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Growth, Electronic and Optical Properties of Si-Ge-Sn Alloys for Silicon Photonics Applications

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Abstract. The primary bottleneck facing silicon-based optoelectronic integration is the absence of high-efficiency light sources due to silicon's indirect bandgap. Si-Ge-Sn alloys can undergo an indirect-to-direct bandgap transition by adjusting the Sn content, providing a CMOS-compatible solution for on-chip light sources. This paper provides a systematic review of research progress on Si-Ge-Sn alloys across three areas: growth control, band engineering, and device applications. In terms of growth, the two major technological approaches—molecular beam epitaxy (MBE) and chemical vapor deposition (CVD)—both operate within the non-equilibrium low-temperature window, complementing each other in practice. While strategies such as gradient-composition buffer layers and pulsed laser annealing can effectively manage strain and defects, they are limited by critical thickness and a narrow process window. In terms of energy bands and optical properties, the synergistic control of composition and strain enables bandgap engineering of the bandgap from the short-wave infrared (SWIR) to the mid-wave infrared (MWIR). Meanwhile, the Urbach tail effect and defect-assisted nonradiative recombination thus become the primary loss mechanisms limiting luminescence at room temperature. In terms of device applications, waveguide-type GeSn photodetectors are now capable of operating across the SWIR-to-MWIR spectral range. SiGeSn/GeSn quantum well lasers have achieved lasing at low temperatures and at specific wavelengths. The review concludes that the realization of room-temperature electrically pumped continuous-wave lasers depends on the synergistic optimization of non-equilibrium post-processing, quantum well band engineering, and high-Q microcavities.

Keywords: Silicon-Based Optoelectronics, Si-Ge-Sn Alloy, Band Project, Direct Bandgap, Optoelectronic Devices

1. Introduction

In recent years, as the computational demands of large artificial intelligence models and high-performance computing have grown exponentially, the parasitic effects and Joule heating losses associated with traditional copper interconnects have pushed their bandwidth density close to its physical limit, making it difficult to meet the demand for high-speed, low-power transmission of massive amounts of data. Optical interconnects, with their high bandwidth, low latency, and low

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power consumption, are regarded as a disruptive technology for inter-chip and on-chip communication in the post-Moore's Law era. Silicon-based optoelectronics aims to achieve monolithic integration of optoelectronic devices on silicon substrates using mature CMOS processes, and represents the inevitable path toward the large-scale commercialization of optical interconnects. However, silicon is an indirect-bandgap semiconductor: its conduction band bottom lies at point X in the Brillouin zone, while its valence band top lies at point Γ, resulting in a mismatch in momentum space. This results in radiative recombination requiring the participation of phonons, leading to extremely low luminescence efficiency and making it difficult to achieve a highly efficient on-chip light source. This "light-emitting bottleneck" means that commercial silicon optical modules still rely on hybrid integration with external III-V lasers, which significantly increases packaging costs and limits their adoption in short-distance data centers.

To overcome this challenge, there has been a great interest in the Group IV Si-Ge-Sn alloy system in recent years. The main advantage of its band structure is the high tunability of the energy gap between the Γ-band valley and the L-band valley of the alloy by tuning the Sn content. Theoretical and experimental investigation has demonstrated that Si-Ge-Sn alloys have an indirect-to-direct bandgap transition at Sn content above ~6-8 at. % which dramatically improves the radiative recombination efficiency [1, 2]. It is a direct-bandgap material compatible with silicon processes which offers an entirely new materials physics platform for the solution of on-chip light sources.

Photodetectors using Si-Ge-Sn alloys have been demonstrated at the device level to have high sensitivity over a wide spectral range from short-wave infrared (SWIR) to mid-wave infrared (MWIR). In the meantime, research on lasers has slowly matured from the optically pumped pulsed lasing to the electrically pumped continuous-wave (CW) operation. Seidel et al. in 2024 realized CW lasing at room temperature (77 K) in a SiGeSn/GeSn multi-quantum-well laser (MQW-L) at ~2.32 μm, and this has now been regarded as the first such achievement for practical application in all-IV-group semiconductor lasers [3]. Alloys are also good choices for MOSFETs and TFETs because they have high carrier mobility, and thus are suitable for electronic applications [4].

