Dielectric constant of gray Tin: A first-principles study

Jinsong Duan[1] and Stephanie Chastang
KBRWyle, 2601 Mission Point Blvd, Suite 300, Dayton, OH 45431

Arnold Kiefer
Air Force Research Laboratory, Wright-Patterson AFB, OH 45433

Rigo Carrasco and Stefan Zollner
Department of Physics, New Mexico State University,
MSC 3D, P. O. Box 30001 Las Cruces, NM 88003
(Dated: May 19, 2022)

α-Sn (gray tin) is a group-IV, zero-gap semiconductor with potential use in infrared detectors, necessitating a clear understanding of its dielectric properties. We report the first-principles calculations of the band structure and dielectric function of α-Sn using density functional theory, emphasizing the effects of strain, spin-orbit interaction, and pseudo-potentials on the electronic and optical properties of α-Sn in the infrared region (photon energy < 1 eV). In α-Sn, spin-orbit coupling greatly influences the electronic band structure that leads to unusual optical behavior. We explain an apparently anomalous absorption at ~ 0.41 eV caused by interbank transitions within the valence band. Infrared spectroscopic ellipsometry on several α-Sn films grown by molecular beam epitaxy validate our band-structure calculations. Our computational methods and results are discussed in detail.

I. INTRODUCTION

α-Sn (gray tin) is the diamond-crystalline phase of elemental tin and a so-called “zero-gap semiconductor”. [1] Owing to its unusual band structure, extensive investigations were carried out primarily in the 1960s on bulk samples [2, 3] and in the 1980s and 1990s on epitaxial films. [4, 5] More recently, the prediction and verification of α−Sn as a topological insulator (under strain) [7] and the inclusion of Sn in group-IV alloys for CMOS-compatible photonic devices provide new impetus to understand α−Sn’s electronic structure and properties in greater detail [8]. As an endpoint element in the SiGeSn alloy system, a clear understanding of α−Sn’s band structure and optical properties is desired to allow deliberate design of optoelectronic devices of various compositions.

Of primary interest for device applications is the dielectric function of α−Sn which is strongly influenced by allowed electronic transitions between bands. Recent observation of an optical transition in the infrared region at ~0.43 eV (~ 2.7 μm) in α−Sn using spectroscopic ellipsometry that corresponds with a ‘negative’ band gap. [11] However, the exact origin of this transition, and its dependence on strain and spin-orbit interaction is not fully understood yet, calling for a renewed effort for a first-principles calculation of the optical properties which can be determined largely from its electronic band structure.

The band structure of α−Sn has many unusual features, including a degeneracy at the Γ-point that closes the gap between the valence and conduction bands. Because of the strong relativistic Mass-Darwin effect on the α-Sn in 5s electrons, the Γc level moves down in the energy and dips below the Γv level, resulting in band inversion. [10] Moreover, the strain and spin-orbit interaction influence the band structure considerably. [11] The band gap at the Γ-point can be opened, however, through epitaxial strain or by alloying with Ge. In-plane compressive strain (~0.164%) in α−Sn grown on InSb substrate can lift the band degeneracy at the Γ point creating a small band gap of 30 meV. [7] Careful consideration of many factors are needed to create an accurate fundamental model that manifests these several unusual features.

In this paper, we report the first-principles calculation of the band structure and optical properties of α−Sn. The emphasis is on the transition in the infrared region and the effect of the spin-orbit interaction and strain on the band structure and optical properties. Our calculations provide insight into the fundamental physics in the optical properties of α-Sn in the infrared region and are compared with experimental measurements.

The paper is organized as follows. In section [II] we describe the theory and computational methods. In section [III] we present the calculated band structure and optical properties. The results are compared with previous calculations and recent experiments.

