SiGeSn Growth Studies Using Reduced Pressure CVD Towards Optoelectronic Applications

S. Wirths[1*], D. Buca[1], Z. Ikonic[2], P. Harrison[2], A.T. Tiedemann[1], B. Holländer[1], G. Mussler[1], U. Breuer[3], D. Grützmacher[1], and S. Mantl[1]

[1]Peter Grünberg Institute (PGI 9-IT) and JARA-FIT, Forschungszentrum Juelich, 52425, Germany

[2]Institute of Microwaves and Photonics, School of Electronic and Electrical Engineering, University of Leeds, Leeds LS2 9JT, United Kingdom

[3]Central Institute for Engineering, Electronics and Analytics (ZEA-3) Forschungszentrum Juelich, 52425, Germany

*Tel: +49-2461-61-3149, Fax: +49-2461-61-4673, E-mail: s.wirths@fz-juelich.de

1. Introduction

Complete photonic integrated circuits on Si would strongly benefit from the development of appropriate direct band-gap group IV semiconductors such as strained Ge. Recently, both theoretical and experimental studies have shown that Ge, an indirect-gap semiconductor, can be band-engineered into a quasi direct-gap semiconductor [1]. It has been predicted that a direct band-gap can be achieved in strained Ge with 2% tensile strain without a need for heavy n-type doping [2]. However, the use of strained Ge as active laser medium demands the development of suitable barrier layers. The SiGeSn alloys are ideal solutions for forming promising quantum-well structures with strained Ge as active well.

In this contribution we first present, based on electronic band-structure calculations, the Si and Sn concentration ranges for the $Si_xGe_{1-x-y}Sn_y$ ternary alloys which offer the best band-offsets between strained $Si_xGe_{1-x-y}Sn_y$ and tensile strained Ge. Then, we present the epitaxial growth of $Si_xGe_{1-x-y}Sn_y$ layers directly on Si(100) and on thin Ge virtual substrates on Si(100). The aim is to show the possibility of realization of laser structures as indicated by simulations.

2. Experimental

The epitaxial growth studies were performed using a 200 mm AIXTRON Tricent® Reduced Pressure CVD (RPCVD) tool with showerhead technology. Since low growth temperatures are essential for the single crystal growth of $Si_xGe_{1-x-y}Sn_y$ semiconductors, Si_2H_6 and Ge_2H_6 in combination with $SnCl_4$ and N_2 as carrier gas were employed. At a constant chamber pressure of 60 mbar and a few slm total gas flow, the growth temperature was varied between 350°C and 450°C. The epitaxial growth of the Ge buffer layers was carried out at 425°C using Ge_2H_6 [3]. Several analysis methods, like Rutherford Backscattering Spectrometry in the ion channeling mode (RBS/C) and X-Ray reciprocal space mapping, were employed to investigate the composition, crystal quality and morphology of the grown layers.

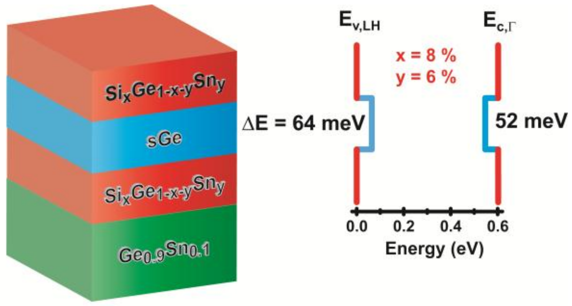

Fig. 1 Layer structure and electronic band structure of a pseudomorphic $Si_{0.08}Ge_{0.86}Sn_{0.06}$/sGe quantum-well grown on a relaxed $Ge_{0.9}Sn_{0.1}$ buffer.

3. Results and Discussion

Our approach for a group IV semiconductor laser design is based on a SiGeSn/strained Ge/SiGeSn quantum well, with a direct band-gap of highly strained Ge as optically active layer. Thereby, a relaxed $Ge_{0.9}Sn_{0.1}$ buffer layer is grown first to set the lattice constant, followed by the pseudomorphic growth of the laser structure which induces elastic strain in

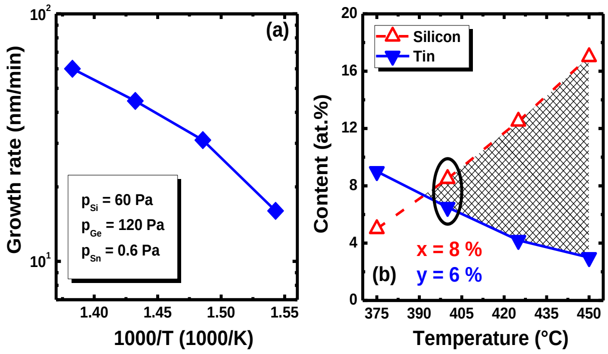

Fig. 2 (a) Arrhenius plot for the SiGeSn epitaxial growth on Si(100). (b) Si and Sn content as a function of the growth temperature at constant partial pressure ratios. The shaded area denotes suitable Si-Sn ratios for SiGeSn cladding layers.

