

Report

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Tin-based IV-IV heterostructures by using Molecular Beam Epitaxy

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Highlights

The main objective of the program is to investigate Sn-based IV-IV compounds which have been considered as direct bandgap material. We have made significant progress towards the growth and characterization of GeSn/Ge heterostructure. (The reason for choosing GeSn/Ge is discussed in the text.) As a collaborated effort between NTU, UMass Boston, and AFRL at Hanscom, USA, we have produced important results that have been published in refereed journals. This report summarizes our accomplishments, future direction of work, and publications produced as a result of this project.

1. Accomplishment

(a) Growth of GeSn/Ge by Molecular Beam Epitaxy

In this project, tin-based SnGe/Ge heterostructures was developed using molecular beam epitaxy (MBE). A systematic growth of GeSn with various Sn compositions up

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to 30% was successfully performed. (The reason for choosing GeSn on Ge is discussed below. Growth using MBE affords flexibility in the growth of the materials system, whereby conditions such as growth temperature, etc., can be varied over a wide range.) The key issues affecting the growth of the alloy and its heterostructure are: (1) the instability of cubic α -Sn at high temperature and the low surface free energy, which can lead to segregation on the surface, and (2) the large lattice mismatch between Sn and the wafer materials of Ge(Si).

The second issue affecting the growth of the alloy and its heterostructure is the lattice mismatch between α -Sn (6.49 Å) and Ge (5.65 Å) or Si (5.43 Å), which is approximately 15% and 17%, respectively. The mismatch between these elements can be reduced by growing binary SnGe alloys with a moderate Sn content or ternary $\text{Ge}_{1-x-y}\text{Si}_x\text{Sn}_y$ alloys on Ge wafers. In the former case, the lattice mismatch is modulated by the Sn composition. In the latter case, the mismatch is tuned by incorporating Si of smaller lattice constant. In the past, we have dealt with the mismatched heterostructure of a SiGe/Si superlattice (the lattice mismatch between Ge and Si is 4.2%). Several techniques were developed to realize the growth of a defect-free SiGe layer with high Ge content. (Defect-free in a cross-sectional transmission electron microscope (TEM) image.) Among these techniques, we achieved a high-quality relaxed SiGe film using a so-called SiGe virtual substrate. The structure consisted of two layers: (a) a thin Si layer grown at low temperature (LT-Si layer) and (b) a $\text{Si}_{1-x}\text{Ge}_x$ layer grown at a normal temperature of 600°C. The Ge layer was grown at a low temperature. Broadly speaking, the effect of the LT-Si layer was (a) to reduce the surface diffusivity of the deposited Si atom forming the low energy center for the epilayer grown on top and (b) to confine the misfit dislocation networks within the interface.

Based on the growth techniques briefly described above, we carried out growth on a $\text{Ge}_{1-x}\text{Sn}_x/\text{Ge}$ heterostructure. A series of (a) $\text{Ge}_{1-x}\text{Sn}_x/\text{Ge}$ heterostructure and (b)

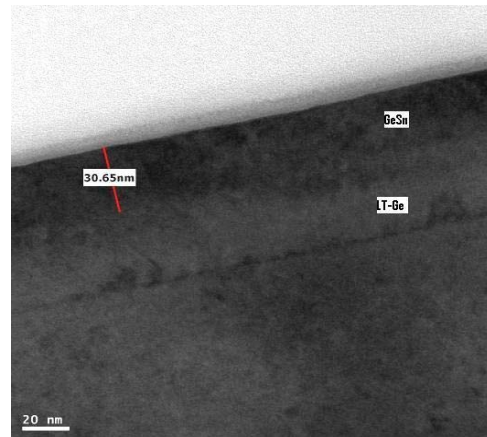


Fig. 1. Cross-sectional TEM images of GeSn/Ge heterostructure with 20% Sn content.

$\text{Ge}_{1-x}\text{Sn}_x/\text{Ge}$ multiquantum wells with various Sn compositions were fabricated. The structure consisted of two layers: (a) a Ge layer grown at low temperature (LT-Ge layer) and (b) a $\text{Ge}_{1-x}\text{Sn}_x$ layer grown at a normal temperature of 600°C . A cross-sectional TEM image of the heterostructure with 20% Sn content is shown in Fig. 1. The TEM image reveals that both the LT-Ge and the GeSn layers are dislocation free. To examine the Sn profile in the GeSn film, the TEM is switched to the scanning (S) TEM mode. A typical STEM image is depicted in Fig. 2(a). A dislocation-free GeSn film is also observed, which is consistent with the TEM measurement. Energy-dispersive spectroscopy (EDS) measurement is performed at various locations labeled 1–13, as marked in Fig. 2(a). The measured Sn composition result is plotted in Fig. 2(b). Along the in-plane (growth direction) direction, the Ge composition is $\sim 10\%$ (10%). Taking the Sn composition from these measured points, the average Ge composition is determined; it is $10 \pm 0.3\%$. This reveals that Sn is nearly uniformly distributed in the GeSn film. A similar pattern is also observed in other samples.