II. METHODS

All first-principles calculations are performed with the Vienna ab initio simulation package (VASP) (Version 5.4). [12] The results depend on the pseudopotentials chosen for a specific problem. To this end, the exchange-correlation is modeled with local density approximation and hybrid functional the projector augmented wave
pseudopotentials (PAW). We set the energy cutoff of the plane wave basis set to 500 eV. The frequency dependence of the dielectric function is calculated using the independent particle approximation provided within the VASP package. The $32 \times 32 \times 32$ $k$-points are used in LDA calculation, while $16 \times 16 \times 16$ $k$-points are used in HSE calculation using an averaging over multiple grids method.

To incorporate strain into the band structure calculation, the deformation of the unit cell is set using the theory of linear elasticity. We explicitly calculate the experimentally relevant case of $\alpha$-Sn grown epitaxially on an InSb (001) substrate. The lattice parameter of $\alpha$-Sn and InSb is 6.4892 Å (20 °C) and 6.4794 Å (25 °C), respectively. Due to the lattice mismatch, the InSb sublattice introduce in-plane compressive strain to the $\alpha$-Sn film on the top of it. First-principles calculation is performed at 0 K. To simulate the strain effect, the volume of crystal is fixed by changing the ratio of lattice constant in the x-y axis, $a_\parallel$, and that in z axis, $a_\perp$. The $\alpha$ phase of Sn has the cubic diamond crystal structure with a lattice parameter of $a = 6.4746$ Å at 0K estimated with LDA and $a = 6.5801$ Å estimated with HSE functional. When a film of $\alpha$-Sn is coherently constrained to the InSb substrate lattice, it has a biaxial in-plane compressive strain, $\epsilon_\parallel$ of $-0.164\%$, which is chosen to represent a reasonable strain effect and does not reflect the real value of the compressive strain because the linear thermal expansion fails when the temperature approaches 0 K. Thus, the corresponding lattice constant in the x-y axis $a_\parallel = 6.4640$ Å. Assuming a linear elastic response, the out-of-plane strain is then $\epsilon_\perp = -2(C_{12}/C_{11}) \cdot \epsilon_\parallel = 0.00138$, where $C_{11} = 0.69$ GPa and $C_{12} = 0.29$ GPa resulting in an out-of-plane lattice constant of $a_\perp = 6.4836$ Å.

It is worth noting that the deformation due to a biaxially symmetric, in-plane strain is different from a uniaxial strain applied along the orthogonal direction. In the former case, $\epsilon_\perp = (-2C_{12}/C_{11})\epsilon_\parallel$; in the latter case, $\epsilon_\perp = -[(C_{12} + C_{11})/C_{11}]\epsilon_\parallel$. Our strain-dependent results should not be confused with calculations by others using different boundary conditions and definition of the compressive and tensile strain.

### III. RESULTS

We discuss the first-principles calculation of the band structure $\alpha$-Sn in section IIIA and its dielectric function in section IIIB focusing on the infrared transition and the influences of the spin-orbit interaction and in-plane compressive strain.

![FIG. 1. Band structure of $\alpha$–Sn calculated with LDA, (a) without, and (b) with spin-orbit interaction. The orbital character is encoded by a cyan and red color code, respectively, for 4s and 4p orbital character in (b).](image)

#### A. Band structure of $\alpha$-Sn with strain and spin-orbit interaction

The first-principles calculation are performed on $\alpha$-Sn to understand the relative influences of spin-orbit interaction and strain on electronic band structure of $\alpha$–Sn regarding relative energy of bands. Of particular interest is the $E_0$ transition at $\sim 0.41$ eV in our ellipsometric measurements. Previous experimental measurements typically cut-off above 1 eV. Kufner et al. calculated the dielectric function of $\alpha$–Sn using HSE hybrid functional, and compared the results with and without the
spin-orbit interaction. The $E_0$ peak is not pronounced in the calculated dielectric function. [21] Pollak et al. calculated the band structure of $\alpha$–Sn and assigned $E_0$ of 0.4 eV to the transition between $\Gamma^-_{7c} \rightarrow \Gamma^+_{8c}$. This transition has not been considered in any great detail.

