

Theoretical Analysis of GeSn Alloys as a Gain Medium for a Si-Compatible Laser

Birendra Dutt, *Senior Member, IEEE*, Hai Lin, Devanand S. Sukhdeo, *Student Member, IEEE*, Boris M. Vulovic, Suyog Gupta, Donguk Nam, *Student Member, IEEE*, Krishna C. Saraswat, *Fellow, IEEE*, and James S. Harris Jr., *Fellow, IEEE*

Abstract—In this paper, a theoretical analysis of unstrained GeSn alloys as a laser gain medium was performed. Using the empirical pseudopotential method, the band structure of GeSn alloys was simulated and verified against experimental data. This model shows that GeSn becomes direct bandgap with 6.55% Sn concentration. The optical gain of GeSn alloys with 0–10% Sn concentration was calculated with different n-type doping concentrations and injection levels. It is shown theoretically that adding Sn greatly increases the differential gain owing to the reduction of energy between the direct and indirect conduction bands. For a double-heterostructure laser, the model shows that at a cavity loss of 50 cm^{-1} , the minimum threshold current density drops 60 times from Ge to $\text{Ge}_{0.9}\text{Sn}_{0.1}$, and the corresponding optimum n-doping concentration of the active layer drops by almost two orders of magnitude. These results indicate that GeSn alloys are good candidates for a Si-compatible laser.

Index Terms—Diode lasers, GeSn alloy, infrared lasers, optoelectronic materials, semiconductor lasers, semiconductor materials, theory and design.

I. INTRODUCTION

AS ELECTRONIC devices continue to scale down in accordance with Moore's law [1], a large portion of the performance limitations in speed, crosstalk, dispersion, and power consumption have been found to result from the electrical interconnects for both intrachip and interchip data links [2]. In an effort to overcome these limitations, optical interconnects have been proposed [3]–[7]; however, this requires that electronic and optical devices be integrated on the same chip. With the ultimate goal of monolithic integration with the current silicon

(Si) CMOS electronics platform, group-IV photonics has been widely investigated, and significant progress has been made. This has included the development of waveguides [8], [9] as well as various types of modulators [2], [10]–[12] and photodetectors [13]–[15]. However, the monolithic integration of group-IV electrically injected laser diodes with the CMOS platform remains a key component that has been missing thus far.

Silicon's indirect bandgap presents the greatest challenge to building an efficient light source. Therefore, other group-IV materials have been investigated for their potential to achieve direct bandgap. In particular, germanium (Ge) has recently been playing an increasingly important role in group-IV lasers because of its pseudodirect gap behavior: the energy difference between its direct Γ and indirect L valleys is only 136 meV [16]. Thus far, three different approaches have been proposed to achieve stimulated emission: biaxial tensile strain [17]–[19], n-doping [18], [20], and GeSn alloys [21]–[25].

Over the past decade, enhanced photoluminescence from Ge has been demonstrated, and in 2009 an MIT group demonstrated direct bandgap electroluminescence [26] and optical gain [27]. In 2010, the same group demonstrated a room-temperature electrically pumped Ge-on-Si laser using a combination of 0.25% tensile strain and n-type doping of $4 \times 10^{19} \text{ cm}^{-3}$ [28], [29]. However, the laser's threshold current density was unacceptably high at 280 kA/cm^2 , several orders of magnitude higher than in current III–V lasers.

Highly tensile strained Ge (larger than 0.25%) can be achieved by means of external mechanical force or lattice mismatch [17], [18]. Although strain redshifts the peak wavelength, it diminishes the requirement for large n-doping, thereby greatly decreasing the Auger recombination and free carrier absorption (FCA) responsible for the high-threshold current density [30]. However, the drawback in terms of the practicality of this approach is that highly strained Ge structures are difficult and expensive to fabricate [31]. Consequently, an approach in which the need for mechanical straining is lessened, but with the same lasing benefits, is highly desirable.

GeSn alloys have recently attracted considerable attention because GeSn becomes a direct bandgap semiconductor with around 6–10% Sn without external mechanical strain. This new alloy has been successfully grown by MBE [23] and chemical vapor deposition (CVD) [21], and enhanced direct bandgap luminescence has been demonstrated up to 8% Sn [24], [32]. In this paper, we show that alloying with Sn has effects analogous to adding tensile strain to reduce the minimum threshold current density and the optimum n-doping concentration [30].

