Final Report for AOARD Grant **FA2386-11-1-4037** “Development of direct band gap group-IV semiconductor with the incorporation of Sn”

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Abstract:

The indirectness of its energy band of group IV materials of Si and Ge prevents the use of these materials and their alloys for optical devices. In this project, direct bandgap group IV alloy of GeSn alloy is developed. This report covers: (a) growth techniques of GeSn alloy with various Sn compositions, (b) characterization of the alloy, and (c) physical properties of the alloy and identifying direct optical transitions. From the analysis, we show that a direct bandgap group IV alloy of GeSn can be obtained at a Sn composition above ~11%.

Introduction:

Sn-based - compound can be made to be direct bandgap for group material. In this project, we focus on GeSn material system and we propose to engineer the energy bands of its optical transition of to establish the crossover of indirect-to-direct transition. By resolving both the indirect and direct optical transition, this enable us to identify the direct optical transition unambiguously which is desired in the application for optical emitters.

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14. ABSTRACT

Due to the indirect energy band of group IV materials of Si and Ge, these materials and their alloys can?t be used to make optical devices. In this project, direct bandgap group IV alloy of GeSn alloy was developed. This report covers: (a) growth techniques of GeSn alloy wiith various Sn compositions, (b) characterization of the alloy, and (c) physical properties of the alloy and identification of direct optical transitions.

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Experiment, Results and Discussion: Describe the results obtained during the period of performance and what work may be performed in the future as follow on.

This section is organized as following sub-sections: (1) growth techniques of GeSn alloy with various Sn compositions, (2) characterization of the alloy, and (3) physical properties of the alloy and identifying direct optical transitions.

1. Growth techniques of GeSn alloy with various Sn compositions

In this project, several types of Sn-based IV-IV compounds are developed. Here, we focus on the growth techniques of GeSn alloy with various Sn compositions. We have successfully demonstrated the growth of GeSn thick film without defect with Sn composition up 12% using Molecular Beam Epitaxy (MBE). Employing the low temperature growth technique, the two key issues in relating to the growth of GeSn film is resolved, namely (a) Sn segregates during the growth of GeSn film and (b) the misfit dislocations develop at GeSn/Ge interface as due to the large lattice mismatch between Sn and the Ge wafer. A series of $Ge_{1-x}Sn_x$ films with various Sn compositions up to 30% and thickness of 30 nm was grown. A typical Cross-sectional transmission electron microscopy (XTEM) image of the film is plotted in Fig. 1(a). It shows that the film is defect free. To probe the Sn profile in the GeSn film, STEM is used instead of XTEM. The STEM image is depicted in Fig. 1(b). Dislocations are not observed, consistent with the XTEM measurement. Energy-dispersive X-ray spectroscopy (EDS) measurements were performed at various locations labeled 1–13, as marked in Fig. 1(b). The measured result is plotted in Fig. 1(c). The result shows that, along the in-plane direction, the Sn composition is ~10%. Along the growth direction, the Sn composition is also approximately ~10%. Taking the Sn composition from these measured points, the average Ge composition is determined to be 9.3±0.6%. This reveals that Sn is nearly uniformly distributed in the GeSn film.

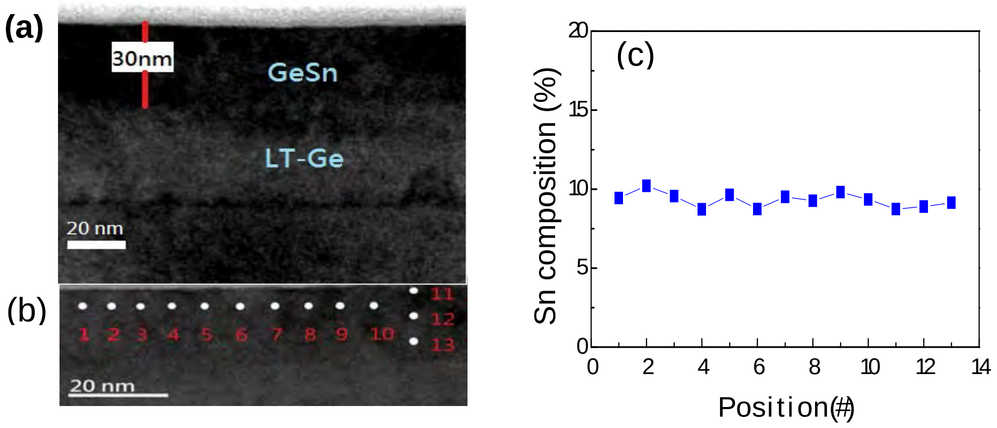

Fig. 1. (a) XTEM imagine of GeSn grown on on Ge buffer layer, showing that the GeSn film is defect free. (b) STEM imagine of the GeSn film. (c) Position-dependent Sn composition of the GeSn, indicating Sn is uniformly distributed without segregation.

