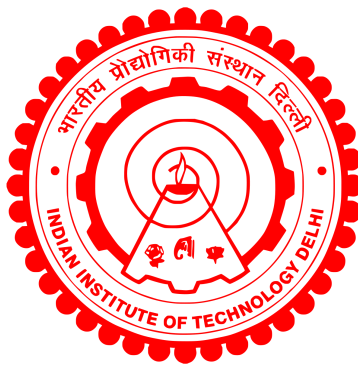


INVESTIGATION OF SUPERCONDUCTIVITY IN Th_3P_4 - TYPE NONCENTROSYMMETRIC LANTHANUM CHALCOGENIDES

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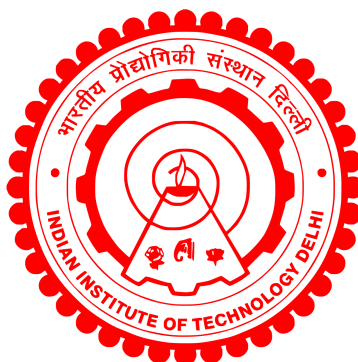
MOUMITA NASKAR

Department of Physics

Submitted

in fulfillment of the requirements of the degree of Doctor of Philosophy

to the



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*Dedicated to my family, friends & teachers
for their endless support and encouragement.*

Certificate

This is to certify that the thesis entitled **“Investigation of superconductivity in Th_3P_4 -type noncentrosymmetric lanthanum chalcogenides”** is being submitted by **Ms. Moumita Naskar** to the **Indian Institute of Technology Delhi** for the award of the degree of **Doctor of Philosophy in Physics** is a record of bonafide research work carried out by her. Ms. Moumita Naskar has worked under our guidance and supervision and has fulfilled the requirements for the submission of the thesis, which to our knowledge, has reached the requisite standard. The results contained in this dissertation have not been submitted in part or full to any other university or institute for the award of any degree or diploma.

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Abstract

The discovery of superconductivity by Heike Kamerlingh Onnes in 1911 is one of the major breakthroughs in the field of condensed matter physics. A number of superconducting materials such as intermetallics, cuprates, iron oxypnictides, bismuth chalcogenide, and transition metal dichalcogenide based systems have been extensively investigated in the last few decades. Recently, the area of superconductivity has been rejuvenated after the discovery of superconductivity in the noncentrosymmetric crystal structures [1]. The absence of inversion symmetry introduces an antisymmetric spin-orbit coupling (ASOC) which lifts the original spin degeneracy at the Fermi level, splitting it into two spin-ordered subsurfaces. This allows the admixture of spin-singlet and spin-triplet pairing states within the same orbital channel [2–4].

In this thesis, we have discussed the synthesis, characterization, and physical properties of rare earth chalcogenides La_3Se_4 , $\text{La}_{2.75}\text{Y}_{0.25}\text{Se}_4$, and La_3SeTe_3 . Polycrystalline chalcogenides were synthesized by solid state sealed tube technique. This thesis discussed the detail characterization of La_3Se_4 and its derivatives in the context of noncentrosymmetric superconductivity. All the systems crystallize in noncentrosymmetric cubic body-centered Th_3P_4 -type structure with space group $I\bar{4}3d$. We have discussed the superconducting properties of La_3Se_4 with superconducting transition temperature $T_c \sim 8.5$ K in detail by means of X-ray diffraction, electrical transport, magnetization, heat capacity measurements, and density functional theory calculations. The specific heat jump at T_c , $\Delta C/\gamma T_c \sim 2.04$, exceeds the value for weakly coupled BCS superconductor, suggesting superconductivity in La_3Se_4 is in the strong-coupling regime. From the density functional theory based first-principles studies, we observe that the number of states at the Fermi energy is dominated by d and f electrons of La, and is found to be highly sensitive to the La deficiency in La_3Se_4 .

Superconductivity is found in $\text{La}_{2.75}\text{Y}_{0.25}\text{Se}_4$ below $T_c \sim 7.4$ K. Bulk

superconductivity is confirmed by the jump at T_c of the specific heat with $\Delta C/\gamma T_c \sim 0.7$, and the value is much smaller than the isotropic weak coupling BCS value of 1.43. Therefore, $\text{La}_{2.75}\text{Y}_{0.25}\text{Se}_4$ is a weakly coupled superconductor. Detailed superconducting characteristic parameters have been estimated.

Superconducting transition below 2.3 K has been observed in La_3SeTe_3 . From the temperature dependent DC susceptibility measurement, it has been observed that the onset of diamagnetism occurs at 2.4 K in ZFC measurement. Normal-state properties such as Sommerfeld coefficient, phonon specific heat coefficient, Debye temperature, electron-phonon coupling constant, and density of states have been discussed. In the final chapter, we summarize all the major results that have been discussed in the preceding chapters and provide the future prospect in this area.

