AN INVESTIGATION OF THE MAGNETO-TRANSPORT AND SUPERCONDUCTING PROPERTIES OF HALF HEUSLER THIN FILMS

SHIVANGI SRIVASTAVA

DEPARTMENT OF PHYSICS
INDIAN INSTITUTE OF TECHNOLOGY DELHI
SEPTEMBER 2025

An Investigation of the Magneto-Transport and Superconducting Properties of Half Heusler Thin Films

by

Shivangi Srivastava

DEPARTMENT OF PHYSICS

Submitted

In fulfilment of the requirement of the degree of

Doctor of Philosophy

INDIAN INSTITUTE OF TECHNOLOGY DELHI

SEPTEMBER 2025

DEDICATION

This thesis is lovingly dedicated to my papa, Late Dr. Prabha Shankar

(my hero, my strength, my role model).

It was his unfulfilled dream to reach the pinnacle of academic pursuit, to earn the highest degree in science. Though he is no longer here to witness this moment, every step of this journey has been carried on the foundation of his unwavering support, quiet sacrifices, and the values he instilled in me.

He taught me to move forward with courage, hope, and a heart full of positivity, even in the darkest of times. His values and principles became my strength. His dreams became my purpose.

I feel his presence in every heartbeat, every achievement, and I know, somewhere beyond this world, he is smiling with pride.

This accomplishment is not mine alone; it is his. With all my love and the deepest gratitude, I offer it to him.

“Love you, Papa.”

Department of Physics
Indian Institute of Technology
Delhi Hauz Khas, India-110016

Certificate

This is to certify that this thesis entitled **"An Investigation of the Magneto-Transport and Superconducting Properties of Half Heusler Thin Films"** being submitted by **Ms. Shivangi Srivastava** to the Indian Institute of Technology Delhi for the award of the degree of **"Doctor of Philosophy (Ph.D.)"**, is a record of bonafide research work carried out under my guidance and supervision. The work or any part of the thesis have not been submitted in part or full to any other University or Institute for award of any degree or diploma.

Supervisor

Prof. Ratnamala Chatterjee
Department of Physics
Indian Institute of Technology Delhi
India - 110016.

Declaration

I certify that

a. The work contained in the thesis is original and has been done by me under the guidance of my supervisor;
b. The work has not been submitted to any other institute for any other degree or diploma;
c. I have followed the guidelines provided by the Institute in preparing the thesis;
d. I have conformed to ethical norms and guidelines while writing the thesis;
e. Whenever I have used materials (data, models, figures and text) from other sources, I have given due credit to them by citing them in the text of the thesis, and giving their details in the references, and taken permission from the copyright owners of the sources, whenever necessary.

Shivangi Srivastava

ACKNOWLEDGMENTS

With deep reverence, I bow to Lord Krishna, the supreme guide in my life.

I sincerely thank everyone who has supported me throughout my academic journey. Without their direct and indirect contributions, reaching this milestone would not have been possible. While it is difficult to name everyone individually, I would like to express my heartfelt gratitude to a few key individuals.

First and foremost, I express my deepest thanks to my teacher and supervisor, Prof. Ratnamala Chatterjee, for her unwavering guidance, encouragement, and trust in me. Her insights and support, especially during challenging times, kept me focused and motivated to give my best.

I am equally grateful to my SRC members, Prof. Pankaj Srivastava, Prof. Sujit Manna, and Prof. Debanjan Bhowmik, for their valuable discussions and mentorship, which helped shape my scientific thinking and sharpen my presentation skills.

I feel fortunate to have worked with inspiring collaborators, Late Prof. Vinay Gupta, Prof. Aftab Alam and Dr. Niladari Banerjee, whose expertise and perspectives enriched my research.

I gratefully acknowledge the Central Research Facilities (CRF)**,** Nanoscale Research Facilities (NRF)**,** and the Department of Physics, IIT Delhi, for providing me with the infrastructure and support necessary for my research. I also thank the Ministry of Education, Government of India**,** and IIT Delhi for the financial support and opportunities to attend conferences and workshops both in India and abroad. I am also thankful to IIT Delhi for providing financial support through the Institute Fellowship.

To my lab mates, Dr. Devendra Pandey, Dr. Mithun Majhi, Dr. Deepika Rani, Dr. Vishal Bhardwaj, Dr. Divya Prakash Dubey, Dr. Anupam Bhattacharya, Dr. Hitesh Gulati, Dr. Priyanka Sharma, Dr. Durgesh Ojha, Vikas Chahar, Balwant Chauhan**,** and Rinku, thank you for your companionship, support, and encouragement throughout the Ph.D. journey. A special thanks to Dr. Risabh Shukla, who has stood by me since my master's days, offering constant support and positivity.