Manuscript received November 30, 2012; revised December 27, 2012 and January 14, 2013; accepted January 14, 2013. This work was supported in part APIC Corporation and PhotonIC Corp., CA, USA, who funded this effort using their internal research-and-development funds, in part by a National Science Foundation Graduate Research Fellowship under Grant DGE-0645962, and in part by a Stanford Graduate Fellowship.

B. R. Dutt is with the APIC Corporation and PhotonIC Corporation, Culver City, CA 90230 USA (e-mail: dutt@apichip.com).

H. Lin is with the PhotonIC Corp., Culver City, CA 90230 USA (e-mail: lin@photonic-corp.com).

D. D. S. Sukhdeo, S. Gupta, D. Nam, K. C. Saraswat, and J. S. Harris are with the Department of Electrical Engineering, Stanford University, Stanford, CA 94305 USA (e-mail: dsukhdeo@stanford.edu; suyog@stanford.edu; dw-nam@stanford.edu; saraswat@stanford.edu; harris@snow.stanford.edu).

B. M. Vulovic is with the APIC Corporation, Culver City, CA 90230 USA (e-mail: vulovic@apichip.com).

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Digital Object Identifier 10.1109/JSTQE.2013.2241397

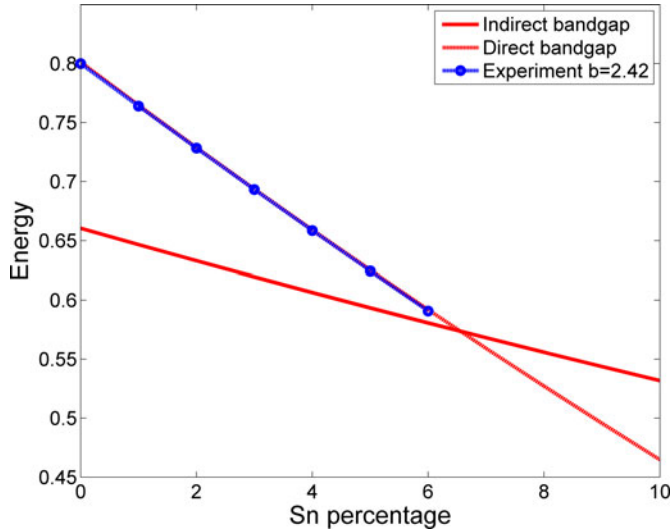


Fig. 1. Calculated direct and indirect bandgap energies of GeSn alloys as a function of Sn fraction. The direct bandgap has the same bowing parameter as that from experimental data.

II. THEORETICAL MODEL

In this effort, the empirical pseudopotential method (EPM) with spin-orbit interaction was used to calculate semiconductor band structures for GeSn alloys of varying Sn fractions. Reciprocal lattice vectors up to the eighth nearest neighbor from the origin are considered in the calculation, which yields satisfactory bulk Ge and bulk alpha-Sn band structures. The calculated energies of the direct and indirect bandgaps as well as the spin split band are consistent with the literature [33].

In order to accurately simulate the band structure of GeSn alloys, the virtual crystal approximation (VCA) with corrections was used to account for alloy disorder-induced crystal potential fluctuations [34]. As shown in Fig. 1, the simulated GeSn alloys' bandgap dependence on Sn fraction has the same bowing parameter b of 2.42 eV as experimental measurements [25]. As a result, the simulated crossover point of the direct and indirect band is at 6.55% Sn. This value is close to other predictions made in the literature [22], [24], [35]. Using this model, band structures of GeSn alloys with 0–10% Sn were calculated and then utilized as the input for optical simulations.

To simulate the optical gain of GeSn alloys, we adopted the method employed in [30]. The gain coefficient of the direct band transition of GeSn alloys at a given photon energy $h\nu$ is described by

$$\gamma_{\Gamma}(h\nu) = |\alpha_{\Gamma}(h\nu)|(f_c - f_v) \quad (1)$$

where $(f_c - f_v)$ is the population inversion factor for direct band transition and is related to the carrier densities in the conduction and the valence bands, and $|\alpha_{\Gamma}(h\nu)|$ is the absorption coefficient of the direct band transition of the GeSn alloy. The experimental absorption spectra of GeSn alloys from [36] were fitted using

$$|\alpha_{\Gamma}(h\nu)| = A\sqrt{h\nu - E_g^{\Gamma}} \quad (2)$$

where E_g^{Γ} is the direct bandgap energy and A is a constant related to the transition matrix element and the effective mass of the material. Despite a small difference in Sn concentration, the fitted prefactors are very similar, with $A \approx 2 \times 10^4 \text{ cm}^{-1} \text{ eV}^{-0.5}$. The FCA was calculated using the relation for pure Ge [19].

