Strain-mediated Sn incorporation and segregation in compositionally graded $Ge_{1-x}Sn_x$ epilayers grown by MBE at different temperature

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Group IV alloys of Ge and Sn are extensively studied for various electronic and optoelectronic applications on a Si platform. $Ge_{1-x}Sn_x$ with α-Sn concentrations as low as 6% [1] allows for a transition from an indirect bandgap to a direct optical. Higher Sn content makes possible mid and even long-range infrared optical emission and detection [2]. At the same time, due to the low solid solubility of Sn in Ge (~1%), as well as the large lattice mismatch of α-Sn with Ge (~14%), the realization of high-quality Sn-rich $Ge_{1-x}Sn_x$ structures has proved challenging. In this study, we demonstrate enhanced Sn content using molecular beam epitaxy (MBE) growth of compositionally graded $Ge_{1-x}Sn_x$ on Ge (001). High-quality GeSn alloys with Sn composition reaching 6% at constant temperature. The maximal fraction of Sn was further increased to 9.0% when the growth temperature was continuously lowered while increasing the Sn flux. The analysis of surface droplets and SIMS (secondary ion mass spectrometry) profiles of elemental composition give evidence of Sn rejection during the growth, potentially associated with a critical energy of elastic strain. The intentional reduction of the coherent strain by decreasing the Sn flux near the sample surface has shown to trap a higher fraction of Sn in the $Ge_{1-x}Sn_x$ layer and lower surface segregation. Supporting data (Fig.2) shows an approach for XRD spectra simulation was developed for strain and composition characterization.

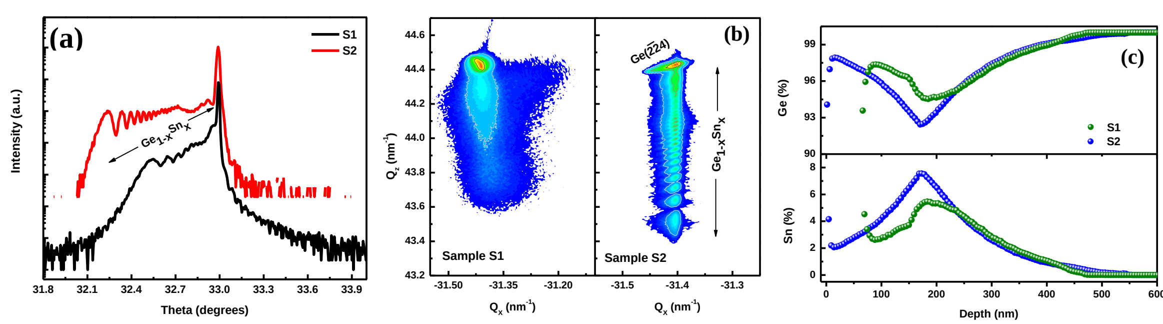

Fig. 1. (a) XRD (004) ω/2θ scans, (b) $(\bar{2}\bar{2}4)$ RSMs of samples G1 and G2 and (c) The SIMS profiles of Sn and Ge in the $Ge_{1-x}Sn_x$ epilayer of samples S1 and S2.

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[2] J. Bass, H. Tran, W. Du, R. Soref, S.-Q. Yu, Opt. Exp. 2021, 29 (19),30844-30856.

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Supplementary Pages (Optional)

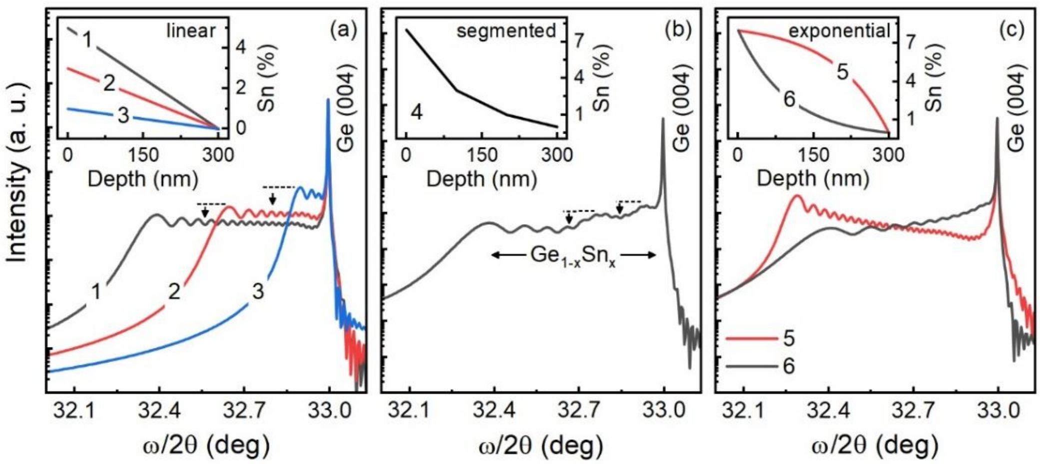

Fig. 2. Calculated X-ray diffraction 004 ω/2θ spectra for several pseudomorphic compositionally graded $Ge_{1-x}Sn_x$/Ge heterostructures showing the effect of (a) linear grading, (b) stepwise grading, and (c) exponential grading on the scattered intensity.