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Topical Review

Towards monolithic integration of germanium light sources on silicon chips

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Abstract

Germanium (Ge) is a group-IV indirect band gap semiconductor, and therefore bulk Ge cannot emit light efficiently. However, the direct band gap energy is close to the indirect one, and significant engineering efforts are being made to convert Ge into an efficient gain material monolithically integrated on a Si chip. In this article, we will review the engineering challenges of developing Ge light sources fabricated using nano-fabrication technologies compatible with complementary metaloxide-semiconductor processes. In particular, we review recent progress in applying high-tensile strain to Ge to reduce the direct band gap. Another important technique is doping Ge with donor impurities to fill the indirect band gap valleys in the conduction band. Realization of carrier confinement structures and suitable optical cavities will be discussed. Finally, we will discuss possible applications of Ge light sources in potential photonics-electronics convergent systems.

Keywords: germanium, silicon, photonics, electronics, CMOS, light source, monolithic integration

(Some figures may appear in colour only in the online journal)

1. Introduction

Feynman precisely predicted the emergence of hand-held mobile computers with human face recognition systems [1] in 1959, when historical patents for integrated circuits (ICs) were filed by Kilby [2] and Noyce [3]. Currently, more than 1 billion complementary-metal-oxide-semiconductor (CMOS) field-effect transistors (FETs) are integrated in a large-scale IC (LSI), and the semiconductor industry has been



continuously scaling down the channel length of FETs in the last four decades towards sub-10 nm technology nodes [4, 5]. In addition to the electronic integration, various photonic devices have also been integrated on silicon (Si) [6–17].

Currently, a laser-diode (LD) using a group III–V compound semiconductor is used in a commercially available Si photonic chip [6–17]. In this device, the coherent light from the III–V LD propagates through an optical fibre, which is coupled to a Si waveguide (WG) through a grating coupler [18]. Another scheme is to employ a hybrid integration of III– V materials on Si, where a propagating mode in a Si WG is evanescently coupled to an optical gain medium made of a III–V material [19–22]. While the use of III–V materials [15, 17, 19, 22, 23] is a practical option available in the

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near-term, there are growing needs to develop monolithic light sources compatible with CMOS processes in order to reduce the cost for manufacturing, while ensuring the scalability and high yields [5, 24–31]. Therefore, significant efforts are being made to develop group-IV LDs, however group IV materials like Si and Ge are in-direct band gap semiconductors.

After the discovery of efficient light emission from porous-Si by quantum confinements [32, 33], the performance of Si-based light sources has steadily improved over the years [6, 7, 9, 30, 34–40]. In particular, a quantum efficiency exceeding 23% was achieved by passivating the surface using high-pressure water vapour annealing [35, 38]. These Sibased light sources would be useful for applications with wide wavelengths over a wide range of visible to near-infrared (NIR). However, they are not compatible with Si photonic passive devices using a Si WG, since the emitted light from a quantum confined Si nano-structure is blue-shifted compared with the band gap energy of Si (1.1 eV), and thus it will be strongly absorbed in a Si WG.

Germanium (Ge) is an another promising material compatible with CMOS processes; the band gap of Ge is around 0.8 eV [41, 42], corresponding to a wavelength of 1550 nm, which is commonly used in glass fibres due to the minimum in absorption losses at this wavelength. Ge has already been introduced in CMOS processes for strain-engineering at the source and the drain of p-channel MOSFETs [4, 43-45], and Ge is also used for photo-detectors (PDs) in Si photonics [5, 46, 47]. If a practical Ge LD is available, we can realize full monolithic integration of opto-electronic integrated circuits with Ge LDs, Ge PDs, Si WGs, modulators, and many other optically passive components like splitters and gratings [6–16]. Currently, there are several reports on successful laser operation of Ge Fabry-Perot (FP) WGs by optical pumping [48] and by electrical pumping [49–51] at room temperature, in addition to Terahertz (THz) lasers in Ge at low temperatures [52–54]. The recent success on germanium-tin $(Ge_{1-x}Sn_x)$ lasers by optical pumping at low temperatures [55] also proved the theoretical prediction of the directindirect transition upon changing the composition, x [56, 57]. There are many review articles [5, 24-31, 58, 59] covering recent progress on the development of Ge-based light sources, which prove significant attention has been directed to this area. In order to avoid duplicating other reviews, our focus in this article is to introduce wide varieties of technological options for enabling direct recombination in Ge. Some pedagogical introductions to light-emission, waveguides, and strain-engineering are summarized in the appendices. We will also raise and discuss many unknown fundamental issues such as requirements for positive optical gain from Ge, which must be addressed by research communities for the future.

2. Various technological approaches for Ge-based light sources

In this section, we will overview various technical approaches to develop Ge-based light sources using Si processes, and we will discuss technical details in the later sections. Figure 1 shows a schematic summary of various options to fabricate Ge-based light sources. Of course, there are many other process options, which are not covered in figure 1. The conventional wisdom for developing a new LD is to heavily rely only on epitaxial growth techniques [60, 61]. Whilst fully respecting the importance of the process developments in epitaxial growth, however, we feel that other routes towards the development of Ge-based light sources will also be important, since various nano-fabrication technologies are available in Si processes in addition to epitaxial growth. However, the technical hurdle of converting an indirect band gap semiconductor to a direct band gap semiconductor is not easy to overcome, and the use of all available technologies in

The first big choice is material selections to be used for the active gain media and cladding layers. Pure Ge is the most widely used material [5, 25–30, 59] in this area, while there is an increasing number of publications on GeSn as well [31, 55, 58]. In order to grow these materials various deposition process technologies are used such as ultra-highvacuum-chemical-vapour-deposition (UHV-CVD) [24, 46– 48, 50, 62–65], molecular-beam-epitaxy (MBE) [51, 66–69], reduced-pressure-chemical-vapour-deposition (RP-CVD) [70–74], low-energy plasma-enhanced-chemical-vapourdeposition (LEPE-CVD) [75–78], and so on.

Si processes should be considered for Ge-based light sources.

The next choice is the structure of the active materials. Most of the research activities are based on bulk Ge [5, 25-31, 58, 59]. However, considering the history of III-V LDs, there are significant advantages in reducing the dimensionality (D) [60, 61, 79] from bulk (3D) to quantum-well (QW, 2D) [80], nano-wire (NW, 1D) and down to quantum-dot (QD, 0D) architectures to achieve lower threshold currents for laser operation and improve high temperature operation [79]. GeSn [31, 58] is particularly promising in this regard, since the double heterostructures with type-I band alignments are theoretically proposed [81]. Here, we would like to emphasize the possibilities of using patterning techniques such as lithography and etching to make these quantum nano-structures [30, 82-84]. Currently, dry-etched vertical Si QWs called fins [82, 85] were successfully introduced in mass production as FinFETs for CMOS [4]. The structures like fins, NWs, or QDs, can be patterned using standard Si processes, and top-down pattering technologies will play an important role for the development of Ge-based light sources in addition to conventional epitaxial growth technologies [30].

Other key piece for the fabrication of Ge light sources is n-type doping and stress-engineering [5, 25, 26, 28–30, 59], which are certainly different from the III to V LDs technologies. This is coming from the quasi-direct band gap character of Ge, which has a conduction minimum at the *L* point [28, 59, 86–90], whose energy is about 0.14 eV smaller than the bottom of the conduction band minimum at the Γ point. It was proposed by Liu [86] to dope with n-type impurities to fill the *L*-valley with carriers, while additional electrons and holes populated by optical or electrical pumping will be efficiently injected to the Γ point. Following the proposal, there were many experimental reports confirming the



Figure 1. Various combinations to fabricate Ge-based light sources. (a) Various options are shown for materials, fabrication processes, active structures, doping recipes, strain engineering methods, cavities structures, and carrier injection procedures. (b) An example of selected options is shown for Ge fin LED.

enhanced light emission from Ge by various processes such as *in situ* doping during growth [24, 63–65], ion implantation [91], spin-on-dopant (SOD) [67–69, 92], and so on. There is no consensus on the exact values of how much doping would be required to expect positive optical gain values from Ge [30, 31, 59, 77, 90]. The emergence of positive optical gain also depends on the lifetime of excess carriers [93–97], which is quite sensitive to the quality of Ge. We will further review doping processes in section 5.

Moreover, it was theoretically predicted that Ge becomes an intrinsic direct band gap semiconductor, if we apply a tensile strain of about 2% [86–88, 98, 99], which is not impossible using various strain-engineering technologies in Si industries [4]. Hetero-epitaxial growth was the classical way to apply stress to the optically active layer during the growth due to the mismatch of the lattice constant [60, 61], while a tensile strain of about 0.25% is applied to Ge grown on Si by the difference in the thermal expansion coefficients between Ge and Si [5, 30, 47]. Even stronger stress can be applied by depositing a Si₃N₄ stress liner [100–102], or employing a membrane structure to fabricate micro-electro-mechanicalsystems (MEMSs) [59, 78, 103, 104]. We will discuss these stress-engineering technologies in section 4.