Next, the recombination current in the material is calculated, including Auger recombination, radiative recombination, and defect-assisted recombination, using the unsaturated gain in accordance with accepted practices [37]. Under a steady state, the carrier increase rate through electrical pumping is equal to the recombination rate due to all recombination mechanisms. All recombination coefficients in this calculation are adopted from Ge, assuming that a small amount of Sn will not significantly change the features of Ge [19]. All the carriers will recombine in the active region.

From this, the threshold current density of an edge-emitting Sn-Si/GeSn/p-Si double-heterostructure (DH) laser is calculated. The thickness of the GeSn active layer is assumed to be 300 nm. Since the light hole (LH) and heavy hole (HH) bands are degenerate and most carriers are in the HH band, the transverse electric (TE) mode dominates. The optical confinement for the TE mode is simulated to be about 0.9 by photon design. Thus, absorption out the active region was considered. Because the emitted photon has less energy than Si bandgap, absorption by interband transitions in the top and bottom Si layers is neglected. FCA from the Si regions, on the other hand, is considered with the doping concentrations of p^+ and n^+ Si of 1×10^{20} and $5 \times 10^{19} \text{ cm}^{-3}$, respectively. Finally, mirror loss is a function of the cavity length and mirror reflectivities. Here, we adopt a device length of $100 \mu\text{m}$ for the DH structure and assume that one end of the facet is coated with antireflection coating with 98% reflectivity, while the other is just an uncoated facet. The corresponding mirror loss is about 50 cm^{-1} .

III. SIMULATION RESULTS: CARRIER DISTRIBUTION

In this simulation, the Fermi level was swept from midgap to 0.5 eV above the conduction band edge and calculated the electron distributions for GeSn alloys with different Sn concentrations. The ratio of the electron concentration in the Γ valley to the total electron concentration is plotted in Fig. 2. With increasing Sn concentration, the energy difference between the Γ and L valleys reduces, so this ratio increases greatly. Especially, at the low electron concentration range, where most of the electrons stay in the L valley for low Sn concentration cases, this ratio increases 10^3 times from Ge to GeSn alloy with 10% Sn. Thanks to this feature, GeSn alloys can more easily reach direct band population inversion with increasing Sn concentration.

Population inversion begins when the difference between the electron and hole quasi-Fermi levels equals the direct bandgap energy [38]. For undoped GeSn alloys, Fig. 3 shows the required injected carrier density to reach population inversion for different Sn concentrations. The required injected carrier density drops from $4.58 \times 10^{19} \text{ cm}^{-3}$ for bulk Ge to $2.8 \times 10^{18} \text{ cm}^{-3}$ for 10% GeSn alloy. This large reduction of carrier density indicates that the threshold current density of the GeSn laser will be

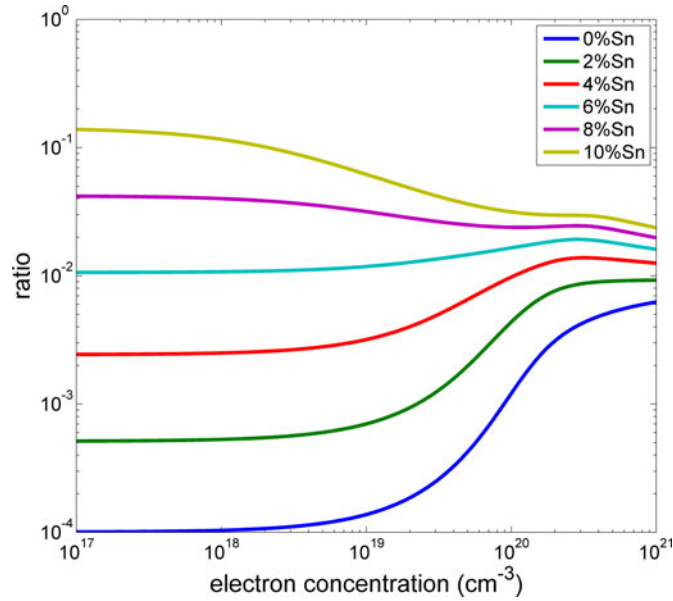


Fig. 2. Ratio of Γ valley electron concentration to total electron concentration for GeSn alloys with 0–10% Sn.