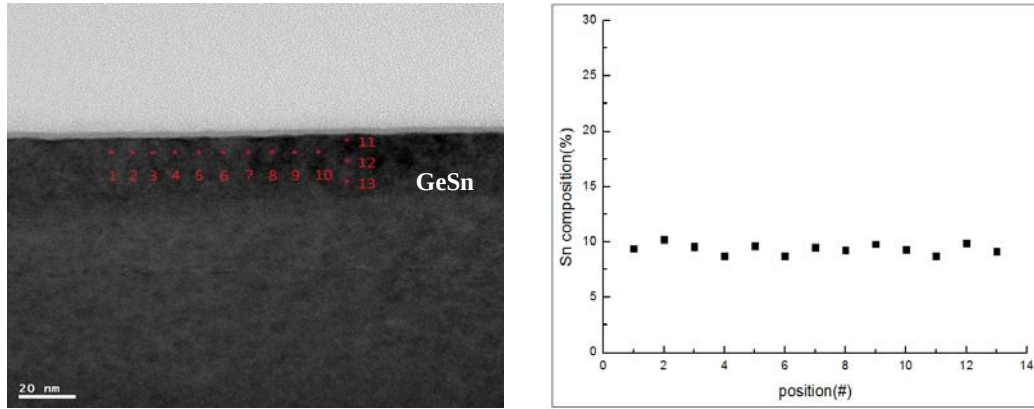


Fig. 2. (a) Left: STEM images of GeSn/Ge heterostructure with 10% Sn content. Dislocation associated with lattice misfit between GeSn and Ge is not observed in the GeSn layer showing the high quality of the growth. (b) Right: Sn content at various positions, as labeled in the left plot.

(b) Characterization of GeSn/Ge

Various measurements have been performed to characterize these samples,

including high resolution X-ray, Raman spectroscopy, photoluminescence (PL) etc. High resolution X-ray data on a series of samples is depicted in Fig. 3. From the shift with respect to the main Ge peak, the lattice constant of the SnGe film is deduced. Based on the X-ray and Raman measurement, we show that pseudomorphic growth of $\text{Ge}_{1-x}\text{Sn}_x$ with thickness beyond the critical thickness which is desired for application can be obtained by MBE growth.

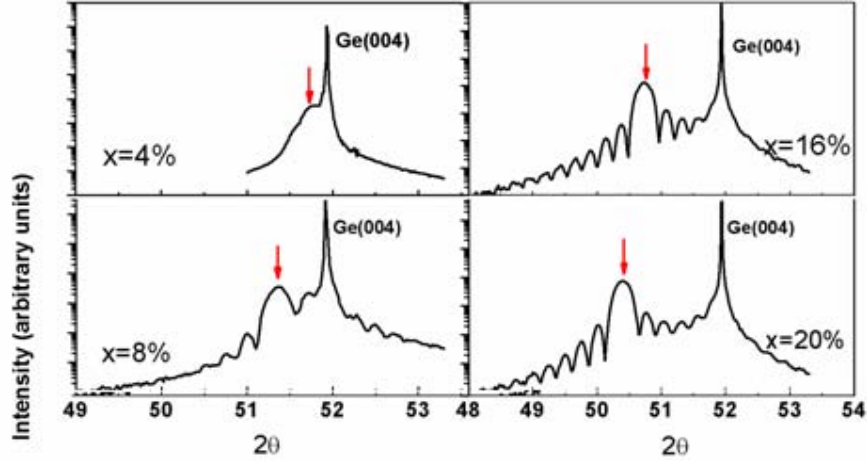


Fig. 3. High angle diffraction patterns of $\text{Ge}_{1-x}\text{Sn}_x$ film for different Sn compositions. Solid arrows indicate the shift trend of $\text{Ge}_{1-x}\text{Sn}_x$ (004) reflection.

2. Future work

In the last year, we focus on exploring the technique of the growth of Sn-based IV-IV compounds and heterostructures. We have successfully demonstrated that pseudomorphic growth of thick $\text{Si}_x\text{Ge}_y\text{Sn}_{1-x-y}$ with uniform Sn distribution can be achieved by Molecular Beam Epitaxy (Fig. 2). As described above, PL measurement has been performed to probe the indirect-to-direct transition. Nevertheless, conclusive evidences haven't been drawn. Further experimental measurement will be performed to tail the energy bands of Sn-based group-IV compound. In the next stage, we will perform absorption measurement to probe different bands of the material. This will enable us to (1) construct indirect-to-direct transition, (2) more importantly, to provide a systematic knowledge to design direct band gap Sn-based group-IV compound.

3. Publications

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- [3] Carrier dynamics of terahertz emission based on strained SiGe/Si single quantum well, K. M. Hung, J.-Y. Kuo, C. C. Hong, H. H. Cheng, G. Sun, and R. A. Soref, *Appl. Phys. Lett.* **96**, 213502 (2010).
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- [5] Pseudomorphic growth of Ge_{1-x}Sn_x thick film at low temperature, submitted to APL