both the SiGeSn barriers and the Ge well. The band-gaps and band-offsets to the strained Ge of strained $Si_xGe_{1-x-y}Sn_y$ layers have been calculated from the supercell empirical pseudopotential method [4], together with linear interpolation of deformation potentials and band offsets of elemental Si, Ge, and Sn, for x and y ranging from 0-20 at.% and 0-10 at.%, respectively. The simulation results indicated that appropriate band alignments, with reasonable band-offsets between $Si_xGe_{1-x-y}Sn_y$ barrier and strained Ge well are obtained for $y < x$. In Fig. 1 we show an example of the simulated heterostructure, for 6at.% Sn and 8at.% Si. The conduction (Γ-valley) and valence band offsets above 50 meV were calculated, which may sustain population inversion and hence make lasing possible. The results of the SiGeSn growth study on Si(100) substrates are shown in Fig. 2. Several stoichiometries for the SiGeSn alloys have been synthesized at fixed partial pressure ratios and temperatures ranging between 450°C and 375°C. The growth rate strongly depends on the growth temperature (Fig. 2a) which indicates a kinetically controlled growth regime. Similar to the GeSn growth [3], the Sn content increases as the temperature decreases (Fig. 2b), whereas the Si concentration decreases due to the lower Si_2H_6 cracking efficiency at lower temperatures. For the applied partial pressure ratios and $T_{growth} \geq 400°C$, $Si_xGe_{1-x-y}Sn_y$ layers with $x \geq 8$at.% and lower Sn than Si concentrations were grown (shaded area in Fig. 2b). These layers are suitable candidates for our proposed SiGeSn/sGe quantum-well laser design. RBS channeling measurements (Fig. 3) reveal a low minimum channeling yield for SiGeSn/Si(100) heterostructures grown at a temperature of 375°C-450°C, evidence of high single crystal quality. Due to the large lattice mismatch dechanneling towards the SiGeSn/Si interface is observed (Fig. 3a), indicating strain relaxation. The use of Ge buffer layers enables the growth of such SiGeSn alloys at even lower temperatures down to 350°C. The RBS/C spectra in Fig.3 correspond to a SiGeSn/Ge /Si(100) structure grown at 350°C, with 10.5at.% Sn and 4.5at.% Si.

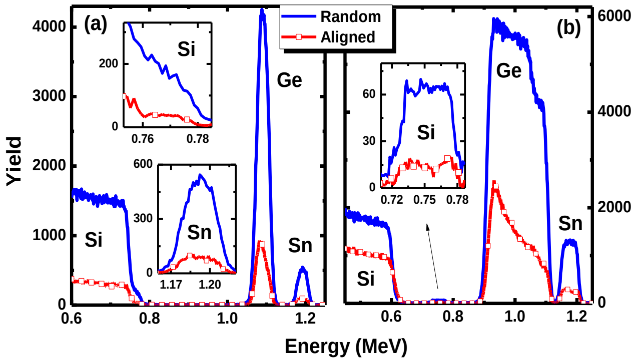

Fig. 3 RBS random and aligned spectra for SiGeSn layers grown on (a) Si(100) at 425°C and (b) Ge buffered Si(100) at 350°C.

4. Conclusion

SiGeSn/strained Ge heterostuctures for optoelectronic applications have been proposed based on empirical pseudopotential method and linear interpolation of deformation potentials and band offsets. The epitaxial growth of $Si_xGe_{1-x-y}Sn_y$ ternary alloys has been studied on Si(100) and Ge-buffered Si(100). Based on the simulation results, ternaries with the appropriate Si to Sn concentrations have been grown and characterized.

References

[1] J. Liu, X. Sun, R. Camacho-Aguilera, L. C. Kimerling, and J. Michel, Optics letters, 35 (2010) 679,

[2] M. El Kurdi, G. Fishman, S. Sauvage, and P. Boucaud, Journal of Applied Physics, 107 (2010) 013710,

[3] S. Wirths, D. Buca, A.T. Tiedemann, B. Holländer, P. Bernardy, T. Stoica, D. Grützmacher, and S. Mantl, ECS Transactions, 50 (2012) 885.

[4] P. Moontragoon, P. Pengpit, T. Burinprakhon, S. Maensiri, N. Vukmirovic, Z. Ikonic, and P. Harrison, J. Non-Cryst. Solids, 358 (2012) 2096.