(2) Characterization of the alloy

Various measurements have been performed to characterize these samples, including: high resolution X-ray, Raman spectroscopy, etc. Typical high resolution X-ray trace is plotted in Fig. 2. For sample with Sn=2%, which had the lowest Sn composition, two features are resolved: (a) a sharp Ge line associated with the Ge substrate and the HT-Ge/LT-Ge buffer layer and (b) a broad line located at the shoulder of the sharp Ge line, marked by the solid arrow, which is attributed to the GeSn film. With increasing Sn composition, the position of the sharp Ge line remains unchanged for all the samples, while the main position of the GeSn line moves to a lower angle with fringes shown in Fig. 2(b). This suggests that the lattice constant of the GeSn film increases with increasing Sn concentration. Similar behavior is also observed in the (202) scan. From the separation of the two main features, the in-plane lattice constant and the lattice

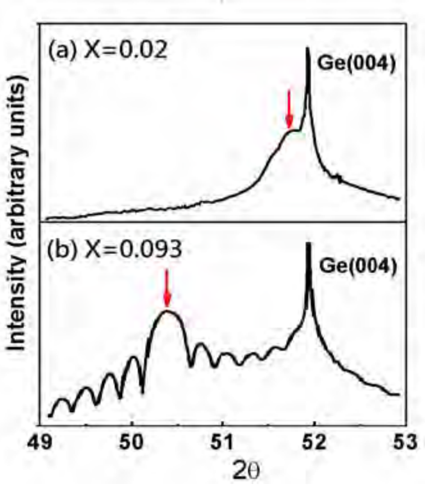

Fig. 2. High-resolution diffraction patterns of two samples of N1 and N5. It shows that, the position of the GeSn line moves to lower angle as Sn composition increases as marked by the solid red arrow lines.

constant along the growth direction of the films can be deduced. Using these measured lattice constants (b), the in-plane strain ($\varepsilon_{//}$) and strain along the growth direction ($\varepsilon_{\perp}$) are calculated by $(b - a_{\mathrm{GeSn}})/a_{\mathrm{GeSn}}$. The results shows that these alloy are partially strained which will be use for the later discussion in identifying the energy bandgap.

(3) Physical properties of the alloy and identifying direct optical transitions

After establishing the characteristic of the alloy, we now move to the energy band of the alloy. Fourier transform infrared spectroscopy (FTIR) is employed for probing both indirect and direct optical transitions. Here, we like to point out a technique detail on the measurement. In the conventional FTIR measurement, the incident light source is normal to the sample (parallel to the growth direction). The light penetrates through the sample and collected by detector. The collected signal is dominated by the signal from the wafer material as the thickness of the wafer is much thicker than the thickness of the film. In here, the technique of multi-reflection is developed. A schematic diagram of the setup is plotted in Fig. 3. The sample is polished a ~ 45 degree at the edge and the incident light source is focused at the edge in which the incident light propagate through the film with multi-reflection as indicated by the solid arrow lines. This enhances the absorption strength on the samples yielding a reasonable collected signal level.

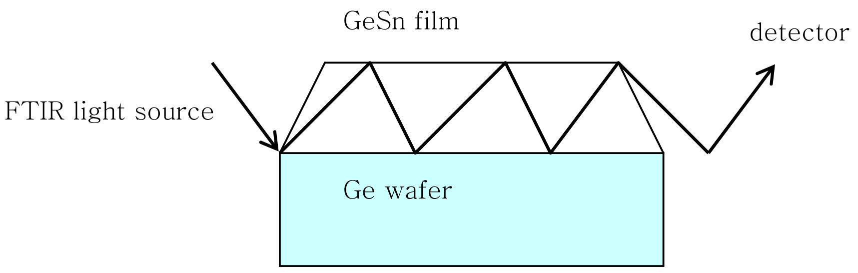

Fig. 3. Experimental setup for the FTIR absorption measurement.

