Waveguide Simulation of a THz Si/SiGe Quantum Cascade Laser*

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Abstract: The waveguide design is one of the most important parts in a terahertz quantum cascade laser (QCL). Si/SiGe QCL waveguides, based on the Drude model and finite-difference time-domain (FDTD) method, are designed by the traditional refractive index waveguide structure, the single-sided metal structure, the double-metal clad structure, and a novel metal/metal silicide structure. The metal/metal silicide structure, showing high modal confinement, is convenient in process engineering and is expected to be a viable waveguide solution for Si/SiGe QCLs in the THz range.

Key words: terahertz; Si/SiGe; quantum cascade laser; waveguide
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1 Introduction

Research on Si/SiGe quantum cascade lasers (QCL) is of particular interest due to the development of silicon-based optoelectronic integration. Si/SiGe QCL operates via hole intersubband transitions to overcome the indirect bandgap character of Si and SiGe alloy and can achieve a silicon LED[1]. The main challenges of a long-wavelength QCL are: improved injection efficiency, increased electron oscillation intensity during transition, reduced modal losses, and increased modal confinement.

The thickness of the active layer should not be less than half of the wavelength if the traditional refractive index waveguide structure for QCL[2] is used. For instance, the active layer thickness of QCL operating at 3THz requires 15μm. It seems impossible for Si and Ge to achieve such thickness because of their large lattice mismatch. So, the adoption of metal as a confining layer can not only enhance the confinement of THz waves, but also help to cool the active layer faster.

Based on the Drude model and finite-difference time-domain (FDTD) method[3], a waveguide simulation of a Si/SiGe QCL has been carried out. This paper compares the TM modal losses and confinement of four waveguide structures: the traditional refractive index waveguide, the single-sided metal, the double-metal clad, and a novel metal-metal silicide structure. Finally, we optimize the structure for the design of Si/SiGe terahertz QCLs.

2 Waveguide structure and Drude model

As Figure 1 shows, Si/SiGe QCL includes an active layer, a doped layer, and a confining layer. According to our primary study on Si/SiGe QCL active layer band engineering[4], the active layer here is 3nm Si and a 3nm $Si_{0.7}Ge_{0.3}$ quantum cascade structure, which operate via an intersubband transition between LH1 and HH1. The boron-doped layer is $Si_{0.85}Ge_{0.15}$ with a concentration of $5\times10^{19}cm^{-3}$. This layer acts as a buffer layer for relaxation and provides a good ohmic contact. The upper confining layer is Al. For the four structures discussed in this paper, the bottom confining layers are: silicon substrate, silicon substrate, and Al or WSi_2 layer.

There is surface plasma in a metal-coated waveguide. This paper mainly discusses the TM waveguide mode because the plasma has an impact on the TM mode[5]. Metal dielectric primarily depends on the change of electric dipole. In the IR range, all the metals' optical properties are similar, which is accurately described by the Drude model.

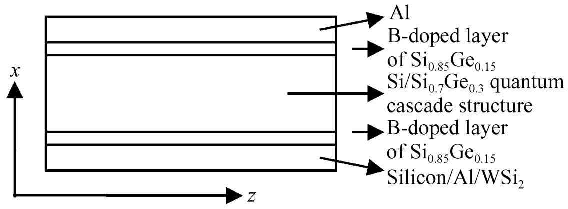

Fig.1　Schematic diagram of the Si/SiGe THz waveguide structure

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Table 1 Complex refractive index of materials

Wavelength/μm	50	100	200
Al	190.923 + 257.323i	300.308 + 349.217i	444.737 + 479.691i
WSi_2	20.217 + 59.453i	49.707 + 91.698i	92.347 + 127.217i
Heavily doped $Si_{0.85}Ge_{0.15}$	5.878 + 5.167i	8.060 + 7.559i	11.222 + 10.867i
Intrinsic $Si_{0.7}Ge_{0.3}$	3.4804 + 0.0003i	3.4804 + 0.0007i	3.4804 + 0.0010i

$$\begin{cases}\varepsilon_1 = \varepsilon_\infty - \omega_p^2/(\omega^2+\gamma^2)\\ \varepsilon_2 = \gamma\omega_p^2/[\omega(\omega^2+\gamma^2)]\end{cases} \quad (1)$$