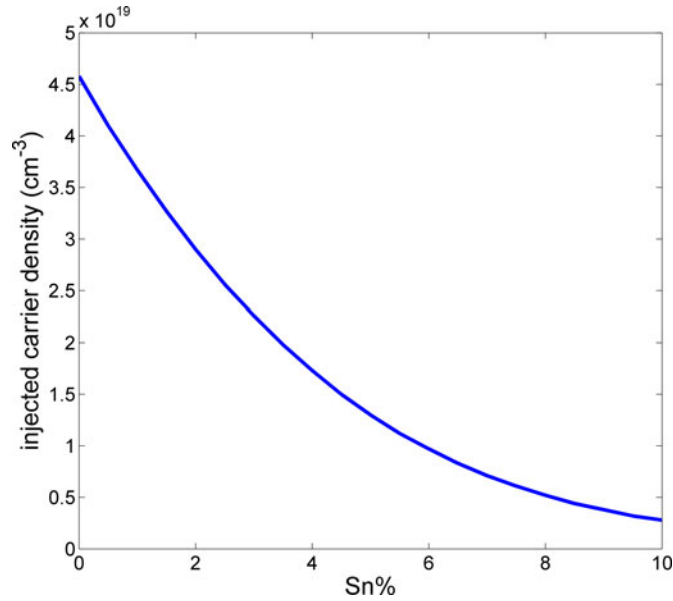


Fig. 3. Required injected carrier density to achieve population inversion as a function of Sn concentrations.

reduced significantly as well, as will be shown in greater detail in Section V.

IV. SIMULATION RESULTS—OPTICAL GAIN

The optical gain of GeSn alloys without FCA was simulated for different n-type doping concentrations as well as for different Sn concentrations. Fig. 4 shows the gain coefficients of 4% GeSn as a function of photon energy with two injected carrier densities: 2.63×10^{19} and 6.61×10^{19} cm^{-3} . The blue dashed

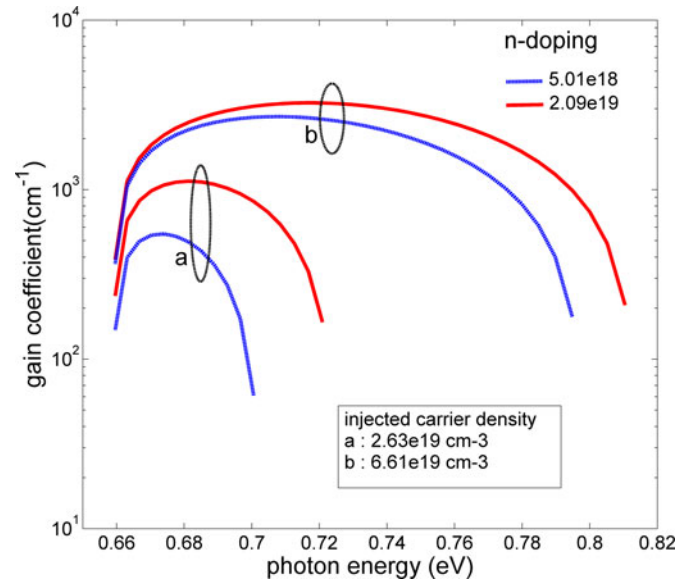


Fig. 4. Optical gain coefficients for the direct transition of 4% GeSn alloy at two different injected carrier densities and two different n-doping concentrations.

