different metal claddings on the performance of terahertz quantum cascade lasers. The experimental results show that by using a metal cladding made of Ta/Cu/Au to replace that of Pd/Ge/Ti/Pt/Au, the maximum lasing temperature of the devices is increased from 132 to 172 K, and the threshold current density of the devices at 10 K can be reduced from 0.74 to 0.68 kA cm⁻². The improvement of the device performance is attributed to lower optical losses associated with the metal cladding layers. The different effects of the metal contacts on device optical properties and electrical properties are also discussed.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

After nearly a decade of intense research on terahertz (THz) quantum cascade lasers (QCL), still one of the biggest challenges is to improve the maximum operating temperature ($T_{\max}$), toward room temperature operation. Many groups have been working on designing active-region gain medium with a sufficient gain at high temperatures [1–4] and engineering low-loss waveguides [5, 6]. The metal–metal (MM) waveguide structure, proposed by Williams *et al* [7], has a very high mode confinement factor and hence improves device performance of THz lasers with a sub-wavelength structure. Belkin *et al* showed that application of copper (Cu)-based MM waveguides slightly improves $T_{\max}$, compared with gold (Au)-based waveguides [8]. Later, Kumar *et al* demonstrated the record breaking $T_{\max}$ of 186 K by using Cu-based waveguides and the resonant phonon-based active region scheme with a diagonal intersubband lasing transition [1]. However, the fabrication of Cu-based MM waveguides is very demanding, due to adhesion and oxidation problems. The stack of contact

metals in such a waveguide also results in a Schottky barrier and drops 1–2 V across the metal contacts. Such an extra voltage drop could generate up to a few watts of Joule heat when the device is in continuous-wave operation. An ohmic contact is highly desired in order to minimize the voltage drop across the laser device.

In a typical III–V semiconductor diode laser (such as GaAs or InP based) that works in the visible-light or near-infrared range, a stack of Ti/Pt/Au is usually employed to form an ohmic contact with p-type semiconductors and a stack of Ni/Ge/Au for that with n-type semiconductors [9]. Since the electron collision frequencies of most metals are in the range of 1–10 THz [10], the optical loss of contact metals in the near-infrared range becomes negligible. As the lasing frequency approaches to the THz range, the high tangent loss of the metals makes a significant contribution to the overall waveguide loss despite small penetration depth of the electromagnetic mode into the metal layers. As a result, the stack of contact metals needs to be carefully selected based on not only their electrical properties, but also their optical properties.

This paper experimentally studies and compares the electrical and optical behaviors of THz QCLs with four different Au- and Cu-based metal contacts: Pd/Ge/Ti/Pt/Au, Ti/Pt/Au, Ti/Au and Ta/Cu/Au. The device with a stack of non-alloyed Ta/Cu/Au exhibits the lowest threshold current density (J_{th}) and the highest T_{max} in pulsed mode. The non-alloyed Ti/Au contact with a thinned Ti layer shows competitive results as also suggested in [12]. The high performance of the devices with these two non-alloyed contacts is attributed to the lower optical losses of the waveguides in spite of the formation of Schottky electrical contacts. The Ti/Pt/Au contact includes a Pt layer between Ti and Au to prevent inter-diffusion of Ti and Au atoms and hence the laser device can be annealed for metal alloying [13]. Thermal annealing the contact at 350 °C for 15 s lowers the contact resistance [14]. The Pd/Ge/Ti/Pt/Au metal combination is believed to form an ohmic contact on n^+ GaAs [9, 15] with a short diffusion of excess Ge in GaAs [16], but its higher optical losses at THz frequencies cause the overall device performance to deteriorate.

2. Device fabrication

The THz QCLs employed in this study are based on a GaAs/ $Al_{0.15}Ga_{0.75}As$ three-well cascade module similar to the one reported in [1]. The layer thicknesses are **45**/ 87/ **29**/ 83/ **44**/ 159 Å—the barriers are indicated in bold fonts. The quantum well of 159 Å is doped with Si dopant atoms to a two-dimensional carrier concentration of $3 \times 10^{10} \text{ cm}^{-2}$ per module that translates into $6.7 \times 10^{15} \text{ cm}^{-3}$ doping concentration for this structure. The whole QCL structure consists of 224 repeats (10 μm thick) of this module and is grown on a semi-insulating (SI) GaAs substrate by molecular beam epitaxy. To facilitate the electrical contacts, the active region is sandwiched between 100 nm of $3 \times 10^{18} \text{ cm}^{-3}$ bottom n^+ GaAs and top stack of 50 nm of $5 \times 10^{18} \text{ cm}^{-3}$, 10 nm of $5 \times 10^{19} \text{ cm}^{-3} n^+$ and 3.5 nm of low-temperature (LT) grown GaAs. The last two layers are used to form a non-alloyed ohmic contact [17]. Generation of THz emission is from the optical transition between a pair of anti-crossed double well states, with a low oscillator strength of 0.35 similar to [1]. Depopulation of carriers from the lower lasing state is mediated by coupling to a wide and doped subsequent well, relaxing by longitudinal-optical (LO) phonon emission and the injection to the following module.