Here $\varepsilon_\infty = n^2\omega$, ω_p, and γ are wave number, plasma frequency, and damping parameter. The relationship between complex dielectric permittivity ε and complex refractive index N is: $\varepsilon \equiv \varepsilon_1 + i\varepsilon_2 \rightarrow N \equiv (n + i\kappa)^2$. So we obtain:

$$\begin{cases} n = \sqrt{\varepsilon_1 + \sqrt{\varepsilon_1^2+\varepsilon_2^2}}/\sqrt{2}\\ k = \sqrt{-\varepsilon_1 + \sqrt{\varepsilon_1^2+\varepsilon_2^2}}/\sqrt{2}\end{cases} \quad (2)$$

κ is the imaginary part of the complex refractive index, also known as the extinction coefficient. ω_p and γ of Al and WSi_2 are taken from Refs. [6,7]. For the heavily doped $Si_{0.85}Ge_{0.15}$ alloy, according to the Drude model, we have

$$\omega_p^2 = N_h e^2/(m_h\varepsilon_\infty\varepsilon_0), \quad \gamma = e/(m_h\mu_h) \quad (3)$$

$N_h = 5\times10^{19}\,cm^{-3}$ is the doped concentration, $m_h = (m_{HH}^{3/2} + m_{LH}^{3/2})/(m_{HH}^{1/2} + m_{LH}^{1/2})$, the mass of heavy-hole and light-hole are $m_{HH} = (0.537 - 0.207x)m_0$ and $m_{LH} = (0.153 - 0.110x)m_0$, m_0 is the mass of electron, and the hole mobility μ_h is $49cm^2/(V\cdot s)$[8]. For the intrinsic SiGe alloy, the real refractive index in the IR range is $n \approx 3.42 + 0.37x + 0.22x^2$ (where x is the Ge mole fraction) the imaginary part is obtained by linear interpolations from that of Si and Ge[9], and the effective Ge mole fraction x in the active layer is 0.15.

3 FDTD method

FDTD is one of the most successful methods for the numerical calculation of electromagnetic fields[4]. For 2D TM polarization, the Maxwell equation can be expressed as:

$$\frac{\partial H_y}{\partial t} = -\frac{1}{\mu_0}\left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x}\right),$$

$$\frac{\partial E_x}{\partial t} = -\frac{1}{\varepsilon}\times\frac{\partial H_y}{\partial z}, \frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon}\times\frac{\partial H_y}{\partial x} \quad (4)$$

In order to carry out numerical calculation, the Yee's grid space can be dispersed. Here, Δx and Δz are the grid space step of direction and Δt is the time step.

$$(i,k,n) = (i\Delta x, k\Delta z, n\Delta t),$$

$$\text{and } c\Delta t \leqslant \sqrt{\left(\frac{1}{\Delta x}\right)^2 + \left(\frac{1}{\Delta z}\right)^2} \quad (5)$$

Therefore, the Maxwell equation can be expressed as:

$$H_y^n(i,k) = H_y^{n-1}(i,k) - \frac{\Delta t}{\mu_0\Delta z}[E_x^{n-1/2}(i,k+1/2) - E_x^{n-1/2}(i,k-1/2)] + \frac{\Delta t}{\mu_0\Delta x}[E_z^{n-1/2}(i+1/2,k) - E_z^{n-1/2}(i-1/2,k)]$$

$$E_x^{n+1/2}(i,k+1/2) = E_x^{n-1/2}(i,k+1/2) - \frac{\Delta t}{\varepsilon\Delta z}[H_y^n(i,k+1) - H_y^n(i,k)]$$

$$E_z^{n+1/2}(i+1/2,k) = E_z^{n-1/2}(i+1/2,k) + \frac{\Delta t}{\varepsilon\Delta x}[H_y^n(i+1,k) - H_y^n(i,k)] \quad (6)$$

One important characteristic of FDTD is to set Yee's grid for computing space. However, it is impossible to calculate all spaces because the limitation of computer memory. An absorbent boundary is added to remove the impact of cutting off the border. The absorbing boundary installs a special border where the incident wave can pass through layers without reflection and rapid decay. Here, we use the un-split perfect matched layer (UPML). The dielectric constant and magnetic conductivity is expressed as:

$$\hat{\varepsilon} = \varepsilon\hat{S}, \hat{\mu} = \mu_0\hat{S}, \hat{S} = \begin{pmatrix} s^{-1} & 0 & 0\\ 0 & s & 0\\ 0 & 0 & s\end{pmatrix}, s = \kappa - i\frac{\sigma}{\varepsilon_0\omega} \quad (7)$$

If the PML thickness is L', we must meet the following conditions in order to converge.

$$\sigma(x) = \sigma_{max}\left(\frac{x}{L'}\right)^m, \kappa(x) = 1 + (\kappa_{max} - 1)\left(\frac{x}{L'}\right)^m \quad (8)$$

$2 \leqslant m \leqslant 4$ and a detailed description of PML can be found in Refs. [10,11].

