STRUCTURAL, ELECTRONIC, AND MAGNETIC PROPERTIES OF Co-BASED FULL HEUSLER ALLOYS: A FIRST-PRINCIPLES STUDY

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Structural, Electronic, and Magnetic Properties of Co-based Full Heusler Alloys: A First-Principles Study

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Submitted

in fulfilment of requirements of degree of the Doctor of Philosophy

to the



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Dedicated

to

My Beloved Parents

and

My Brother

Certificate

This is to certify that the thesis entitled **"Structural, Electronic, and Magnetic Properties of Co-based Full Heusler Alloys: A First-Principles Study"**, which is being submitted by **Mr. Amar Kumar** to the **Indian Institute of Technology Delhi**, New Delhi, for the award of the degree of **Doctor of Philosophy** in Physics, is a record of bonafide research work carried out by him. He has worked under our supervision and guidance, and has fulfilled the requirements for the submission of this thesis, which, in our opinion, has reached the requisite standard.

The results contained in this thesis 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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Amar Kumar
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Abstract

Co-based Heusler alloys are among the leading material classes for achieving the desirable physical properties required in spintronic memories, such as very high spin polarization with half-metallic character, high Curie temperature, low damping parameter, large magnetic anisotropy, *etc*. However, all these properties are highly sensitive to the structural phase of the Heusler alloy, and the presence of structural imperfections can significantly alter them. It is noteworthy that, owing to the thermodynamic synthesis conditions, structural imperfections are almost inevitably present in experimentally fabricated Heusler alloys. Therefore, to develop these materials as viable candidates for spintronic memory applications, their structural, electronic, and magnetic characteristics must be thoroughly understood and optimised in the presence of various kinds of structural imperfections. The present thesis examines the impact of various structural imperfections - namely point defects, lattice distortions, surface terminations, and interface formations - on the physical properties of two technologically important Co-based Heusler alloys: Co_2MnAl and CoFeCrGa. The investigated properties include the electronic structure, magnetism, magnetic anisotropy, anomalous Hall conductivity, and spin Hall conductivity. These physical properties have been computed using density functional theory in combination with Wannier-interpolation-based tight-binding methods.

Regarding the structural imperfections within Co_2MnAl Heusler alloy, it is observed for a broad range of the point defects - including B2-disorder (Mn-Al swap disorder), binary antisite disorders (Co_{Mn}, Co_{Al}, Mn_{Co}, Mn_{Al}, Al_{Co}, and Al_{Mn}), ternary antisite disorders (($Mn_{Co} + Al_{Co}$), ($Co_{Mn} + Al_{Mn}$), and ($Co_{Al} + Mn_{Al}$)) - the electronic nature and total magnetism are nearly unchanged and closely resemble those of the bulk Co_2MnAl, independent of defect concentrations. In contrast, the presence of vacancy defects (V_{Co}, V_{Mn}, and V_{Al}) results in drastic modifications to both electronic and magnetic properties, with a strong dependence on the types and degree of vacancy defects. In the presence of lattice distortions, the compressive uniform strains and tetragonal distortions with small distortion values ($|\Delta c/a| < 0.1$) did not affect the electronic structure and magnetic properties; on the other hand, tensile uniform strains and the tetragonal distortions with the larger distortion values induce substantial alteration in the electronic structure and magnetic properties. Analysis of various surface geometries of Co_2MnAl with (100)-, (110)-, and (111)-orientations revealed that the several surface geometries, such as - MnAl-(100), CoCoMnAl-(110), Al-(111), and Co-Mn-(111), retain bulk-like electronic behaviour, with MnAl-(100) and Co-Mn-(111) surface geometries also exhibiting out-of-plane magnetocrystalline anisotropy. In contrast, CoCo-(100), Mn-(111), and Co-Al-(111) surfaces show

