How Does the Incorporation of Sn Affect the Structure of a Ge Matrix?

This report features the work of Yun-Liang Soo, Shih-Lin Chang, Hung-Hsiang Cheng and their co-workers published in Semicond. Sci. Technol. ***29****, 115008 (2014).*

Group-IV semiconductor germanium has a great potential for the development of novel electronic devices compatible with conventional Si-based semiconductor technology, but the indirect band gap of Ge has appeared to be a limiting factor for the performance of such devices. To achieve direct band gaps, alloys of Ge and other group-IV elements have been extensively studied. In 2014, Yun-Liang Soo, Shih-Lin Chang, Hung-Hsiang Cheng and their co-workers from National Tsing Hua University and National Taiwan University investigated the crystal structure and local structures surrounding Sn in Sn-Ge alloy samples of Sn concentration varying up to 20 at. %. The structural information derived from the use of X-ray techniques with synchrotron radiation is of central importance for understanding the electronic properties of the material. They reported that Sn atoms occupy Ge sites in these thin-film samples for which the lattice parameters of the films are distinctly larger than that of the Ge substrate and depend linearly on the Sn concentration in the out-of-plane direction; such increased lattice parameters were not observed in the in-plane direction.

Their film samples of $Ge_{1-x}Sn_x$ (thickness 30 nm; Sn concentrations 8, 12, and 20 at. %) were deposited with molecular beam epitaxy (MBE) from a solid source.[1] The local structures surrounding Sn atoms were probed with the extended X-ray absorption fine structure (EXAFS) technique at **BL01C1** of Taiwan Light Source at the NSRRC in Taiwan. A conventional fluorescence mode of detection was adopted with an energy-dispersive 13-element Ge fluorescence detector for all samples. The X-ray diffraction (XRD) patterns were measured near the Ge (004), (040) and (400) signals for all samples at **BL07A1**.

Figure 1 shows that the Fourier transform of the EXAFS χ-function for the 20% sample has two pronounced peaks, whereas those of the 8% and 12% samples have only one pronounced peak. Local structural parameters were quantitatively extracted from the χ-functions with an improved curve-fitting procedure. The final values of derived parameters reveal that the first pronounced peak in all samples is due to the nearest-neighbor shell of 4.8-6.2 Ge atoms at distances 2.56 Å to 2.58 Å from the central Sn atoms. The second pronounced peak in the 20% sample is a composite peak arising from the second and third nearest shells, both of 12 Ge atoms, at distances 4.17 Å and 4.80 Å, respectively. Except for the slightly longer bonds and somewhat larger coordination numbers, the local struc-

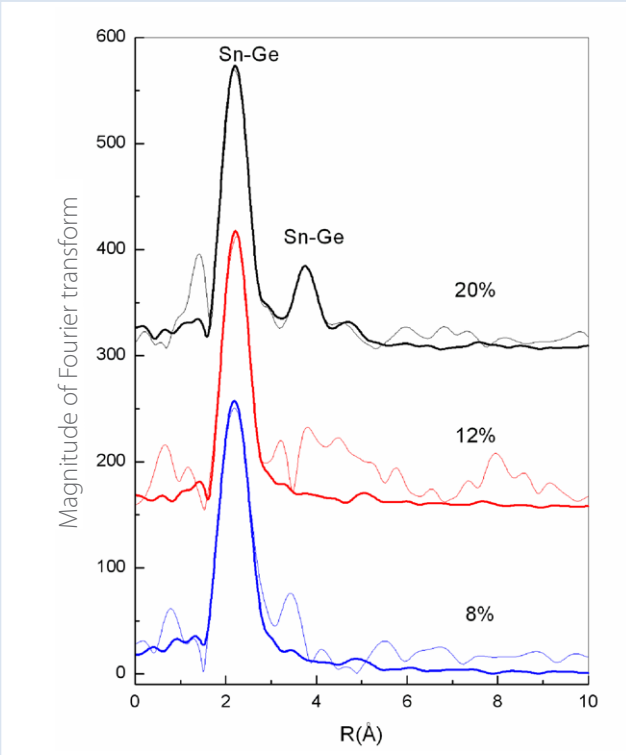

Fig. 1: Fourier transform of the weighted Sn K-edge EXAFS χ-functions. Fine lines: experiment; Coarse lines: curve fitting. (Reproduced from Ref. 2)

tures of Sn obtained in their analysis resemble that of the standard Ge crystal, in which Ge atoms are surrounded by 4, 12 and 12 Ge neighboring atoms at distances 2.45, 4.00 and 4.69 Å, respectively. The apparent resemblance of Sn and Ge local environments, especially those in the 20% samples, indicates that Sn atoms most likely substitute for Ge atoms in these $Ge_{1-x}Sn_x$ films.