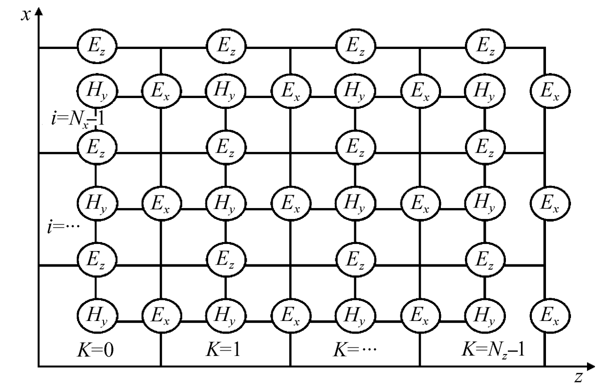

Fig.2 Location of the TM fields in the computational domain by FDTD

Table 2 Structure of Si/SiGe THz quantum cascade laser

Sturcture		(a) Traditional refractive index waveguide	(b) Single-sided metal structure	(c) Double-metal clad structure	(d) Metal-metal silicide structure
Width /μm	Al	0.00	0.20	0.20	0.20
	B-doped layer	0.05	0.05	0.05	0.05
	Active layer	6.00	6.00	6.00	6.00
	B-doped layer	0.05	0.05	0.05	0.05
	Nether confining layer	10.00	10.00	0.20	0.40
κ		0.182	0.066	0.025	0.053
α/cm^{-1}		114.35	41.47	15.71	33.30
Γ/%		27.65	61.32	96.46	95.00
$g_{th}=\alpha/\Gamma$(cm^{-1})		413.56	67.63	16.29	35.05

The nether confining layers of different structures are (a) silicon substrate, (b) silicon substrate, (c) Al, (d) WSi_2.

4 Results and discussion

We aimed to minimize the relevant figure-of-merit α/Γ, the ratio of modal losses α to the modal confinement factor Γ, in the QCL waveguide design. This is useful for an approximate comparison of different structures,

$$g_{th} = \alpha/\Gamma = (\alpha_w + \alpha_m)/\Gamma \qquad (9)$$

$\alpha_w = 4\pi\kappa/\lambda$, $\alpha_m = -\ln R/L$, λ is the wavelength, R is the reflectivity, and L is the length of waveguide. Since the waveguide length is far larger than the wavelength, α_m is very small (1cm^{-1} approximately). We ignore it in the following discussion.

4.1 Comparison of different waveguide structures

Table 2 shows the comparison of the traditional refractive index waveguide structure, the single-sided metal structure, the double-metal clad structure, and the novel metal-metal silicide structure. The wavelength of the QCL is 200μm.

Table 2 shows that the mode mainly leaks to the silicon substrate and makes confinement in traditional refractive index waveguide (a) very poor. A 6μm active layer only confines about 30% of the mode. The active layer can be increased to enhance the confinement. But achieving a thick active layer is difficult because of the lattice mismatch between Si and Ge.

In contrast, the single-sided metal waveguide (b) shows superiority in restrictions in the THz region. Due to surface plasma, light is confined on the interface of the semiconductor and metal. Second, the heavily doped layer decreases the coupling between plasma and the mode[12]. The first III-V QCL in the world adopted this method.

However, because the hole mass of a heavily doped semiconductor is large and the migration rate is low, at the bottom of the waveguide we cannot build an effective limitation. So, the single-sided metal structure only restricts half the mode. Compared with (b), the double-metal clad structure (c), which is clamped by two metal layers, avoids substrate carrier absorption and gives a high confinement factor ($\Gamma \approx 1$).

The double-metal clad structure can greatly increase the confinement, but are difficult to achieve because the semiconductor material cannot grow on the metal layer. Therefore, we should use bonding, which greatly increases the difficulty of the process. Due to the large size of metal silicide substrate development, a metal/metal silicide structure becomes the first choice. Examining Table 2 (d), the performance of the metal/metal silicide structure has been greatly improved. Because the plasma effect of metal silicide is weaker than that of metal, it is necessary to increase the thickness of metal silicide. The introduction of metal silicide, which is suitable for Si/SiGe QCL, confines the mode properly and simplifies the process.