notable deviations in electronic character, including a transition from bulk-like nearly half-metallic behaviour to metallic behaviour. Concerning magnetization, all surface geometries except Al-(111), the total magnetization is enhanced relative to bulk Co_2MnAl, due to modifications in the atomic magnetic moments in the proximity of near-surface atoms. On the other hand, Al-(111) surface shows a reduction in magnetization, due to decreased atomic magnetic moments of near-surface atoms. For the interfacial properties of Co_2MnAl, different interfacial morphologies emerging from the Co_2MnAl/MgO and Co_2MnAl/GaAs heterostructures have been examined. It is observed that interfaces comprising Mn-, Al-, or MnAl-termination of the Co_2MnAl slabs largely preserve the nearly half-metallic character of bulk Co_2MnAl, whereas interfaces with Co- or CoCo-terminations of Co_2MnAl-slab exhibit significantly altered electronic properties. For magnetic properties, all interfacial morphologies show enhanced magnetization as compared to bulk-slabs, regardless of their atomic arrangements.

Considering all structural imperfections in Co_2MnAl, these results collectively indicate that Co_2MnAl can preserve bulk-like physical properties even in the presence of most of the structural imperfections studied. In other words, Co_2MnAl exhibits remarkable resistance against structural imperfections, contrary to the typical behaviour of most of Heusler alloys, where the presence of structural imperfections leads to the degradation of spintronic properties. Therefore, upon integrating Co_2MnAl as a ferromagnetic electrode in spintronic devices, its favourable bulk-like spintronic properties are expected to be preserved.

In case of CoFeCrGa, uniform strain preserves its spin-gapless semiconducting nature, along with magnetic isotropic nature, small anomalous and spin Hall conductivities. However, under tetragonal distortion, the distorted structures show a nearly half-metallic or metallic nature, accompanied by a very large magnetocrystalline anisotropy ($\approx 10^6$ J/m^3), large anomalous Hall conductivity, and moderate spin Hall conductivity – and all these properties depending on the axial ratio (*c/a*) of the distorted structures. In context of the thin-film, CoFeCrGa thin film displays a nearly half-metallic nature for the (220) orientation. Thus, besides the spin gapless semiconducting nature for the Y-I ordered bulk structure, CoFeCrGa exhibits favourable spintronic properties - even under lattice distortions and surface termination - which underscore its promise for next-generation spintronic applications.

In summary, the findings of this thesis provide valuable insights into the tailoring of the physical properties of experimentally realised (fabricated) bulk structures, thin films, and heterostructures of Co_2MnAl and CoFeCrGa. Consequently, these results can also provide guidance for optimising the performance of spintronic devices by employing these materials in spintronic memory technologies.

सार

कोबाल्ट-आधारित ह्यूसलर (Heusler) मिश्रधातुएँ स्पिन्ट्रॉनिक मेमोरी में आवश्यक वांछनीय भौतिक गुणों को प्राप्त करने हेतु प्रमुख पदार्थ वर्गों में से एक हैं, जैसे कि - अर्ध-धात्विक प्रकृति के साथ अत्यधिक उच्च स्पिन ध्रुवीकरण, उच्च क्यूरी तापमान, निम्न डैम्पिंग (damping) पैरामीटर, उच्च चुंबकीय विषमदिशात्मकता (magnetic anisotropy), आदि। यद्यपि, ये सभी गुण ह्यूसलर मिश्रधातु के संरचनात्मक अवस्था के प्रति अत्यधिक संवेदनशील होते हैं, तथा संरचनात्मक अपूर्णताओं (structural imperfections) की उपस्थिति इन्हें महत्वपूर्ण रूप से परिवर्तित कर सकते हैं। यह ध्यान देने योग्य है कि ऊष्मागतिकीय संश्लेषण परिस्थितियों के कारण, प्रयोगात्मक रूप से निर्मित ह्यूसलर मिश्रधातुओं में संरचनात्मक अपूर्णताएँ लगभग अनिवार्य रूप से उपस्थित रहती हैं। इसलिए, इन पदार्थों को स्पिन्ट्रॉनिक मेमोरी अनुप्रयोगों के लिए व्यवहार्य उम्मीदवारों के रूप में विकसित करने हेतु, विभिन्न प्रकार की संरचनात्मक अपूर्णताओं की उपस्थिति में उनके संरचनात्मक, इलेक्ट्रॉनिक तथा चुंबकीय गुण धर्मों का गहन अध्ययन एवं समायोजित किया जाना आवश्यक है। प्रस्तुत शोधप्रबंध दो तकनीकी रूप से महत्वपूर्ण कोबाल्ट-आधारित ह्यूसलर मिश्रधातुओं - Co_2MnAl तथा CoFeCrGa - के भौतिक गुणों पर विभिन्न संरचनात्मक अपूर्णताओं, यथा - बिंदु दोष (point defects), lattice distortions, surface terminations, तथा interface formations, के प्रभाव का अध्ययन करता है। अध्ययन किए गए गुणों में इलेक्ट्रॉनिक संरचना, चुंबकत्व, चुंबकीय विषमदिशात्मकता, असामान्य (anomalous) हॉल चालकता, एवं स्पिन हॉल चालकता शामिल हैं। इन भौतिक गुणों की गणनाएँ Density Functional Theory तथा Wannier-interpolation आधारित tight-binding विधियों के संयोजन का उपयोग करके की गई हैं।