Over the past few years, extensive research around the world has been conducted on this material system, covering epitaxial growth, fabrication, physical property characterization, and prototype device validation. Some results have been obtained so far, but at present, there is no general and applicable study that connects defect evolution, band structure and carrier properties in epitaxial growth with the performance of macroscopic optoelectronic devices.

Based on the deficiencies mentioned above, this paper will systematically review the preparation, electronic and optical properties of Si-Ge-Sn alloys, etc. The organization of this paper is as follows. Chapter 2 introduces the main epitaxial methods, strain engineering and defect control techniques, and analyzes the key physical challenges involved in the growth process. Chapter 3 will first present the synergistic control of composition and strain to study the band structure, carrier transport properties and heterojunction band alignment of the alloy in detail, with a focus on the suppression of optical transitions by defect states. Chapter 4 shows application cases of photodetectors and lasers. Chapter 5 summarizes the key progress and outlook on the problems that will affect the future development of highly efficient electrically pumped lasers.

2. Growth control and material quality of Si-Ge-Sn alloys

The epitaxial growth of Si-Ge-Sn alloys is both a prerequisite and a key bottleneck for their application in optoelectronic devices. The challenges stem from two sources of incompatibility: the large lattice mismatch between Si and Sn-containing alloys, and the extremely low equilibrium

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solubility of Sn in Ge and Si. As shown in Figure 1, a typical Si-Ge-Sn alloy device structure starts with a silicon substrate (lattice constant of Si 5.431 Å) and, via a compositionally graded Si buffer layer and SiGe virtual substrate, terminates in an active layer of GeSn or SiGeSn alloy on the top layer. This layered gradient strategy is designed to mitigate the lattice mismatch of up to 15–20% between silicon and the high-Sn-content alloy (the lattice constant of α-Sn reaches 6.489 Å) [5]. However, this system faces three fundamental growth constraints. First, the equilibrium solubility of Sn in Ge and Si is less than 1% and 0.1%, respectively, which is far short of the >8 at.% Sn composition needed to obtain a direct bandgap [1]. Second, the surface diffusion barrier for Sn atoms is extremely low; thus, it is expected that surface segregation and co-precipitation will occur during high-temperature growth [5]. Thirdly, there is an endogenic contradiction in that the low-temperature requirement for non-equilibrium growth (generally <400 °C) does not provide sufficient atomic mobility to achieve good epitaxy.

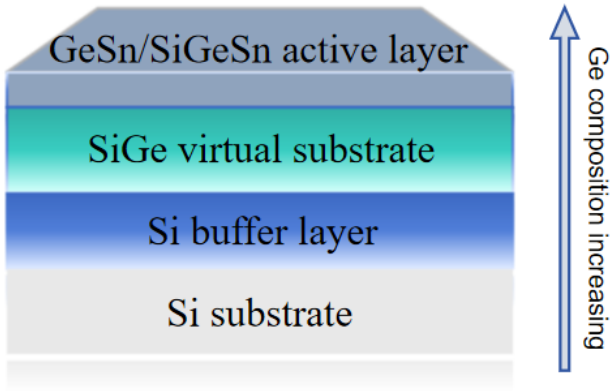


Figure 1. Schematic cross-section of a typical Si-Ge-Sn epitaxial structure grown on a Si substrate

These constraints dictate that the growth of Si-Ge-Sn alloys must be strictly confined to a process window far from thermodynamic equilibrium. Therefore, the core scientific challenge in this field is to reduce the lattice mismatch strain and at the same time reduce defect generation under non-equilibrium conditions. Based on the above, it needs to achieve a uniform substitution incorporation of high-tin-content elements ultimately to obtain device-grade epitaxial films. With this objective in mind, this chapter will first introduce the principles and latest developments in the two primary epitaxial techniques, Molecular Beam Epitaxy (MBE) and Chemical Vapor Deposition (CVD). Then it will analyse the effect of strain engineering and defect control on threading dislocations and other problems in materials. Finally, it summarizes the key challenges and outlines future research directions toward room-temperature device applications.

2.1. Key epitaxial technologies

Epitaxial growth of Si-Ge-Sn alloys should be carried out at a low temperature and far from thermodynamic equilibrium, and as a result, the two main technological routes mentioned above have been developed: molecular beam epitaxy (MBE) and chemical vapour deposition (CVD).

