High-resolution X-ray diffraction study of (001)-oriented SnTe and $Pb_{1-x}Sn_xTe$ layers, MBE-grown on commercial GaAs substrate

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Introduction

SnTe-related alloys, compounds and nanostructures are promising and currently investigated candidate materials for topological crystalline insulators or semimetals, as well as thermoelectrics or superconductors [1-5]. Some of their crucial properties are protected by crystal symmetry thus it is important to study their crystallographic quality, extended defects amount and spatial distribution, lattice strain and chemical homogeneity.

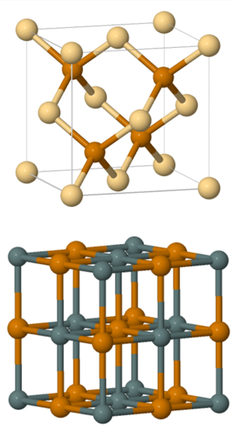
Comprehensive structural characterization of (001)-oriented SnTe and $Pb_{1-x}Sn_xTe$ layers deposited on commercial GaAs substrate with special CdTe(001) buffer layer was performed using laboratory high-resolution X-ray diffractometer equipped with $CuK_{\alpha 1}$ irradiation (λ = 1.5404 Å).

[1] G. Tan et al., J. Am. Chem. Soc., 137 (2015) 11507.
[2] T. M. Schmidt and G. P. Srivastava, physica status solidi (RRL)–Rapid Research Letters, 14 (2020) 2000362.
[3] A.S. Tarasov et al., Applied Surface Science, 569 (2021) 150930.
[4] A. Sulich et al., Journal of Materials Chemistry C, 10 (2022) 3139.
[5] S. Dad et al., Scientific Reports 14.1 (2024) 589.

Summary

- ✓ Crystallographic quality of the characterized materials is good (the values of FWHM of X-ray diffraction curves measured by us are comparable with published in literature);
- ✓ Although CdTe buffer is fully relaxed in all of the samples, SnTe and $Pb_{1-x}Sn_xTe$ layers are partially strained (the minimal percentage relaxation is 86% and the maximal 98%);
- ✓ The following types of defects have been detected in CdTe, $Pb_{1-x}Sn_xTe$ and SnTe: distortion of the unit cells, misfit dislocations presence and misorientation between the substrate and the layers: CdTe-GaAs, SnTe-CdTe and $Pb_{1-x}Sn_xTe$-CdTe;
- ✓ Azimuthal defects distribution in all of the studied layers is anisotropic;
- ✓ Unit cell distortion in $Pb_{1-x}Sn_xTe$ is tetragonal but in some SnTe layers alternative, monoclinic distortion occurs which may affect the topological properties of the heterostructure (SnTe lattice strain ~10^{-3} is large enough to open an energy gap in topological surface states, secured by the crystal symmetry).

Unit cells of GaAs, CdTe, SnTe and PbTe



Figures created by ICSD database

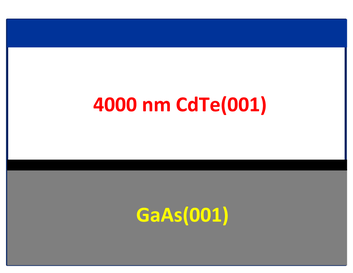
zinc-blende structure

GaAs:
a = 5.6535 Å
CdTe:
a = 6.480 Å

rock-salt structure

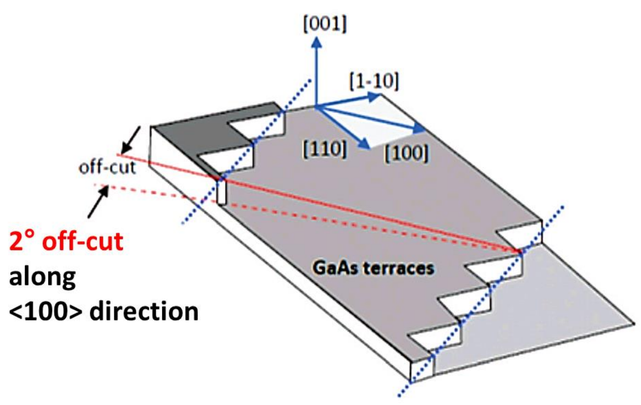
SnTe and $Pb_{1-x}Sn_xTe$:
a (SnTe) = 6.300 Å
a (PbTe) = 6.460 Å