4.2 Structural optimization of a metal/metal silicide waveguide

The relationship between TM modal losses α and WSi_2 thickness in metal/metal silicide structure is shown in Fig. 3 (a). We assume that the Al and the active layer thicknesses are 0.2 and 6μm, the doped layer is 0.05μm, and the laser wavelengths are 50, 100, and 200μm. The diagram illustrates that a short wavelength corresponds to larger modal losses. Depending on different wavelengths, as the metal silicide layer thickness increases, the modal losses α decreases significantly. The loss reaches a plateau when the thickness of silicide is more than 0.4μm.

Figure 3 (b) are TM modal losses α (solid line) and the modal confinement factor Γ (dashed line), for wavelengths of 50, 100, and 200μm, as a function of SiGe active layer width, for an Al layer thickness of 0.2μm, a WSi_2 layer of 0.4μm, and a contact layer

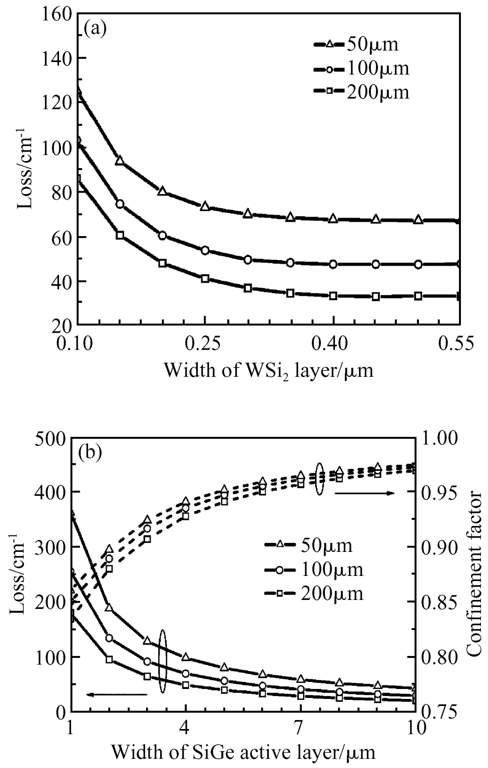

Fig.3 (a) TM modal losses in Al-SiGe-WSi_2 waveguides with a 6μm thick active layer, as a function of the width of metal silicide (The wavelengths are 50, 100, and 200μm.); (b) TM modal losses (solid line) and the modal confinement factor (dashed line) in Al-SiGe-WSi_2 waveguides, with 0.05μm thick contact layer ($N_h = 5 \times 10^{19}$ cm^{-3}), as a function of the active region width (The wavelengths are 50, 100, and 200μm.)

of 0.05μm. According to the calculations, the waveguide loss is greater and the model confinement factor is slightly larger for shorter wavelengths. For different wavelengths, as the active layer thickness increases, the modal losses decrease and the confinement factor becomes larger. Therefore, we should increase the active layer thickness to enhance the performance of waveguide.

5 Conclusion

The Drude model and the FDTD method are used to simulate the TM modal losses and confinement factor in a traditional refractive index waveguide structure, a single-sided metal structure, a double-metal clad structure, and a novel metal-metal silicide structure in the THz range. The results show that the usage of a metal/metal silicide structure not only reduces the modal losses, but also has a high modal confinement factor. At the same time, it is easier to achieve the structure which can be adopted for Si/SiGe QCLs. Finally, we optimize the structure by comparing modal losses and confinement factor with the change of metal/metal layer, active layer thickness, and wavelength.

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太赫兹 Si/SiGe 量子级联激光器波导模拟*

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摘要：波导层结构设计是制备太赫兹(THz)量子级联激光器的关键问题之一.本文基于德鲁得(Drude)模型，利用时域有限差分(FDTD)法，对 Si/SiGe 量子级联激光器的波导层进行优化设计，从理论上对传统的递变折射率波导、单面金属波导、双面金属波导以及金属/金属硅化物波导横磁模(TM 模)的模式损耗和光场限制因子进行了对比分析.结果表明，金属/金属硅化物波导不但可以减小波导损耗，而且有很高的光学限制因子，同时其工艺也比双面金属波导容易实现，为 Si/SiGe 太赫兹量子级联激光器波导层的设计提供了一定的理论指导.

关键词：太赫兹；Si/SiGe；量子级联激光器；波导
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