To understand the origin of the $E_0$ transition, we calculate the band structure with and without the spin-orbit interaction, and the density of states of $\alpha$–Sn around the $\Gamma$ point, and present the results in Figure 1. The bands are labeled using the notation of Pollak et al. [4] and +, – superscripts denote the parity. Optical transitions are determined using selection rules, meaning transitions can only connect states with opposite parities. [22] Without spin-orbit interaction, the transition $E_0$ occurs between $\Gamma^+_{7c}$ and $\Gamma^-_{7c}$, which is lower than the valence band $\Gamma^+_{8c}$, demonstrating an inversed band structure shown in Figure 1 (a). The band structure (the position of light hole and heavy hole) of $\alpha$–Sn is modified by spin-orbit interaction, shown in Figure 1 (b). $\Gamma^+_{7c}$ subband is split from the valence band $\Gamma^+_{8c}$ and $\Gamma^-_{7c}$ band is shifted down by spin-orbit interaction. [7] This is caused by the quantum mechanical repulsion that the $\Gamma^+_{8c}$ and $\Gamma^-_{7c}$ band are pushed apart by the split-off band $\Gamma^-_{16a}$. [23]

$\alpha$–Sn demonstrates the inversed band structure that the conduction band $\Gamma^-_{7c}$ at the $\Gamma$ point is lower than the valence band $\Gamma^+_{8c}$, as shown in Figure 1 and 2. [2] The possible transitions are indicated in these Figures and listed in Table I. In Figure 1(b), the band ordering calculated with LAD is $\Gamma^+_{7c} > \Gamma^-_{8c} > \Gamma^-_{7c}$, where $\Gamma^+_{7c}$ is 4p orbital character, and is a split-off valence band from $\Gamma^+_{8c}$, which is mixed 4s and 4p orbital character, but is 4p orbital character near the $\Gamma$ point shown in red line. $\Gamma^-_{7c}$ is a conduction band of 4s orbital character, which is lower than the valence band $\Gamma^+_{8c}$ by 0.69 eV corresponding to $E_0$ interband transition.

The band order is $\Gamma^+_{8c} > \Gamma^-_{7c} > \Gamma^-_{8c}$ calculated with HSE hybrid functional as shown in Figure 2 which is consistent with $\mathbf{k} \cdot \mathbf{p}$ calculation, [4] but is different from the results obtained with LDA, where split-off band $\Gamma^+_{7c}$ is higher than $\Gamma^-_{7c}$. $E_0$ transition occurs between $\Gamma^-_{7c}$ and $\Gamma^+_{8c}$. Our value is 0.58 eV which is close to 0.52 eV reported in. [10] Both calculations using LDA and HSE hybrid functional show that the $E_0$ is interband transition between inverted the valence band $\Gamma^+_{8c}$ and $\Gamma^-_{7c}$ conduction band.

The calculated band structure of $\alpha$–Sn under $-0.164\%$ biaxial compressive strain is presented in Figure 3. The symmetry from the $O_h$ (cubic) unit cell to $D_{4h}$ (tetragonal) caused by strain, see Figure S12 the supplementary material in. [9] The band structure in Figure 3 refers to the direction perpendicular to the plane of applied strain, i.e. the surface plane of the film.

The in-plane compressive strain changes the band structures. The most notable feature is that the strain opens a gap between the conduction band $\Gamma^+_{8c}$ and valence

---

**TABLE I.** Band gap (in eV) in $\alpha$–Sn calculated using LDA and HSE hybrid functional compared with computational data reported in literature.

