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Electrically Active Defects in GeSnSi/Ge Junctions Formed at Low Temperature

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Abstract
Defects in GeSnSi/Ge junctions formed at various temperatures were investigated by XRD and *I-V* characteristics. Diffuse scattering due to defects (DSD) increases with deposition temperature (T_d) of the GeSnSi layers. On the other hand, it was found that electrically active defects are formed in the depletion layer at low T_d. This strongly indicates that formation at high T_d reducing DSD is required for GeSnSi device applications.

Introduction
GeSnSi is an attractive material for Group IV electrical and optical devices for monolithic integration on ULSI because the energy band structure and lattice constant can be controlled without depending on each other such as III-V compound semiconductors. For realizing GeSnSi devices, control of defect density in the GeSnSi layer and at the GeSnSi/Ge interface is important because the defects significantly impact on the control of carrier concentration, life time of carriers, and mobility.

Point defects such as vacancy are often introduced into GeSn layer formed at low temperatures[1]. Incorporation of Si with high melting point (MP) of 1430°C and Sn atoms with low MP of 230°C in Ge could give modulation of defect structures. However, in a GeSnSi system, defect concentration and structures have been rarely investigated.

In this study, defects in GeSnSi layers, which formed at various temperatures and annealed at various temperatures, are systematically investigated by 2 dimensional x-ray reciprocal space mapping (2DRSM) and *I-V* characteristics of GeSnSi/Ge junctions.

Experimental procedure
After chemical cleaning with an alkaline solution and thermal cleaning at 430°C of n-type Ge (001) substrate with resistivity of 1-3 Ω·cm, GeSnSi layers were formed from 200°C to 350°C on Ge substrates (Sn and Si contents:~4% and ~20%, respectively). GeSnSi/Ge diodes with mesa isolation of the GeSnSi layer, a SiO_2 isolation layer and Al electrodes were fabricated by conventional lithography technique and vacuum evaporation. The structure is shown in the inset of Fig. 7(a).

Results and discussion
Ternary alloy system, low MP and low solubility limit of Sn could make it difficult to form a high quality GeSnSi layer. First, GeSnSi layer structure formed at 200°C was confirmed by TEM (Fig. 1). For g_{004}, a GeSnSi layer with uniform contrast is observed, while, for g_{220}, columnar shape contrast is observed. These results mean that the GeSnSi layer has an anisotropic defect structure.

A Bragg diffraction point consists of interference of scattered x-ray from lattice planes with averaged periodicity in a layer. Lattice tilt and small domain induce broadening of a diffraction peak, which can be observed in full width at half maximum (FWHM) in omega rocking curves. Scattered x-rays from defects and phonon, which are called diffuse scattering (DS), are slightly deflected from the Bragg point. Since the scattered x-rays do not induce strong interference, the intensity of DS is much weaker than the Bragg diffraction point. As a result, DS can be observed in the tails of a Bragg peak. Figures 2 (a) to 2(c) show 2DRSMs for the GeSnSi layers formed at 200°C, 250°C and 300°C, respectively. The weak streaks elongated to the [110] direction are clearly observed[2]. This could be owing to the columnar defect structures shown in Fig. 1(b). The elongation for the 300°C deposition seems to become weak. In order to make clear the change of the peak shapes for T_d and the annealing temperatures (T_a), the extracted profiles for the [110] direction from 2DRSMs are shown in Figs. 3 and 4. It should be noted that T_d has a significant impact on DS, as shown in Fig. 3. On the other hand, although DS seems to increase after 600°C annealing, the peak shapes hardly change below T_a of 500°C as shown in Fig. 4. These results mean that Sn atoms located in diamond lattice sites are stable below 500°C. Figure 5 shows omega rocking curves for the GeSnSi layer around 004 diffraction peaks. Although FWHMs for 200°C to 300°C are approximately twice larger than that for Ge substrate, FWHMs hardly depend on T_d except for 350°C. This means that macroscopic crystallinities are almost identical. In order to quantitatively indicate DS, the ratios of I_d/I_G as a function of T_d are plotted in Fig. 6. It is found that the ratios increase with increasing T_d, and that 400°C annealing is effective for reducing DS except for T_d of 350°C.

