Epitaxy and design of GeSn/SiGeSn heterostructure LEDs

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1. Introduction

Since the first report on lasing from GeSn/Ge/Si [1], optically-pumped lasing has been demonstrated from GeSn heterostructures with maximum Sn contents of 17.5 at. % and operating temperatures up to 180 K, thus paving the way for the use of GeSn in monolithically grown group IV optoelectronic devices [2,3,4].

In line with the development of III-V lasers since the sixties, the next logical step is to use hetero- and nanostructures to enhance radiative processes occurring in the active regions [5]. Along this line, we have recently demonstrated the increase of optical output brought about by the use of SiGeSn/GeSn multi quantum well (MQW) LEDs [6]. Though far from being optimized in respect to carrier confinement, optically pumped lasing was demonstrated from undoped, direct bandgap heterostructures for the first time in 2017 [6].

Several hurdles have to be overcome in order to demonstrate an electrically pumped laser. On one hand, higher Sn concentrations (and high Si contents, in cladding layers) have to be achieved, to increase the “directness” of the active material and the confinement of charge carriers in heterostructures. Here, it is also necessary to choose the material parameters carefully, designing an “ideal” strain-balanced device. On the other hand, electrical contacts have to be designed in a way that enables efficient charge carrier injection and preserves the lasing mode confinement.

This contribution discusses the epitaxial growth of direct bandgap GeSn/SiGeSn LED structures via reduced-pressure CVD. Moreover, using 8 band k·p calculations, material design of GeSn/SiGeSn MQWs will be discussed to find an optimal parameter space in terms of carrier confinement.

2. Experiments & Results

2.1. CVD growth

Two LED structures, namely a double heterostructure (DHS) and a MQW, have been grown at 350 °C on top of a Ge strain relaxed buffer layer. GeSn:B buffer layers with an average thickness of 220 nm have been grown as a first step for both structures at 360 °C, in order to reduce the heteroepitaxial strain in the active material, increasing the energy band “directness”, and to define the bottom electrical contact. The B doping was graded to zero near to the first SiGeSn cladding/barrier, in order to prevent the emitted light from being absorbed in highly doped regions. At the same time, while lowering the B flow to zero, Disilane (Si_2H_6) was introduced in increasing amounts into the reaction chamber to grow the first SiGeSn barrier. After that, the active region of LED structures was grown, i.e. a 110 nm thick GeSn layer in the case of the DHS and 6 x 20 nm GeSn wells sandwiched between 20 nm SiGeSn barriers in the case of the MWQ. Similarly to the bottom part, the top cladding/barrier was grown such that an inverted Si concentration profile compared to the bottom layer was achieved. While reducing the Si_2H_6 precursor flow to zero, the PH_3 flow was simultaneously increased to grow a 150 nm thick GeSn:P top contact.

Both LED structures were investigated in terms of their morphology and material properties using X-Ray Diffraction, Rutherford Backscattering Spectrometry, Transmission Electron Microscopy, Energy Dispersive X-Ray Spectroscopy (EDX), Atom Probe Tomography and Secondary Ion Beam Mass Spectrometry (SIMS).

Figure 1 shows the EDX line scan of the DHS LED structure. The GeSn:B buffer layer contains around 8.6 at. % Sn, while the active layer and top contact have about 11 at. % Sn. The Sn/Si concentration in the claddings were around 12.0/4.5 at. % with Si content increasing when going from GeSn:B to

SiGeSn and decreasing from SiGeSn to GeSn:P, as intended.

From SIMS measurements we derive a maximum Boron concentration of $3{\cdot}10^{18}$ cm^{-3} and a maximum Phosphorous concentration of $1.5{\cdot}10^{19}$ cm^{-3}. A grading opposite to the above described Si grading has been achieved here, which is supposed to keep the dopants away from the optically active region.

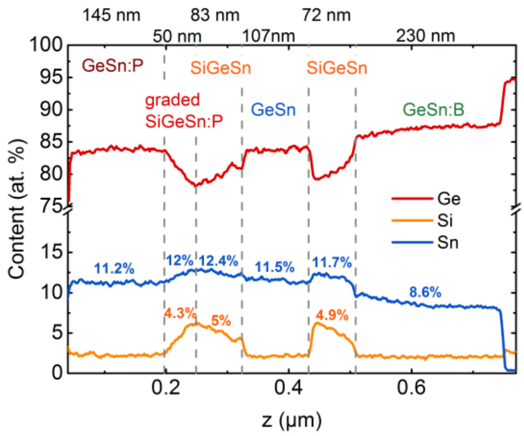

Fig. 1. EDX line scan of a DHS LED showing Si/Ge/Sn elemental profiles.