| Energies Transitions | This work w.SO | k · p | HSE |
|----------------------|----------------|-------|-----|
| $E_0$ $\Gamma^+_{7c} \rightarrow \Gamma^-_{8c}$ | 0.69 | 0.70 | 0.58 | 0.40 | 0.52 |
| $E_1$ $\Gamma^+_{43c} \rightarrow \Gamma^-_{4c}$ | 0.84 | 0.80 | 1.00 | 1.10 | – |
| $E_1 + \Delta_1$ $\Gamma^+_{6c} \rightarrow \Gamma^-_{6c}$ | 1.28 | 1.24 | 1.48 | 1.55 | – |
| $E_2$ $\Gamma^-_{8c} \rightarrow \Gamma^-_{8c}$ | 3.24 | 3.11 | 3.73 | 3.25 | – |

*a* The calculated data from Ref. [4]

*b* The calculated data from Ref. [10]

*c* The data calculated with in-plane compressive strain of $-0.164\%$
band $\Gamma_8^\pm$ at the $\Gamma$ point \cite{24}, as shown in the inlay in Figure \text{[3]} The magnitude of the gap opening depends on the computation method. The PAW-LDA pseudopotential gives 31 meV, which is closer to the value of 30 meV calculated under a in-plane compressive strain of $-0.14\%$ using QW quasi-particle calculation, \cite{7} but larger than 13 meV calculated under the in-plane strain of $-0.13\%$ using Pikus-Bir Hamiltonian, \cite{25}

To gain insight into how the band structure changes with strain, we consider the general Luttinger Hamiltonian of an electron (or hole) in a semiconductor including only the four low-energy bands around the $\Gamma$ point.\cite{25, 26}

The four low-energy bands of strained $\alpha-$Sn around the $\Gamma$ point can be written becomes \cite{19}

$$H = H_L + H_{strain},$$

where $H_{strain}$ is an additional perturbation term $H_{strain}$ created by externally applied strain and written as follows,

$$H_{strain} = -g \left( J_2^2 - \frac{5}{4} \right),$$

where $g$ is determined by the strength of the strain and $g > 0$ for biaxial compressive strain.

$\alpha-$Sn is an inverted band structure materials, where the light hole band $\Gamma_8^+$ moves up become unoccupied. Under the biaxial compressive strain, the light hole ($J_z = \pm \frac{3}{2}$) band, $\Gamma_8^+$, is pushed up ($H_{strain} > 0$, and $H$ increases), while the heavy hole band, $\Gamma_8^+$ ($J_z = \pm \frac{3}{2}$), is pushed downward ($H_{strain} < 0$, and $H$ decreases). A small gap thus opens between $\Gamma_8^+$ and $\Gamma_8^+$ under a in-plane compressive strain. This result quantitatively agrees with the computational and theoretical prediction, as shown in Figure \text{[3]}.

The magnitudes of optical transitions such as $E_0$, $E_1$, and $E_2$ also are changed between 8.5 meV and 25 meV in $\alpha-$Sn under $-0.164\%$ in-plane compressive strain. This result is in consistent with the energy peaks estimated from the calculated dielectric function and our ellipsometry experiment discussed in \text{III B}.

**B. Dielectric function of $\alpha-$Sn**

The imaginary part of the frequency dependent dielectric constant, $\epsilon''(\omega)$, is calculated within the independent-particle approximation and is expressed as, \cite{27, 29}

$$\epsilon''_{\alpha\beta}(\omega) = \frac{4\pi q^2}{\Omega} \lim_{q \rightarrow 0} \frac{1}{q^2} \sum_{c,v,k} 2u_k \delta(\epsilon_{ck} - \epsilon_{vk} - \omega) \times <u_{c+k+e,q}|u_{vk}> <u_{v+k+e,q}|u_{vk}>'^*, \quad (3)$$

where $\Omega$ is the volume of the primitive cell, $q$ the Bloch vector of the incident wave, $k$ a wavevector within the first Brillouin zone, the indices $c$ and $v$ the conduction and the valence band states, respectively, $u_k$ the $k$ point weights, the unit vectors $e_{\alpha}$ for the three Cartesian directions.