A spectrum on $Ge_{0.98}Sn_{0.02}$ film with a thickness of 30 nm is depicted in Fig. 4. Both indirect (located at ~ 0.55 eV, conduction X band to the valence Γ band X—Γ) and direct optical transition (located at ~ 0.68 eV, conduction Γ band to the valence Γ band Γ—Γ) is resolved as marked by the two dotted arrow lines.

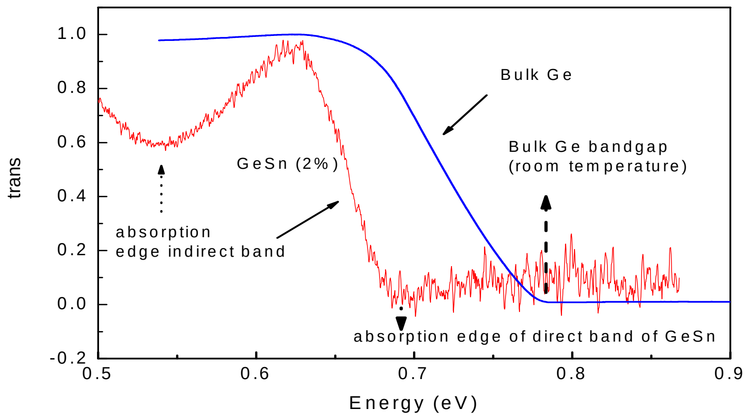

Fig. 4. A typical FTIR spectrum showing both indirect and direct optical transition on GeSn thick film.

Taking the measured value of all the samples and plotted in Fig. 5, it shows that the indirect optical transition become the lowest transition for sample with Sn composition of ~ 11%. (The black solid line indicates the change of the direct optical energy of Γ—Γ transition while the red solid line indicates the change of the indirect optical energy of X—Γ transition.) From the analysis, we can say that the critical Sn composition of the indirect-direct crossover occurs at a Sn composition of ~ 11% as indicates by dashed arrow line.

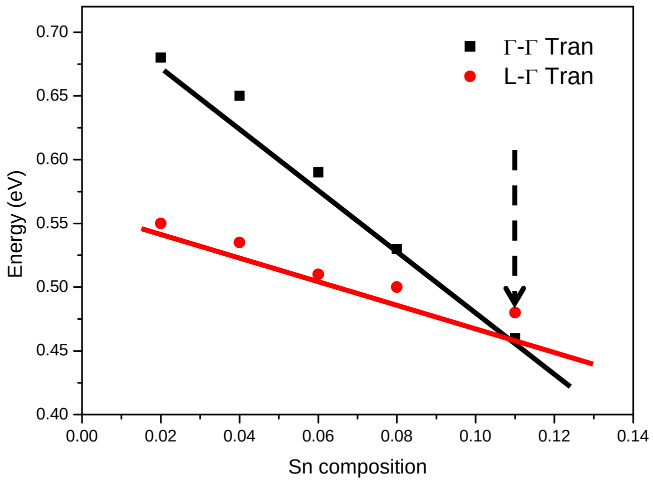

Fig. 5. Optical energy for both direct and indirect optical transitions.

List of Publications:

[1] Local intermixing on Ge/Si heterostructures at low temperature growth, H. H. Cheng, W. P. Huang, V.I. Mashanov, and G. Sun J. Appl. Phys. 108, 044314 (2010). Selected paper by American Institute of Physics and the American Physical Society. Published by Virtual Journal of Nanoscale Science & Technology, http://www.vjnano.org, September 6, (2010).

[2] G. Sun, R. A. Soref, and H. H. Cheng, "Design of an electrically pumped SiGeSn/GeSn/SiGeSn double-heterostructure mid-infrared laser," *J. Appl. Phys.* **108**, 033107 (2010).

[3] G. Sun, R. A. Soref, and H. H. Cheng, "Design of a Si-based lattice-matched room-temperature GeSn/GeSiSn multi-quantum-well mid-infrared laser diode." Opt. Express 18, 19957-19965 (2010).

[4] Pseudomorphic growth of Ge1-xSnx thick film at low temperature, AIP ADVANCES **1**, 042118 (2011).

[5] Formation of Ge-Sn nanodots on Si(100) surfaces by molecular beam epitaxy, Nanoscale Research Letters, publication date 12 January (2011).

[6] Clustering Effect on The Band Gap of GeSn Alloys, H. H. Cheng, submitted to JAP.