The choice of a suitable substrate is another important aspect. Considering the cost requirement for future products, the use of a bulk Si substrate is the most attractive option. However, if we use a bulk Si substrate, the Ge light source cannot be compatible with standard Si photonic devices, which require a silicon-on-insulator (SOI) substrate. It will be relatively straightforward to transfer the technologies developed using Si bulk substrates to the technologies based on SOI substrates. Another substrate is a Ge-on-insulator (GOI) substrate [105-112], which would have better crystalline quality compared with Ge directly grown on Si or SOI. The third option is the use of III-V substrate such as galliumarsenide (GaAs) for the growth of Ge [113–116]. The lattice constants of Ge and GaAs are almost the same, and heteroepitaxy is one of the most reliable and traditional way to make a QW. It will also be useful to investigate the impact of tensile strain [117]. These research activities would be mainly to investigate fundamental material properties of Ge rather than near-term applications, but Ge grown on III-V materials may be useful for high-value products such as extremely efficient solar cells [116] for space applications in satellites or advanced CMOS circuits with Ge channels.

After the completion of the active layers, optical cavities [60, 61] suitable for Ge-based LDs must be designed and fabricated. FP cavities using bulk Ge WGs are simple yet useful structures [65]. For single mode operation in the future, distributed-feedback (DFB) cavities or distributed-Bragg-reflector (DBR) mirrors will be integrated [60, 61]. For direct coupling to optical fibres, structures similar to a vertical-external-cavity surface-emitting-laser (VECSEL) [60, 118] will be quite attractive, although the deposition of thick DBR

mirrors on both sides of the substrate will be challenging, since Si CMOS processes are based on planar technologies. We can also utilize more exotic cavities like disks, rings, or photonic-crystals (PhCs) [60]. These cavities typically have a large quality (Q)-factor, compared with other cavities, therefore they are suitable for analysing fundamental material properties as well as for applications to quantum technologies. These cavities will be reviewed in section 6.

The final issue is the scheme for carrier injection. Traditional III–V LDs are based on vertical injection, since the key process technology is epitaxial growth [60]. On the other hand, for planar Si technologies, lateral carrier injection is easier to implement in terms of designs and fabrications [29, 30, 83, 101, 102]. There are many other possibilities, e.g., the combination of lateral and vertical injections [104, 118, 119].

As an example, we show in figure 1(b) what kind of options we chose to make a Ge fin-type light-emitting diode (LED) [83]. We chose Ge as an active material and the structure was multi-fins, which are multiple-quantum-wells (MQWs) made vertically to the substrate. In order to make the Ge fins, first, we used conventional lithography and dry etching to make Si fins. Then, RP-CVD was used to selectively grow SiGe epitaxially on top of the sidewalls of the Si fins, followed by the oxidation condensation technique [83] to make pure Ge fins [83, 120–124]. The fabricated Ge fins are expected to have better crystalline quality, since the 3D Ge fins can release the strain during the condensation oxidation by stretching the fins vertically to the substrate. Thus, low dark current was confirmed by lateral carrier injection [83]. In the next sections, we will review more technological details.

3. Active materials and structures

Active materials and their structures are one of the most important issues for Ge-based light sources, and we summarized the structure and fabrication processes in table 1. The emission wavelengths actually depend on the stress engineering techniques, and therefore, the listed values just stand for approximate wavelengths range published in references.

3.1. Virtual substrate (VS): a brief history of strained Si

The difference in the lattice constant between bulk Si and Ge is about 4.2%, which is too huge to overcome during Ge growth on Si [158–160]. The growth of single crystalline $Si_{1-x}Ge_x$ layers [158–160] is an important research area and it is still quite a challenging classical topic [27]. Here, we briefly discuss the historical background of $Si_{1-x}Ge_x$ growth technologies developed for bipolar transistors and CMOSFETs.

Under lattice-matched conditions, the epitaxially grown layer can be perfectly aligned with the original substrate, which is known as *pseudomorphic* growth [27, 158–160]. However, such growth is difficult: if the grown epi-layer exceeds the *critical thickness*, we expect significant densities of defects, such as threading dislocations, misfit dislocations,

and stacking faults [27, 158-160]. The critical thickness depends on the Ge content, x, and larger x results in smaller critical thickness, as expected [27, 158–160]. Therefore, a graded buffer layer with a gradual increase of x upon growing is often prepared before the target channel layer is formed [27, 158–160]. The graded buffer layer is fully relaxed, and typically around 1 μ m or more is required to secure excellent crystalline quality [27, 158-160]. A substrate with such a graded buffer layer is called VS, since we can assume the substrate is made of the crystal at the top surface (figure 2(a)). Nevertheless, it has proved quite difficult to grow excellent strained-Si layer with tens of nano-meters on top of VS for application as the channels in MOSFETs due to stringent requirements to secure CMOS circuitry with billions of FETs. The wafer-scale uniform epitaxial growth process is denoted global strain technology, and according to the ITRS roadmap around 2000, it was expected to be introduced in mass production around 2005 [4]. However, global strain technologies have not been commonly introduced in CMOS. Instead, local strain technologies using Si₃N₄ stress liners were widely introduced around 2001, even earlier than predicted by the roadmap [161, 162].

3.2. Direct Ge growth on Si

Considering the above history of global strain engineering in CMOS, it is quite surprising that Si photonic industries [18] could use a Ge PD for mass production, which is grown directly on Si [5, 27, 30, 46, 47]. There are several deposition techniques, as shown in table 1, but the overall strategies are the same (figure 2(b)). First, a thin buffer layer of Ge was deposited at low-tempearture (LT, ~400 °C) directly on Si. The LT layer contains a lot of defects [46, 47]. Subsequently, the second Ge layer is deposited at high-temperature (HT, ~700 °C) with a higher growth rate. After deposition, postdeposition annealing is carried out [5, 30, 46, 47]. The annealing conditions are critical to improve the quality of the film, which is evidenced by increased PL intensities [102, 125]. It was reported that multiple hydrogen annealing heteroepitaxy (MHAH) [110, 126] improved the crystalline quality. Among various process technologies, RP-CVD is the commonest process in industries ready for mass production [70-74], while UHV-CVD [24, 46-48, 50, 62-65] and MBE [51, 66–69] are quite useful in universities. There are many other tools, e.g., hot-wire CVD, which is useful for the growth of a large area at low temperatures [127]. Oxidation condensation and subsequent growth is also a very interesting and unique growth technique for Si [129, 130].

3.3. Bulk Ge substrate and bonding to Si

We think that gaining a fundamental understanding of material properties and physics of Ge is still important. In this regards, the use of bulk Ge substrates are useful, since we can assume almost perfect crystalline quality, while we need to think about the process technologies for transfer of the Ge light sources made on bulk Ge substrates for the future.

Structure	D	Process	Wavelengths (nm)	Reference
Ge on Si	3	2-steps growth by UHV-CVD	1400 ~ 2200	[24, 46–48, 50, 62–65]
Ge on Si	3	2-steps growth by MBE	$1400 \sim 1700$	[51, 66–69]
Ge on Si	3	2-steps growth by RP-CVD	$1400 \sim 1700$	[70–74]
Ge on Si	3	LEPE-CVD	$1400 \sim 2200$	[75–78]
Ge on Si	3	Cold-wall thermal CVD	$1400 \sim 1700$	[102, 125]
Ge on Si	3	MHAH by RP-CVD		[126]
Ge on Si	3	Hot-wire CVD		[127]
Ge on Si	3	Bulk Ge bonding and polishing	_	[128]
Ge on Si	3	Oxidation condensation and growth	$1400 \sim 1700$	[129, 130]
Ge WG on a Si rib	3	RP-CVD	_	[131]
Ge (100) bulk	3	Bulk Ge substrate	$1400 \sim 2000$	[132]
Ge (110) bulk	3	Bulk Ge substrate	_	[49]
n-Ge bulk	3	Growth by MOCVD for doping	$1400 \sim 2200$	[133]
GeOI	3	Layer transfer with SiO ₂	$1500 \sim 2200$	[105–108]
GeOI	3	Layer transfer with Al ₂ O ₃ /SiO ₂	$1500 \sim 2200$	[109, 110]
GeOI	3	LPE on Si ₃ N ₄		[44, 134]
GeOI	3	LPE on SiO ₂		[111, 112]
poly Ge on metal	3	MIC		[135]
Ge on GaAs	3	Ge on GaAs by UHV-CVD		[113]
Ge on GaAs	3	Ge on GaAs by MOCVD	$1400 \sim 1800$	[114, 115]
SiGe/Si MQW	2	MBE	$1400 \sim 1700$	[136]
Ge/SiGe MQW	2	LEPE-CVD	1000 ~ 1300 (10 K)	[137]
Ge/SiGe MQW	2	LEPE-CVD	$1400 \sim 1700$	[138]
Ge/SiGe MQW	2	UHV-CVD	$1400 \sim 1700$	[139–141]
Ge/SiGe MQW	2	RP-CVD	$1400 \sim 1600$	[142]
Ge QW on IIII-V	2	Growth on $In_xGa_{1-x}As/GaAs$ by MBE	$1400 \sim 2000$	[116, 117]
Ultrathin GOI	2	Oxidation condensation of $Si_{1-x}Ge_x$	$1400 \sim 1700$	[120–122, 124, 130, 143]
Ge fin	2	Dry etching and oxidation condensation	$1400 \sim 1700$	[83, 84]
Ge fin	2	LPE and dry-etching	_	[44]
SiGe/Ge MQW	2	MBE	$1100 \sim 1300$	[144]
a-Ge pillar	1	a-Ge deposition and lift-off	$1400 \sim 2600$	[145]
Ge nano-wire on Si	1	MHAH by RP-CVD	$1400 \sim 2200$	[110, 126]
Si/Ge core/shell QD	0	MBE	$1300 \sim 2000$	[146]
Ge QD powder	0	Mechanical motor-grinding	$1000 \sim 1700$	[147]
Ge QD on Si	0	Ge QDs by MBE	$1300 \sim 1600$	[148–153]
SiGeSn/GeSn	3	UHV-CVD		[154]
GeSn/GeSi	3	MBE	_	[155]
Ge/GeSn/Ge	3	Double heterostructure by MBE	$1800 \sim 2300$	[156]
GeSn/Ge	3	RP-CVD	$2000 \sim 2400$	[55]
Ge/GeSn	3	UHV-CVD	_	[157]