सार

1911 में हाइक कामेरलिंग ओन्स द्वारा अतिचालकता की खोज संघनित पदार्थ भौतिकी के क्षेत्र में प्रमुख सफलताओं में से एक है। एक संख्या सुपरकंडक्टिंग सामग्री जैसे इंटरमेटेलिक्स, कप्रेट्स, आयरन ऑक्सीप्रिकटाइड्स, बिस्मथ चेल्कोजेनाइड, और ट्रांज़िशन मेटल डाइक्लोजेनाइड आधारित सिस्टम पिछले कुछ दशकों में व्यापक रूप से जांच की गई है। हाल ही में, का क्षेत्र सुपरकंडक्टिविटी की खोज के बाद सुपरकंडक्टिविटी का कार्याकल्प किया गया है नॉनसैंट्रोसिमेट्रिक क्रिस्टल संरचनाएं [1]। उलटा समरूपता का अभाव एक एंटीसिमेट्रिक स्पिन-ऑर्बिट कपलिंग (ASOC) पेश करता है जो मूल स्पिन को उठाता है फर्मी स्तर पर अधः पतन, इसे दो स्पिन-आदेशित उपसतहों में विभाजित करता है। इस स्पिन-सिंगलेट और स्पिन-ट्रिपलेट पेयरिंग स्टेट्स के मिश्रण को उसी के भीतर अनुमति देता है कक्षीय चैनल [2-4]।

इस थीसिस में, हमने संश्लेषण, लक्षण वर्णन और भौतिक पर चर्चा की है रेयर अर्थ चाकोजेनाइड्स La_3Se_4 , $\text{La}_{2.75}\text{Y}_{0.25}\text{Se}_4$, और La_3SeTe_3 के गुण। पॉलीक्रिस्टलाइन चाकोजेनाइड्स को सॉलिड स्टेट सीलबंद ट्यूब तकनीक द्वारा संश्लेषित किया गया था। इस थीसिस ने La_3Se_4 और इसके डेरिवेटिव के विस्तृत लक्षण वर्णन पर चर्चा की नॉनसैंट्रोसिमेट्रिक सुपरकंडक्टिविटी का संदर्भ। सभी प्रणालियाँ क्रिस्टलीकृत होती हैं अंतरिक्ष के साथ नॉनसैंट्रोसिमेट्रिक क्यूबिक बॉडी-केंद्रित Th_3P_4 -प्रकार की संरचना में समूह $I\bar{4}3d$ । हमने La_3Se_4 के अतिचालक गुणों पर चर्चा की है अतिचालक संक्रमण तापमान टीसी 8.5 के एक्स-रे के माध्यम से विस्तार से विवर्तन, विद्युत परिवहन, चुंबकीयकरण, ताप क्षमता माप, और घनत्व कार्यात्मक सिद्धांत गणना। टीसी, $\Delta C/\gamma T_c$ पर विशिष्ट गर्मी कूद 2.04, कमजोर युग्मित बीसीएस सुपरकंडक्टर के लिए मूल्य से अधिक है, सुझाव दे रहा है La_3Se_4 में सुपरकंडक्टिविटी मजबूत-युग्मन शासन में है। घनत्व से कार्यात्मक सिद्धांत आधारित प्रथम-सिद्धांत अध्ययन, हम देखते हैं कि राज्यों की संख्या Fermi ऊर्जा में La के d और f इलेक्ट्रॉनों का प्रभुत्व होता है, और यह अत्यधिक पाया जाता है La_3Se_4 में La की कमी के प्रति संवेदनशील।

$T_c \sim 7.4$ K के नीचे $\text{La}_{2.75}\text{Y}_{0.25}\text{Se}_4$ में अतिचालकता पाई जाती है। थोक अतिचालकता की पुष्टि $\Delta C/\gamma T_c$ के साथ विशिष्ट ऊष्मा के T_c पर कूदने से होती है। 0.7, और मूल्य आइसोट्रोपिक कमजोर युग्मन बीसीएस मूल्य से बहुत छोटा है 1.43 का। इसलिए, $\text{La}_{2.75}\text{Y}_{0.25}\text{Se}_4$ एक कमजोर युग्मित सुपरकंडक्टर है। विस्तृत सुपरकंडक्टिंग विशेषता मापदंडों का अनुमान लगाया गया है। La_3SeTe_3 में 2.3 K से नीचे का अतिचालक संक्रमण देखा गया है। से तापमान पर निर्भर डीसी संवेदनशीलता

माप, यह देखा गया है कि प्रतिचुंबकत्व की शुरुआत ZFC माप में 2.4 K पर होती है। सामान्य-राज्य गुण जैसे सोमरफेल्ड गुणांक, फोनन विशिष्ट ताप गुणांक, डेबी तापमान, इलेक्ट्रॉन-फोनन युग्मन स्थिरांक, और राज्यों के घनत्व पर चर्चा की गई है। में

अंतिम अध्याय में, हम उन सभी प्रमुख परिणामों को संक्षेप में प्रस्तुत करते हैं जिन पर चर्चा की गई है पिछले अध्यायों और इस क्षेत्र में भविष्य की संभावना प्रदान करते हैं।

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