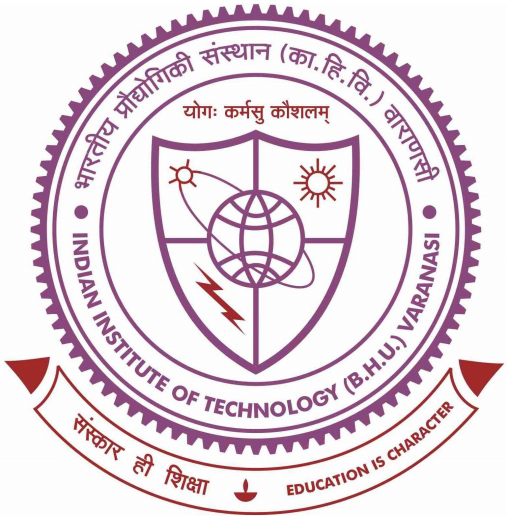
Anomalous Hall and Topological Properties of Co-based Heusler Alloys



Thesis submitted in partial fulfilment

for the Award of

DOCTOR OF PHILOSOPHY

in

MATERIALS SCIENCE

by

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ROLL NUMBER
18111502

YEAR OF SUBMISSION
2024

Chapter 8

Summary and suggestions for future work

8.1 Summary

In this thesis, we investigated the anomalous Hall effect (AHE) and topological properties of Co-based Heusler alloys using experimental techniques and theoretical calculations. This thesis involves the study of the polycrystalline intermetallic samples, which were prepared using the standard arc-melting furnace followed by vacuum annealing as per the requirements. The investigation employed several experimental methods like laboratory-based x-ray diffraction (XRD), scanning electron microscope, DC magnetization, ac-susceptibility, and anomalous transport measurements (resistivity, magnetoresistance, and Hall) using in-house experimental facilities. The synchrotron X-ray diffraction measurement was performed at PETRA -III, DESY-Germany; to capture the amount of disorder by measuring the accurate intensities of superlattice reflections. The theoretical calculations were conducted using the Quantum Espresso code in the framework of density functional theory (DFT). The Wannier90 package and WANNIERTOOL software were used for the Berry curvature-related calculations. The key findings of the present study are summarized below-

1. By using both experimental and theoretical methodologies, we investigated AHE in Co_2FeGe Heusler compound. While this compound had been theoretically predicted to show intrinsic anomalous Hall conductivity (AHC) due to a gapped nodal line, experimental confirmation was not present. Our study represents the inaugural experimental exploration of AHE in this compound, where we found an intrinsic AHC of approximately 78.6 S/cm. Additionally, using theoretical calculations employing maximally localized Wannier functions, we found an intrinsic AHC of about 77.29 S/cm due to the gapped nodal lines, which is in good agreement with the experimental intrinsic AHC.

2. We investigated the anomalous Hall response of a polycrystalline Co_2FeAl Heusler compound. Synchrotron X-ray diffraction data reveals a large degree of Fe-Al antisite disorder. Experimental values of AHC were found to be 227 S/cm at 2 K and 219 S/cm at 300 K with an intrinsic AHC of 155 S/cm. The experimental analysis shows that the AHE in Co_2FeAl is dominated by an intrinsic Berry phase mechanism. Our theoretical calculations suggest that the enhanced Berry curvature-induced intrinsic AHC in the Co_2FeAl Heusler compound is linked with the antisite disorder present in the system.

3. We have experimentally measured the AHC in the NiCoMnGa quaternary Heusler compound and theoretically calculated the intrinsic part of the AHC due to the Berry curvature of the dispersion bands. The extrinsic and intrinsic mechanisms contribute equally to the AHC of the present system. We found a good agreement between the experimentally extracted intrinsic AHC (about 120 S/cm) and the theoretically calculated AHC (about 100 S/cm). The reduction of the number of mirror symmetries in NiCoMnGa in comparison to Co_2MnGa leads to the absence of nodal lines. Hence, AHC reduces about 10 times in NiCoMnGa to the Co_2MnGa nevertheless, the band splitting in the presence of spin-orbit coupling (SOC) at the Fermi energy leads to the finite Berry curvature and intrinsic AHC in the system. The presence of a significant contribution of the extrinsic mechanism in the AHE, despite the longitudinal conductivity being of the order of 10^4 S/cm, suggests that the relation of the origin of the AHE solely with the longitudinal conductivity may not be strictly valid.

4. We theoretically investigated the electronic, magnetic, and anomalous transport properties of Cu_2CoSn full Heusler compound. We have shown that the gapped nodal lines at the Fermi energy lead to the large AHC of about 1000 S/cm and anomalous Nernst conductivity (ANC) of about 3.98 A/m-K in the system. Therefore, the Cu_2CoSn is added as a new candidate in the family of Heusler compounds with high AHC and ANC. Our work provides a comprehensive understanding of the anomalous transport properties in the nodal line hosting magnetic materials and motivates the further exploration of the Cu_2CoSn Heusler compound through experimental studies.

5. We studied the topological Hall effect (THE) in bulk Co_2FeAl Heusler compound through magnetotransport measurements. We found that THE stabilizes in a wide temperature range (2 K to 300 K), with a maximum value of 0.22 μΩ-cm at 300K. The THE varies rather slowly with temperature suggesting its correlation with the skyrmions present in the compound. Furthermore, the hump anomaly in AC-susceptibility (AC-χ(H)) measurement, which aligns with the field where THE reaches its peak, provides further evidence of skyrmion formation in this system. The micromagnetic simulations demonstrate the emergence of a skyrmionic state resulting from competition among magnetic anisotropy, exchange interaction, and dipolar interactions. Owing to the high Curie temperature and significant THE, this material is useful

for potential technological applications at room temperature as well as high temperatures.

8.2 Future work

A detailed investigation of AHE and topological properties of Co-based Heusler alloys has been performed using experimental techniques and theoretical calculations. The results open several possibilities for future experimental and theoretical investigations. We outline a few of them given below:

1. The Fermi level dependent AHC of Co_2FeGe Heusler compound shows an intrinsic AHC about 3000 S/cm above the 100 meV of Fermi energy, which has not been investigated experimentally. We plan to dope electrons in the system to shift the Fermi energy towards the nodal line to achieve the giant AHC.

2. The theoretically calculated intrinsic AHC for disordered Co_2FeAl remains lower than the experimental value. This underscores the imperative for an in-depth exploration of the AHE within the Co_2FeAl Heusler compound. Furthermore, the impact of the disorder on AHE has yet to be extensively investigated, highlighting the essential need for a more comprehensive examination of this phenomenon.

3. We plan to synthesize the Cu_2CoSn Heusler compound and study the anomalous Hall and Nernst effect experimentally. The realization of large AHC experimentally can put this material for spintronic application.

4. Since our study on Co_2FeAl suggests the presence of skyrmion in the system. We plan to confirm the presence of skyrmion by observing through Lorentz transmission electron microscopy.