Table 1. Active Ge structures	and fabrication	processes.
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One concern of using bulk Ge substrates is producing an optical confinement in a cavity. The refractive index of Ge is around 4.2, and so the deposition of amorphous (a)-Si or poly crystalline (poly)-Si does not make a WG on top of Ge. Alternatively, it was reported that a Ge bulk substrate was successfully bonded onto a Si substrate for a Ge PD at a process temperature less than 450 °C, and the Ge layer was polished to thin down to 5.4 μ m [128]. This substrate would also be useful for investigating Ge-based light sources.

3.4. GOI

A possible alternative technology to use a bulk Ge substrate is to make GOI by using Smart-CutTM technology [163]. This involves using hydrogen (H) ion implantaion to transfer the Ge layer to the handle Si wafer with or without an oxide

(SiO₂). In principle, this works, however, the size of available Ge wafers is much smaller than that of Si wafers, and therefore, the size limitation will prevent wafer scale bonding in larger scale production. To avoid this issue, we must transfer the grown Ge layer onto a Si substrate which has the same size of the handle wafer. Successful transfers of Ge layer grown on thick VS to make a GOI substrates was reported by several groups [105–110]. There was a concern about the weak adhesion between Ge and SiO₂, and existing commercially available prototypes of GOI substrates were found to be too fragile to make reliable devices [92, 107]. By using Al_2O_3 on top of SiO₂, the adhesion has been improved substantially [109, 110]. The tensile strain of Ge accumulated during the growth is usually preserved during the bonding process [107].



Figure 2. Tensile strain engineered Ge structures. (a) Epitaxially grown Ge layer on the graded buffer virtual-substrate (VS). (b) Two-steps grown Ge layers with the low-temperature (LT) grown buffer layer and the high-temperature (HT) grown epi-layer. (c) Ge Fabry–Perot (FP) waveguide (WG) with the patterned Si₃N₄ stressor [169]. (d) Ge FP WG with the un-patterned Si₃N₄ stress liner [101]. (e) Ge microdiks with the surrounding Si₃N₄ stressor [176]. (f) Ge microdiks grown on GaAs with the Si₃N₄ stressor [115]. (g) Free-standing Ge bridge on insulator [78, 106, 172]. (h) Ge microdiks on free-standing oxide bridge [177].

Liquid-phase-epitaxy (LPE) is also a possible option to make a local GOI structure on a Si substrate by melting Ge on top of an insulator like Si_3N_4 or SiO_2 , and then re-growing single crystalline Ge through a window to the seed Si substrate [30, 44, 111, 112, 134]. Excellent single crystalline structures have been confirmed, paving the way for an investigations into the use of LPE grown Ge for light emissions.

3.5. Quantum wells and quantum dots

Considering several reports on successful laser operations with bulk (3D) Ge [48–51] and GeSn [55], the next challenge would be to improve the performance by reducing the threshold pump power for laser operation. MQWs or QDs are suitable for reducing the threshold, and various process

technologies have been used [116, 117, 136–142, 148–153]. The emission wavelength becomes slightly longer due to the quantum confinement, and therefore, applications to the wavelengths in the 1.3 μ m region should be possible by optimizing the size of the quantum nano-structures. The use of fins or NWs by combining lithography and etching techniques could also be useful for quantum confinement [83, 84, 110, 126, 145].

3.6. GeSn growth

There are two approaches for using GeSn: one is to use GeSn as an active layer with a direct band-gap [56, 57], and another is to use GeSn as a buffer layer to apply tensile-strain to Ge, which is on top of GeSn [81]. The first approach has been

Process	Anisotropy	Strain (%)	Reference
Thermal expansion of Ge on Si in UHV-CVD	Biaxial	0.25	[47, 50, 164–166]
Un-patterned Si ₃ N ₄ on a Ge FP cavity	Uniaxial	1.07	[114]
Un-patterned Si ₃ N ₄ on a Ge microdisk	Biaxial	1	[115]
Un-patterned Si ₃ N ₄ on a Ge microdisk	Biaxial	1.5	[176]
Patterned Si ₃ N ₄ on a Ge FP cavity	Uniaxial	0.4	[168]
Patterned Si ₃ N ₄ on a Ge FP cavity	Biaxial	0.9	[169, 170]
Patterned Si ₃ N ₄ on a Ge FP cavity	Biaxial	0.4	[102]
Hetero-epitaxy of Ge on $In_xGa_{1-x}As/GaAs$	Biaxial	2.33	[117]
Membrane of polyimide	Biaxial	2.0	[145, 167]
Mechanical stress on a Ge membrane	Biaxial	0.6	[171]
Ge membrane	Biaxial	1.13	[104]
Ge membrane with Si ₃ N ₄	Biaxial	1.13	[118]
Ge membrane with Si ₃ N ₄	Uniaxial	0.98	[106]
Ge bridge	Uniaxial	2.77	[172]
Ge bridge	Uniaxial	3.1	[78]
Ge bridge	Uniaxial	5.7	[173]
Ge bridge	Uniaxial	2.3	[110]
Ge microdisk on a SiO ₂ bridge	Uniaxial	0.92	[177]

Table 2. Strain-engineering technologies for Ge.

employed using $Si_{1-x-y}Ge_xSn_y/Ge_{1-x}Sn_x$ [154], $Ge_{1-y}Sn_y/Ge_{1-x}Si_x$ [155], $Ge/Ge_{1-x}Sn_x/Ge$ [156], and $Ge_{1-x}Sn_x/Ge$ [55]. The latter approach was taken using $Ge/Ge_{1-x}Sn_x$ [157]. For both approaches, it will be required to use a double-heterostructure or similar carrier confinement structure in MQWs or QDs for practical applications, considering almost all commercially available III–V LDs are based on MQWs or QDs and do not use a bulk semiconductor as an optically active gain medium.

4. Strain engineering

In the last few years, significant progress has been made in understanding and technologies for strain-engineering in Ge [47, 50, 78, 92, 104, 106, 114, 115, 117, 118, 145, 164–173]. Raman spectroscopy is usually used to analyse the amount of strain from the red-shift of the phonon energy upon the application of the tensile strain [174]. The peak position of the Raman spectrum in the Bulk Ge is located at 301 cm⁻¹, and the shift $\Delta \omega$ is given by

$$\Delta \omega = S\epsilon,\tag{1}$$

where ϵ is the strain and *S* is a coefficient. *S* was reported to be 390 cm⁻¹ for biaxial strain [169, 170], and for uniaxial strain, *S* was 152 cm⁻¹ [78, 173, 175].

Various strain-engineering technologies are summarized in table 2 and figure 2 and will be discussed in more detail in this section.