Subsequent calculation of the real part of the dielectric function, $\epsilon'(\omega)$, is done by applying the Kramers-Kronig relationship,\cite{29}

$$\epsilon''_{\alpha\beta}(\omega) = 1 + \frac{2}{\pi} P \int_{0}^{\infty} \frac{\epsilon''_{\alpha\beta}(\omega')\omega'}{\omega'^2 - \omega^2} d\omega', \quad (4)$$

where $P$ denotes the principal value.

We use the PAW-LDA pseudopotential to calculate the electronic states in equation \text{[3]}

\text{FIG. 4. Computed dielectric function (the imaginary part) of $\alpha-$Sn using PAW-LDA pseudopotential presented together with experimental measurement (red line) \cite{9}. Without (a) and with (b) the spin-orbit interaction.}

The computed imaginary part $\epsilon_{\alpha\beta}(\omega)'''$ of the frequency dependent dielectric function of $\alpha-$Sn, without and with spin-orbit coupling calculated in the LDA scheme for exchange and correlation, are presented together with derived from spectroscopic ellipsometry measurements in Figure \text{[4](a) and [4](b), respectively. In general, except for}
some deviations, the calculated imaginary part of dielectric functions $\epsilon_\alpha(\omega)'''$ agree well with the experimental measurement with respect to the line shape, peak positions, and peak intensities. The main optical features are indicated by arrows and labeled with $E_0$, ..,$E_1'$ being assigned to peaks according to the band gaps calculated in the electronic band structure in Figure 4 (a) without and with spin-orbit interaction.

Figure 4 (b) shows that spin-orbit interaction has effects on $\epsilon'$ of $\alpha$–Sn, in particular, in lower energy region, in three respects. First, finer lineshape is obtained. The calculated dielectric function captures transitions such as $E_0'$, $E_0' + \Delta_0'$, which are not clearly observed in the ellipsometric measurements shown in red line in Figure 4 (b). Second, calculated $E_1$ and $E_1 + \Delta_1$ peaks agree better with the ellipsometric measurements. Third, the magnitude of calculated peaks are comparable with these experimental values, with the largest difference in the $E_0$ peak, whose magnitude is three times higher than the value without spin-orbit interaction. These changes may be because, as we discussed earlier, split-off band $\Gamma_{7\nu}$ modifies the band structure at $\Gamma$ point, where $E_0$, $E_1$, and $E_1 + \Delta_1$ transition occur (see $E_0$ calculated without and with spin-orbit interaction in Figure 4 (a) and (b), respectively). However, there is no remarkable change in band structure at $X$ point, thus, $E_2$ peak is unchanged. Therefore, the inclusion of spin-orbit interaction leads a better agreement with experimental measurement, and the following discussion focuses on the results with spin-orbit interaction.

The energies of transitions in unstrained $\alpha$–Sn shown in Figure 4 (a) and (b) are estimated using the method mentioned in [29], and are presented in Table 1 together with available experimental data. We calculated $E_1$ and $E_1 + \Delta_1$ to be 1.30 eV and 1.78 eV, close to our experimental value 1.278 eV and 1.73 eV, respectively.[9] The calculated $E_0$ value is higher than our experimental value by 0.35 eV. The calculated $E_2$ is 3.26 eV, and is lower than our experimental value by 0.19 eV.[9]