MBE evaporates high-purity solid-state sources (Si, Ge, Sn) in an ultra-high vacuum (UHV) environment by means of an independently controlled beam-source furnace to obtain atomic-scale precision in the composition and thickness of the film. Its most notable advantage lies in its ability to support growth at ultra-low temperatures, less than 200 °C, which effectively suppresses surface segregation of Sn. Therefore, it is often used as a test case to explore new material systems and

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verify band theory. However, MBE involves high equipment maintenance costs and extremely low growth rates (typically < 1 μm/h), making it difficult to meet the demands of large-scale integration.

In contrast, CVD is a method of chemical reaction to deposit thin films on the surface of a heated substrate using gaseous precursors, such as Ge_2H_6, Si_2H_6, $SnCl_4$, etc. Among them, reduced-pressure chemical vapour deposition (RP-CVD) technology has good growth efficiency in the typical CVD process window of 300–450°C and has been employed as one of the main ways to produce device-grade active layers. However, for the growth of alloys with high Sn content, this temperature range must be further narrowed and precisely controlled to suppress Sn segregation and ensure uniform substitution doping. Seidel and others have realised the electrical pumping of continuous-wave lasers in RP-CVD-grown active regions in 2024. CVD has been successfully implemented in the industry on the 200mm standard silicon platform and is expected to be applied in large-scale mass production.

Although there are significant differences in the technical details of the two, they both face the same physical constraint: to achieve high Sn (>8 at.%) substitutional incorporation, the growth temperature was strictly maintained below the Sn segregation threshold (approximately 350°C). However, such low temperatures inevitably decrease the surface mobility of adatoms, and thus the growth mode will be in the critical region between 2D layer-by-layer growth and 3D island growth. Addressing this constraint remains a central challenge for both techniques.

2.2. Strain engineering and defect control

Growing high-Sn alloys on a Si substrate involves a lattice mismatch of approximately 4% relative to a Ge virtual substrate. Managing the strain and defects arising from this mismatch is a key challenge in growth control [2].

The main and direct way of lattice mismatch control is the use of a gradient buffer layer. The typical scheme begins with a Si substrate and then, a composition gradient is designed in Si buffer layer and SiGe virtual substrate, so that the active layer GeSn or SiGeSn can be grown on the top layer. A unique advantage of the SiGeSn ternary alloy is that, by controlling the composition to precisely match the Si/Sn ratio of ~3.7:1, a lattice-matched ternary alloy can be achieved which will match exactly the lattice constant value of Ge (~5.658 Å) and thus allows the decoupling of bandgap engineering and lattice engineering [6].

The misfit dislocations (mainly edge dislocations) that are formed at the Ge/GeSn interface can effectively release the compressive strain, which is beneficial to the incorporation efficiency of Sn. SiGeSn grown directly on Si (100) develops periodic edge dislocations at the interface to accommodate the lattice mismatch with the substrate [6].

In order to control defects, low-temperature growth is desirable, because it allows high Sn incorporation, but this growth results in the introduction of point defects and dislocations, which decrease the crystalline quality. Rapid annealing can be used to enhance the quality of the crystalline structure, but attention needs to be paid to prevent Sn segregation. In recent years, another technique to synergistically enhance the surface properties of SiGe has been developed by amorphising the SiGe surface using Sn ion implantation and then irradiating with nanosecond level laser pulses. The process can be used to suppress long-term thermal diffusion of Sn, and to complete melt recrystallization in a very short time. With optimized laser energy density, up to 62% fraction of substitutional Sn and up to 80% fraction of substitutional Ge is achieved and a compressive strain of ~ -1.15% was introduced. This technology has been successfully used for strain engineering and application to high mobility devices under stress [7].

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2.3. Key challenges to growth

Although epitaxial technology has made significant strides over the past three decades, the growth of Si-Ge-Sn alloys continues to be limited by two fundamental problems that have not been solved yet. The first is the critical thickness set by lattice matching, and the second is the thermodynamic limit of the temperature process window.

The main reason there is a limit to the thickness of good epitaxial layers is lattice mismatch. The lattice mismatch of about 15-20% between the Si substrate (5.431 Å) and the high-Sn alloy (α-Sn: 6.489 Å) is too large; thus, the thickness of the epitaxial layer cannot exceed the critical thickness. When the critical thickness is reached, the accumulated strain energy will cause a change in the growth mode from a 2D layer to a 3D island, and as a result, a large number of misfit dislocations and threading dislocations will be formed at the interface [2]. This results in a fundamental conflict between high Sn content (>8 at.%) and thick active layers: the former requires a high Sn content to obtain a direct bandgap, while the latter needs a sufficiently large thickness for the formation of optical waveguide or quantum well devices.