Heterostructure's scheme

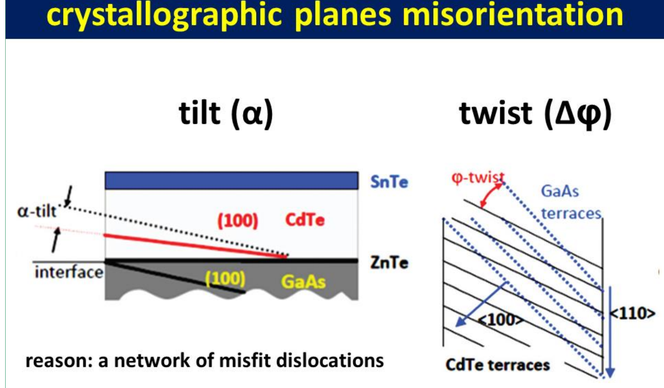


Growth technique: **Molecular Beam Epitaxy**

GaAs(001) substrate's scheme

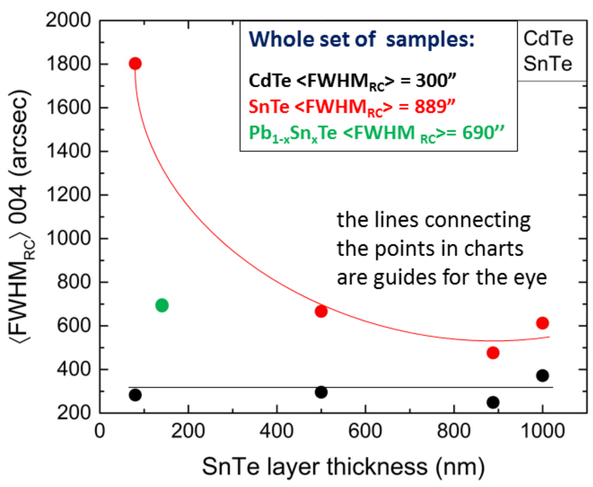


GaAs-CdTe interface: crystallographic planes misorientation



reason: a network of misfit dislocations

General crystallographic quality of the samples



(001) plane misorientation

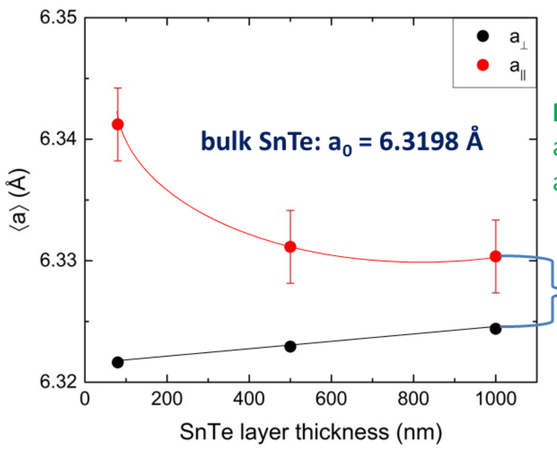
CdTe–GaAs :
tilt: up to 0.8°
twist: up to 23°

SnTe–CdTe :
tilt: up to 0.12°
twist: up to 2°

$Pb_{1-x}Sn_xTe$–CdTe :
tilt: 0.29°
twist: 0.09°

SnTe unit cell distortion magnitude and order

the lines connecting the points in charts are guides for the eye

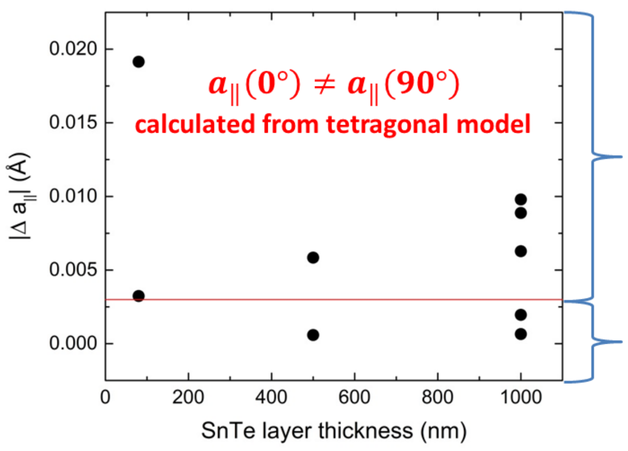


$Pb_{1-x}Sn_xTe$:
$a_\perp$ = 6.4091(± 0.0002) Å
$a_\parallel$ = 6.417 (± 0.003) Å