As demonstrated in Fig. 2, a satellite peak appearing at the left of the intense substrate peak of Ge (004) for each sample represents the (004) reflection from the $Ge_{1-x}Sn_x$ layer, in which the larger Sn atoms produce a lattice parameter larger than that of the pure Ge substrate. As the Sn concentration increases from 8 at. % to 20 at. %, such a satellite signal shifts to smaller angles indicating that the $Ge_{1-x}Sn_x$ lattice parameter in the direction of the film surface normal increases with Sn concentration. In contrast to the (004) reflection, no satellite peak is observed near the Ge (040) and (400) peaks, indicating that the in-plane lattice parameters of $Ge_{1-x}Sn_x$ are indistinguishable from those of the Ge buffer layer.

Figure 3 shows that the lattice parameter of $Ge_{1-x}Sn_x$ films calculated from the (004) Bragg reflection increases linearly from the value for the crystalline Ge to that for metallic Sn as the Sn concentration increases. Such a linear dependence conforms to Vegard's law.

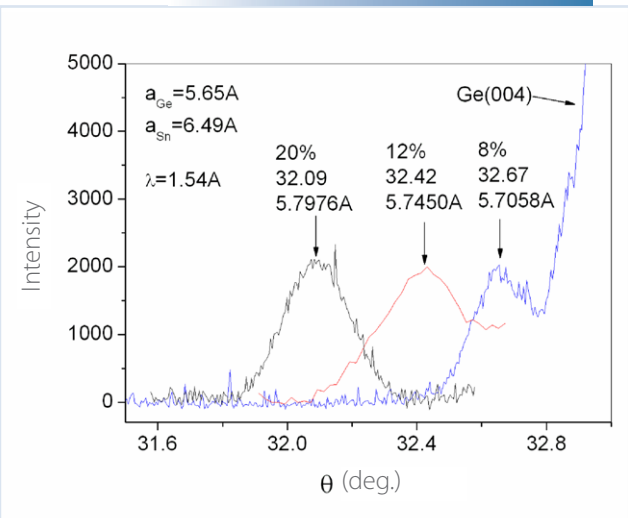

Fig. 2: X-ray powder diffraction patterns near the Ge (004) peak. (Reproduced from Ref. 2)

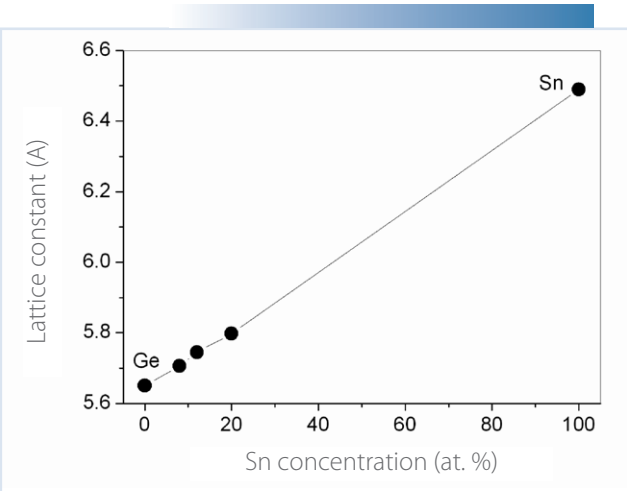

Fig. 3: Lattice parameter vs Sn concentration calculated from XRD patterns.

In summary, local structures surrounding Sn in MBE-grown $Ge_{1-x}Sn_x$ thin films probed with EXAFS resemble those surrounding Ge atoms in Ge crystal, indicating a substitutional incorporation of large concentration of Sn in the Ge host. As the Sn dopant atoms are larger than Ge, the Sn-Ge bond appears to be longer than the Ge-Ge bond. As revealed by XRD from the (004) atomic planes, such a longer bond produces a linearly increased lattice parameter in the out-of-plane direction as the Sn concentration increases, consistent with Vegard's law. That no sign of increased lattice parameter in the in-plane directions was observed with XRD from the (040) and (400) planes indicates that a compressive strain might be present for the alloy layer to match the in-plane atomic arrangement of the Ge substrate. The synchrotron-radiation X-ray results obtained by the research groups of Soo, Chang and Cheng have revealed the structural variation of the Ge matrix due to incorporation of Sn, and demonstrated the successful fabrication of substitutional $Ge_{1-x}Sn_x$ thin films with a large Sn concentration. (Reported by Yun-Liang Soo)

References

1. H. H. Tseng, K. Y. Wu, H. Li, V. Mashanov, H. H. Cheng, G. Sun, and R. A. Soref, Appl. Phys. Lett. **102**, 182106 (2013).
2. Y. L. Soo, T. S. Wu, Y. C. Chen, Y. F. Shiu, H. J. Peng, Y. W. Tsai, P. Y. Liao, Y. Z. Zheng, S. L. Chang, T. S. Chan, J. F. Lee, G. E. Sterbinsky, H. Li, and H. H. Cheng, Semicond. Sci. Technol. **29**, 115008 (2014).