4.1. Thermal expansion mismatch

It is quite commonly observed that the Ge directly grown on Si has a tensile strain of around 0.25%, using various epitaxial

growth techniques including UHV-CVD [47, 50, 102, 125, 164-166], MBE [51, 66-69] RP-CVD [70-74], LEPE-CVD [75-78], cold-wall thermal CVD [102, 125], and so on. Therefore, this is a genuine phenomenon, although it is surprising that it is a tensile strain rather than a compressive strain, since the lattice constant of bulk Ge is larger than the lattice constant of Si. This means the direct growth of Ge on Si cannot be a pseudomorphic growth with complete lattice matching between Ge and Si. The strain was expected to be relaxed in the LT layer, abut if so, why does the tensile strain remain after the growth? The mechanism was investigated, and it was found that the difference in their thermal expansion coefficients of Si and Ge is responsible for the tensile strain [47, 164], which is crucially important for applications to Ge PDs where the efficient absorption of photons at a wavelenth of 1550 nm is key.

During the growth of a HT layer, both Ge and Si are fully relaxed at high temperatures, where no strain is expected to be remain. Then, during the cooling down to room temperature, both Ge and Si must shrink according to their respective thermal expansion coefficients. However, the thermal expansion coefficient of Ge is larger than that of Si, which means that the Ge layer must shrink more than the Si substrate, while the elastic bonds between Ge and Si will prevent deformation of the layer arriving at the fully relaxed state. As a result the lattice constant of the Ge layer must be slightly larger than that of the equilibrium point in the bulk. The expected tensile strain values depend on the starting temperature for cooling during the growth, and they were calculated in excellent agreement with experiments [164]. In fact, the remaining strain values can be controlled from compressive to tensile by increasing the post-deposition annealing temperature [5, 30, 102, 125]



Figure 3. Finite-element simulations of the stress profile for (a) uniaxial beam, and (b) biaxial beam.

4.2. Tensile stress liner

It is quite natural to think about the application of *local strain* engineering technologies, using a Si_3N_4 stress liner [4, 161, 162] developed for CMOS to Ge-based light sources [102, 114, 115, 168–170] (figures 2(c)–(f)). The internal stress of the Si_3N_4 stress liner can be controlled to be either compressive or tensile, depending on the hydrogen content of the film [161, 162]. Here, it is very important that the structures are patterned, otherwise the expected strain on the flat interface, which can be estimated by the famous Stoney's formula [178, 179], is very weak due to the huge difference in thickness between the stressor film and the supporting substrate. The patterning can be made into the Si_3N_4 layer [102, 168–170] (figure 2(c)), or vice versa i.e., the Ge layer can be patterned, while the Si_3N_4 layer is un-patterned [30, 114, 115, 176] (figures 2(d)–(f)).

It is also very important to recognize that the intensities of the stress strongly depend on the position. Finite-element simulations were employed to calculate the strain profile [30, 169, 177], and it was found that the stress is stronger at the interface [169] and at the corner of the WG [30]. Depending on the structures of Ge and the stressor, both tensile strained and compressive strained regions can appear within the same Ge WG [30]. This local profile of the strain would result in a local change of the band structure at the nano-scale. If the strain profile is optimally designed, the locally tensile stressed region will have a lower direct bandgap compared with the surrounding region with a type-I band alignment [172], which is similar to double-heterostructures in a III-V QW LD. This means that we cannot expect that the entire bulk Ge WG can become a direct band-gap structure, and the cladding region with a lower tensile strain or compressive strain would have a positive absorption coefficient. Therefore, the net optical gain would be significantly reduced, if the optical propagation mode in a WG has a large overlap with the lossy region. Thus, special care must be taken to design a Ge FP WG if the WG is n-type doped due to the increase of the free-carrier absorption. Optimistically, the donated electrons can automatically accumulate into the region where the tensile strain is strong. Then, the actual electron concentration at the tensile stressed region can be even larger than the average impurity doping concentration, while the free electrons in the cladding region can be reduced, contributing to reduction of the loss. However, we still need to further optimize the design of the Ge FP WG, both for impurity and stress profiles.

4.3. Micro-bridge

The use of a MEMS structure for applying stronger stress is attracting great attention these days [59, 78, 104, 106, 110, 118, 145, 167, 171–173, 177]. The mechanical deformations of a free-standing bridge would certainly change the bond lengths of neighbouring Ge atoms. The theoretical proposal to use a MEMS structure for Ge light-emission was made by Lim [103]. Using finite element simulations, he showed the application of biaxial strain of the order 2% is feasible with the possibility of positive optical gain [103]. Examples of the finite-element simulations [177] are shown in figure 3. Later, strong tensile-strain was actually confirmed in various free-standing membrane structures [59, 78, 104, 106, 110, 118, 145, 167, 171–173, 177].

In particular, Jain [106], Nam [172], and Süess [78] successfully fabricated micro-bridge structures almost at the same time. Their designs are quite ingenious, in which a narrow micro-bridge is connected to a wider bridge girder. As discussed in section 4.1, epitaxially grown Ge is tensile strained with about 0.25% larger lattice expansion [164], which means that the Ge has a tendency to be compressed by its own internal force. If the wider bridge grider is movable, the force to pull the connected narrower micro-bridge is stronger, and thus a tensile strain is applied to the microbridge to further expand the bond length of the Ge [59, 78, 106, 110, 172, 173]. A very strong tensile-strain was confirmed, as summarized in table 2.

While these micro-bridge ideas are interesting, it is not obvious how to combine the free standing structure with optical confinement in a cavity. One of the simplest solutions is to prepare two separate materials for a cavity and a bridge [177]. We have used the thermally grown buried-oxide (BOX) of a SOI substrate for making a micro-bridge to apply

Table 3. Process technologies to dope Ge.

Process	Impurity	Concentration (cm ⁻³)	Sheet resistance (Ω)	Reference
In situ by UHV-CVD	Р	1×10^{19}		[65]
In situ by LEPE-CVD	Р	2.5×10^{19}	_	[77]
In situ by RP-CVD	Р	7.5×10^{18}	_	[71]
In situ by RP-CVD	Р	1×10^{19}		[180]
In situ by MOCVD	Р	1×10^{19}	_	[133]
In situ by MOCVD	Р	3×10^{19}		[168]
In situ by MBE	Sb	5×10^{18}	_	[66]
δ -doping by MBE	Sb	2×10^{20}	_	[183]
δ -doping by MBE	Sb	7×10^{19}	_	[184]
δ -doping by MBE	Р	1×10^{20}	120	[108]
δ -doping by UHV-CVD	Р	5×10^{17}	_	[48]
δ -doping by UHV-CVD and annealing	Р	4.5×10^{19}	_	[<mark>166</mark>]
Multiple δ -doping by MBE	Р	7.4×10^{19}	280	[181]
Implantation	Р	6×10^{19}	_	[185]
Implantation and RTA	Р	_	_	[<mark>91</mark>]
Implantation with Co capping	Р	2.7×10^{20}	_	[186]
Implantation and laser annealing	Р		73	[187]
Implantation and laser annealing	Р	_	57	[43]
Implantation and laser annealing	Р	6.5×10^{19}	55	[188]
Co-implantation and RTA	P and Sb	1.3×10^{19}		[189]
Gas phase doping	As	4×10^{19}		[<mark>190</mark>]
GILD	Р	$1.5 imes 10^{20}$	12	[<mark>19</mark> 1]
GILD	Р	5×10^{19}	_	[182]
SOD to bulk Ge	Р	3×10^{19}	36	[192]
SOD to GOI	Р	1×10^{19}	166	[92]
SOD to GOI	Р	1×10^{20}	—	[67, 68]
SOD to Ge on Si	Р	4×10^{19}	—	[<mark>69</mark>]

tensile-strain to the Ge micro-disk on it [177]. Whisperinggallery-modes (WGMs) were successfully observed from the tensely strained Ge microdisk [177].

Another problem of the micro-bridge structure is heating during measurements due to the free-standing structure [110, 177]. Recently, Petykiewicz made a structure where the Ge bridge was bent and connected to the BOX to allow the dissipation of heat during the measurements. They successfully observed FP modes with a *Q*-factor exceeding 2000 [110]. Exciting progress is expected with these ideas for the future.

5. Electron doping

As we discussed above, n-type doping to fill the *L*-valley certainly enhances the spontaneous light-emission probability [86], which was confirmed by many groups and thus is well established [48, 65–69, 71, 77, 91, 92, 133, 166, 168, 180–182]. On the other hand, the impact of doping on the emergence of the optical gain is still controversial [31, 77, 110]. In fact, the crystalline qualities of actual Ge samples depend on the process technologies used, and thus the carrier life-time can vary substantially, which would affect the complex carrier dynamics upon pumping. This makes the impact of doping highly non-trivial [31, 95]. Moreover, some impurities are not activated upon doping, which would further reduce the carrier

life-time, and the inhomogeneous strain profile would further affect the actual carrier profile. At this moment, there is no consensus on how much we should dope Ge with n-type impurities to increase the gain value.

Nevertheless, n-type doping has been shown to improve the quantum efficiency of LEDs. Here, we will discuss various technological options for n-type doping of Ge, as summarized in table 3. In addition to the carrier concentration reported, the sheet resistance is also listed in table 3, although the actual sheet resistance also depends on the depth of the impurity profile.