To my dear friends who became family at IIT Delhi, Dr. Ranjana, Dr. Vandana, and Shobha, thank you for the shared weekends, comforting food, endless conversations, and

unforgettable memories. Your support during difficult times and your patience with my sarcasm meant more than words can say.

I deeply cherish the love and encouragement from my school and college friends at BHU and IIT Kanpur, who celebrated every small and big success of mine with genuine happiness.

Words cannot express the immense love and gratitude I have for my mother, Dr. Vandana Srivastava**,** my sister, Dr. Trishla Srivastava**,** and my brother, Dr. Trishek Srivastava, for their constant belief in me and for being my unwavering pillars of strength throughout this journey and beyond.

My heartfelt thanks to my family and my extended family, especially my sister-in-law, Shikha Sharma, whose motherly care for my toddler during the most demanding phase of thesis writing was a true blessing. Her selfless support played a crucial role in the completion of this journey.

This journey would have been much more difficult without the unwavering support of my husband, Dr. Suraj Prakash. I feel truly blessed to have him by my side through every phase, from M.Sc. to Ph.D., and beyond. His constant encouragement, strength, and wisdom inspired me to keep moving forward. I am deeply grateful for his love, patience, and belief in my dreams.

Finally, my utmost and most special thanks to my son, Shivank Madhav, whose birth brought light into my life. His innocent smile wipes away every sorrow, and his presence fills my heart with boundless joy and completeness. I thank him for choosing me as his mother.

Shivangi Srivastava

ABSTRACT

This thesis presents a systematic investigation of the magneto-transport, superconducting, and topological properties of doped and strained half-Heusler (HH) thin films based on rare-earth alloys. The study focuses on three alloy systems: (i) Er-doped YPdBi, (ii) Y-doped HoPdBi, and (iii) strained GdPdBi, grown using pulsed laser deposition (PLD), with the aim of tuning their electronic structure via *f*-electron doping, magnetic dilution, and lattice strain.

The first part of this thesis investigates the $Y_{1-x}Er_xPdBi$ (x = 0.2(E2), 0.5(E5), 0.8(E8)) thin films to study the effect of *f*-electron doping on the otherwise topologically trivial, diamagnetic YPdBi. All the films exhibit semimetallic behavior with clear signatures of superconductivity at low temperatures. The optimally doped E5 film (x = 0.5) showed a maximum superconducting transition temperature (T_c ~ 4.4 K), with a high quantum mobility, and a large phase coherence length. While E2 and E8 films exhibited T_c values of ~2.2 K and ~3.7 K, respectively. Detailed magneto-transport measurements revealed features characteristic of non-trivial topological materials, such as weak anti-localization (WAL) and Shubnikov–de Haas (SdH) oscillations. The power law fitting of phase coherence lengths, the extracted α value confirmed the presence of 2D surface state. The extracted Berry phase (~π) confirmed the presence of Dirac fermions. First-principles DFT calculations validated the non-trivial topological band ordering in all compositions, with band inversion strength increasing with Er content due to *s–f* exchange interactions. The optimally doped film (E5) showed enhanced quantum coherence and mobility, attributed to more *f* bands near the Fermi level. These findings indicate that Er-doped YPdBi thin films exhibit a strong interplay between superconductivity and topological band structure.

The second part investigates $Ho_{1-x}Y_xPdBi$ (x = 0(Y2), 0.2(Y2), 0.8(Y8)) thin films, where substitution of magnetic Ho^{3+} ions by non-magnetic Y^{3+} modifies both magnetism and transport characteristics. Electrical resistivity measurements revealed semimetallic nature and superconducting transitions in all films, with the x=0.8 (Y8) film achieving a zero-resistivity state at T_c~2.8 K.While Y0 and Y2 films exhibited T_c values of ~0.9K and ~2.1 K, respectively Bulk superconductivity in the Y8 film was confirmed through AC susceptibility measurements, showing a strong diamagnetic response and an upper critical field $H_{c2}(0) \sim 5.7$ T. Magneto-resistance measurements displayed weak anti-

localization (WAL)-like behavior at low fields. Using HLN model, the α and l_{φ} value extracted. The unphysical value of α at different temperatures and value of $l_{\varphi}(4K) <$ thickness of HYPB films, which reflects that WAL originates from 3D bulk conduction.l_{φ} analysis revealed that *electron–electron (e–e)* scattering dominates in Y0 and Y8 films, while the Y2 film exhibited additional *electron–phonon (e–ph) scattering*, suggesting a coexistence of scattering mechanism.

