Atomic disorder and Berry phase driven anomalous Hall effect in Co$_2$FeAl Heusler compound

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Co$_2$-based Heusler compounds are the promising materials for the spintronics application due to their high Curie temperature, large spin-polarization, large magnetization density, and exotic transport properties. In the present manuscript, we report the anomalous Hall effect (AHE) in a polycrystalline Co$_2$FeAl Heusler compound using combined experimental and theoretical studies. The Rietveld analysis of high-resolution synchrotron x-ray diffraction data reveals a large degree (~ 50 %) of antisite disorder between Fe and Al atoms. The analysis of anomalous transport data provides the experimental anomalous Hall conductivity (AHC) about 227 S/cm at 2 K with an intrinsic contribution of 155 S/cm, which has nearly constant variation with temperature. The detailed scaling analysis of anomalous Hall resistivity suggests that the AHE in Co$_2$FeAl is governed by the Berry phase driven intrinsic mechanism. Our theoretical calculations reveal that the disorder present in Co$_2$FeAl compound enhances the Berry curvature induced intrinsic AHC.

Hall effect is defined as the realization of transverse electric field when a magnetic field is applied to a current-carrying conductor [1]. Ferromagnetic materials show anomalous Hall effect (AHE) due to the interaction between spin-orbit coupling (SOC) and magnetization. [1-4]. AHE finds renewed attention in condensed matter physics due to huge application in magnetic sensors, random access memory, and spin logic devices [2, 5, 6]. Two possible mechanisms have been proposed to explain the origin of AHE. An extrinsic mechanism related to the scattering events, which includes skew scattering and side jump, another one is an intrinsic mechanism related to the band structure of the material [2, 7, 8]. The intrinsic mechanism was proposed by Karplus and Luttinger (K-L theory of intrinsic mechanism), which is connected with the role of SOC in electronic band structure of ferromagnetic material and results into the anomalous velocity of electrons perpendicular to the electric field direction [2, 9, 10]. Later, K-L theory was well understood in terms of Berry phase and Berry curvature [11]. The Berry curvature is identical to a fictitious magnetic field in momentum space related to the geometrical phase of the electronic wave function [12]. Berry curvature in momentum space introduces the transverse momentum to the electrons and gives intrinsic AHE [13, 14].

Berry curvature is highly sensitive to the electronic band structure of material and modulation in the band structure can influence the Berry curvature and hence intrinsic anomalous Hall conductivity (AHC) [15]. The disorder may change the topology of the Fermi-surface or position of the Fermi level or modify the local potential environment that breaks the translational symmetry, inevitably modifying the band structure, which may reshape the AHE [15-19]. An increased AHC has been reported in the thin film of Co$_2$MnAl$_{1-x}$Si$_x$ due to increased L2$_1$ ordering within the lattice [18]. Recently, the enhancement in the AHC has been observed in Fe$_2$-based high Curie temperature Heusler compounds due to the increase in the crystal symmetry, when the system transforms from inverse Heusler to B2 type (CsCl) structure [20].

Co$_2$-based full Heusler compounds got enormous attention for their half-metallic behaviour, and 100% spin-polarization around Fermi level, which are the most prominent properties useful in spintronics devices and other memory-based applications [21-24]. Additionally, Co$_2$-based Heusler compounds are of current interest, because of their large AHE due to the large Berry curvature linked with their band structure [17-28]. Among Co$_2$-based Heusler compounds, Co$_2$FeAl is the most prominent candidate for the data processing and storage based applications due to its large Curie temperature (~ 810 K to 900 K), high spin-polarization, low Gilbert damping factor, and ultrafast magnetization dynamics [30-33]. As literature suggest that the Co$_2$FeAl is generally crystallizes in B2-type [31, 33, 36] disordered structure, therefore, this compound provides an opportunity for the investigation of the disorder effect on the Berry curvature and intrinsic AHC. Attempts to investigate anomalous transport in Co$_2$FeAl thin films report controversial result concerning to the origin of AHE [34, 35, 37].

