Superconductivity and Topological Insulator Characteristics of $(Pb_{1-x}Sn_x)_{1-y}In_yTe$

Ishaan Aggarwal

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Abstract

This study delves into the impact of indium doping on $(Pb_{1-x}Sn_x)_{1-y}In_yTe$, a topological crystalline insulator. It's found that low indium levels, around 2%, retain weak-metallic characteristics, while a 6% doping leads to bulk-insulating resistivity and hints at nontrivial topological surface states. Higher indium concentrations induce superconductivity, with the transition temperature escalating up to 4.7 K[1], directly proportional to the indium content. The analysis emphasizes how indium-induced impurity levels pin the Fermi level, affecting the bulk electronic structure, offering insights into the topological and superconducting properties of these materials.

1 Introduction

Topological Crystalline Insulators (TCIs) represent a fascinating frontier in condensed matter physics, combining unique electronic properties with topological concepts. Since the discovery of topological insulators, the exploration into TCIs has unfolded a new dimension in understanding material properties[2]. Superconductivity, discovered over a century ago, continues to

intrigue scientists due to its potential for lossless energy transmission and other revolutionary applications[3]. The interplay between superconductivity and topological states of matter opens avenues for novel quantum phenomena and applications. The focus of this report is the TCI sys-

tem $(Pb_{1-x}Sn_x)_{1-y}In_yTe$, chosen for its intriguing electronic properties and transitions under indium doping. The material exhibits a spectrum of behaviors, from weak-metallic to superconducting states, based on indium concentration, making it a prime candidate for studying the relationship between structure, doping, and electronic properties. The report will explore the crystal structure, bulk band structure, and topological characteristics of $(Pb_{1-x}Sn_x)_{1-y}In_yTe$, concluding with a discussion on its superconductive characteristics and a summary of the research findings, emphasizing their relevance to the broader field of condensed matter physics.

2 Crystal Structure

SnTe, a semiconductor in the IV-VI group, crystallizes in a cubic rocksalt structure at room temperature. This structure remains stable even when Sn is partially substituted with Pb and/or In, crucial for maintaining topological surface states (Figure 1). The lattice parameters of $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ compounds adjust with the concentrations of Pb and In, as seen in Figure 1b of Zhong 2017[1]. The pristine SnTe has a lattice constant of 6.32 Å. When doped with Pb (Pb0.5Sn0.5Te, x = 0.5, y = 0), the lattice constant increases to 6.39 Å. Conversely, further doping with In ((Pb0.5Sn0.5)0.7In0.3Te, x = 0.5, y = 0.3) decreases the lattice constant to 6.36 Å, aligning with Vegard's law. This lattice parameter variation, influenced by the different ionic radii, becomes more pronounced with increasing In substitution, eventually leading to structural distortion and the appearance of a secondary phase, InTe, indicating the solubility limit.

3 Bulk Band Structure

SnTe and related IV-VI rocksalt structure materials are significant for their role as small band gap semiconductors. The contrasting band structures of SnTe, which is topologically nontrivial at $x = 1$, and trivial PbTe at $x = 0$(shown in Figure 22, are characterized by a change in the ordering of the conduction and valence bands at the L points in the Brillouin zone. As x increases in the Pb1-xSnxTe alloy, the band gap first closes and then reopens, signifying a topological quantum phase transition. This transition is observed near $x \approx 0.35$[1] at low temperatures, marking a critical juncture in the study of the electronic properties of Pb1-xSnxTe. This inversion leads to a reversal in the s-like conduction band and p-like valence band energy levels, altering the band topology and resulting in topologically protected surface states[4]. Indium doping in the material is responsible for the resistivity behaviours of the material. The pinning of the Fermi level by indium doping in $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ is crucial for understanding its superconductivity and resistivity. Indium-induced impurity states alter the electronic density of states near the Fermi level, affecting electron pairing and the superconducting transition. This

pinning also influences bulk resistivity, dictating electronic transport characteristics crucial for understanding the material's superconductive behavior under various doping levels[1][4].