Holes with concentrations of more than 10^{18} cm^{-3} and 10^{17} cm^{-3} at room temperature (RT) and 200K, respectively, are generated in the GeSn layer formed at 170°C[1]. Although carrier concentrations in the GeSnSi layers are still unclear, depletion layer widths (W_d) in the GeSnSi layers at low temperature could be wider than those at RT. The wider W_d makes it easy to evaluate the electrical properties of the GeSnSi layer. Figure 7 shows *I-V* characteristics of the GeSnSi/Ge diodes. Clear rectifying properties are observed for all samples. It is found that, from the rectifying properties, the formed GeSnSi layers are p-type, whose conduction could be due to defects with shallow energy level upon the valence band maximum. At RT, the reverse bias currents (I_R) of the samples for T_d of 200°C to 300°C are almost identical, while I_R for 350°C is largest. Besides, it should be noted that, at 200K, I_R for T_d of 200°C is larger than I_R for T_d of 250°C and 300°C. Figure 8 shows Arrhenius plots of I_R. At near RT, I_R from T_d of 200°C to 300°C are almost same, meaning that the influence of defects in the GeSnSi layer is hardly observed in I_R because of formation of one-side abrupt p+/n junction. At around 200K, I_R for T_d of 200°C and 350°C is larger than I_R for the other samples. The activation energy (E_a) evaluated from the slope of the Arrhenius plot around 200K is 0.3 eV. This value is approximately half of the bandgap evaluated by the optical properties[3], suggesting that the dominant currents are generated from generation current through the defects. Ideality factors evaluated from the forward bias currents measured at RT and 200K get worse at T_d of 200°C (Fig.9). These results show that the sample for T_d of 200°C has a large amount of defects with energy level of near midgap or large capture cross-section of carriers.

Conclusions
Formation of GeSnSi layer at low T_d can suppress defect density as shown in the XRD results, while the low T_d induces electrically active defects in the depletion layer. In order to apply GeSnSi layer to future electrical and optical devices, formation at high T_d reducing DSD is strongly required.

References: [1]T. Ohmura *et al.*, JSAP meeting 2013, 18p-B4-8. [2]T. Asano *et al,*. ISTDM 2014, *to be presented.* [3]T. Terashima *et al.*, JSAP meeting 2014, 18p-F6-20.
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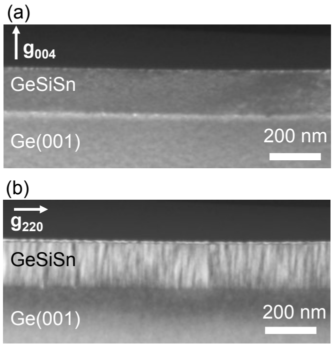

Fig.1: Dark field TEM images of GeSnSi layer grown at 200°C taken by diffraction vectors (g) of (a) 004 and (b) 220.

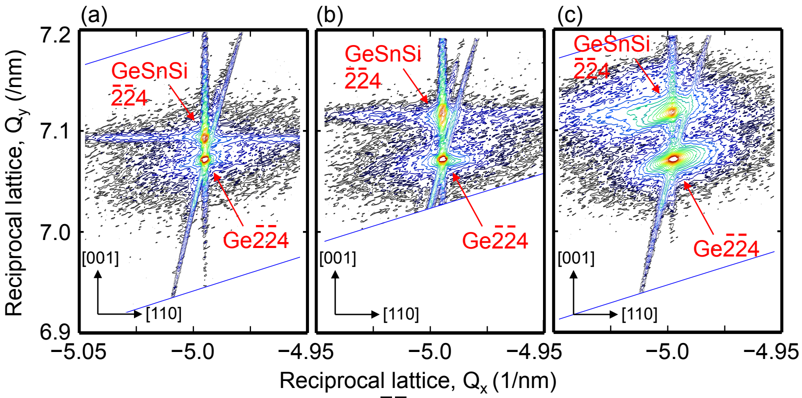

Fig.2: 2DRSMs measured around $\bar{2}\bar{2}4$ reflections for GeSnSi layers formed at (a) 200°C, (b) 250°C and (b) 300°C.

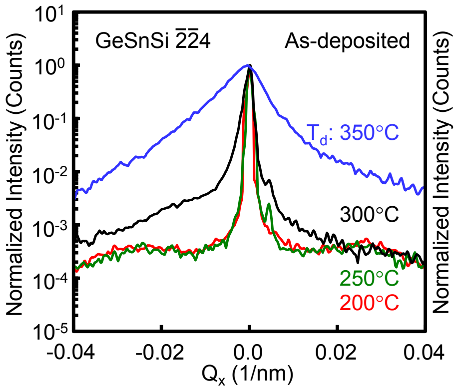

Fig.3: XRD profiles extracted from GeSnSi $\bar{2}\bar{2}4$ peaks for [110] direction in 2DRSMs for various deposition temperatures (T_d).