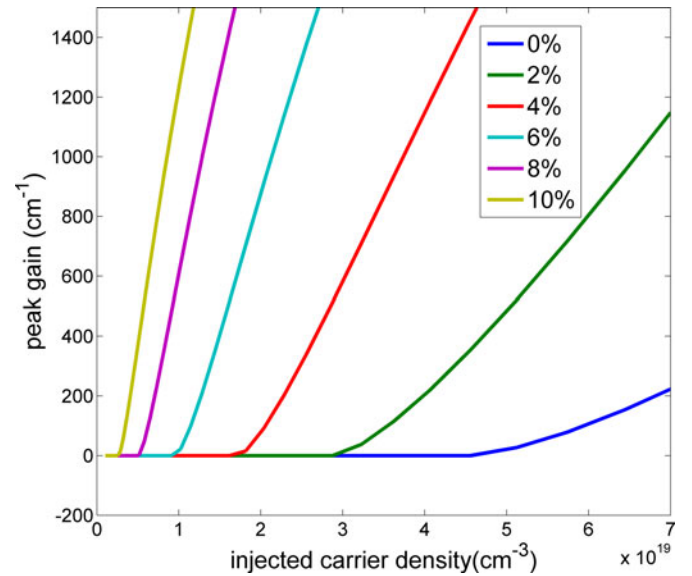


Fig. 5. Maximum gain coefficient for different GeSn alloys with fixed n-doping of 1×10^{17} cm^{-3} .

lines represent the alloy with n-doping of 5×10^{18} cm^{-3} , and the red solid lines represent the alloy with n-doping of 2×10^{19} cm^{-3} . Unlike in strained Ge, the LH and HH bands are still degenerate in GeSn alloys, and therefore, only one smooth curve is observed in each scenario. Increasing the injected carrier density and n-type doping can both increase the gain coefficient and shift the maximum gain coefficient to occur at higher photon energy.

First, the effect of Sn concentration to the gain coefficient is studied. With a fixed n-doping concentration of 1×10^{17} cm^{-3} , Fig. 5 shows the maximum gain coefficient as a function of injected carrier densities for different Sn concentrations. Negative

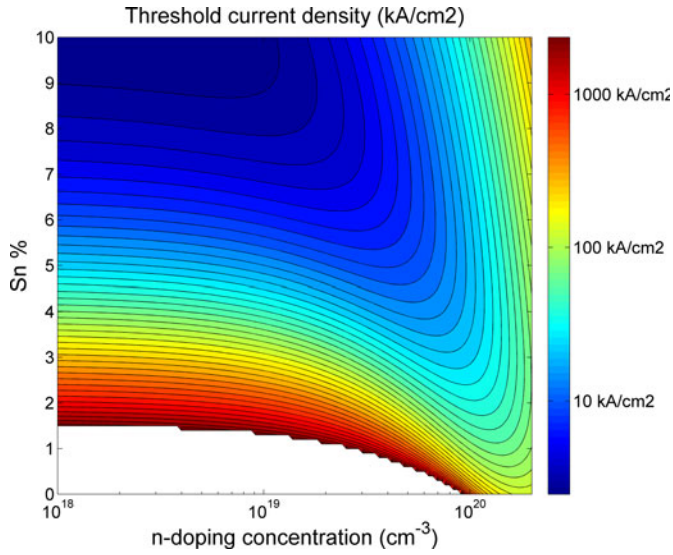


Fig. 6. Threshold current density map for combination of Sn concentration and n-doping concentration with a mirror loss of 50 cm^{-1} .

gain at lower injection levels is ignored. The peak gain data can be linearly fit to the first order, and the slope of the line is defined as the differential gain $d\gamma/d\Delta n$. The differential gain increases two orders of magnitude, from $2.14 \times 10^{-18} \text{ cm}^2$ for Ge to $1.77 \times 10^{-16} \text{ cm}^2$ for GeSn alloy with 10% Sn. In addition, the injected carrier density to achieve transparency, i.e., where the lines intercept with the x -axis, decreases greatly with increasing Sn concentration as well. Thanks to such a huge increase in differential gain and reduction in injected carrier density for transparency, GeSn alloys can reach a high gain coefficient with a much lesser injection level than Ge. The reduction of injection level also decreases the FCA and Auger recombination, which will further reduce the threshold current density. In comparison, including n-type doping reduces the injected carrier density for transparency, but it has little effect on the differential gain.