4 Topological Characteristics

The resistivity characteristics of the material are portrayed in Fig 3 of the paper. In Figure 3, we observe the resistivity effects due to variations in PbTe and SnTe ratios in $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ (Figure 3).We see, in Figure 3a For $x = 0.50$, the material behaves as a weak metallic-like substance. At $x = 0.40$ and $x = 0.35$, an increase in resistivity indicates a transition to bulk resistivity phase. Particularly at $x = 0.30$, there's a significant spike in resistivity, approximately five orders of magnitude, likely due to the proximity of Pb and Sn concentrations to the band inversion region, revealing topological insulator characteristics. $x = 0.25$ mirrors the behavior of $x = 0.40$, while $x = 0.20$ acts more like an n-type semiconductor with higher resistivity than $x = 0.50$ but not sufficient to be classified as an insulator, in this concentration levels the PbTe semiconductor is dominant. Figure 3b demonstrates a significant increase in resistivity for each concentration variance in $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ with an increase in In doping from 3% to 6%. This marked elevation across all values highlights the profound effect of indium doping in enhancing the material's topological characteristics. The changes in resistivity with varied In concentrations showcase the dopant's critical role in modulating the topological properties of the material. The resistivity behaviors in In-doped $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ demonstrate a com-

plex interplay between indium concentration and electronic properties. Initially, with up to about 1% indium doping, the material exhibits weak-metallic behavior, akin to pure SnTe or Pb1-xSnxTe without indium. Upon increasing indium concentration to 6%, there's a dramatic rise in resistivity at 10 K, indicative of a transition to a bulk-insulating state. This shift in resistivity, which is nonmonotonic and dependent on the specific Pb/Sn ratio, is attributed to the chemical potential being pinned within the band gap. Such a pinning effect is significant across different $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ compositions, where maximum resistivities surpassing $10^6\Omega$cm are observed for certain ranges of x, particularly between 0.25 and 0.30. Even at $x = 0.35$, a 6% In doping leads to an increase in resistivity by six orders of magnitude at low temperatures. The phenomenon of long relaxation times in bulk resistance, especially in samples exhibiting true bulk-insulator behavior, is also observed. This relaxation, which can last days until reaching a stable resistivity value, aligns with previous findings in similar materials doped with group-III elements, where it's explained by interactions between the crystal lattice and non-equilibrium electron densities related to the pinned chemical potential at the impurity level[1].

5 Superconductive Characteristics

The superconductivity in $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ is deeply influenced by indium doping. Indium introduces key changes in the material's electronic structure, notably through the pinning of the Fermi level[1]. This pinning is critical for the transition from a normal insulator to a superconducting state. With higher levels of indium doping, the material exhibits a marked increase in superconductivity. The studies suggest that this transition correlates with the indium concentration, where higher concentrations yield a stronger superconducting response. Figure 4

in the study illustrates the resistivity behaviors of $(PbSn)_{1-y}In_yTe$ as a function of indium concentration (y). figure 4 showcases the bulk resistivity behaviour of the material when the

Indium concentration is lower than 10 percent. It shows that for $y \leq 0.10$, the material does not exhibit superconductivity at low temperatures. However, at higher concentrations of indium, particularly $y > 0.10$ (as measured at $y = 0.13, 0.16, 0.20, 0.30$), the material becomes superconductive with very low resistivity at low temperatures. We see that these curves behave like conventional superconductors in the temperature zone of 4-5 degrees K. The lowest resistivity, achieved at $4.7K$, is observed with an indium concentration of 35 percent. The

superconductivity of $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ is linked to its transition from an insulator to a superconductor as indium concentration increases. This transition is associated with the instability in the 3-dimensional Dirac semimetal state and the flattening of bulk valence and conduction bands[4]. The study suggests that these flattened bands, showing a Mexican hat-like dispersion, might contribute to pairing instability, potentially leading to superconductivity under certain conditions. The concept of flattened bands in the context of superconductivity in $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ is crucial. These flattened bands, characterized by a Mexican hat-like dispersion, are seen on the inverted side of the phase diagram. This unique band structure is hypothesized to enhance pairing instability, which is a key factor in the emergence of superconductivity. The specific conditions under which these flattened bands contribute to superconductivity are a significant focus of the study.

6 Summary of Research

The research on $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ has revealed critical insights into the role of indium doping in electronic transitions. Indium's incorporation significantly alters the material's electronic properties, facilitating a transition from weak-metallic behavior to superconductivity. The study highlights the Fermi level pinning and band inversion phenomena, critical in these transitions. With indium concentrations up to 6%, resistivity increased by five orders of magnitude at 10 K, indicating a shift towards bulk-insulating behavior[1]. Furthermore, higher concentrations of indium, specifically around 35%, led to a marked decrease in resistivity and the emergence of superconductivity at temperatures around 4.7 K. The concept of flattened

bands, as seen in the Mexican hat-like dispersion, plays a pivotal role in the material's topological and superconducting properties. These bands, resulting from indium doping, contribute to the stabilization of topologically nontrivial states. The band structure transformation, linked to superconductivity, suggests an intrinsic connection between topological characteristics and superconducting behavior. The research indicates that the flattened bands enhance pairing instability[4], a crucial factor for the emergence of superconductivity, particularly in regions close to the band inversion. Resistivity in $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ shows significant variation