5.1. In situ doping during growth

In situ doping during Ge growth was reported using various processes, including UHV-CVD [65], LEPE-CVD [77], RP-CVD [133, 180], MOCVD [168], MBE [66, 184], and so on (table 1). Independent of deposition method, there is a trade-off relationship between the crystalline quality and doping concentration, and above $2-4 \times 10^{19}$, significant degradation is observed [5, 30, 102].

5.2. δ -doping

In order to overcome the trade-off, δ -doping was used to achieve even higher doping concentration, while minimizing the deposition thickness of the Ge layer with poor crystalline quality [48, 108, 166, 181, 183, 184]. The δ -doped layer can

Table 4. Novel photonic cavities for Ge.		
Structure	Q-factor	Reference
Micororing on Si	620	[103, 197]
Microdisk on Si	932	[180]
Microdisk on BOX	150	[<mark>67</mark>]
Microdisk on BOX	800	[198, 199]
Microdisk on SiO ₂ bridge	192	[177]
Free-standing microdisk	700	[200]
Free-standing microdisk	794	[<mark>66</mark>]
Free-standing microdisk	1350	[115]
Nano-wire with DBR mirrors	2000	[110]
PhC ring resonator	3085	[153]
2D PhC	220	[201]
2D PhC	540	[129]
2D PhC	560	[202]
2D PhC	600	[203]
2D PhC	5000	[151]
2D PhC	16 000	[204]
3D PhC	13 600	[152]

be removed after the diffusion to the Ge layer by chemicalmechanical-polishing (CMP) [29, 166, 193]. The segregation of Sb was also controlled by optimizing the temperature during the growth to achieve a high density of active dopants [184].

5.3. Ion implantation

Ion implantation is the standard process doping in Si CMOS technologies. Ge is a promising material for the channel in the future generations of CMOS technologies, and therefore researchers are developing processes of ion implantation and activation for Ge [43, 91, 185-189]. For a short channel MOSFET with a channel length as small as 10 nm, an extremely shallow junction is required to avoid the short channel effects in MOSFETs, which result in a decrease of the threshold voltage due to an increase of the leakage current [194, 195]. On the other hand, for Ge light sources, we want to dope the entire Ge layer, which may require different process optimization from the conditions for Ge MOSFETs. If we increase the power and the dose for the ion implantation, the surface of the Ge layer will become amorphous. Usually, the damaged amorphous region will be recovered by annealing [194, 195], while the crystalline quality of the bottom region underneath the a-Ge would be the LT layer with poor crystalline quality, if we use Ge directly grown on Si. If we can use the bulk Ge substrate, we will be able to recover the crystalline quality, however the issue of compatibility with SOI based Si photonics arises, again. We need more ideas to utilize ion implantation technologies for Ge light sources.

5.4. Gas phase doping and spin-on doping

Considering the above difficulties of using conventional ion implantation technologies, we consider going back to the legacy technologies based on diffusion of impurities upon heating. The gas phase doping of As was reported [190], and gas immersion laser doping (GILD) technology was developed [182, 191]. In principle, the diffusion process will enable doping up to the solid solubility density of the order of 10^{20} cm⁻³ without significant degradation of the crystalline quality [194, 195].

SOD is another process to dope Ge with impurities from a solution-based oxide [67–69, 92, 192]. In spite of the relatively simple recipes, there are several issues to do with SOD processes such as stress induced degradation of Ge due to the weak adhesion between Ge and BOX [92]. The Ge desorption as GeO during the annealing also degrades the active Ge layer [92]. By optimizing the SOD processes, a huge optical gain of 5300 cm^{-1} has been reported by Xu [69].

6. Optical cavities

An optical cavity is a crucial component to integrate for developments of a Ge-based LD beyond the performance of an LED, in terms of the efficiency and coherence towards practical applications [60, 61]. For short-reach optical communications, we need decent optical outputs comparable to those from III-V LDs. Then, standard optical cavities like FP, DFB, DBR, or VECSEL structures will be required [60, 61]. FP, DFB, and DBR structures can be fabricated by using a bulk Ge WG. In fact, all devices with the claims of successful laser operations are based on a bulk FP WG [48-51, 55]. Laser operations with a QW or MQWs as well as the clear experimental proof of the reproducibility from different groups will be the next academic target, while the fabrication a FP WG with embedded Ge MQWs will be quite challenging. With the GeSn-based materials, the growth of MQWs is quite promising.

For fundamental understanding and possible future applications to quantum technologies, novel photonic cavities [196] would be even more suitable, as summarized in table 4. In order to demonstrate laser operations from Ge-based light sources, the gain must be larger than the loss, while these cavities will enable a very strong optical confinement. Among them, micro-rings [103, 197] and micro-disks [66, 67, 115, 177, 180, 198–200] have very simple structures, yet exhibit high *Q*-factors of WGMs. The compatibility of optical confinements with strain-engineering has been demonstrated in Ge disks on a SiO₂ bridge [177] and Ge NWs with DBR mirrors [110].

PhC is another route to high-*Q* cavities, and the planar processes of CMOS are quite appropriate to fabricate these PhC by using conventional lithography and dry-etching [196]. Various PhC structures are examined [129, 151–153, 201–204] with Ge QDs [151–153, 201–204] or using GOI [129]. In addition to the strong optical confinements, these cavities will enhance recombination through the Purcell effects [153, 205–212].



Figure 4. Future applications of Ge-based light sources.

7. Applications

Future applications of Ge-based light sources are summarized in figure 4. The internet-of-things (IOTs) is expected to revolutionize the way we communicate using global sensor networks, and the demands of the communication in a data centre are exponentially increasing. It is highly desirable to realize monolithic light sources integrated on a Si photonic chip for global data centres, cloud computing, and fibre-tothe-home (FTTH), however severe power requirements must be overcome for applications to optical interconnections [11]. active optical cables (AOCs) using Si photonics are already widely used [18], and those technologies will also be implemented in consumer products like USB memory sticks with optical input/output (I/O). The main advantage to the use of an optical interconnection rather than metal wiring is the power reduction in addition to the higher data transmission rate. A quantum efficiency as high as that of a III-V LD is required for it to be replaced by a Ge-based LD. If the developed Ge LD in the future can be operated very fast, which means at least as fast as 10 Gbps and ideally beyond 25 Gbps, direct modulation without using a modulator will be possible. In that case, the energy consumption estimated for a modulator will not be needed, which would slightly relax the requirement for the quantum efficiency.

There are many other possible applications of Ge-based light sources, like local-area-network (LAN) in cars or biosensing. For these applications, a laser operation may not be necessary, as far as the quantum efficiency of Ge-based LED is reasonable. For example, a LED is used for LAN in a car, due to the relatively slow data rate of around 25 Mbps. The advantage of using Ge-based light sources will be the cost and the integration capabilities using CMOS processes. Applications to quantum technologies as a single photon source will also be interesting. It will be very important to identify the first target for a real product of Ge-based light sources.

8. Conclusion

We have reviewed the current status of the developments of Ge-based light sources towards monolithic integration in a Si chip. There are many technological options for fabricating Ge-based light sources. Suitable material choice and design of the structure will be very important, and epitaxial growth processes should be further improved with the help of various patterning techniques. Stress-engineering and doping will be further developed to increase the optical gain values upon pumping. The optical confinements must be considered together with the structure of the active layer and the scheme of carrier injections. At this moment, there is no standard process to fabricate Ge-based light sources, and more innovative ideas are needed. We would like to encourage more researchers ranging from condensed-matter physicists to process/device engineers to join this rapidly growing area.

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Appendix A. List of abbreviations

AOC	Active optical cable
BOX	Buried oxide
CMOS	Complementary metal-oxide-semiconductor
CMP	Chemical-mechanical-polishing
D	Dimensional
DBR	Distributed-Bragg-reflector
DFB	Distributed-feedBack
EM	Electro-magnetic
FET	Field-effect transistor
FP	Fabry–Perot
FTTH	Fibre-to-the-home
GaAs	Gallium arsenide
Ge	Germanium
GeSn	Germanium-tin
GILD	Gas immersion laser doping

(Continued.