In the present manuscript, we studied AHE in a polycrystalline bulk Co$_2$FeAl Heusler compound. Synchrotron x-ray diffraction (SXRD) data reveals a large degree of antisite disorder between Fe and Al atoms. The experimental value of AHC was found to be about 227 S/cm at 2 K and 219 S/cm at 300 K with an intrinsic contribution of 155 S/cm. This intrinsic value of AHC is an order of magnitude larger than the theoretically predicted AHC for an ordered L2$_1$ phase of Co$_2$FeAl. Our theoretical calculations show that the antisite disorder present in Co$_2$FeAl enhances the Berry curvature
induced intrinsic AHC.

A polycrystalline Co$_2$FeAl Heusler compound was synthesized using conventional arc melting technique using stoichiometric amount of its high pure constituent elements. The compound was melted four times to ensure the chemical homogeneity. A very small weight loss of 0.32% was noted after melting. Further, the ingot was sealed in quartz ampoule under Ar atmosphere and then annealed at 800°C for 12 hours for the better homogeneity. The energy dispersive x-ray (EDX) analysis reveals the composition ratio of 2:1:1 within the standard deviation (3 to 5 %) of EDX measurement. A small piece was cut from the annealed ingot and crushed into powder for SXRD measurement. The SXRD measurement was performed at PETRA-III, DESY for structural analysis using wavelength of 0.207 Å. Magnetic field-dependent magnetization measurements were carried out using the Magnetic Property Measurement System (MPMS) from Quantum Design, U.S.A. A small polished rectangular piece was used for four-probe and five-probe magneto-transport measurements to obtain the longitudinal resistivity ($\rho_{xx}$) and the Hall resistivity ($\rho_{H}$), respectively. To obtain the actual $\rho_{H}$, raw Hall resistivity data ($\rho_{H}^{raw}$) was anti-symmetrized by averaging the difference of $\rho_{H}^{raw}$ at the positive and negative magnetic fields.

Electronic structure calculations were carried out using pseudo-potential based density-functional theory and plane-wave basis sets as implemented in Quantum ESPRESSO (QE) [38], whereas the exchange-correlation potential is approximated through PBE-GGA functional [39]. Optimized norm-conserving Vanderbilt pseudo-potentials [40] are used in the calculations and the kinetic energy cutoff for the plane-wave is taken as 80 Ry. The electronic integration over the Brillouin zone is approximated by the Gaussian smearing of 0.01 Ry both for the self-consistent (SC) and non-self-consistent (NSC) calculations. The threshold for the SC energy calculations is taken as $10^{-8}$ Ry. The projections of Bloch wave functions are made into maximally localized Wannier functions. Wannier90 tool (implemented within QE) has been used to compute the Wannier interpolated bands and AHC [38, 41, 42]. SOC is introduced in all the calculations. The Monkhorst-Pack k-grid of $8 \times 8 \times 8$ are considered in the SC, NSC and Wannier90 calculations. The transition metal-d and Al-p orbitals are used as the projections for the Wannier90 calculations. The AHC calculation is carried out with a dense k-grid of $75 \times 75 \times 75$. Further, through the adaptive refinement technique a fine mesh of $5 \times 5 \times 5$ is added around the points wherever the mode of the Berry curvature ($|\Omega(k)|$) exceeds 100 bohr$^2$. The calculations are carried out using experimental lattice parameter.

The SXRD pattern of Co$_2$FeAl compound was col-
FIG. 3. (a) Temperature dependent longitudinal resistivity $\rho_{xx}$. (b) Field dependent Hall resistivity $\rho_H$ at different temperatures. (c) Temperature dependent normal Hall coefficient $R_0$. Inset shows temperature variation of carrier concentration $n$. (d) Experimental data (black dots) plotted between $\log \rho_{AH}$ and $\log \rho_{xx}$ and the fitted curve is shown in red color.