with changes in Pb and Sn concentrations. At lower Pb/Sn ratios (x = 0.20 to 0.50), the material exhibits weak-metallic characteristics. However, as the Pb concentration increases (x = 0.25 to 0.35)[4], the resistivity spikes dramatically, indicating a transition towards an insulating state. This change is particularly notable at x = 0.30, where resistivity increases by six orders of magnitude at low temperatures, highlighting the material's sensitivity to compositional changes. Superconductivity in $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ is predominantly influenced by

the concentration of indium doping. As indium content increases, particularly beyond 10%[1], the material transitions from a non-superconducting to a superconducting state at low temperatures. The highest superconducting transition temperature recorded is approximately 4.7 K at an indium concentration of 35%[1]. This correlation between indium concentration and

superconducting behavior underscores the critical role of indium in modulating the material's electronic and superconductive properties. The ternary phase diagram in Figure 5[1] effectively

summarizes the impact of indium substitution on $(Pb_{1-x}Sn_x)_{1-y}In_yTe$ materials. It displays trends like low-temperature resistivity character and the solubility limit, highlighting three distinct regions: weak metallic resistivity with low indium doping (blue), insulation at moderate indium levels (orange), and superconductivity at higher concentrations (green). The diagram also denotes the solubility limit of indium in the system (dashed line), beyond which additional In leads to the formation of a secondary phase. It shows that superconductivity emerges rapidly with indium doping in SnTe, but requires more indium for Pb-rich compositions.

Figures

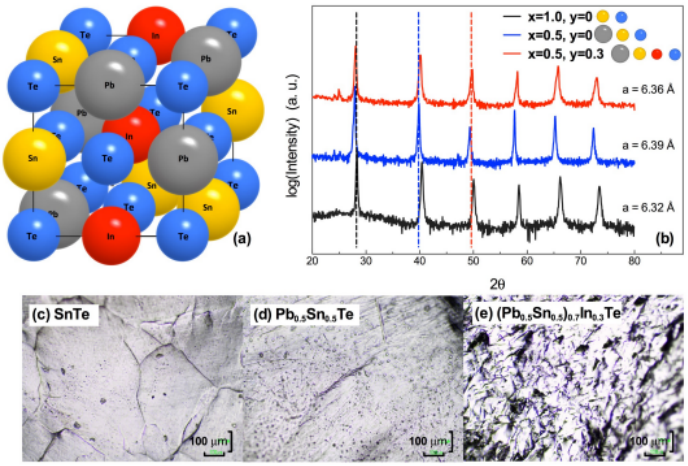

Figure 1: Illustration of crystallographic changes in SnTe upon partial substitution with Pb and In. Part (a) shows the crystal structure with Sn, Pb, and In atoms, (b) presents X-ray diffraction patterns for SnTe, $Pb_{0.5}Sn_{0.5}Te$, and $(Pb_{0.5}Sn_{0.5})_{0.7}In_{0.3}Te$, and (c-e) depict optical microscope images of their pristine surfaces.

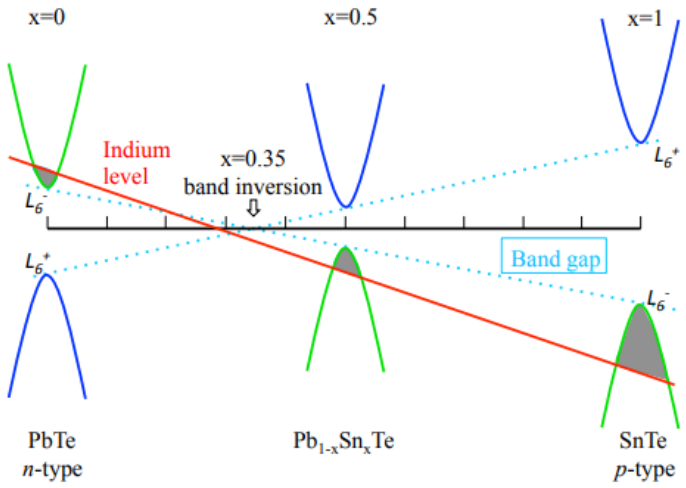

Figure 2: Energy diagrams depicting the conduction and valence bands, and the indium-induced impurity band in $Pb_{1-x}Sn_xTe$ alloys with low In doping. These diagrams demonstrate the evolution of the band structure throughout the series, emphasizing the band inversion and dynamics of the Fermi level.