Н	Hydrogen
IC	Integrated circuit
I/O	Input/output
IOT	Internet-of-things
III–V	group III-V compound semiconductor
InGaAs	Indium gallium arsenide
LAN	Local-area network
LED	Light-emitting diode
LEPE-	Low-energy plasma-enhanced chemical vapour
CVD	deposition
LPCVD	Low pressure chemical vapour deposition
LPE	Liquid phase epitaxy
LSI	Large-scale integrated circuit
MBE	Molecular beam epitaxy
MEMS	Micro electro mechanical systems
MHAM	Multiple hydrogen annealing heteroepitaxy
MIC	Metal-induced crystallization
MQW	Multiple quantum well
MOCVD	Metal-organic chemical vapour deposition
MOS	Metal-oxide-semiconductor
NIR	Near-infrared
PhC	Photonic crystal
QM	Quantum mechanical
RP-CVD	Reduced pressure chemical vapour deposition
RTA	Rapid thermal annealing
SOD	Spin-on dopant
SOI	Silicon on insulator
Si	Silicon
SiGe	Silicon germanium
UHV-	Ultra-high vacuum chemical vapour deposition
CVD	
VECSEL	Vertical-external-cavity surface-emitting-laser
WG	Waveuuide
WGM	Whispering-gallery-mode

Appendix B. Introduction to quantum field theory for spontaneous and stimulated emissions

The generation of an elementary particle, a photon, by recombination of an electron and its anti-particle, a hole, in a semiconductor is a highly quantum mechanical (QM) phenomenon. However, the modern quantum field theoretical treatments in condensed matter physics are not necessarily popular among engineers working for CMOS and Si photonics. Therefore, we briefly review the second quantized formulation for spontaneous and stimulated emissions, which are suitable to analyse the gain for bulk Ge. Interested readers should follow more advanced textbooks [61, 213].

In general, many body Hamiltonian for electrons is described by

$$H = \sum_{i,j} \langle \mathbf{i} | \mathcal{H} | j \rangle c_i^{\dagger} c_j, \tag{B.1}$$

where c_i^{\dagger} and c_i are the creation and annihilation operators for the *i*th state, which run over all states including spins σ , and $\langle i|\mathcal{H}|j\rangle$ is the one-body Hamiltonian, which becomes in the coordinate representation

$$\langle \mathbf{x} | \mathcal{H} | \mathbf{x}' \rangle = \left[-\frac{\hbar^2 \nabla^2}{2m_{\rm e}} + V_{\rm lattice}(\mathbf{x}) \right] \delta(\mathbf{x} - \mathbf{x}'), \qquad (B.2)$$

where m_e is the bare electron mass in a vacuum, and $V_{\text{lattice}}(\mathbf{x})$ is a periodic potential from a crystal lattice.

The one-body problem can be solved by the $\mathbf{k} \cdot \mathbf{p}$ method or *ab initio* calculations, and the solution of the Schrödinger equation

$$\left[\frac{\mathbf{p}^2}{2m_{\rm e}} + V_{\rm lattice}(\mathbf{x})\right]\psi_i(\mathbf{x}) = \epsilon_i\psi_i(\mathbf{x}), \qquad (B.3)$$

is given by the Bloch state

$$\psi_{\mathbf{k}n}(\mathbf{x}) = u_{\mathbf{k}n}(\mathbf{x}) \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}},\tag{B.4}$$

where $u_{\mathbf{k}n}$ describes the rapidly oscillating atomic wavefunction, for the *n*th band with the band dispersion, $\epsilon_{\mathbf{k}n}$, and *V* is the volume of a bulk active material. Then, the Hamiltonian for electrons without the electro-magnetic (EM) fields is given by

$$H_0 = \sum_{\mathbf{k}n\sigma} (\epsilon_{\mathbf{k}n} - E_{\mathrm{F}n}) c_{\mathbf{k}n\sigma}^{\dagger} c_{\mathbf{k}n\sigma}, \qquad (B.5)$$

where E_{Fn} is the quasi-Fermi level (more precisely, chemical potential) for the *n*th band. What is unusual in a semiconductor, is we can apply different Fermi levels for the conduction band (E_{Fc}) and the valence band (E_{Fv}) by electrical or optical pumping. Fortunately, the non-interacting many-body Hamiltonian H_0 can be solved exactly and the partition function, *Z*, is given by

$$Z = \prod_{\mathbf{k}n\sigma} \exp\left(-\frac{\sum_{\mathbf{k}n\sigma}(\epsilon_{\mathbf{k}n} - E_{\mathbf{F}n})n_{\mathbf{k}n\sigma}}{kT}\right),\tag{B.6}$$

considering all the possible combinations of states, which are occupied $n_{\mathbf{k}n\sigma} = 1$ or not $n_{\mathbf{k}n\sigma} = 0$. As a result, we can calculate all thermodynamic properties, including the statistical QM occupation probabilities for the conduction band $\epsilon_{\mathbf{k}c}$ and the valence band $\epsilon_{\mathbf{k}v}$

$$\langle c_{\mathbf{k}c\sigma}^{\dagger}c_{\mathbf{k}c\sigma}\rangle = \frac{1}{1 + \exp(-\frac{\epsilon_{\mathbf{k}c} - E_{\mathbf{F}c}}{kT})} \equiv f_{\mathbf{c}}(\epsilon_{\mathbf{k}c}),$$
 (B.7)

$$\langle c_{\mathbf{k}\nu\sigma}^{\dagger}c_{\mathbf{k}\nu\sigma}\rangle = \frac{1}{1 + \exp(-\frac{\epsilon_{\mathbf{k}\nu} - E_{\mathbf{F}\nu}}{kT})} \equiv f_{\nu}(\epsilon_{\mathbf{k}\nu}),$$
 (B.8)

which are both given by Fermi–Dirac distribution functions.

Similarly, the classical EM Hamiltonian in a bulk semiconductor of the dielectric constant of ϵ ,

$$H_{\rm EM} = \int_{V} d^{3}\mathbf{x} \left(\frac{\epsilon}{2} \mathbf{E}^{*}(\mathbf{x}) \cdot \mathbf{E}(\mathbf{x}) + \frac{1}{2\mu_{0}} \mathbf{B}^{*}(\mathbf{x}) \cdot \mathbf{B}(\mathbf{x}) \right), \tag{B.9}$$

can be diagonalized to obtain the second quantized form

$$H_{\rm EM} = \sum_{\mathbf{k}s} \hbar \omega_k \left(b_{\mathbf{k}s}^{\dagger} b_{\mathbf{k}s} + \frac{1}{2} \right), \tag{B.10}$$

where $b_{\mathbf{k}s}^{\dagger}$ and $b_{\mathbf{k}s}$ describe the creation and the annihilation operators for a photon with the polarization *s* (1 or 2). This can be achieved by inserting the vector potential

$$\mathbf{A}(\mathbf{x}, t) = \sum_{\mathbf{q}s} \sqrt{\frac{\hbar}{2\epsilon\omega_q V}} \mathbf{e}_s(b_{\mathbf{k}s} \mathbf{e}^{\mathbf{i}\mathbf{k}\cdot\mathbf{x} - i\omega t} + b_{\mathbf{k}s}^{\dagger} \mathbf{e}^{-\mathbf{i}\mathbf{k}\cdot\mathbf{x} + i\omega t}),$$
(B.11)

into the electric field $\mathbf{E}(\mathbf{x}, t) = -\partial \mathbf{A}(\mathbf{x}, t)/\partial t$ and the magnetic field $\mathbf{B}(\mathbf{x}, t) = \nabla \times \mathbf{A}(\mathbf{x}, t)$ under the Coulomb gauge $\nabla \cdot \mathbf{A}(\mathbf{x}, t) = 0$.

The electron-photon interaction can be generated by via the electron charge of -e through $\mathbf{A}(\mathbf{x}, t)$, in the Schrödinger equation

$$\left[\frac{(\mathbf{p} + e\mathbf{A}(\mathbf{x}, t))^2}{2m_{\rm e}} + V_{\rm lattice}(\mathbf{x})\right]\psi_i(\mathbf{x}) = \epsilon_i\psi_i(\mathbf{x}), \quad (B.12)$$

and therefore, the one-body interaction Hamiltonian is

$$\mathcal{H}_{\rm int}(\mathbf{x}) = \frac{e}{m_{\rm e}} \mathbf{A}(\mathbf{x}, t) \cdot \mathbf{p}, \qquad (B.13)$$

which can be converted to show

$$\mathcal{H}_{\text{int}}(\mathbf{x}) = e\mathbf{E}(\mathbf{x}, t) \cdot \mathbf{x} \equiv -\mathbf{E}(\mathbf{x}, t) \cdot \boldsymbol{\mu}, \qquad (B.14)$$

that the EM waves couple and oscillate the electric dipole $\mu = -e\mathbf{x}$. Therefore, light-emissions by the recombinations of electrons and holes are described by the dipole radiations.