The MM waveguide of the THz QCLs was fabricated by using In–Au wafer bonding technology [18] and standard photolithography. Reactive ion etch (RIE) was performed to etch through the entire thickness of the 10 μm thick active region, which minimizes the lateral spreading of current flow. Other details of the device fabrication can be found in [19]. Figure 1 shows the schematic cross-section of fabricated QCL devices with a MM waveguide. Using scanning electron microscopy, the area of the tested laser facets was measured; the average width of the ridge waveguides varies between 141 and 147 μm and the top metal width is 120 μm . The variations in the ridge size and shape can be accounted to the reproducibility of the RIE that is not fully controlled. The substrate of the samples was thinned down to $\sim 150 \mu\text{m}$ to

Figure 1. Schematic diagram of the cross section of fabricated THz QCLs with a metal–metal waveguide. The active region (AR) is based on a three-well cascade module that is repeated 224 times. The thickness of the active region is $\sim 10 \mu\text{m}$. The top semiconductor contact layer is 100 nm thick n^+ GaAs doped at $3 \times 10^{18} \text{ cm}^{-3}$. The bottom semiconductor contact layers consist of 50 nm thick n^+ GaAs doped at $5 \times 10^{18} \text{ cm}^{-3}$, 10 nm thick n^+ GaAs doped at $5 \times 10^{19} \text{ cm}^{-3}$ and 3.5 nm of LT GaAs. The semiconductor active region is sandwiched by two metal claddings from the top and the bottom.

facilitate heat dissipation from the active region to a heat sink underneath [19]. The sample was cleaved into laser bars with an $\sim 1 \text{ mm}$ long Fabry–Perot resonator. The laser bars were indium soldered (epi-layer side up) on oxygen-free copper packages and then mounted in a Janis closed-cycle cryostat for measurements.

Four groups (A–D) of QCL devices with different metal stacks for the electrical contacts were fabricated and tested to examine their effects on device performance. The metal stack employed in group A is Pd/Ge/Ti/Pt/Au (55/100/25/55/300 nm), which was annealed at 380 °C for 15 s and formed an ohmic contact with the n -type GaAs contact layer. The metal stack employed in group B is Ti/Pt/Au (25/55/300 nm), annealed at 350 °C for 15 s. The annealing of the first two groups yielded alloyed contacts. The metal stack employed in group C is the simplest, consisting only two layers Ti/Au (5/300 nm, non-annealed). The metal stack employed in group D is Ta/Cu/Au (10/500/100 nm, non-annealed). As we will show later, the optical loss of the last two metal stacks is relatively low and Cu is believed to be one of the least lossy metals in the THz frequency range. To ensure the comparison of the results, four small wafer pieces (1 cm by 1 cm) were cut from the same wafer and processed under the exactly same conditions.

3. Results and discussions

In THz QCLs with MM waveguides, the waveguide losses can vary to a large extent depending on the different constituent metals in the metal claddings. Figure 2 compares the calculated temperature-dependent waveguide losses for the structure with the metal claddings made of the four aforementioned metal stacks. The waveguide losses were calculated from simulating the complete 2D structure of the device shown schematically in figure 1, at a lasing

Figure 2. Calculated waveguide losses of THz QCLs with different metal claddings. The curves from the top to the bottom correspond to metal claddings made of Pd/Ge/Ti/Pt/Au, Ti/Pt/Au, Ti/Au and Ta/Cu/Au. The waveguide losses increase with temperature for all cases. The device with a metal cladding made of Ta/Cu/Au has the lowest waveguide loss. The right vertical axis shows the simulated optical gain based on a simplified density matrix model [4], which includes intersubband LO-phonon, ionized impurity and interface roughness scatterings. At $T_{\max}$ (136, 146, 170, 172 K) the disagreement between the simulated waveguide loss and optical gain is represented by the vertical double arrows. This disagreement is too high to be solely accounted by the mirror loss. This could be explained by the inaccuracy of the models used for optical gain and waveguide loss, as well as waveguide imperfections.