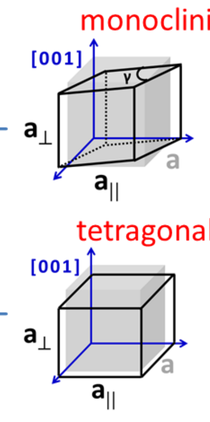
$a_\perp \neq a_\parallel$

SnTe unit cell distortion magnitude and order

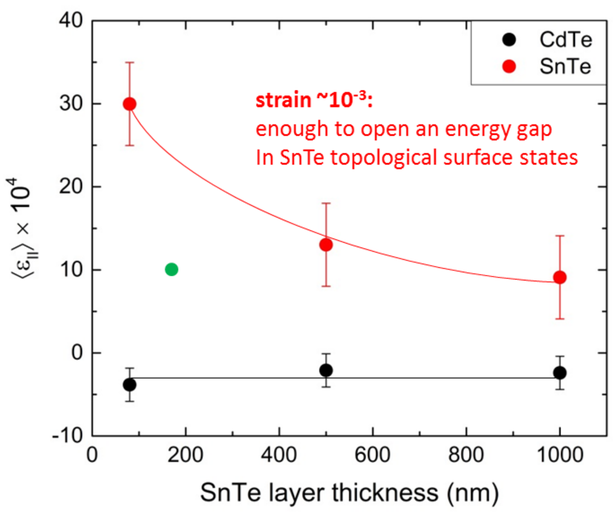
$Pb_{1-x}Sn_xTe$: only tetragonal distortion was detected



γ ≠ 90°
monoclinic
tetragonal



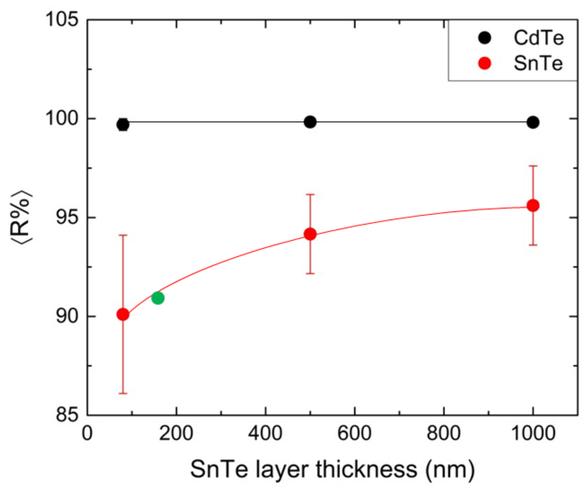
Impact of a SnTe layer thickness on horizontal strain magnitude in SnTe



$Pb_{1-x}Sn_xTe$:
$\langle \varepsilon_\parallel \rangle = 10 \times 10^{-4}$

the lines connecting the points in charts are guides for the eye

Impact of a SnTe layer thickness on horizontal strain relaxation in SnTe

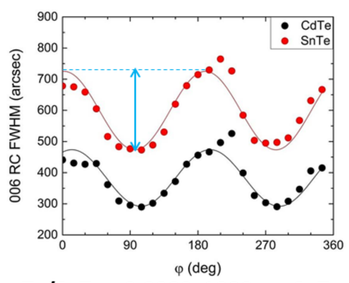


$Pb_{1-x}Sn_xTe$:
<R% > = 90.7%

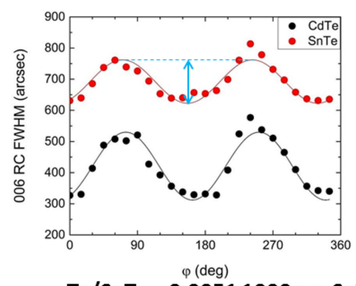
the lines connecting the points in charts are guides for the eye

$$R\% = \frac{a_\parallel^{L1} - a_\parallel^{L2}}{a_\parallel^{L1} - a_{relax}^{L2}} \times 100\%$$

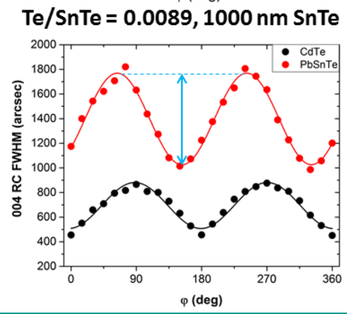
Azimuthal defects distribution in CdTe and SnTe



Te/SnTe = 0.0089, 1000 nm SnTe



Te/SnTe = 0.0051 1000 nm SnTe



$Pb_{1-x}Sn_xTe$

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