lected at room temperature for detail structural study. In the first step, the Rietveld refinement of SXRD pattern was carried out using the $L_2_1$ ordered cubic structure with space group $Fm\bar{3}m$. For the refinement, all the atoms were considered at special positions i.e. Co at 8c (0.25, 0.25, 0.25), Fe at 4b (0.5, 0.5, 0.5) and Al at 4a (0, 0, 0) Wyckoff positions, respectively. The result of refinements is shown in FIG. 1(a). We noticed the presence of (111) superlattice reflection in the calculated x-ray diffraction (XRD) pattern (black lines of FIG. 1(a)), while this reflection is completely absent in the observed XRD pattern (red dots in FIG. 1(a)), which indicates the presence of antisite disorder in the Co$_2$FeAl compound. Recently the mixed $L_2_1$ and $B_2$ phase was observed in Co$_2$FeAl ultrathin film [43]. We would like to mention here that attempt to anneal the Co$_2$FeAl at different temperature could not show the different XRD pattern as compared to the observed in FIG. 1(a). It is important to remark here that atomic disorder is a common phenomenon in Heusler compounds [16, 18, 44].

The available literature also suggests that the most stable structure of Co$_2$FeAl is the $B_2$ type structure i.e. there is antisite disorder between Fe and Al atoms [31, 34, 36]. So, in the next step we simulated the XRD pattern of Co$_2$FeAl considering Fe-Al antisite disorder in such a way that total number of Fe and Al atoms remain same. For the XRD simulation, we used PowderCell software [45]. It is clear from FIG. 1(b), the intensity of (111) peak decreases with increase in amount of disorder and vanishes completely about 50% antisite disorder between Fe-Al atoms. Therefore, finally we performed the Rietveld refinement of the SXRD data assuming 50% antisite disorder between Fe-Al atoms, which could fit the Bragg peaks very well (FIG. 1(c)) and confirms the phase purity (cubic) as well as large antisite disorder ($B_2$ type) in the sample. Moreover, the presence of (200) Bragg peak primarily indicates the formation of ordered Co sublattice and also precludes the possibility of $A2$ disorder (atomic disorder among all sites) in the sample. The intensity ratio of superlattice reflection (200) and
the AHE in the Co based Heusler compounds \[25, 51, 52\]. The Fermi energy is set to 0 eV. Bottom: Calculated Berry curvatures along the high-symmetry path.

We carried out detailed magneto-transport measurements in a wide temperature range of 2 K-300 K to study the AHE in the Co$_2$FeAl. The Hall resistivity ($\rho_H$) can be given by the equation, $\rho_H = R_0 H + R_s n$, where $R_0$, $R_s$ are the normal and anomalous Hall coefficients respectively. $\rho_H$ versus $H$ were measured at different temperatures up to field of 7 Tesla (T). From Fig.3(b), it is evident that $\rho_H$ steeply increases with field upto 1 T, which can be observed due to AHE. However, under the application of higher fields (>1 T), a negative slope is noted due to ordinary Hall effect. The normal Hall coefficient ($R_0$) was calculated from the slope of the high field $\rho_H$ curve. Fig.3(c) shows temperature variation of $R_0$. The negative value of $R_0$ indicates the electrons are the majority charge carriers. Inset of Fig.3(c) shows the magnitude of carrier concentration ($n$) at different temperatures, calculated using the relation, $R_0 = \frac{1}{n e}$ and $n$ was found to be around $3 \times 10^{21}$ at 300 K and variation of $n$ with temperature is little scattered. The anomalous Hall resistivity ($\rho_{AH}$) was calculated by extrapolating the high field $\rho_H$ curve on $y$ axis at zero field.