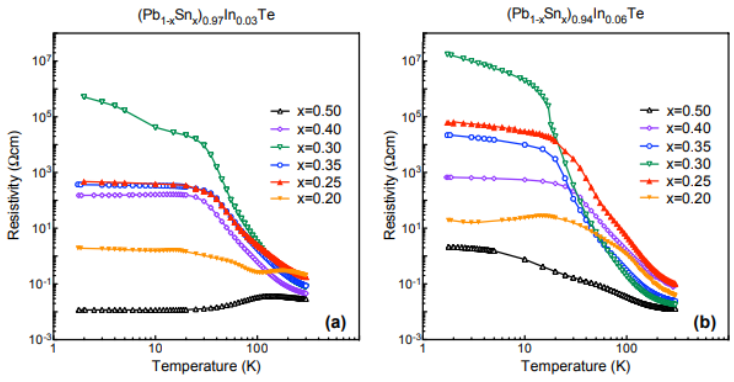

Figure 3: Logarithmic display of the temperature dependence of resistivity for $(Pb_{1-x}Sn_x)_{0.97}In_{0.03}Te$ and $(Pb_{1-x}Sn_x)_{0.94}In_{0.06}Te$ single crystals. The graph aids in comprehending the resistivity changes across various compositions and temperatures.

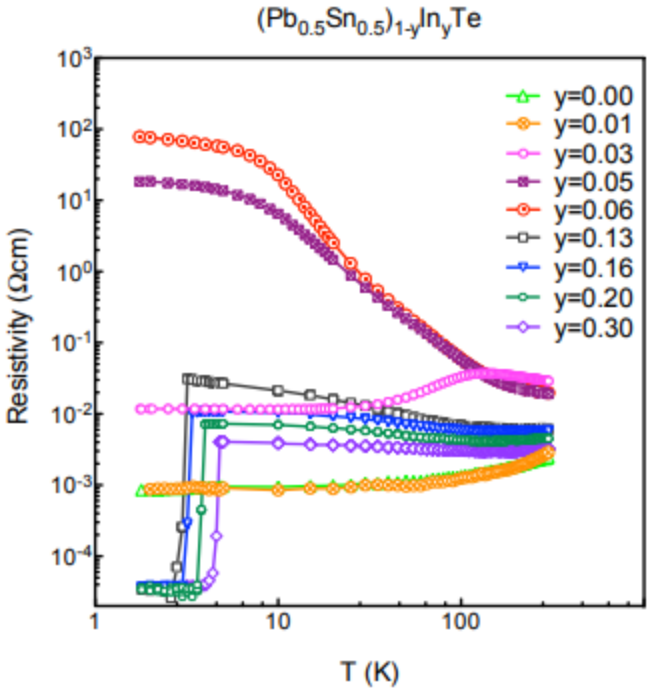

Figure 4: Temperature-dependent resistivity of $(Pb_{0.5}Sn_{0.5})_{1-y}In_yTe$ crystals for various indium contents, from 0% to 30%. This graph reveals the alteration in resistivity at different temperatures correlating with the increase in indium concentration.

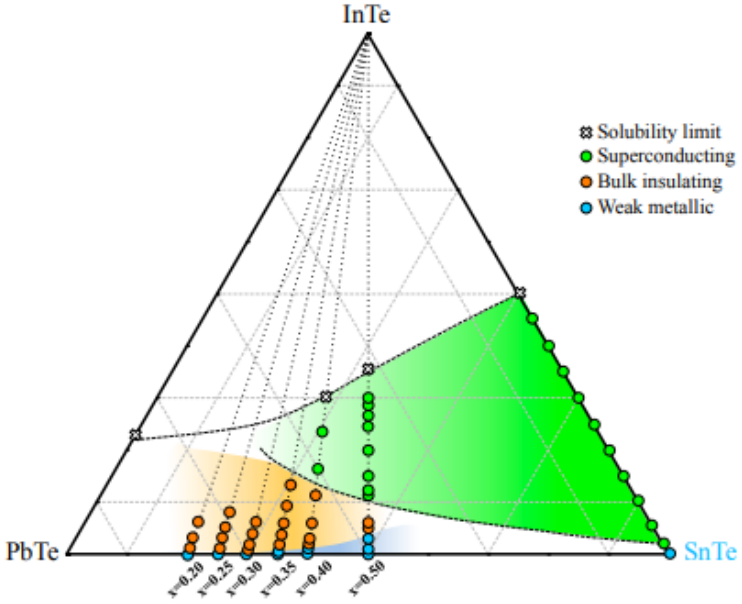

Figure 5: Ternary phase diagram representing resistivity behaviors in $(Pb_{1-x}Sn_x)_{1-y}In_yTe$. This diagram delineates low-temperature resistivity characteristics (metallic, insulating, superconducting) and indium solubility limits, demarcating three distinct regions depending on indium concentration.

Bibliography

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