Co_2MnAl ह्यूसलर मिश्रधातु में संरचनात्मक अपूर्णताओं के संदर्भ में यह पाया गया कि बिंदु दोषों की एक विस्तृत श्रेणी - जिनमें B2-disorder (Mn-Al swap दोष), binary antisite disorders (Co_{Mn}, Co_{Al}, Mn_{Co}, Mn_{Al}, Al_{Co}, तथा Al_{Mn}), एवं ternary antisite disorders (($Mn_{Co} + Al_{Co}$), ($Co_{Mn} + Al_{Mn}$), तथा ($Co_{Al} + Mn_{Al}$)) शामिल हैं - के लिए इलेक्ट्रॉनिक प्रकृति तथा कुल चुंबकत्व लगभग अपरिवर्तित रहते हैं तथा दोष सांद्रता से लगभग स्वतंत्र होकर bulk-Co_2MnAl के अनुरूप पाए जाते हैं। इसके विपरीत, रिक्ति दोषों (V_{Co}, V_{Mn}, and V_{Al}) की उपस्थिति इलेक्ट्रॉनिक तथा चुंबकीय गुणों में अत्यधिक परिवर्तन उत्पन्न करती है, जो रिक्ति दोषों के प्रकार तथा उनकी सांद्रताओं पर अत्यधिक निर्भर करता है। Lattice distortions की उपस्थिति में, compressive uniform strains तथा छोटे विकृति मानों ($|\Delta c/a| < 0.1$) वाले tetragonal distortions इलेक्ट्रॉनिक संरचना तथा चुंबकीय गुणों को प्रभावित नहीं करतीं; वही दूसरी ओर, tensile uniform strains तथा बड़े विकृति मानों वाले tetragonal distortions इलेक्ट्रॉनिक संरचना तथा चुंबकीय गुणों में महत्वपूर्ण परिवर्तन उत्पन्न करती हैं। Co_2MnAl की (100)-, (110)-, तथा (111)-अभिविन्यासों (orientations) की विभिन्न surface geometries के विश्लेषण से यह ज्ञात हुआ कि अनेक surface geometries, जैसे - MnAl-(100), CoCoMnAl-(110), Al-(111), तथा Co-Mn-(111), bulk-like इलेक्ट्रॉनिक व्यवहार को बनाए