frequency of 3.75 THz. It consists of 10 μm thick and 144 μm wide MM THz QCL waveguides. The temperature-dependent permittivity and mobility of the active and n^+ regions were calculated using the data in [20, 21], respectively. The optical constants for the metals (plasma and carrier collision frequencies) were taken from [10] and the complex permittivity of various layers was calculated using the Drude–Lorentz approximation as [10]

$$\epsilon(\omega) = \epsilon_{\infty} - \frac{\omega_p^2}{\omega^2 + j\omega\omega_0}, \quad (1)$$

where ϵ_{∞} is the high-frequency limit of the material permittivity, and ω_p and ω_0 are the plasma and electron collision frequencies, respectively. For the sake of simplicity, the waveguide loss values are estimated using an isotropic Drude model for the laser active region, whereas a more rigorous approach would include (i) the Drude model only in the quantum-well plane [11] and (ii) use of an intersubband absorption model in the growth direction [22]. The temperature dependence of metal permittivity is extracted from the conductivity temperature dependence data in [23]. The full details of the waveguide structure, including the thin highly doped GaAs layers below and above the 10 μm thick active region and the thin metal layers of platinum, gold and copper in the metal stacks, were taken into account in the simulation. Due to lack of information about the metal layers (titanium, palladium germanium and tantalum), these layers are modeled by using the temperature-independent parameters of tungsten. The calculated waveguide losses in figure 2 are in good agreement with the experimental results reported by other groups [24, 25]. The simulation of the optical gain, on the other hand, was performed using the simplified density matrix model

presented in [4]. The gain model includes intersubband LO-phonon, ionized impurity and interface roughness scattering mechanisms. Some key simulation parameters deployed in our simulations are electron heating temperature (90 K), pure dephasing time constant (0.36 ps) and lasing dephasing time constant (1.15 ps). Other simulation parameters can be found in [4].

As shown in figure 2, the metal cladding of Pd/Ge/Ti/Pt/Au exhibits the highest waveguide loss (α_w) over the temperature range of the simulation. The metal cladding of Ti/Pt/Au shows the second-highest waveguide loss, with a small reduction of $\sim 3\text{--}5\text{ cm}^{-1}$ in α_w compared to that of Pd/Ge/Ti/Pt/Au over the temperature range from 90 to 250 K. The metal cladding of Ti/Au shows a further reduction of $> 10\text{ cm}^{-1}$ in waveguide loss. The metal cladding of Ta/Cu/Au has the lowest waveguide loss, $\sim 18\text{ cm}^{-1}$ even at 160 K. The effects of the mirror losses of the different metal contacts are not taken into account in the following discussion. This is because that the mirror loss is much smaller compared to the waveguide loss in MM THz QCLs [5], and the variation of the mirror loss due to different metal contacts is therefore negligible. Since the J_{th} and the $T_{\max}$ of the THz QCLs are strongly affected by the waveguide losses, it is expected that the performance of the devices with different metal claddings could be significantly different.

Figure 3 shows the light–current (LI) characteristics of the THz QCLs (A–D) at temperatures from 10 to 170 K. The devices were biased in pulsed mode with a pulse duration of 250 ns and repetition rate of 1 kHz. The pulse duty cycle is so small (only 2.5×10^{-4}) that the average device electrical power consumption is in the milli-watt range and thus the Joule heating in the device is negligible. At $T = 10\text{ K}$, the J_{th} values are 0.74 kA cm^{-2} for device A (with Pd/Ge/Ti/Pt/Au metal claddings), 0.69 kA cm^{-2} for device B (with Ti/Pt/Au metal claddings), 0.66 kA cm^{-2} for device C (with Ti/Au metal claddings) and 0.68 kA cm^{-2} for device D (with Ta/Cu/Au metal claddings). Device A clearly shows a higher J_{th} value, which is correlated to the highest value of the calculated waveguide losses of the four different structures.

Maximum lasing temperature is an important performance indicator of THz QCL devices. $T_{\max}$ is determined when the temperature-degrading optical gain reaches the optical waveguide loss (figure 2). Devices with lower loss are hence expected to show higher lasing temperatures. The experimental results show $T_{\max}$ of 136 K for device A, 146 K for device B, 170 K for device C and 172 K for device D. The improvement in temperature performance from devices A to D could mainly be attributed to the reduction of waveguide losses, due to the different metal contacts [8]. Device D has the lowest waveguide loss so it attains the highest $T_{\max}$.