Conflict in the temperature process window is a thermodynamic bottleneck to growth. High Sn doping requires low-temperature growth, usually below 350 °C and as low as 190-220 °C, to reduce Sn surface segregation and the phase transition from α-Sn to metallic β-Sn. However, if the growth temperature is too low, there will be insufficient atomic surface diffusion, and point defects will be introduced to degrade the crystal structure. Moreover, although low-temperature growth has been achieved successfully, the post-growth annealing temperature will still be limited to 550 °C or lower and will be far from the thermal budget of standard CMOS production. The equilibrium solubility of Sn in Ge and Si is less than 1% and 0.1%, respectively. Si-Ge-Sn alloys are essentially metastable artificial materials in which the Sn concentration far exceeds the solubility limit, resulting in an extremely narrow operating window between compositional stability and heat treatment temperature [8].

3. Band structures, optical transitions, and carrier dynamics

A defining feature of Si-Ge-Sn alloys is the exceptional tunability of their band structure. Si, Ge, and α-Sn are all Group IV elements with the diamond crystal structure. Among them, Si and Ge are indirect-bandgap semiconductors. α-Sn, in contrast, is a semimetal—its valence band and conduction band overlap slightly at the band extrema, resulting in a negative bandgap. These band-structure characteristics enable the indirect-to-direct bandgap crossover in Group-IV elements. Moreover, the composition range of Si-Ge-Sn alloys is very broad, and the bandgap and lattice constant can be controlled independently by adjusting the Si and Sn contents [2].

3.1. Synergistic control of composition and strain

The band structure of Si-Ge-Sn alloys is synergistically controlled by composition and strain, both of which determine whether the bandgap is indirect or direct, the bandgap width, and the band offset.

The most common way to convert an indirect bandgap to a direct bandgap is to tune the composition. The direct bandgap (E_0) at the Γ point in SiGeSn redshifts monotonically as the Sn content is increased, and the indirect bandgaps at the L and X points decrease at different rates. With the Sn content about 6-8 at. %, the transition from indirect band gap to direct band gap occurs as the Γ- valley energy is lowered in relation to the L- valley energy.

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Buffer Layer Engineering is used for Strain control, to introduce compressive strain, tensile strain or even full relaxation into the Si-Ge-Sn epitaxial layer. The strain state directly defines the type of bandgap and the band offset, and can cause the indirect to direct band gap transition.

3.2. Optical transitions and band-edge absorption

The optical transition characteristics directly determine the application potential of Si-Ge-Sn alloys in active devices such as lasers and detectors.

The indirect-to-direct bandgap crossover leads to a significant increase in the oscillator strength of the Γ-point direct transition. The fundamental explanation of the remarkable improvement of the probability of radiative recombination is that the oscillator strength at the direct Γ-point transition is sharply increased as a function of Sn content in direct-bandgap GeSn alloys. In the case of SiGeSn ternary alloys, the oscillator strength is not only a function of the Sn content, but also is closely related to the width of the quantum well and the composition of the SiGeSn barrier. Optimization of the well width (e.g. 11–12 nm) can give a high absorption contrast ratio, very important for high efficiency electro-absorption modulators [9].

In edge characteristics, The Urbach tail effect is an important effect influencing the absorption-edge properties. It has been demonstrated by experiments that the band-tail effect due to the structural disorder can reduce the optical band gap by over 50% compared to its intrinsic value in the case of GeSn samples with 8% Sn content. When the Sn content is increased the competition between the direct transitions and the indirect transitions and the Urbach tail comes in. The contribution of indirect transitions decreases. The tail-width broadening is of great importance for the sensitivity of the detector to low energy photons, and is a design criterion for infrared detectors [10].

3.3. Carrier transport and doping

Carrier transport links electronic structure to device performance, and the two-dimensional hole gas in quantum wells serves as the ideal platform for studying this phenomenon. Lidsky et al. conducted a systematic study of the transport properties of two-dimensional hole gases in GeSn/SiGeSn quantum wells and achieved the highest mobility record to date for Sn-containing systems. In the two heterostructure field-effect transistors fabricated in this study, the peak 2D hole mobility reached 19,000 cm^2/Vs (at 2 K), setting a record high for Sn concentrations of 6% or higher [4].