2.2. Band alignment calculations

Band structure calculations have been performed to investigate GeSn/SiGeSn heterostructures in respect to the requirements for efficient carrier confinement. These are not only a maximal band discontinuity between barrier and well at Γ and L ($V_{Γ,L}$), but also a direct bandgap active region, while maintaining an indirect barrier material. Conduction and valence band energies have been calculated using a Sn/Si concentration dependent linear interpolation with parameters extracted from the empirical pseudopotential method [8].

From these calculations, particular combinations of GeSn/SiGeSn have been chosen to investigate the material gain g and its dependence on doping and injected charge carrier density N_{inj}.

Figure 2a shows the band alignment at Gamma for a $Ge_{0.84}Sn_{0.16}$ well, as it depends on the Sn and Si content in the barrier. The previously mentioned confinement requirements are fulfilled only in the small green region. The calculated gain of a $Ge_{.84}Sn_{.16}/Si_{.10}Ge_{.75}Sn_{.15}$ MQW is plotted in figure 2b for different injected charge carrier densities. The free carrier absorption (FCA) of bulk $Ge_{.875}Sn_{.125}$ for the same injected charge carrier densities is shown in dashed lines, which is a reasonable approximation for the FCA in the $Ge_{.84}Sn_{.16}/Si_{.10}Ge_{.75}Sn_{.15}$ MQWs. These calculations indicate that a minimum of $4{\cdot}10^{17}$ cm^{-3} carriers needed to achieve material gain and overcome losses due to free carrier absorption.

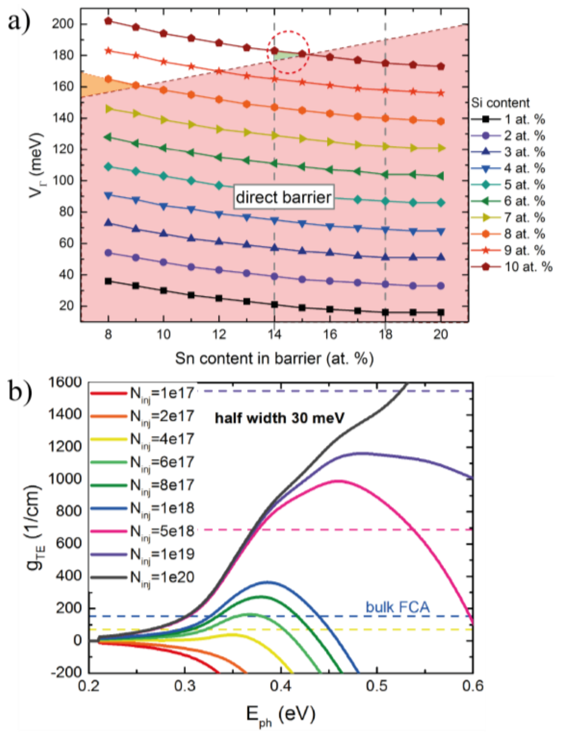

Fig. 2 a) Band alignment map for GeSn/SiGeSn showing regions, where the barrier is direct (red area), the band alignment in L is negative (orange area) and the Sn content of barrier and well differs strongly (dashed lines). b) Gain spectra for $Ge_{.84}Sn_{.16}/Si_{.10}Ge_{.75}Sn_{.15}$ with different injected charge carrier densities and FCA levels (dashed lines).

3. Conclusions

This contribution demonstrates the growth of GeSn/SiGeSn heterostructure LEDs with graded contact layers. Efficient carrier confinement and gain calculations show the possibilities and limitations in creating efficient laser structures.

Acknowledgements

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References

[1] S. Wirths et al., Nature Photonics, **9**, 88 (2015).
[2] V. Reboud et al., Appl. Phys. Lett. **111**, 092101 (2017).
[3] J. Margetis et al., ACS Photonics, (2017).
[4] S. Al-Kabi et al., Applied Physics Letters, **109**, 171105 (2016).
[5] Z.Alferov, IEEE, **6**, 832-840 (2000)
[6] D. Stange et al., OPTICA, **4**, 2334-2536 (2017)
[7] D. Stange et al., IEDM17, 589 (217)
[8] P. Moontragoon et al., J. Appl. Phys. **112**, 073106 (2012);