Growth Orientation Analysis of SnTe Epitaxial Layers on GaAs(001) Substrates by XRD Pole Figure Measurements

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SnTe, a representative IV-VI rocksalt compound, exhibits a mirror-symmetry-protected topological crystalline insulator (TCI) phase with confirmed bulk band inversion and surface Dirac states [1-3]. For the band engineering, high-quality single-domain epitaxial films are crucial. Although the GaAs(001)/ZnTe buffer system enables SnTe growth [4], it often shows orientation competition and twinning. Hence, x-ray diffraction (XRD) pole figure analysis was used to identify those domains and their relation to growth parameters.

SnTe films were formed on GaAs(001) by molecular beam epitaxy with ZnTe buffer layers. As a representative case, sample A was grown at $T_{\mathrm{sub}} = 220°C$ with a thickness of 0.2 um. Using the X-ray diffraction (XRD) θ-2θ scan, the dominant phase of the layer aligned to the substrate surface was (001). However, this technique alone cannot fully characterize complex microstructures because it is insensitive to orientations that deviate from the substrate normal. To overcome this limitation, we further performed XRD pole-figure analysis, with measuring peaks of GaAs111, SnTe200, and SnTe222 and resolving the three-dimensional configuration. It was confirmed that (001), (011), and (111) oriented domains were included in most layers. As shown in Fig. 1, the SnTe200 pole figure exhibits (001), (011), (111) oriented domains normal to the substrate surface. The SnTe (111) component became dominant when the SnTe buffer layer was extensively annealed. An insufficient annealing duration enhances the (022) component. These findings provide an experimental basis for fabricating high-quality, single-domain SnTe epitaxial layers and will facilitate device research based on SnTe as a TCI.

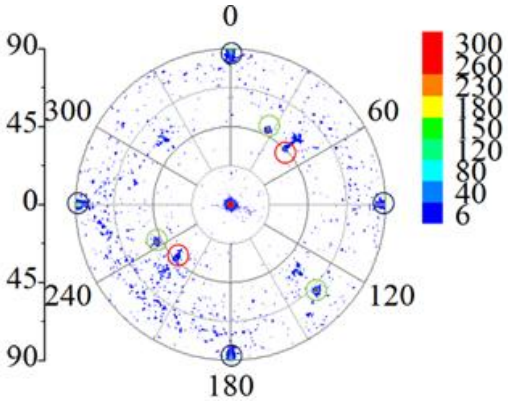

Figure 1. SnTe200 pole figure exhibits 3 different components of SnTe. They are (001) (black circles), (011) (red circles), and (111) (green circles) components, respectively.

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[2] Zhang Y., Liu Z., Zhou B., *et al.*, J. Electron Spectrosc. Relat. Phenom. 219 (2017) 35–40.
[3] Tanaka Y., Ren Z., Sato T., *et al.*, Nat. Phys. 8 (2012) 800–803.
[4] Kobayashi M., Nan S., J. Cryst. Growth 628 (2024) 127531.

Supplementary information:

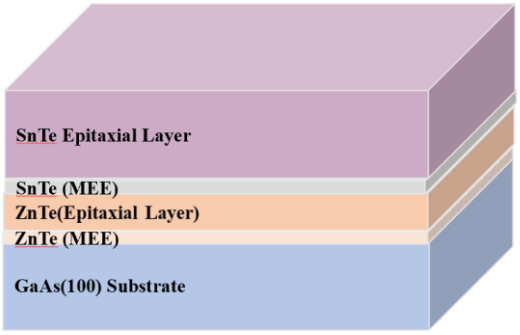

Figure 2. a schematic cross-section of sample A the ZnTe layer is approximately 100 nm thick, and the SnTe layer is approximately 200 nm thick.

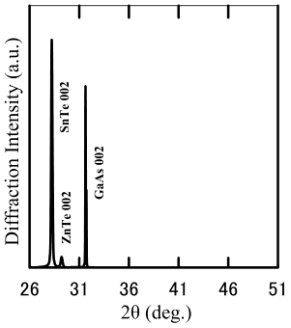

Figure 3. θ-2θ scans result of Sample A.

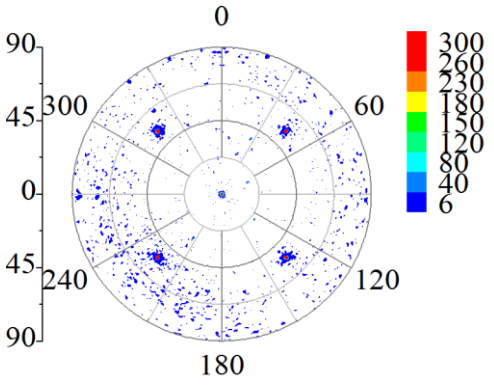

Figure 4. GaAs111 pole figure.

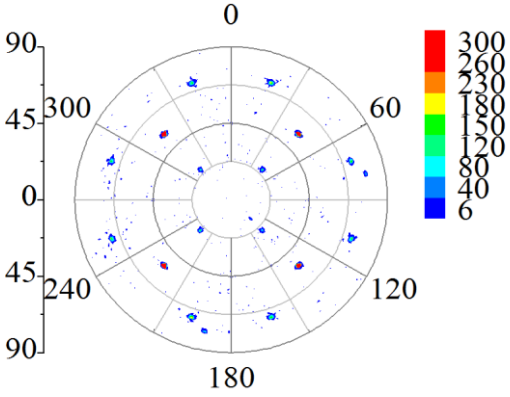

Figure 5. SnTe222 pole figure