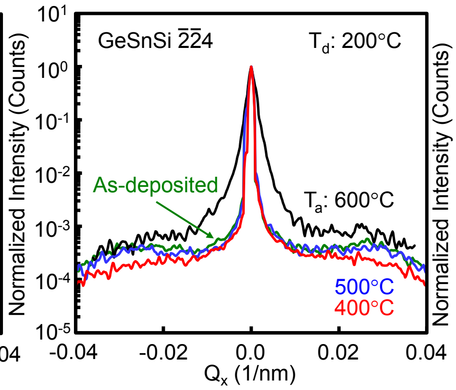

Fig.4: XRD profiles extracted from GeSnSi $\bar{2}\bar{2}4$ peaks for [110] direction in 2DRSMs for various annealing temperatures (T_a).

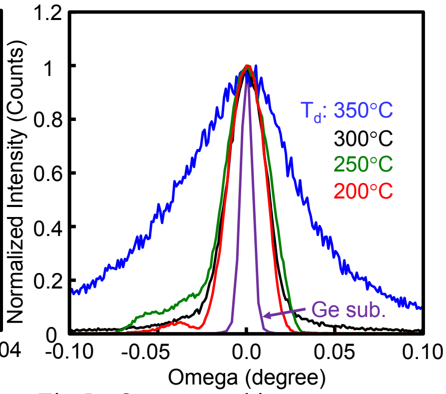

Fig.5: Omega rocking curves around 004 diffraction peaks of GeSnSi layers grown at various temperatures and Ge substrate without GeSnSi layer.

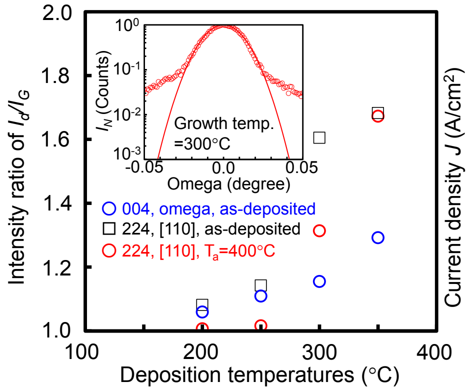

Fig.6: Intensity ratio of I_d/I_G as a function of growth temperatures. Here, I_d and I_G were integrated intensities of the measured data and the fitted curves with Gaussian as shown in inset.

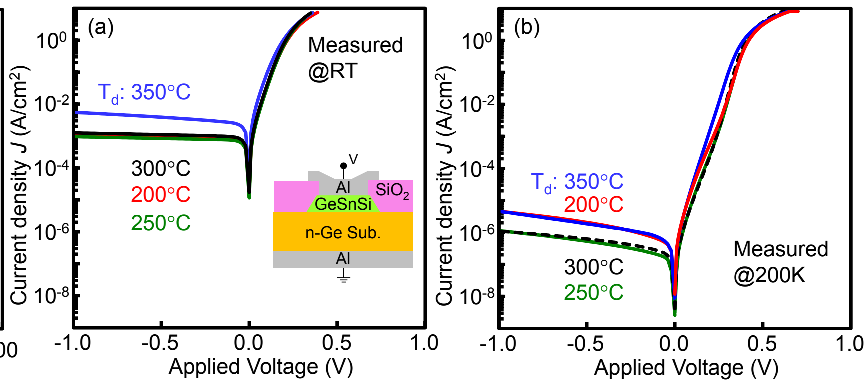

Fig.7: J-V characteristics of GeSnSi /n-Ge diodes measured at (a) RT and (b)200K. Here, indicated temperatures are growth temperatures.

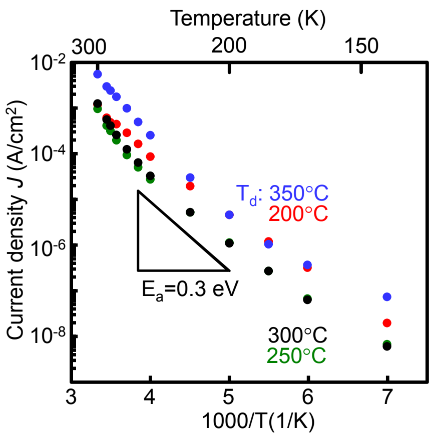

Fig.8: Arrhenius plots of current densities measured at a reverse bias of -1V.

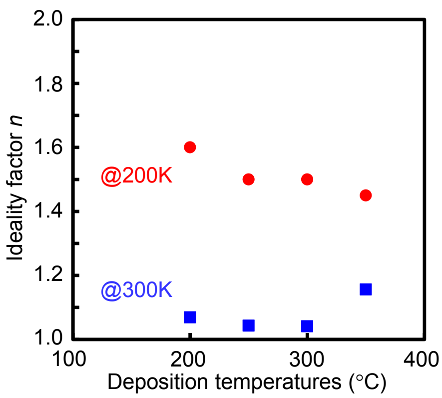

Fig.9: Ideality factor as a function of growth temperatures. Here, the ideality factors evaluated by fitting an ideal forward current to the measured forward current.