Achieving controlled and efficient doping of epitaxially grown Si-Ge-Sn alloys is key to applying these materials in practical devices. Doping of Si-Ge-Sn alloys differs from that of conventional Si and Ge because of the presence of Sn. Research on doping has focused primarily on p-type doping, which is related to the requirements of photodetectors and lasers. In fact, researchers primarily use two doping methods: in-situ doping during the epitaxial growth process and post-growth ion implantation doping. In contrast, there has been little research on n-type doping of Si-Ge-Sn alloys. The primary difficulty lies in the low solubility of donor impurities in Sn-containing alloys, which results in poor activation efficiency.

3.4. Band alignment and defect state control in heterojunctions

The modulation of the aforementioned band structure and the enhancement of optical transitions both rely on the crystal having sufficiently high quality. However, the epitaxial growth defects

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described in Section 2 introduce band-tail states (Urbach band tails) within the bandgap, with an energy broadening on the order of 50 meV.

Not only do these defect states broaden the absorption edge, as discussed in Section 3.2, but their deeper impact lies in providing a nonradiative recombination channel, which fundamentally limits the carrier lifetime and the performance of the gain medium. Therefore, the types and densities of defect states, as well as their effects on carrier dynamics, must be considered as independent variables in device bandgap design.

The type of band alignment in a heterojunction determines the degree of carrier localization and serves as the core basis for the design of quantum-well optoelectronic devices. Theoretical calculations show that short-range order can modulate the energy bands. Research has shown that Type-I band alignment can be achieved in material systems with identical chemical compositions by controlling the degree of short-range ordering of Si atoms in Si-Ge-Sn alloys [5]. This discovery offers a new approach to building heterostructures: creating band barriers through atomic-level order rather than compositional differences, which may represent a new direction for future research.

Misfit dislocations and deep-level defects associated with Sn clusters are the primary nonradiative recombination centers, which degrade carrier lifetime. Although high-temperature annealing can reduce the hole density, it may also accelerate Sn diffusion and cause interface blurring. A theoretical analysis by Pareek et al. of SiGeSn/GeSn quantum well infrared detectors further indicates that Sn concentration and bias conditions have a decisive influence on carrier trapping, thermal emission, and tunneling escape behavior. At a low bias voltage of 0.28 V, a single $Ge_{0.83}Sn_{0.17}$ quantum well can achieve a bandwidth of 200 GHz [11]. It is clear that optimizing device performance requires a comprehensive consideration of alignment type, defect density, and carrier dynamics.

4. Silicon-based optoelectronic devices and applications

The rapid development of the Si-Ge-Sn alloy system has made it one of the most promising active materials in the field of silicon-based optoelectronic integration. Thanks to breakthroughs in low-temperature epitaxial technology, it is now possible to grow device-grade GeSn and SiGeSn thin films on Si substrates, and based on this, prototype devices such as light-emitting diodes, photodetectors, and lasers have been developed [12]. In this chapter, the emphasis will be on the latest developments in this material system in the two most relevant applications of infrared photodetection and light emitting devices. The former has the advantage of tunability of the bandgap in the short-wave to mid-infrared region, while the latter takes advantage of the fact that the radiative recombination efficiency increases considerably after the bandgap changes from being indirect to direct.

4.1. Infrared photodetector

The main strength of Si-Ge-Sn alloy infrared detector technology is the ability to continuously tune the detector bandgap between 1.6 and 3.7 μm or even longer, covering the short-wave infrared (SWIR) to mid-wave infrared (MWIR) bands. GeSn detectors could be tuned to an absorption edge that goes beyond the near-infrared to 2200–2700 nm by changing the Sn content [13].

Significant recent progress has been made in waveguide-type PIN detectors. The responsible microwave annealing ridge-type GeSn waveguide photodetector (WGPD) fabricated on a (001) Si substrate showed a responsivity of 0.16 A/W at 2745 nm. This device is compatible with CMOS process and can serve as an important part in the integration of electron-photon for short-wave

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infrared. Moreover, the avalanche photodiode architecture is constantly being optimized, and by controlling the lattice mismatch between the GeSn absorption layer and Si substrate, it is expected to be possible to obtain infrared detection with low dark current and high gain. Another class of detectors has been developed by introducing quantum well (QW) structures, which further broaden the design possibilities. By band alignment design, SiGeSn/GeSn multi-quantum wells can be designed to be Type-I carrier localization, which can also suppress the dark current and maintain high absorption coefficient. Carrier capture, thermal emission, and tunneling escape can be controlled by varying the Sn concentration and the bias conditions, which leads to high-speed infrared detection [12].