V. SIMULATION RESULTS—THRESHOLD CURRENT DENSITY

With the inclusion of FCA and the other loss mechanisms, the threshold current density is plotted on a log scale in Fig. 6 for different combinations of n-doping and Sn concentration for a mirror loss of 50 cm^{-1} . As shown in the figure, for each Sn concentration, n-type doping helps reduce the threshold current density, but doping becomes less advantageous at higher Sn concentrations. Similar to the case of strained Ge, there is an optimum n-type doping for each Sn concentration, and the threshold current density increases again when the doping is larger. The minimum threshold current density and the corresponding optimum n-type doping concentration are plotted in Fig. 7. When the Sn concentration increases from 0 to 10%, the minimum threshold current density drops 60 times, from 143.6 to 2.4 kA/cm^2 , while the optimum n-type doping concentration also drops dramatically, from 1.82×10^{20} to $3.16 \times 10^{18} \text{ cm}^{-3}$. The blank white areas in the left bottom of Figs. 6 and 8 are due to the cutoff of the simulation. In addition, alloying with Sn

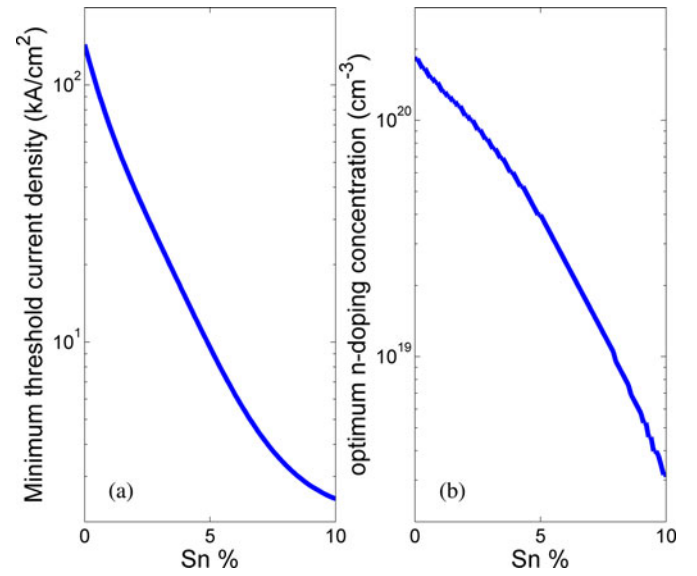


Fig. 7. (a) Minimum threshold current density for different Sn concentrations with a cavity loss of 50 cm^{-1} and (b) corresponding optimum n-doping concentrations.

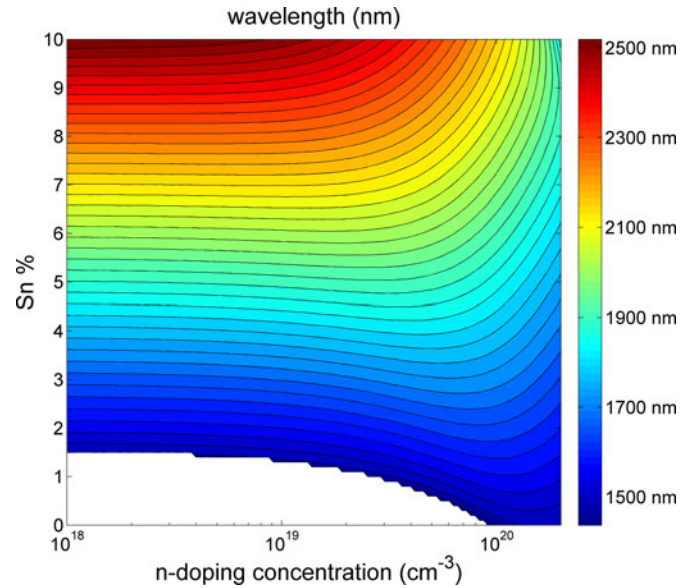


Fig. 8. Wavelength of the emitted photon at the condition of minimum threshold current density.

increases the emitted wavelength to 2500 nm, as shown in Fig. 8. The increase in wavelength unfortunately has a negative effect because the FCA increases with wavelength but is more than overcome by the benefit of increasing the fraction of carriers in the direct valley.

VI. CONCLUSION

In this paper, band structures of GeSn alloys have been simulated using EPM and corrected VCA. The model shows results consistent with experimental data. GeSn alloys are shown to become direct bandgap materials with 6.55% Sn concentration.

Owing to the reduction of the energy difference between direct and indirect conduction band with increasing Sn concentrations, a larger ratio of electrons reside in the direct valley, and so the differential gain increases two orders of magnitude from Ge to GeSn alloys with 10% Sn. The threshold current density of the DH laser was calculated for different combinations of Sn and n-doping concentrations with a cavity loss of 50 cm^{-1} . The results show that the minimum threshold current density drops 60 times from bulk Ge to 10% Sn, and the corresponding optimum n-doping concentration drops greatly as well. Though not considered in this analysis, GeSn alloys can be combined with tensile strain to further improve laser performance. Thus, employing GeSn alloys is part of a viable path to a low-threshold Si-compatible laser.