रखती हैं, जबकि MnAl-(100) तथा Co-Mn-(111) surface geometries out-of-plane magnetocrystalline anisotropy भी प्रदर्शित करती हैं। इसके विपरीत, CoCo-(100), Mn-(111), तथा Co-Al-(111) surfaces इलेक्ट्रॉनिक गुणों में उल्लेखनीय विचलन प्रदर्शित करते हैं, जिनमें bulk-like लगभग-अर्ध-धात्विक व्यवहार से धात्विक व्यवहार की ओर परिवर्तन भी शामिल है। चुंबकीकरण के संदर्भ में, Al-(111) को छोड़कर सभी surface geometries में bulk-Co_2MnAl की तुलना में कुल चुंबकीकरण में वृद्धि देखी गई, जिसका कारण सतह के समीप स्थित परमाणुओं के परमाण्विक चुंबकीय आघूर्णों में परिवर्तन है। दूसरी ओर, Al-(111) surface चुंबकीकरण में कमी प्रदर्शित करता है, जो surface के निकट स्थित परमाणुओं के घटे हुए परमाण्विक चुंबकीय आघूर्णों के कारण उत्पन्न होती है। Co_2MnAl के interfacial गुणों के अध्ययन हेतु Co_2MnAl/MgO तथा Co_2MnAl/GaAs heterostructures से उत्पन्न विभिन्न interfacial morphologies का विश्लेषण किया गया। यह पाया गया कि Co_2MnAl slab के Mn-, Al- अथवा MnAl-समापन रखने वाले interfaces, bulk-Co_2MnAl के लगभग अर्ध-धात्विक गुणों को काफी हद तक संरक्षित रखते हैं, जबकि Co_2MnAl slab के Co- अथवा CoCo-समापन रखने वाले interfaces उल्लेखनीय रूप से परिवर्तित इलेक्ट्रॉनिक गुण प्रदर्शित करते हैं। चुंबकीय गुणों के संदर्भ में, सभी interfacial आकृतियाँ अपने atomic arrangements से स्वतंत्र, bulk-slabs की तुलना में बढ़ा हुआ चुंबकीकरण प्रदर्शित करती हैं।

Co_2MnAl के लिए सभी संरचनात्मक अपूर्णताओं को ध्यान में रखते हुए, ये परिणाम सामूहिक रूप से संकेत करते हैं कि यह अध्ययन की गई अधिकांश संरचनात्मक अपूर्णताओं की उपस्थिति में भी, Co_2MnAl bulk-like भौतिक गुणों को संरक्षित रख सकता है। अर्थात्, Co_2MnAl संरचनात्मक अपूर्णताओं के प्रति उल्लेखनीय प्रतिरोध क्षमता प्रदर्शित करता है, जोकि अधिकांश ह्यूसलर मिश्रधातुओं के सामान्य व्यवहार के विपरीत है, जहाँ संरचनात्मक अपूर्णताओं की उपस्थिति स्पिन्ट्रॉनिक गुणों के ह्रास का कारण बनती है। अतः, स्पिन्ट्रॉनिक उपकरणों में Co_2MnAl को एक फेरोमैग्नेटिक इलेक्ट्रोड के रूप में सम्मिलित करने पर इसके अनुकूलित bulk-like स्पिन्ट्रॉनिक गुणों के संरक्षित रहने की अपेक्षा की जा सकती है।

CoFeCrGa के विषय में, uniform strain इसकी spin-gapless semiconducting प्रकृति, समदैशिक चुंबकीय प्रकृति, तथा निम्न असामान्य और स्पिन हॉल चालकताओं, के साथ संरक्षित रखती है। हालाँकि, tetragonal distortion के अंतर्गत, विकृत संरचनाएँ लगभग अर्ध-धात्विक अथवा धात्विक अवस्था, अत्यधिक उच्च चुंबकीय विषमदिशात्मकता ($\approx 10^6$ J/m^3), उच्च असामान्य हॉल चालकता तथा मध्यम स्पिन हॉल चालकता, के साथ प्रदर्शित करती हैं - तथा ये सभी गुण विकृत संरचनाओं के axial ratio पर निर्भर करते हैं। Thin film के संदर्भ में, (220)-अभिविन्यास (orientation) के लिए, CoFeCrGa-thin film, लगभग अर्ध-धात्विक प्रकृति प्रदर्शित करती है। इस प्रकार, Y-I ordered bulk structure के लिए spin gapless semiconducting प्रकृति के अतिरिक्त, CoFeCrGa lattice distortions तथा surface termination की उपस्थिति में भी स्पिन्ट्रॉनिक उपकरण अनुकूलित गुण प्रदर्शित करता है, जो अगली पीढ़ी के स्पिन्ट्रॉनिक अनुप्रयोगों के लिए इसकी संभावनाओं को रेखांकित करता है।