The dielectric function of $\alpha$–Sn is also calculated using HSE functional and presented in Figure 5. The major difficulty of HSE functional is that the calculation is computationally demanding and slow to converge. To overcome the difficulty, the calculation is performed with improved dielectric method to moderate the number of $\mathbf{k}$ points and without spin-orbit interaction to accelerate converge. In consequence, the calculated dielectric function demonstrates wiggles and higher magnitude specifically $E_1$ and $E_1 + \Delta_1$. Their positions are red-shift compared with experimental results and this seems to agree with the trend shown in Figure 4 (a), where spin-orbit interaction is not included. Peaks $E_0$ and $E_2$ demonstrate clearly. The estimated $E_0$ is 0.480 eV, which is close to our experimental value of 0.416 eV. The significant difference in calculated $E_0$ value (representing the transition $\Gamma_{8\nu} \rightarrow \Gamma_{7\nu}$) with LDA and HSE hybrid functional can be understood from the different band order of $\Gamma_{8\nu}, \Gamma_{7\nu}$, and $\Gamma_{7\nu}$ near the $\Gamma$ point in the band structure, as shown in Figure 4 (a) and (b). The better agreement with experiment can be expected by increasing the number of $\mathbf{k}$ points and including spin-orbit interaction.

The dielectric function of $\alpha$–Sn with $-0.164\%$ in-plane compressive strain is calculated and presented together with results without strain in Figure 6. The strain does not significantly change the dielectric function of $\alpha$–Sn, which agrees with our recent ellipsometric measurement that showed critical points by 5 meV by in-plane strain of $-0.13\%$ using deformation formalism.[9] More importantly, it provides evidence that the $E_0$ transition does not arise from externally applied strain, but instead from a direct interband transition $\Gamma_{8\nu} \rightarrow \Gamma_{7\nu}$.

The real part of the dielectric function $\epsilon'$ is shown in Figure 7 along with the experimentally determined $\epsilon'$. A sum rule [22] is used to estimate $\epsilon_\infty$ as 23.4,[9] which is close to $\epsilon_\infty = 24$ measured by infrared polarized reflectance.[30] The calculated dielectric constant $\epsilon_\infty$ is 28, which is larger than the experimental value by 4. The $\epsilon'$ becomes negative at 3.2 eV and continue to the minimum point at 3.45 eV, which relates to $E_2$ transition.

**TABLE II.** Energies (in eV) of peaks in $\alpha$–Sn extracted from the imaginary part dielectric function shown in Figure 4 and 5. The values are compared with available experimental results.

| Energies | This work | Exp. | Exp. |
|----------|-----------|------|------|
| $E_0$    | 0.769     | 0.30 | 0.480 | 0.410 |
| $E_1$    | 1.30      | 1.00 | 1.129 | 1.278 |
| $E_1 + \Delta_1$ | 1.78 | 1.48 | 1.489 | 1.73 |
| $E_2$    | 3.26      | 3.10 | 3.602 | 3.45 |

a The experimental data from Ref. [9]

b The experimental data from Ref. [3]

**FIG. 5.** Computed the imaginary part of dielectric function (cyan line) of $\alpha$–Sn using HSE hybrid functional without spin-orbit interaction presented together with experimental measurement (red line). [9]
In this paper, we explore the dielectric function of α-Sn with focus on the infrared wavelength (photon energy < 1 eV) using the first-principles method. The optical transition at 0.41 eV observed in the our ellipsometric experiment originates from the interband transition $\Gamma_8^+ \rightarrow \Gamma_7^-$ and is explained by combining first-principles calculation of the band structure and dielectric function. The spin-orbit interaction changes the band structure. The biaxial compressive strain induced by epitaxial growth on InSb(001) opens a small band gap at the $\Gamma$ point.

**Appendix A: The refractive index of α-Sn**

The refractive index ($n$) and extinction coefficient ($k$) is calculated for α-Sn using the following equations, and demonstrated in Figure 8.

$$n = \left( \frac{\epsilon' + \epsilon''}{2} \right)^{1/2},$$  \hspace{1cm} (A1)

$$k = \left( \frac{\epsilon' + \epsilon''}{2} - \epsilon' \right)^{1/2},$$  \hspace{1cm} (A2)

where $\epsilon'$ and $\epsilon''$ are taken from the dielectric function computed using PAW-LDA pseudopotential with inclusion of spin orbit interaction, as discussed in section III B. The extinction coefficient $k$ demonstrates distinct peaks associated with transitions, which are labeled in Figure 8. For example, the peak at 0.71 eV corresponds to $E_0$ transition.