ACKNOWLEDGMENT

The authors thank Dr. Z. Ji of APIC Corp. for the help with optical mode simulations. They also thank R. Chen and E. Fei from Stanford University for discussions on GeSn and hetero-junction properties.

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Birendra (Raj) Dutt (SM'12) received the Graduate degree (with Hons.) from the Indian Institute of Technology, Kharagpur, India, in 1971, and then studied the nonlinear physics of solitons at the University of Southern California (USC), Los Angeles, USA, where he received the Ph.D. degree in experimental fluid mechanics in 1976, with thesis work undertaken at the California Institute of Technology. He received the Master's degree in theoretical applied physics from Virginia Polytechnic Institute, Blacksburg, USA.

He is the founder and CEO of APIC Corporation and PhotonIC Corporation, Culver City, CA, USA. He has a longstanding reputation in the defense and intelligence communities for his ability to suggest novel solutions to a host of challenging technical problems. Most recently, his efforts have encompassed pioneering work in the areas of microelectronics, photonics, and optoelectronic integration. His areas of expertise include theoretical and experimental physics, fluid mechanics, image understanding, robotics, and artificial intelligence. He currently holds several significant patents in the fields of radar, applied physics, and photonics.

Hai Lin received the M.S. and Ph.D. degrees in materials science and engineering from Stanford University, Stanford, CA, USA, in 2009 and 2012, respectively.

She is currently a Senior Photonic Engineer at PhotonIC Corporation, Culver City, CA. Her research interests include modeling, characterization, and growth of optoelectronic materials and devices for use in Si-compatible optical interconnects.

Devanand (Dave) S. Sukhdeo (S'09) received the B.S. degree in electrical engineering from Columbia University, New York, USA, in 2010 and the M.S. degree in electrical engineering from Stanford University, Stanford, CA, USA, in 2012, where he is currently working toward the Ph.D. degree.

His research interests include theory and modeling of germanium photonic devices, such as lasers and detectors, for use in silicon-compatible optical interconnects.

Boris M. Vulovic received the Dipl.-Ing. degree in electrical engineering from the University of Belgrade, Belgrade, Serbia, the M.Eng. degree in engineering physics from McMaster University, Hamilton, ON, Canada, and the Ph.D. degree in electrical engineering from University of California, Los Angeles (UCLA), USA.

He is currently a Senior Research Engineer at APIC Corporation, Culver City, CA, USA, and a Lecturer of nanoelectronics in the Department of Electrical Engineering, UCLA. His research interests include nanophotonics, nanoelectronics, and spintronics.

Suyog Gupta received the Bachelor's and Master's degrees in technology from the Indian Institute of Technology Bombay, Mumbai, India, in 2009. He is currently working toward the Ph.D. degree in the Department of Electrical Engineering, Stanford University, Stanford, CA, USA.

He is a part of Saraswat Group at Stanford working on GeSn alloys for high-performance MOSFETs. His research interests include semiconductor device physics and modeling, novel materials and structures for logic and memory.

Mr. Gupta has been a recipient of the IIT Bombay Institute Gold Medal, the Stanford Graduate Fellowship, and the Numerical Technologies Founders Scholarship.

Donguk Nam (S'12) received the B.Eng. degree from Korea University, Seoul, Korea, in 2009 and the M.S. degree from Stanford University, Stanford, CA, USA, in 2012. He is currently working toward the Ph.D. degree in the Department of Electrical Engineering, Stanford University, Stanford, CA, USA.

His current research interests include germanium optoelectronics and nanophotonics for on-chip optical interconnects.

Krishna C. Saraswat (F'89) received the B.E. degree in electronics from the Birla Institute of Technology and Science, Pilani, India, in 1968, and the M.S. and Ph.D. degrees in electrical engineering from Stanford University, Stanford, CA, USA, in 1969 and 1974, respectively.