By inserting the field operators, we obtain the interaction Hamiltonian

$$H_{\text{int}} = \sum_{\mathbf{kq}s\sigma} \sqrt{\frac{\hbar}{2\epsilon\omega_{\mathbf{q}}V}} (\mathbf{e}_{s} \cdot \mathbf{p}_{\text{vc}} \mathbf{e}^{i\omega t} b_{\mathbf{q}s}^{\dagger} c_{\mathbf{k}+\mathbf{q}v\sigma}^{\dagger} c_{\mathbf{k}c\sigma} + \mathbf{e}_{s} \cdot \mathbf{p}_{\text{cv}} \mathbf{e}^{-i\omega t} b_{\mathbf{q}s} c_{\mathbf{k}+\mathbf{q}c\sigma}^{\dagger} c_{\mathbf{k}v\sigma}), \qquad (B.15)$$

where the first (second) term describes the emission (absorption) of a photon through the collision between an electron in the conduction band and a hole in the valence band. We have defined the optical transition matrix element by the integral over the unit cell of the volume $V_{\rm uc}$

$$\mathbf{p}_{vc} = \frac{1}{V_{uc}} \int_{V_{uc}} d^3 \mathbf{x} u_v^*(\mathbf{x}) \mathbf{p} u_c(\mathbf{x}), \qquad (B.16)$$

which describes the optical selection rules, requiring the change of the *parity* and the conservation of the angular momentum, provided by the unit spin of a photon. Note that the momentum is conserved during the collision processes, while the momentum of a photon is low and $\mathbf{q} \sim 0$ dominates without changing the momentum of an electron and a hole.

After obtaining H_{int} , the QM average of the emission and absorption rates from the initial state *i* to the final state *f* can be calculated by Fermi's Golden rule

$$w_{i \to f}^{\text{QM}} = \frac{2\pi}{\hbar} |\langle f | H_{\text{int}} | i \rangle|^2 \delta(E_f - E_i \pm \hbar\omega), \qquad (B.17)$$

where + (-) stands for emissions (absorptions), and the energy conservation is required upon recombinations. To calculate the matrix element, we must remember that each many-body state is described by the direct product of an electronic state and a photonic state. For electronic states, we



Figure B1. Feynman diagram for (a) spontaneous and (b) stimulated emissions.

must also take the statistical average into account for electronic states. In order to calculate the emission rate, the conduction band must be occupied and the valence band must be occupied whose statistical average will give a factor of

$$f_{\rm c}\left(\epsilon_{\rm kc}\right)\left(1 - f_{\rm v}\left(\epsilon_{\rm kv}\right)\right),\tag{B.18}$$

while the absorption process will give a factor of

$$f_{\rm v}(\epsilon_{\rm kv})(1-f_{\rm c}(\epsilon_{\rm kc})). \tag{B.19}$$

On the other hand, a photonic state can be considered to be an essentially pure QM state at zero temperature except for the black body radiations. The matrix element of the bosonic creation operator will give a factor of

$$\langle n_{\mathbf{q}s} + 1 | b_{\mathbf{q}s}^{\dagger} | n_{\mathbf{q}s} \rangle = \sqrt{n_{\mathbf{q}s} + 1},$$
 (B.20)

for the emission process, while for the absorption process it is

$$\langle n_{\mathbf{q}s} - 1 | b_{\mathbf{q}s} | n_{\mathbf{q}s} \rangle = \sqrt{n_{\mathbf{q}s}}.$$
 (B.21)

This difference is especially important, since this explains the difference between spontaneous and stimulated emissions. For spontaneous emissions, a photon is produced from the vacuum where there is no photon

$$\langle 1|b_{\mathbf{q}s}^{\dagger}|0\rangle = 1. \tag{B.22}$$

Thus, a photon is created even without any net average electric fields, while there are vacuum zero-point fluctuations (figure B1 (a)). In stimulated emissions, the number of photons will be increased (or decreased) by the electric fields created by the photons themselves (figure B1(b)), which are trapped in a cavity. Successive productions of copies of photons with the same phase can achieve the macroscopic occupation of the single mode, which is considered to be a Bose–Einstein condensation of photons. Therefore, the radiation from a laser is coherent.

Finally, the total emission and absorption rates are

$$W^{\text{emission}} = \frac{2\pi}{\hbar} \frac{e^2}{m_e} \frac{\hbar}{2\epsilon\omega_q} \frac{1}{V} \sum_{\mathbf{k}\sigma} (n_{\mathbf{q}s} + 1) |\mathbf{e}_s \cdot \mathbf{p}_{vc}|^2 \times f_c (\epsilon_{\mathbf{k}c}) (1 - f_v (\epsilon_{\mathbf{k}v})) \delta(\epsilon_{\mathbf{k}v} - \epsilon_{\mathbf{k}c} + \hbar\omega), \qquad (B.23)$$

$$W^{\text{absorption}} = \frac{2\pi}{\hbar} \frac{e^2}{m_e} \frac{\hbar}{2\epsilon\omega_q} \frac{1}{V} \sum_{\mathbf{k}\sigma} n_{\mathbf{q}s} |\mathbf{e}_s \cdot \mathbf{p}_{cv}|^2 \times f_v(\epsilon_{\mathbf{k}v})(1 - f_c(\epsilon_{\mathbf{k}c}))\delta(\epsilon_{\mathbf{k}c} - \epsilon_{\mathbf{k}v} - \hbar\omega).$$
(B.24)

Therefore, we obtain spontaneous and stimulated emission rates

$$W^{\text{spon.}} = \frac{2\pi}{\hbar} \frac{e^2}{m_e} \frac{\hbar}{2\epsilon\omega_q} \frac{1}{V} \sum_{\mathbf{k}\sigma} |\mathbf{e}_s \cdot \mathbf{p}_{vc}|^2 \times f_c(\epsilon_{\mathbf{k}c})(1 - f_v(\epsilon_{\mathbf{k}v}))\delta(\epsilon_{\mathbf{k}v} - \epsilon_{\mathbf{k}c} + \hbar\omega), \quad (B.25)$$

$$W^{\text{stim.}} = \frac{2\pi}{\hbar} \frac{e^2}{m_e} \frac{\hbar}{2\epsilon\omega_q} \frac{1}{V} \sum_{\mathbf{k}\sigma} n_{\mathbf{q}s} |\mathbf{e}_s \cdot \mathbf{p}_{cv}|^2 \times (f_c(\epsilon_{\mathbf{k}c}) - f_v(\epsilon_{\mathbf{k}v})) \delta(\epsilon_{\mathbf{k}c} - \epsilon_{\mathbf{k}v} - \hbar\omega), \qquad (B.26)$$

respectively.

Considering the optical power density of $P = \hbar \omega_q v_g n_{qs}$, where the group velocity is $v_g = c/n_r$ with the refractive index of n_r , we can obtain the gain formula

$$g = \frac{W^{\text{stim.}}/V}{P/(\hbar\omega)}$$
(B.27)

$$= \frac{\pi e^2}{m_{\rm e}^2 n_{\rm r} \epsilon_0 c \epsilon \omega_q} \frac{1}{V} \sum_{\mathbf{k}\sigma} |\mathbf{e}_s \cdot \mathbf{p}_{\rm cv}|^2 \times (f_{\rm c}(\epsilon_{\mathbf{k}c}) - f_{\rm v}(\epsilon_{\mathbf{k}v})) \delta(\epsilon_{\mathbf{k}c} - \epsilon_{\mathbf{k}v} - \hbar\omega).$$
(B.28)

We have not explicitly included the degeneracy of valence bands with heavy holes and light holes, but it is straightforward to includes these contributions. The inclusion of the *L*-valley in the conduction band will reduce the gain values significantly due to the free carrier absorptions, while helping the populations in the Γ valley. The quantitative evaluations are currently hot topics in the area of Ge light-emissions.

Appendix C. Optical mode confinement in a FP waveguide : an analogy of photonics with electronics

The starting fundamental equations to describe the electromagnetic waves in a dielectric with the refractive index of nare Maxwell's equations, or their equivalent relativistic form of Poisson equation

$$\left(\nabla^2 - \frac{1}{\nu^2}\right)\mathbf{E} = 0, \tag{C.1}$$

where v = c/n is the velocity of a photon in a dielectric, which is slower than that in vacuum, *c*. If a photon is propagating along *z* with the polarization along *x*, the solution in a uniform dielectric is given by

$$E_x \sim \mathrm{e}^{\mathrm{i}(\omega t - k_z z)},$$
 (C.2)

with the simple *massless* photon dispersion relationship of $\omega = vk_z$ between angular frequency ω and the wavenumber k_z .