4.2. Light-emitting diodes and lasers

Light-emitting devices represent both the most challenging and the most promising application area for this material system. In the field of light-emitting diodes, a GeSn-based p-i-n structure has achieved electroluminescence at room temperature, and the emission wavelength can be continuously tuned within the range of 2200–2700 nm as the Sn content increases. Electroluminescence at room temperature has also been demonstrated in multi-quantum-well structures with in-situ p-i-n doping. Due to its higher thermal stability, the SiGeSn ternary alloy demonstrates better reliability than GeSn in long-wavelength LED applications [13].

Laser research is the core driving force in this field, having evolved from optical pumping to electrical pumping, and from pulsed to continuous-wave operation. The operating temperature of early optically pumped GeSn lasers was gradually increased to 180 K, with an emission wavelength of 2–3 μm. The SiGeSn/GeSn multi-quantum well structure reduces the threshold power density to 33 kW/cm² through improved carrier and optical mode confinement, although the operating temperature remains at 80 K [14]. In 2024, Seidel et al. achieved the first electrically pumped CW lasing, using a 6-cycle SiGeSn/GeSn multi-quantum-well microdisk cavity structure. They obtained a CW output at ~2.32 μm and 77 K, with a threshold current approximately 4 mA. This breakthrough is regarded within the field as a milestone toward the practical application of all IV-group lasers [15].

Currently, the core research efforts in this field are focused on the ultimate realization of room-temperature electrically pumped CW lasers. The main bottlenecks include: the thermal stability of materials with high Sn content at room temperature; non-radiative recombination caused by defects introduced during low-temperature growth; and carrier leakage in p-i-n junction designs at high temperatures. In the future, through the synergistic optimization of non-equilibrium post-processing techniques—such as pulsed laser annealing—along with quantum well band engineering and microcavity photonic design, it is expected that this goal will ultimately be achieved.

5. Conclusion

Over the past thirty years, development in the Si-Ge-Sn alloy system has advanced steadily, and now it has reached the stage of prototype device verification. It is now one of the leading Group IV active materials in the field of silicon-based optoelectronic integration. Centered on the theme of "Growth—Physical Properties—Devices", this paper systematically reviews key advances and core bottlenecks in this field and derives the following general conclusions.

There have been considerable advances in the field of non-equilibrium epitaxial growth. MBE and CVD play complementary roles in exploratory research and engineering-scale production, respectively. However, this system is fundamentally constrained by two boundaries defined by

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thermodynamics and dynamics. First, the equilibrium solubility of Sn in Ge/Si is much lower than the concentration required for a direct bandgap (>8 at.%). The low-temperature growth window is 250-350 °C, but it is not high enough to achieve good atomic mobility and high crystallinity. Second, the critical thickness of the lattice mismatch is relatively small (less than 100 nm at high Sn concentration). It is not in the range of 300-500 nm for the active region thickness of optoelectronic devices. The two constraints together are quite restrictive for good epitaxy.

For energy bands and optical properties, the synergistic control of composition and strain has experimentally realized an indirect-to-direct bandgap transition. The sudden increase in the strength of the Γ-point oscillator provides the physical basis for radiative recombination. These defect states constitute the primary loss mechanism for nonradiative recombination at room temperature. Therefore, the defect states should be taken as independent variables in band structure designs and carrier dynamics models.

In devices, this material system has achieved significant advances in the fields of infrared detection and light emission. Functional verification has now been carried out, ranging from short-wave infrared detection to electrically pumped continuous-wave lasing, fully demonstrating its feasibility as a silicon-based active material. The ultimate realization of room-temperature electrically pumped continuous-wave lasers requires synergistic breakthroughs in three areas: Non-equilibrium post-processing, quantum well band engineering, and high-Q-factor microcavity design. As these challenges are addressed, all IV-group lasers are expected to operate at room temperature in the future, paving the way for the large-scale commercialization of silicon-based optoelectronics.

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