From 1969 to 1970, he worked on microwave transistors with Texas Instruments. Returning to Stanford in 1971, he completed his Ph.D. degree on high-voltage metal-oxide-semiconductor (MOS) devices and circuits. He joined Stanford University, as a Research Associate in 1975 and later became a Professor of electrical engineering in 1983. For the next 15 years, he worked on modeling of chemical vapor deposition (CVD) of silicon, conduction in polysilicon, diffusion in silicides, contact resistance, interconnect delay, and 2-D oxidation effects in silicon. He pioneered the technologies for aluminum/titanium layered interconnects, CVD of tungsten silicide MOS gates, CVD tungsten MOS gates and tunable work function SiGe MOS gates. In 1980s, he became interested in the economics and technology of single-wafer manufacturing. He developed equipment and simulators for single-wafer thermal processing, deposition, and etching and technology for *in situ* measurements, and real-time control. Jointly working with Texas Instruments, he demonstrated a microfactory for single-wafer manufacturing in 1993. Since the mid-1990s, he has been working on new materials, devices and interconnects for scaling MOS technology to sub-10-nm regime. He has pioneered several new concepts of 3-D integrated circuits (ICs) with multiple layers of heterogeneous devices. His group demonstrated the first high-performance germanium MOSFET with high-*k* dielectrics. He has been working on integration of germanium on silicon for high-performance MOSFETs and optical interconnects. He stayed at Stanford as a Researcher and was appointed Professor of electrical engineering in 1983. He also has an honorary appointment of an Adjunct Professor with Birla Institute of Technology and Science, Pilani, India, since January 2004 and a Visiting Professor during the summer of 2007 at the Indian Institute of Technology Bombay, Mumbai, India. From 2000 to 2007, he was an Associate Director of the National Science Foundation/Semiconductor Research Corporation Center for Environmentally Benign Semiconductor Manufacturing. He has been a Technical Advisor, Board Member, and Consultant to several industrial organizations in the U.S., Asia, and Europe. He has also advised several academic and government organizations worldwide. He serves on the leadership council of the Microelectronics Advanced Research Corporation (MARCO)/Defense Advanced Research Projects Agency-funded Focus Center for Materials, Structures, and Nano-Devices. He is currently a Rickey/Nielsen Professor with the School of Engineering, a Professor of electrical engineering, and, by courtesy, a Professor of materials science and engineering, Stanford University. He has graduated more than 70 doctoral students. He is the author or coauthor of more than 630 technical papers. His research interests include new and innovative materials, structures, and process technology of silicon, germanium, and III-V devices and interconnects for very large scale integration and nanoelectronics. His special interests include new device structures to continue scaling MOS transistors, dynamic random access memory devices, and flash memory for nanometer regime, 3-D ICs with multiple layers of heterogeneous devices, and metal and optical interconnections.

Dr. Saraswat was the recipient of the Best Paper Award for six of his technical papers, the Thomas Callinan Award from The Electrochemical Society in 2000 for his contributions to the dielectric science and technology, the 2004 IEEE Andrew Grove Award for his seminal contributions to silicon process technology, the Inventor Recognition Award from MARCO/Focus Center Research Program in 2007, and the Technovisionary Award from the India Semiconductor Association in 2007. He is listed by the Institute for Scientific Information as one of the 250 Highly Cited Authors in his field.

James S. Harris, Jr. (S'66-M'68-SM'77-F'88) received the B.S., M.S., and Ph.D. degrees from Stanford University, Stanford, CA, USA, in 1964, 1965, and 1969, respectively, all in electrical engineering.

In 1969, he joined Rockwell International Science Center, Thousand Oaks, CA, USA, where he was engaged in developing preeminent position in GaAs device technology. In 1982, he joined the Solid State Electronics Laboratory, Stanford University, as a Professor of electrical engineering, where he was the Director of the Solid State Electronics Laboratory from 1984 to 1998, the Director of the Joint Services Electronics Program from 1985 to 1999, and is currently the James and Ellenor Chesebrough Professor of Engineering. He has supervised more than 85 Ph.D. students. He is the author or coauthor of more than 750 publications and holds 18 U.S. patents. His current research interests include the physics and application of ultrasmall structures and novel materials to new high-speed and spin-based electronic and optoelectronic devices and systems.

Dr. Harris is a Fellow of the American Physical Society, the Optical Society of America, and the Materials Research Society. He was the recipient of the 2000 IEEE Morris N. Liebmann Memorial Award, the 2000 International Compound Semiconductor Conference Walker Medal, the IEEE Third Millennium Medal, and the Alexander von Humboldt Senior Research Prize in 1998 for his contributions to GaAs devices and technology.