In our Si photonics applications, the refractive index depends on the positions (x, y) perpendicular to a FP WG [6–10]. Then, the Poisson equation for the transverse-electric

(TE) mode, $E_x^j e^{i(\omega t - k_z^j z)}$, becomes

$$\left(\partial_x^2 + \partial_y^2 - k_z^{j2} + \frac{n(x, y)^2}{c^2}\omega^2\right) E_x^j(x, y) = 0, \quad (C.3)$$

for the *j*th eigenmode. A similar equation is also valid for the transverse-magnetic (TM) mode. By substituting with $k_z^j = \omega n_{\text{eff}}^j/c$, we obtain

$$\left(\partial_x^2 + \partial_y^2 - \frac{\omega^2}{c^2} (n_{\text{eff}}^{j2} - n(x, y)^2)\right) E_x^j(x, y) = 0.$$
 (C.4)

We can compare equation (C.4) with the 2D Schrödinger equation with the effective mass of m_{eff} under the potential $V_{\text{eff}}(x, y)$, whose discrete energy level is E_{eff}^{j} ,

$$\left(\partial_x^2 + \partial_y^2 - \frac{2m_{\rm eff}}{\hbar^2} (V_{\rm eff}(x, y) - E_{\rm eff}^j)\right) \psi(x, y) = 0, \quad (C.5)$$

and we get intuitive equations

$$V_{\rm eff}(x, y) = -\hbar\omega n(x, y)^2, \qquad (C.6)$$

$$E_{\rm eff}^{\ j} = -\hbar\omega n_{\rm eff}^{\ j2},\tag{C.7}$$

$$m_{\rm eff}c^2 = \frac{\hbar\omega}{2}.$$
 (C.8)

This means that a photon propagating along with a FP WG becomes *massive* perpendicular to the WG, and we have the emergence of the *rest* effective mass with the Einstein relationship for the zero-point energy. Moreover, the squared refractive index with a negative sign works as an effective attractive potential for a photon, which means a photon has a tendency to be trapped in a material with a higher refractive index. For example, assuming the photon energy of $\hbar\omega = 1 \text{ eV}$, we get $m_{\text{eff}} = 0.976 \times 10^{-6}m_{\text{e}}$, where m_{e} is the bare electron mass, which means the effective mass of a photon is sixs-orders of magnitude smaller than that of an electron. This estimation is also consistent with the difference of the rest energies between a photon $m_{\text{eff}}c^2 = \hbar\omega/2 = 0.5 \text{ eV}$ and an electron $m_{\text{e}}c^2 = 0.512 \text{ MeV}$.

As an application of this formulation, we can think about the tunnelling leakage from the waveguide to the substrate (figure C1). The tunnelling leakage probabilities from the false vacuum can be calculated by the *instanton* method [214], which is equivalent to the Wentzel–Kramers–Brillouin formula

$$\Gamma \sim e^{-\frac{B}{\hbar}},\tag{C.9}$$

where

$$B = \oint \sqrt{2m_{\rm eff}(V_{\rm eff}(x, y) - E_{\rm eff}^{j})} \,\mathrm{d}y. \tag{C.10}$$

According to the above estimation of the effective mass, in order to avoid the optical leakage, we need to prepare the cladding layer with a thickness of approximately three-orders of magnitude larger than that of an electronic system. In fact, the tunnelling of electrons can be observed in a commercially available MOS with a gate oxide thickness of around 1 nm,



Figure C1. Quantum mechanical behaviours of a photon propagating in a waveguide. A Si_3N_4 waveguide is fabricated on top of a Ge quantum-well with a thin buried oxide. (a) Leakage of the propagating mode into the substrate through the thin buried oxide. (b) Stronger confinement in a waveguide due to the local removal of the substrate.



Figure D1. Deformation of a wafer after the deposition of the tensile stress liner.

while the cladding layer of the Si WG and the box thickness should be around 1 μ m.

Appendix D. Derivation of Stoney's formula

Stoney's formula [178, 179], which was derived in 1909, is quite useful to estimate the *global* strain of the stress liner film. For the *local* strain, we need finite-element simulations. Nevertheless, Stoney's formula is still valuable to estimate the internal stress of the deposited film, experimentally, and it will be also useful in understanding how the deformation will be induced by the film with an internal stress. Therefore, we will derive Stoney's formula in this appendix.

Suppose we have a bulk substrate, which is a Ge or Si substrate in our case, with a thickness of t_{sub} . We will deposit a film with the thickness of t_{film} with an internal stress of σ_{film} , as shown in figure D1. Here, we assume that the surface of

the substrate is *tensely strained*, which means the atomic bond length is expanded, compared with the lattice constant in the bulk. For this inward bending, the deposited film has a tendency to expand, which means that the film is *compressively strained*, internally. The force is always balanced by the action-reaction law, i.e. Newton's third law of motion, so that the words of tensile and compressive are sometimes confusing. Fortunately, both compressive and tensile stress liners are available in CMOS processes prepared for both *n*-MOS and *p*-MOS. Of course, the bending will be outward, if we deposit the film with an internal *tensile strain*.

If we use X_i and X'_i for positions before and after the displacement in the elastic body, the local displacement is described by $u_i = X'_i - X_i$, where i = x, y, z. The deformation is described by the strain tensor

$$u_{ik} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right), \tag{D.1}$$

where i, k = x, y, z.

For example, by using the Yang's modulus, E, and the Poisson ratio, ν , the deformation by the uniaxial compressive stress P along z can be described as

$$u_{zz} = -\frac{1}{E}P,$$
 (D.2)

$$u_{xx} = u_{yy} = -\nu u_{zz} = \frac{\nu}{E} P.$$
 (D.3)

Similarly, the biaxial strain, $\sigma_{xx} = \sigma_{yy} = \sigma$ along the xy plane, will induce the deformation of

$$u_{xx} = u_{yy} = \frac{1-\nu}{E}\sigma,$$
 (D.4)

$$u_{zz} = -\frac{2\nu}{E}\sigma.$$
 (D.5)

In other words, we can define biaxial modulus, $E_{\rm b}$, for the biaxial strain as

$$E_{\rm b} = \frac{E}{1 - \nu},\tag{D.6}$$

which means that the displacement will be larger than the uniaxial strain, because the elastic body is bent along two directions.

Going back to the original problem of the inward bending in figure D1 with the bending radius of *R*, the top surface of the substrate is tensely strained, while the bottom of the substrate is compressively strained. This is apparent, because the length of the arc at the top surface, $2(R + t_{film})\theta$, is larger than the original diameter of the substrate, while the bottom length of the arc, $2R\theta$, is shorter than that. Now, the strain profile is not uniform across the wafer, and it depends on the location along *z*, where we take the origin of *z* at the bottom of the substrate. There exists the stress neutral line at $z = z_0$, where the internal stress is negligible. Assuming the uniform deformation from the neutral line, the strain tensor can be calculated from the ratio of the length of the arc as

$$u_{xx} = u_{yy}, \tag{D.7}$$

$$=\frac{2(R+z)\theta - 2(R+z_0)\theta}{2(R+z_0)\theta},$$
 (D.8)

$$\approx \frac{z - z_0}{R}.$$
 (D.9)

Then, the biaxial strain in the substrate depends on the depth, z, and we obtain it as

$$\sigma_{\rm sub} = \frac{E}{1-\nu} \frac{z-z_0}{R}.$$
 (D.10)

At the top surface of the substrate, $z = t_{sub}$, the bending moment is zero, since the elastic body is not rotating, which leads

$$\int_0^{t_{\rm sub}} (z - t_{\rm sub}) \sigma_{\rm sub} \, \mathrm{d}z = 0. \tag{D.11}$$

Then, we obtain the stress neutral position

$$z_0 = \frac{1}{3} t_{\text{sub.}}$$
 (D.12)

We also have the following identity, which is coming from the balance of the force between the substrate and the film, as

$$\int_0^{t_{\rm sub}} \sigma_{\rm sub} \, \mathrm{d}z = \int_{t_{\rm sub}}^{t_{\rm sub}+t_{\rm film}} \sigma_{\rm film} \, \mathrm{d}z. \tag{D.13}$$

After integrating both sides, we finally obtain the Stoney's formula

$$\sigma_{\rm film} = \frac{E}{1 - \nu} \frac{t_{\rm sub}^2}{6t_{\rm film}R},\tag{D.14}$$

which is useful in estimating the strain from *R*.

It is evident from equation (D.10), that the tensile strain is maximized at the top surface

$$\sigma_{\rm sub}(t_{\rm sub}) = \frac{E}{1-\nu} \frac{2t_{\rm sub}}{3R},\tag{D.15}$$

while it is compressive at the bottom as

$$\sigma_{\rm sub}(0) = -\frac{E}{1-\nu} \frac{t_{\rm sub}}{3R}.$$
 (D.16)

If we calculate the ratios of equations (D.15) and (D.16) to (D.14), we obtain

$$\frac{\sigma_{\rm sub}(t_{\rm sub})}{\sigma_{\rm film}} = \frac{4t_{\rm film}}{t_{\rm sub}},\tag{D.17}$$

$$\frac{\sigma_{\rm sub}(0)}{\sigma_{\rm film}} = -\frac{2t_{\rm film}}{t_{\rm sub}},$$
(D.18)

which means that the impact of a uniform film on a bulk substrate is extremely weak, as long as we are using a standard substrate with a thickness of 100–800 μ m, with a stressor film of thickness less than 1 μ m. We can apply a greater strain if we thin down the wafer with mechanical bending [171]. We can also recognize that the use of a MEMS architecture like a bridge is quite valuable, since the thickness

of the bridge is comparable to the thickness of the strainedlayer, thus, we can expect significant application of the strain to the active Ge [78, 106, 172, 177].

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