संक्षेप में, इस शोधप्रबंध के निष्कर्ष Co_2MnAl तथा CoFeCrGa की प्रयोगात्मक रूप से साकारित (निर्मित) bulk structures, thin films तथा heterostructures के भौतिक गुणों के समायोजन संबंधी महत्वपूर्ण अंतर्दृष्टियाँ प्रदान करते हैं। परिणामस्वरूप, ये निष्कर्ष स्पिन्ट्रॉनिक मेमोरी प्रौद्योगिकियों में, इन पदार्थों का उपयोग करके स्पिन्ट्रॉनिक उपकरणों के प्रदर्शन के अनुकूलन हेतु मार्गदर्शन भी प्रदान कर सकते हैं।

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List of Abbreviation

Abbreviation	Full Form	Abbreviation	Full Form
AHC	Anomalous Hall Conductivity	GGA	Generalised Gradient Approximation
AHE	Anomalous Hall Effect	GMR	Giant Magnetoresistance
AFM	Antiferromagnetic	HA(s)	Heusler Alloy(s)
AMM(s)	Atomic Magnetic Moment(s)	HF	Hartree-Fock
AP	Atomic Spin Polarization	HK	Hohenberg and Kohn
APW	Augmented Plane-Wave	HM	Half-Metallic
BC	Berry Curvature	IMA	In-Plane Magnetic Anisotropy
BOA	Born-Oppenheimer Approximation	KS	Kohn-Sham
CF	Crystal Field	LDA	Local Density Approximation
DFT	Density Functional Theory	MA	Magnetic Anisotropy
DOS	Density of States	MAE	Magnetic Anisotropy Energy
E_F	Fermi Level	MCA	Magnetocrystalline Anisotropy
E_{gap}	Energy Gap	MEA	Magnetoelastic Anisotropy
EI	Exchange Interactions	ML(s)	Monolayer(s)
EoS	Equation of State	MLWF(s)	Maximally Localised Wannier Function(s)
FM	Ferromagnetic	M_S	Total Magnetic Moment
f.u.	Formula Unit	MTJ(s)	Magnetic Tunnel Junction(s)

Abbreviation	Full Form	Abbreviation	Full Form
MRAM	Magnetoresistive Random-Access Memory	SGS	Spin Gapless Semiconductor(s)
MSA	Magnetic Shape Anisotropy	SHE	Spin Hall Effect
NM	Non-Magnetic	SOC	Spin-Orbit Coupling
NSCF	Non-Self-Consistent Field	SOT	Spin-Orbit Torque
OHE	Ordinary Hall Effect	SP	Slater-Pauling
OLP	Optimised Lattice Parameter	SPR	Site-Preference Rule
OMA	Out-of-Plane Magnetic Anisotropy	SPV	Slater-Pauling Valley
P	Spin Polarization	STT	Spin-Transfer Torque
PAW	Projector Augmented Wave	SV(s)	Spin Valve(s)
PBE	Perdew–Burke–Ernzerhof	TB	Tight-Binding
PDOS	Partial Density of States	T_C	Curie Temperature
PMA	Perpendicular Magnetic Anisotropy	TM(s)	Transition Metal(s)
PP	Pseudopotential	TMR	Tunnel Magnetoresistance
PW	Plane Wave	USPPs	Ultrasoft Pseudopotentials
PWP	Plane-Wave Pseudopotential	V	Volume
PZ	Perdew–Zunger	V_0	Optimised Volume
RFE	Relative Formation Energy	WF(s)	Wannier Function(s)
SCF	Self-Consistent Field	XC	Exchange-Correlation
SHC	Spin Hall Conductivity		