In order to elucidate the mechanism giving rise to AHE, we have plotted $\rho_{AH}$ versus $\rho_{xx}$ on a double logarithmic scale and fitting was employed to determine the exponent $\beta$ using the relation $\rho_{AH} \propto \rho_{xx}^\beta$ [25] as shown in inset of Fig.3(d). If $\beta=1$, the origin of AHE is assigned to the skew scattering and if $\beta = 2$, the origin of AHE is due to intrinsic and side jump mechanisms [22, 25]. We found the exponent $\beta = 1.69$, which indicates that the AHE in Co$_2$FeAl is dominated by the intrinsic and side jump mechanisms. The contribution of side jump in AHC can be estimated using an expression ($e^2/(ha)(\epsilon_{so}/E_F)$, where $\epsilon_{so}$ is the spin–orbit interaction and $E_F$ is Fermi energy [63, 64]. The terms $e$, $h$ and $a$ are the electronic charge, Planck constant and lattice parameter, respectively. For the most of the ferromagnetic metals $\epsilon_{so}/E_F$ is order of $10^{-2}$, and hence very small contribution of AHC is expected due to side jump in comparison to the intrinsic part of AHC. However, it is not possible to decouple the intrinsic and side jump mechanism practically because both have similar dependencies on $\rho_{xx}$.

We have calculated the Hall conductivity using tensor conversion $\sigma_{xx} = \frac{\rho_H}{(\rho_{xx}^2 + \rho_{xx}^2)}$ [41, 55] as shown in inset of Fig.4(a). The AHC is calculated by averaging of extrapolated values of the high field Hall conductivity curve at zero field of the positive and negative field directions. Temperature dependent $\rho_{AH}$ (black dots) and AHC (blue...
dots) are shown in FIG. 4(a). The value of AHC is found to be about 227 S/cm at 2 K and does not show appreciable change at 300 K (219 S/cm). The variation of AHC is nearly temperature-independent, suggests that the origin of AHE is intrinsic [50, 57].

To separate the extrinsic and intrinsic part of AHE, we have plotted \( \rho_{\text{AH}} \) versus \( \rho_{\text{ex}} \) and fitted (FIG 4(b)) according to well established equation for AHE, \( \rho_{\text{AH}} = \alpha^{\text{skew}} \rho_{\text{ex}} + \alpha^{\text{int}} \rho_{\text{ex}}^2 \), where \( \alpha^{\text{skew}} \) and \( \alpha^{\text{int}} \) correspond to skew scattering parameter and intrinsic AHC respectively. \( \alpha^{\text{int}} \) was estimated \( \sim 155 \) S/cm, which is about 70\% of total AHC at 2 K. Thus, in the present system intrinsic Berry phase driven K-L contribution dominates along with finite skew scattering [2, 56–58].

After obtaining the experimental value of AHC, we have theoretically calculated AHC for CoFe2Al by setting the magnetization direction along [001]. For CoFe-based Heusler alloys the ground state energy in other magnetization direction like [110] was found close to the [001] direction and the band structure was also found quite similar in both directions, therefore the average picture of AHC is expected close to [001] direction [17, 27, 59, 60]. The intrinsic AHC is proportional to the Brillouin zone (BZ) summation of the Berry curvature over all occupied states. [61]

\[
\sigma^{\alpha\beta} = \frac{e^2}{\hbar} \frac{1}{N} \sum_{k \in \{BZ\}} \Omega_\gamma(k)f(k),
\]

where the indices \( \alpha, \beta \), and \( \gamma \) are the Cartesian coordinates. \( f(k) \) stands for the Fermi distribution function, \( \Omega_\gamma(k) \) denotes the \( \gamma \) component of the Berry curvature for the wave vector \( k \) and \( N \) is the number of electrons in the crystal. Further, the Berry curvature is related to the Berry connection \( \langle A_n(k) \rangle \) as

\[
\Omega_n(k) = \nabla_k \times A_n(k),
\]

where "\( n \)" is the band index and \( A_n(k) \) in terms of cell-periodic Bloch states \( |u_{nk}\rangle = e^{-ikr}|\psi_{nk}\rangle \) is defined as \( A_n(k) = \langle u_{nk} | i\nabla_k | u_{nk} \rangle \) [62]. In the first step of the AHC calculation, we considered the ordered \( L_2 \) structure of CoFe2Al i.e without any disorder. As discussed earlier the intrinsic AHC of a system is strongly connected to its electronic band structure. In FIG. 5 (Top), we have compared the full electronic band structure of \( L_2 \) ordered CoFe2Al with the Wannier interpolated one. The better interpolation suggests that it will provide Wannier90 related properties accurately. The Wannier interpolation is a potential tool to calculate the momentum space integrals of rapidly varying functions [63]. Such integrals are involved in calculating the properties such as anomalous Hall conductivity, spin Hall conductivity, orbital magnetization and optical properties [64]. The most popular technique to construct the Wannier functions is maximally localized method [65] which is implemented in the Wannier90 code [64]. The Wannier functions generated using the unitary transformation of Bloch wave function, so there is no loss of information during the generation. The main advantage of Wannier interpolation over other approaches is that it allows for the most precise interpolation of band energies and matrix elements compared to other methods such as the tight binding approach because there is no limitation in terms of the size of the basis set [66].