**Appendix B: The absorption spectrum of α-Sn**

The absorption coefficient $\alpha$ is calculated using a relation:

$$\alpha = 4\pi k/\lambda,$$

where $\epsilon'$ and $\epsilon''$ are taken from the dielectric function computed using PAW-LDA pseudopotential with inclusion of spin orbit interaction, as discussed in section III B. The extinction coefficient $k$ demonstrates distinct peaks associated with transitions, which are labeled in Figure 8. For example, the peak at 0.71 eV corresponds to $E_0$ transition.
The absorption spectrum captures the critical points in the long wavelength region. In particular, the absorption peak at 1.614 \(\mu m\) corresponds to transition \(E_0\) (\(\Gamma_7\) to \(\Gamma'_{18}\)). Transitions \(E_1, E_2\), and also the transitions due to spin orbit splitting, \(E_1 + \Delta_1, \Gamma'_{14} + \Delta'_{14}\), are clearly obvious.

The absorption spectrum of \(\alpha\)-Sn also provide the information of the band structure. \(\alpha\)-Sn becomes a direct band gap semiconductor in the long wavelength region because an absorption peak at 1.614 \(\mu m\) is observed. The transition \(E_1\) and \(E_1 + \Delta_1\) are indirect because both conduction and valence band edges are not at the center of the Brillouin zone.

ACKNOWLEDGMENTS

Jinsong Duan wishes to thank Air Force Office of Scientific Research for financial support, DoD High Performance Computing Modernized Program for providing computational support, and Catalin Badescu in Sensors Directorate at Air Force Research Laboratory for a fruitful discussion.

