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Epitaxy and Photoluminescence Studies of High Quality GeSn Heterostructures with Sn Concentrations up to 13 at.%

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***Abstract* — We present photoluminescence measurements on highly compressively strained and partially relaxed GeSn alloys with Sn contents up to 13 at.%. Calculations predict a net gain of 572 cm^{-1} for partially relaxed and moderately doped $Ge_{0.88}Sn_{0.12}$.**

***Keywords* — Germanium-Tin; Si photonics; Laser materials; Photoluminescence; Chemical Vapor Deposition; Group IV alloys; low temperature epitaxy**

I. Introduction

Optical interconnects are one of the promising alternatives to copper wires for data transfer, thereby reducing the power consumption in future CMOS technology. Especially group IV semiconductors are highly desirable for such applications due to their straightforward CMOS integration. Unfortunately, column-IV materials exhibit poor light emitting properties. Due to the small energy difference between Γ- and L-valleys in Ge several approaches have been investigated recently to improve its light emission efficiency, such as tensile strain [1] or high n-type doping [2]. In the last decade another approach has emerged, i.e. alloying Ge with Sn. The higher the substitutional Sn concentration in the Ge lattice the smaller the energy difference between the Γ- and L-valleys becomes (see sketch in Fig. 1). However, the epitaxial growth of high quality GeSn is challenging due to the low solid solubility of Sn in Ge (<1% [3]) and the huge lattice parameter mismatch between the two (15%). Here we present structural and optical characterization of high Sn content GeSn binaries that are suitable for group IV photonic devices.

II. Experimental

The GeSn layers under investigation were grown in a 200 mm reduced pressure chemical vapor deposition (RPCVD) tool with showerhead technology. The special design in combination with the developed growth process enables high quality Si-Ge-Sn epitaxy at very low growth temperatures [4]–[6]. We used Ge_2H_6 and $SnCl_4$ as precursors which were led into the reactor chamber by a N_2 carrier gas. Two sets of GeSn epilayers with Sn concentrations ranging between 8 at.% and 13 at.% have been grown on high quality Ge-buffered Si(100) wafer (Ge-VS) [7]. The first series consist of 30-50 nm thick pseudomorphically grown layers while the other set concerns partially relaxed layers with thicknesses ranging between 200 and 300 nm. X-ray diffraction (XRD), Rutherford spectrometry (RBS) and transmission electron microscopy (TEM) have been used to study the crystalline quality and the strain relaxation mechanisms in the grown layers. Reciprocal space maps (RSM) have been acquired to determine the built-in strain. The optical quality and the light emission were investigated by room temperature photoluminescence (PL). The PL peak shift, depending on the Sn content and strain, was compared to theoretical band structure calculations. Finally, 8x8 k.p electronic band structure calculations were used to investigate the optical gain as function of the injected carriers and the doping level.

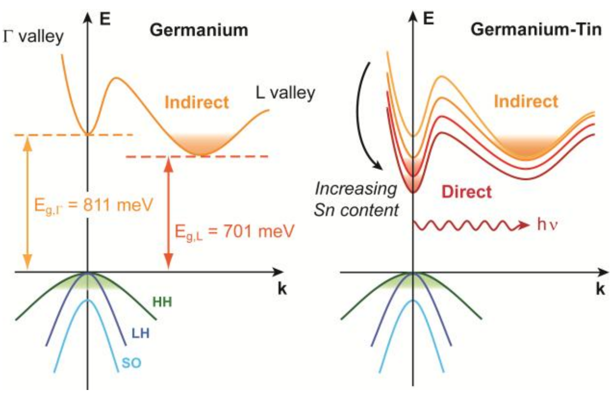
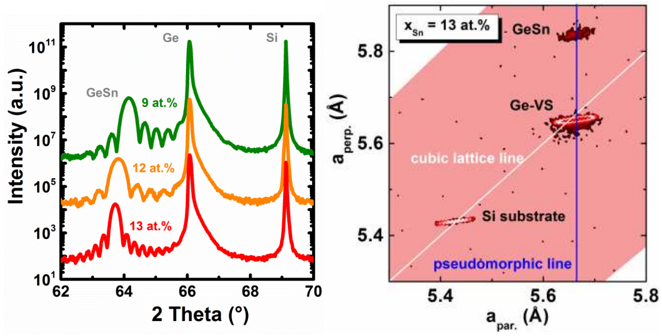
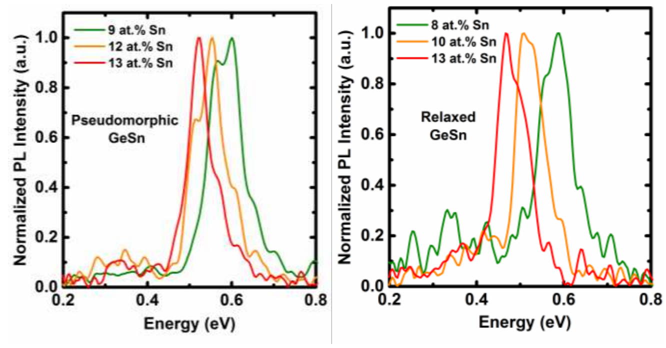