The selection of different metal contacts also affects the electrical behaviors of the THz QCLs. Figure 4(a) shows the measured J_{th} of the four devices (A–D) as a function of temperature from 10 K to their respective $T_{\max}$. Within the experimental uncertainty, one can find a fairly good correlation between the threshold current density and the calculated waveguide loss—the device with a lower waveguide loss

Figure 3. Temperature-dependent LI curves for the THz QCL devices (A–D) with different metal claddings. The ridge waveguides of all devices are $150\ \mu\text{m}$ wide and $1\ \text{mm}$ long and are fabricated using (a) Pd/Ge/Ti/Pt/Au, (b) Ti/Pt/Au, (c) Ti/Au and (d) Ta/Cu/Au metal contacts. The bias is applied in pulsed mode (pulse width = $250\ \text{ns}$, repetition rate = $1\ \text{kHz}$). The Ta/Cu/Au shows the highest T_{max} and lowest J_{th} at $10\ \text{K}$.

exhibits a lower J_{th} , particularly at higher temperatures. The tested devices were lasing at longer lasing wavelengths than the designed value at lower temperatures, while the calculated waveguide losses and optical gain were obtained at the designed lasing wavelength. This could lead to discrepancies between the simulation and experimental results, as shown in figure 2. Device A exhibits the highest J_{th} over the entire temperature range, which stems from the highest waveguide loss as shown in figure 2. The J_{th} of device D, which has the lowest loss, is slightly higher than that of device C at low temperatures. This might be attributed to the different profile of the ridge sidewalls. Indeed, SEM inspection indicates that the sidewalls of device D are much more vertical than the others, which widens the gap between the top metal and the edge of the ridge ($\sim 12\ \mu\text{m}$ for devices D versus $\sim 10\ \mu\text{m}$ for the others). The optical image also shows that device D was cleaved into the shortest Fabry–Perot ridge waveguide ($930\ \mu\text{m}$), and hence its mirror loss should be the highest among the four devices. The higher mirror loss would give rise to a higher threshold current density. Figure 4(b) shows the measured current–voltage (IV) curves of the four devices (A–D). As mentioned earlier, Pd/Ge/Ti/Pt/Au forms an ohmic contact with the n^+ GaAs layer; device A therefore exhibits the lowest bias voltage under any given electrical current among

Figure 4. (a) The threshold current densities of the devices (A–D) as a function of temperature. (b) Current–voltage (IV) curves of the devices at $10\ \text{K}$. Device A exhibits the best IV characteristics due to its ohmic metal contacts. Devices B–D show inferior IV characteristics in which extra bias ($\sim 0.8\ \text{V}$) is needed to overcome the Schottky barrier at the metal/semiconductor interface.

the four devices. Other metal stacks form more or less a similar Schottky contact with the n^+ GaAs layer, so extra bias voltage ($\sim 0.8\ \text{V}$) needs to be applied to overcome the Schottky barrier between the top metals and the semiconductor layer (non-alloyed bottom contact with LT-GaAs should form an ohmic contact). For a given bias of $10\ \text{V}$ (below lasing threshold) the current density was measured to be $0.7\ \text{kA cm}^{-2}$ for device A, $0.66\ \text{kA cm}^{-2}$ for devices B and C and $0.65\ \text{kA cm}^{-2}$ for device D. The IV curves in figure 4(b) indicate that the electrical current is injected into device A most easily, while other devices show similar extra resistance. The extra voltage drop to overcome the Schottky energetic barrier at the metal/semiconductor interface in devices B, C and D leads to extra electrical power consumption, which eventually converts to Joule heat. The active region of the device could be over-heated if the Joule heat cannot be dissipated away quickly and gets accumulated in the core. This can be the case when the device is operated in continuous-wave mode (i.e. under dc bias). The device performance deterioration due to Joule heating may become substantial and completely offsets the benefits arising from the lower waveguide losses in non-ohmic metal claddings. Nevertheless, when the devices are biased in pulsed mode with a low duty cycle (such as in the measurements of this study), the improvement in temperature performance due to lower waveguide losses overwhelms the deterioration in electrical current injection. This explains why device D exhibits the best performance.

4. Conclusion

Four groups of THz QCLs with different metal contacts were fabricated and characterized. The stack of annealed

Pd/Ge/Ti/Pt/Au can form an ohmic contact with an n-GaAs semiconductor layer; however, the metal contact has a high optical loss, which degrades the device performance. On the other hand, other metal stacks, annealed Ti/Pt/Au, non-annealed Ti/Au and non-annealed Ta/Cu/Au, form a Schottky-like junction with the n^+ GaAs layer but exhibit lower waveguide losses. Among them, Ta/Cu/Au has the lowest calculated waveguide losses at 3.75 THz. Consequently, the device with such metal stack claddings exhibits the highest $T_{\max}$ in pulsed mode. The metal stack of Ti/Au with a thinned Ti layer (only 5 nm thick) also shows relatively low waveguide losses (very close to that of Ta/Cu/Au), and exhibits comparable $T_{\max}$ and threshold current density to that of Ta/Cu/Au. It is worth pointing out that it is much less demanding to fabricate the Ti/Au-based metal claddings than the Cu-based ones. The experimental results reveal that lowering the optical losses of the metal claddings in THz QCLs becomes more prominently important for enhancing $T_{\max}$ and reducing J_{th} in pulsed mode operation.

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