By this method, we found the theoretical value of AHC \( (\sigma^{xy}) \) about \( \sim 42 \) S/cm, which is in well agreement with literature [67]. Thus the theoretical AHC considering ordered \( L_2 \) structure is an order smaller than the experimental intrinsic AHC. Therefore, in the next step we incorporated 50 \% anti-site disorder between the Al and Fe sites (as observed from SXRD analysis) in order to compute AHC for the disordered CoFe2Al. In FIG. 6 (Top), we have plotted the full electronic band structure of disordered CoFe2Al with the Wannier interpolated band structure. The Berry curvature along high symmetry path of disordered structure (space group Pm\( \bar{3} \)m) is depicted in FIG. 6 (Bottom). The intrinsic AHC \( (\sigma^{xy}) \) for disordered CoFe2Al calculated from the integration of Berry curvature turned out to be \( \sim 63 \) S/cm, which is interestingly larger than the ordered \( L_2 \) structure. Thus, our theoretical calculations suggest that the disorder can modify the Berry curvature and result into an increased value of intrinsic AHC. Recently, it has been suggested in literature that the presence of B2 disorder lowers the value of AHC in comparison to ordered \( L_2 \) structure [18, 20]. Therefore, our combined experimental and theoretical results suggest that there is no straightforward rule that connects the Berry curvature to the disorder, rather it depends on the disorder induced change in electronic structure, which is different for different Heusler compound as they have different number of electrons. If the effect of disorder is such a way that it

![FIG. 6. Top: Comparison of Wannier interpolated band structure (red) with the full electronic band structure (blue) of disordered CoFe2Al. The Fermi energy is set to 0 eV. Bottom: Calculated Berry curvatures along the high-symmetry path.](image-url)
brings the band crossings or avoided band crossing very close to the Fermi energy then the value of Berry curvature will be large. We would also like to mention here that the experimentally found intrinsic AHC (155 S/cm) is larger than the theoretically predicted intrinsic AHC similar to the other metallic compounds. Hence, our results provide a platform for the systematic investigate of AHE in the disordered Heusler compounds and related materials.

In conclusion, we investigated the anomalous transport properties of polycrystalline Co$_2$FeAl Heusler compound by experiment and theoretical calculations. SXRD data reveals a large degree of Fe-Al antisite disorder. Experimental values of AHC were found to be 227 S/cm at 300 K with an intrinsic AHC of 155 S/cm. Our experimental analysis show that the AHE in Co$_2$FeAl is dominated by intrinsic Berry phase mechanism. Our theoretical calculations suggest that the enhanced Berry curvature induced intrinsic AHC is linked with the antisite disorder present in Co$_2$FeAl Heusler compound.

We gratefully acknowledge UGC-DAE CSR for experimental support. SS thanks Science and Engineering Research Board of India for financial support through the award of Ramanujan Fellowship (grant no: SB/S2/RJN-015/2017) and Early Career Research Award (grant no: ECR/2017/003186) and UGC-DAE CSR, Indore for financial support through “CRS” Scheme. GKS thanks to DST INSPIRE scheme for financial support. Portions of this research were conducted at the light source PETRA III of DESY, a member of the Helmholtz Association. Financial support from the Department of Science and Technology, Government of India within the framework of the India@DESY is gratefully acknowledged. We would like to thank the beamline scientist Dr. Martin Ettel for his help in setting up the experiments.

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