Fig. 1. Sketch of the electronic band structure of Ge and GeSn alloys near the indirect to direct band gap transition. For sufficiently high Sn concentrations the Γ-valley lies energetically below the L-valley.



(a) (b)

Fig. 2. (a) θ/2θ scans for GeSn layers with 9, 12 and 13 at.% Sn. The GeSn peak shifts towards lower angles with the Sn content. (b) XRD-RSM of a biaxially compressively strained GeSn layer (x_{Sn} = 13 %) grown on Ge-VS.



(b) (b)

Fig. 3. Room temperature PL measurements for (a) fully strained and (b) partially relaxed GeSn layers grown on Ge-VS. For higher Sn concentrations and lower compressive strain the peak positions shift towards lower energies.

III. Results and Discussion

θ/2θ-scans of three 30 nm thick GeSn layers of the first series are shown in Fig. 2a. Well-defined, intense GeSn and Ge peaks are observed. The marked thickness fringes around the GeSn peaks are clear signs of the single crystalline quality of the growth. The Sn concentrations are obtained by fitting the θ/2θ-scans. Since Sn has a larger cubic lattice constant compared to Ge, the GeSn peaks for layers exhibiting larger Sn concentrations grown at lower growth temperatures are shifted towards smaller angles due to the larger out-of-plane lattice constant. RSMs of the GeSn/Ge/Si(100) heterostructures have been acquired to determine the latter as well as the in-plane lattice constant. The RSM of a $Ge_{0.87}Sn_{0.13}$ layer is shown in Fig. 2b. The peak of the roughly 2.5 µm thick Ge buffer lies below the cubic lattice line indicating a weak tensile strain of 0.16 %, whereas the GeSn peak is on the pseudomorphic line, proving that its growth was pseudomorphic on the Ge-VS underneath. A large compressive strain of about -1.9 % is obtained by using the bowing corrected Vegard´s law [8].

Room temperature photoluminescence measurements of these highly strained layers are presented in Fig. 3a. Strong photoluminescence, which indicates high optical quality for all investigated Sn concentrations, has not been previously observed for such high Sn concentrations. The observed oscillations in the spectra are due to Fabry-Perot (FP) interferences from the underlying Ge buffer layers. The PL peaks shift to lower energies for higher Sn concentrations, in accordance with the band structure calculations. Luminescence spectra of the partially relaxed layers from the second set are shown in Fig. 3b. The RSM measurements exhibit a degree of relaxation of up to 70 %. Again, we observed strong luminescence at room temperature in spite of strain relaxation induced defects at the GeSn/Ge-VS interface. We otherwise obtained a PL peak shift towards lower energies compared to fully strained layers, due to the reduced strain. Relaxed GeSn layers are highly desirable since the Sn concentration required for the indirect to direct band gap transition becomes lower with increasing strain relaxation, or by introducing tensile strain [4]. Additionally, the layers' thicknesses in combination with the high crystalline quality make these GeSn/Ge heterostructures grown on Si(100) a promising material system for efficient group IV light emitters. Gain calculations were performed for strained and partially relaxed GeSn layers with Sn concentrations up to 14 at.%. Net gain values beyond 500 cm^{-1} at n-doping levels of $3x10^{19}$ cm^{-3} have been found for partially relaxed $Ge_{0.88}Sn_{0.12}$ layers.

IV. Conclusion

In conclusion, we have grown high quality GeSn layers on Ge-VS with high compressive strain values of up to -1.9 % and Sn concentrations up to 13 at.%. Room temperature luminescence measurements prove the high optical quality of partially relaxed, high Sn content layers which theoretically exhibit large gain values for mild doping. These findings evidence the high potential of GeSn alloys to be implemented in future active optoelectronic devices.

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