In the final part, the structural and transport properties of GdPdBi thin films were explored under ~1% strain. X-ray diffraction and microscopic analyses confirm high-quality, single-phase films with ~1% lattice strain relative to the bulk. Temperature-dependent resistivity measurements reveal a two conducting behaviour: metallic behavior ($T < 3.5K$), and semiconducting behavior ($T > 3.5K$) with a reduced energy gap of ~10.2 meV, significantly smaller than the bulk band gap (~70 meV), indicating strain-induced band narrowing in the films. Magneto-resistance measurements displayed weak anti-localization (WAL)-like behavior at low fields. HLN model analysis gives unphysical α-values and coherence lengths smaller than the film thickness, indicating that WAL originates from 3D bulk conduction. Angle-dependent magneto-conductance measurements confirmed that the observed WAL-like features originated from 3D bulk states due to spin-orbit coupling (SOC), not from 2D surface states.

Overall, this thesis demonstrates that *f*-electron doping, magnetic dilution, and lattice strain are effective tuning parameters for manipulating the quantum transport and topological properties of HH thin films. These findings provide valuable insights into the design of topological superconductors and pave the way for future applications in spintronics, quantum computation, and topological device platforms.

सारांश

यह शोधप्रबंध दुर्लभ-पृथ्वी मिश्रधातुओं पर आधारित डोप्ड और तनावित हाफ-ह्यूस्लर (HH) पतली परतों (thin films) के चुम्बकीय-परिवहन, अतिचालक (superconducting) और टोपोलॉजिकल गुणों की एक व्यवस्थित जाँच प्रस्तुत करता है। अध्ययन तीन मिश्रधातु प्रणालियों पर केंद्रित है: (i) Er-डोप्ड YPdBi, (ii) Y-डोप्ड HoPdBi, और (iii) तनावित GdPdBi। इन्हें पल्स्ड लेज़र निक्षेपण (PLD) तकनीक से विकसित किया गया है, जिसका उद्देश्य *f*-इलेक्ट्रॉन डोपिंग, चुम्बकीय पतला करना (magnetic dilution), और लैटिस तनाव के माध्यम से इनके इलेक्ट्रॉनिक संरचना को नियंत्रित करना है।

शोधप्रबंध का पहला भाग $Y_{1-x}Er_xPdBi$ (x = 0.2(E2), 0.5(E5), 0.8(E8)) पतली परतों की जाँच करता है ताकि f-इलेक्ट्रॉन डोपिंग के प्रभाव का अध्ययन किया जा सके, जो सामान्यत: टोपोलॉजिकल रूप से तुच्छ और प्रतिचुम्बकीय (diamagnetic) YPdBi पर लागू होता है। सभी फिल्में अर्ध-धात्विक (semimetallic) व्यवहार प्रदर्शित करती हैं और निम्न तापमान पर अतिचालकता (superconductivity) के स्पष्ट संकेत देती हैं। E5 (x = 0.5) फिल्म ने अधिकतम अतिचालक संक्रमण तापमान (~4.4 K) दर्शाया, साथ ही उच्च क्वांटम गतिशीलता (mobility) और बड़ी चरण-समरूपता लंबाई (phase coherence length) दिखाई। वहीं E2 और E8 फिल्मों ने क्रमशः ~2.2 K और ~3.7 K के Tc मान प्रस्तुत किए। विस्तृत मैग्नेटो-ट्रांसपोर्ट मापनों ने टोपोलॉजिकल पदार्थों की विशिष्ट विशेषताओं, जैसे कि कमजोर प्रतिलोकीकरण (weak anti-localization, WAL) और शुब्निकोव–डी हास (SdH) दोलन, को उजागर किया। चरण-समरूपता लंबाई के पावर-लॉ विश्लेषण से 2D सतही अवस्था की उपस्थिति की पुष्टि हुई। निकाली गई बेरी फेज़ ($\sim\pi$) ने डिराक फ़र्मियॉन्स की उपस्थिति को सत्यापित किया। प्रथम-सिद्धांत DFT गणनाओं ने बैंड उलटफेर (band inversion) के साथ गैर-तुच्छ टोपोलॉजिकल बैंड क्रम की पुष्टि की, जो Er मात्रा के बढ़ने के साथ s–f विनिमय क्रियाओं द्वारा प्रबलित हुआ। विशेष रूप से E5 फिल्म ने अधिक f-बैंड्स के फ़र्मी स्तर के समीप होने से, उन्नत क्वांटम समरूपता और गतिशीलता प्रदर्शित की। यह दर्शाता है कि Er-डोप्ड YPdBi पतली परतों में अतिचालकता और टोपोलॉजिकल बैंड संरचना के बीच मजबूत अंतःक्रिया होती है।