[1] A. Ewald and O. Tufte, Gray tin single crystals, Journal of Applied Physics 29, 1007 (1958).
[2] S. Groves and W. Paul, Band structure of gray tin, Physical Review Letters 11, 194 (1963).
[3] M. Cardona, P. McElroy, F. H. Pollak, and K. L. Shaklee, Electroreflectance and band structure of gray tin, Solid State Communications 4, 319 (1966).
[4] F. H. Pollak, M. Cardona, C. Higginbotham, F. Herman, and J. P. Van Dyke, Energy-band structure and optical spectrum of grey tin, Physical Review B 2, 352 (1970).
[5] L.-W. Tu, G. K. Wong, and J. B. Ketterson, Growth of n-type heteroepitaxial films of gray tin on (001) c-dte, Applied physics letters 54, 1010 (1989).
[6] P. John, T. Miller, and T.-C. Chiang, Core-level photoemission studies of the \(\alpha\)-sn/insb (100) heterostructure system, Physical Review B 39, 3223 (1989).
[7] A. Barfuss, L. Dudy, M. R. Scholz, H. Roth, P. Höpfner, C. Blumenstein, G. Landolt, J. Dil, N. Plumb, M. Radovic, et al., Elemental topological insulator with tunable fermi level: Strained \(\alpha\)-sn on insb (001), Physical Review Letters 111, 157205 (2013).
[8] L. Fu, C. L. Kane, and E. J. Mele, Topological insulators in three dimensions, Physical review letters 98, 106803 (2007).
[9] R. A. Carrasco, C. M. Zamarripa, S. Zollner, J. Menéndez, S. A. Chastang, J. Duan, G. J. Gryniewski, B. B. Claflin, and A. M. Kiefer, The direct bandgap of gray \(\alpha\)-tin investigated by infrared ellipsometry, Applied Physics Letters 113, 232104 (2018).
[10] S. Küffner, J. Furthmüller, L. Matthes, M. Fitzner, and F. Bechstedt, Structural and electronic properties of \(\alpha\)-tin nanocrystals from first principles, Physical Review B 87, 235307 (2013).
[11] J. Reno and L. Stephenson, The stability of \(\alpha\)-sn grown on c-dte by molecular beam epitaxy, Journal of electronic materials 19, 549 (1990).
[12] G. Kresse and J. Furthmüller, Vienna ab-initio simulation package (vasp), Vienna: Vienna University (2001).
[13] P. E. Blöchl, Projector augmented-wave method, Physical Review B 50, 17953 (1994).
[14] M. Bokdam, T. Sander, A. Stroppa, S. Picozzi, D. Sarma, C. Franchini, and G. Kresse, Role of polar phonons in the photo excited state of metal halide perovskites, Scientific reports 6, 1 (2016).
[15] M. Oehme, J. Werner, M. Gollohofer, M. Schmid, M. Kaschel, E. Kasper, and J. Schulze, Room- temperature electroluminescence from gesn light-emitting pin diodes on si, IEEE Photonics Technology Letters 23, 1751 (2011).
[16] M. Straumanis and C. Kim, Lattice parameters, thermal expansion coefficients, phase width, and perfection of the structure of gasb and insb, Journal of Applied Physics 36, 3822 (1965).
[17] P. Moongragoon, Z. Ikoníć, and P. Harrison, Band structure calculations of si-ge-sn alloys: achieving direct band gap materials, Semiconductor science and technology 22, 742 (2007).
[18] J. Hinckley and J. Singh, Influence of substrate composition and crystallographic orientation on the band structure of pseudomorphic si-ge alloy films, Physical Review B 42, 3546 (1990).
[19] J. Ruan, S.-K. Jian, H. Yao, H. Zhang, S.-C. Zhang, and D. Xing, Symmetry-protected ideal weyl semimetal in hgte-class materials, Nature communications 7, 1 (2016).
[20] L. Vina, S. Logothetidis, and M. Cardona, Temperature dependence of the dielectric function of germanium, Physical Review B 30, 1979 (1984).
[21] S. Kühner, J. Furthmüller, L. Matthes, and F. Bechstedt, Optical absorption and emission of α-sn nanocrystals from first principles, Nanotechnology 24, 405702 (2013).
[22] Y. Peter and M. Cardona, Fundamentals of semiconductors: physics and materials properties (Springer Science & Business Media, 2010).
[23] C. Y.-P. Chao and S. L. Chuang, Spin-orbit-coupling effects on the valence-band structure of strained semiconductor quantum wells, Physical Review B 46, 4110 (1992).
[24] L. Yang, J. R. Watling, R. C. Wilkins, M. Borici, J. R. Barker, A. Asenov, and S. Roy, Si/sige heterostructure parameters for device simulations, Semiconductor Science and Technology 19, 1174 (2004).
[25] J. M. Luttinger, Quantum theory of cyclotron resonance in semiconductors: General theory, Physical review 102, 1030 (1956).
[26] D. Zhang, H. Wang, J. Ruan, G. Yao, and H. Zhang, Engineering topological phases in the luttinger semimetal α-sn, Physical Review B 97, 195139 (2018).
[27] B. Adolph, V. Gavrilenko, K. Tenelsen, F. Bechstedt, and R. Del Sole, Nonlocality and many-body effects in the optical properties of semiconductors, Physical Review B 53, 9797 (1996).
[28] G. Grosso and G. P. Parravicini, Optical and transport properties in metals, Solid State Physics 396 (2000).
[29] M. Gajdoš, K. Hummer, G. Kresse, J. Furthmüller, and F. Bechstedt, Linear optical properties in the projector-augmented wave methodology, Physical Review B 73, 045112 (2006).
[30] R. E. Lindquist and A. Ewald, Optical constants of single-crystal gray tin in the infrared, Physical Review 135, A191 (1964).
[31] S. Adachi, Optical properties of α-sn, Journal of applied physics 66, 813 (1989).
[32] K. Hummer, J. Harl, and G. Kresse, Heyd-renzerhof hybrid functional for calculating the lattice dynamics of semiconductors, Physical Review B 80, 115205 (2009).