शोध का दूसरा भाग $Ho_{1-x}Y_xPdBi$ (x = 0(Y0), 0.2(Y2), 0.8(Y8)) पतली परतों पर केंद्रित है, जहाँ चुंबकीय Ho^{3+} आयनों को अचुंबकीय Y^{3+} आयनों से प्रतिस्थापित करने से चुम्बकत्व और

परिवहन गुण दोनों में परिवर्तन आता है। विद्युत प्रतिरोधकता ने सभी फिल्मों में अर्ध-धात्विक प्रकृति तथा अतिचालक संक्रमण दिखाया। विशेष रूप से x=0.8 (Y8) फिल्म ने ~2.8 K पर शून्य प्रतिरोधात्मक अवस्था प्राप्त की, जबकि Y0 और Y2 फिल्मों के लिए यह मान क्रमशः ~0.9 K और ~2.1 K रहा। Y8 फिल्म में बल्क अतिचालकता को AC सुसेप्टिबिलिटी मापन द्वारा पुष्टि मिली, जिसमें प्रबल प्रतिचुम्बकीय प्रतिक्रिया और 5.7 T तक का उच्चतम क्रांतिक क्षेत्र (upper critical field) पाया गया। मैग्नेटो-रेसिस्टेंस मापनों में निम्न क्षेत्रों पर WAL जैसी विशेषताएँ दिखाई दीं। HLN मॉडल से प्राप्त मानों ने दर्शाया कि WAL मुख्य रूप से 3D बल्क कंडक्शन से उत्पन्न होता है। साथ ही, विश्लेषण से स्पष्ट हुआ कि Y0 और Y8 फिल्मों में मुख्यतः इलेक्ट्रॉन–इलेक्ट्रॉन प्रकीर्णन (*e–e scattering*) प्रभावी है, जबकि Y2 फिल्म में इसके अतिरिक्त इलेक्ट्रॉन–फोनॉन (*e–ph*) प्रकीर्णन भी मौजूद है, जो मिश्रित प्रकीर्णन तंत्र की उपस्थिति का संकेत देता है।

अंतिम भाग में, ~1% तनाव के अधीन GdPdBi पतली परतों की संरचनात्मक और परिवहन विशेषताओं का अध्ययन किया गया। एक्स-रे विवर्तन और सूक्ष्मदर्शी विश्लेषणों ने बल्क की तुलना में ~1% लैटिस तनाव वाली एकल-चरण व उच्च गुणवत्ता वाली फिल्मों की पुष्टि की। ताप-निर्भरता अध्ययन में द्वि-चालकता (dual conducting) व्यवहार देखा गया—उच्च तापमान पर धात्विक व्यवहार और T<~3.5 K पर अर्धचालक व्यवहार। यहाँ ऊर्जा गैप ~10.2 meV मापा गया, जो बल्क गैप (~70 meV) से काफी छोटा है, और यह तनाव-प्रेरित बैंड संकुचन को दर्शाता है। मैग्नेटो-रेसिस्टेंस मापनों ने निम्न क्षेत्रों पर WAL जैसी विशेषताएँ दिखाई। HLN मॉडल का विश्लेषण बताता है कि α-मूल्य भौतिक रूप से अवास्तविक हैं और समरूपता लंबाई फिल्म की मोटाई से छोटी है, जिससे यह सिद्ध होता है कि WAL 3D बल्क कंडक्शन से उत्पन्न होता है। कोण-निर्भर मैग्नेटो-कंडक्टेंस ने यह पुष्ट किया कि WAL जैसी विशेषताएँ 2D सतही अवस्थाओं से नहीं, बल्कि प्रबल SOC (spin–orbit coupling) के कारण 3D बल्क अवस्थाओं से उत्पन्न हुई थीं।

समग्र रूप से, यह शोधप्रबंध दर्शाता है कि *f*-इलेक्ट्रॉन डोपिंग, चुम्बकीय पतलापन, और लैटिस तनाव HH पतली परतों में क्वांटम परिवहन और टोपोलॉजिकल गुणों को नियंत्रित करने के लिए प्रभावी साधन हैं। ये निष्कर्ष टोपोलॉजिकल अतिचालकों के डिज़ाइन में महत्वपूर्ण दृष्टिकोण प्रदान करते हैं और स्पिन्ट्रॉनिक्स, क्वांटम कंप्यूटेशन, एवं टोपोलॉजिकल युक्ति प्लेटफॉर्म्स में भविष्य के अनुप्रयोगों का मार्ग प्रशस्त करते हैं।

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