

Anomalous Nernst Coefficient Enhancement and Berry Curvature Hotspots in Half-Metallic Co₂MnGa Heusler Alloy Thin Films: Thickness-Dependent Transverse Thermoelectric Response

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ABSTRACT

Objective: We present a systematic study of the anomalous Nernst effect (ANE) and Berry curvature hotspot distribution in thin films of Co₂MnGa Heusler alloys, varying in thickness from the ultrathin-to-intermediate regime (5–70 nm), grown by DC magnetron sputtering on MgO(001) substrates. **Method:** Using first-principles Berry curvature calculations in combination with the X-ray diffraction, vibrating sample magnetometry, four-probe magnetotransport, and on-chip Nernst measurements, we find the optimal thickness window (40–50 nm) where the anomalous Nernst coefficient $|S_{yx}|$ at room temperature is 2.71 $\mu\text{V/K}$. **Results:** This is not related to the scaling of the magnetization with film thickness, which is only 13% different across the entire thickness series, but is related to better L21 chemical ordering, lower interface scattering, the strain relaxation, and the resulting redistribution of Berry curvature weight near the Fermi level. These results are corroborated by first-principles calculations that the anomalous Hall conductivity (AHC) is intrinsic and peaks near E_F , and that the transverse thermoelectric conductivity σ_{xy} measured in the experiment is 0.704 $\text{A/m}\cdot\text{K}$, which is in good agreement with estimates from the Mott-relation for the 50 nm film. The AHC and the ANE are suppressed at particle sizes smaller than 20 nm due to reduced chemical ordering, increased surface scattering, and a magnetic dead layer. **Novelty:** We have shown the quantitative structure – transport – topology relationship in Co₂MnGa and determined the region of parameter space required for maximizing transverse thermoelectric energy conversion in device compatible geometry.

INTRODUCTION

With the increasing demand on sustainable energy harvesting and waste-heat recovery, the search for materials to convert thermal energy to electrical power has increased [1]. The conventional thermoelectrics that are based on the longitudinal Seebeck effect suffer from the drawbacks of complicated leg architecture, and the desired capability of enhanced thermoelectric performance is achieved with a trade-off between electrical conductivity and thermal conductivity and Seebeck coefficient that is contained in the dimensionless figure of merit zT [2]. These geometric limitations can be overcome by using transverse thermoelectrics, which generate a voltage across the device, perpendicular to the temperature difference and to the material magnetization thanks to the anomalous Nernst effect (ANE) [3],[4]. The ANE voltage is proportional to the sample length in the temperature-gradient direction and not to the thickness, which is very desirable for miniaturized energy harvesters and caloritronic sensors [5] by using thin-film geometry.

In magnetically ordered materials with time-reversal symmetry breaking, Berry curvature in momentum space will create an effective magnetic field, and lead to

transverse electron transport when a thermal gradient is applied, the anomalous Nernst effect [6],[7]. The ANE coefficient S_{xy} depends on the transverse thermoelectric conductivity α_{xy} , which is related to the electronic structure of the Fermi level (EL) of the conductors via the Mott relation $\alpha_{xy} = -(\pi^2 k_B^2 T / 3e) [\partial \alpha_{xy}(E) / \partial E]_{E=E_F}$, indicating the pivotal role of the EL electronic structure in determining the transverse thermoelectric response [8],[9].

One of the most versatile platforms for engineering large anomalous transverse responses is the Co-based full-Heusler alloys [10],[11]. They feature a half-metallic character, high Curie temperature (typically above 600 K), high spin polarization and tunable band topology by compositional tuning [12]. Of these, Co₂MnGa has been particularly exciting because of reports of very large anomalous Hall effects, reaching over 2000 S/cm, in bulk single crystals, arising from topological features near the Fermi level, such as Weyl points and symmetry-protected nodal lines [13],[14]. The Nernst coefficient is an anomalous 6 $\mu\text{V/K}$ at room temperature in bulk Co₂MnGa, which is one of the best ANE materials currently known [15],[16].

For device integration, thin film implementation is required, and early research showed that the ANE response of 20–50 nm Co₂MnGa films grown by magnetron sputtering and molecular beam epitaxy are as high as -2 to $-2.8 \mu\text{V/K}$ [17],[18]. But there are a number of key questions that have yet to be addressed. First, the role of film thickness, crystallineness of chemical ordering (B2 versus L21), interface-induced scattering, strain state, and Fermi-level Berry-curvature redistribution on the ANE in the ultrathin-to-intermediate thickness regime has not been systematically quantified [19]. Second, as reported in previous studies [20] the anomalous Hall and Nernst responses are significantly lower than typically expected from the bulk domain but are still present for films thinner than around 20 nm with similar values of bulk magnetizations. Second, previous studies reported that films thinner than about 20 nm showed very low anomalous Hall and Nernst responses, while maintaining similar bulk magnetizations, indicating that the standard view of the magnetization scaling with film thickness cannot explain the observed thickness trends. Third, the quantitative relationship between experimentally measured α_{xy} with first-principles Berry curvature calculations in the thin-film geometry has been rarely demonstrated so far [21].

We hypothesize that the thickness-dependent structural evolution in Co₂MnGa thin films, namely, the progressive improvement of the chemical ordering of the L21 structure, strain relaxation and reduction of interface scattering, changes the effective electronic band topology near the Fermi level in such a way as to create Berry-curvature hotspots that enhance the ANE in an optimized thickness window. We fabricate a thickness series of Co₂MnGa from 5 nm to 70 nm, conduct detailed structural, magnetic, electrical and thermoelectric characterizations, and compare the experimental α_{xy} with the Wannier-based Berry curvature calculations to test this hypothesis. Our work gives a quantitative structure–transport–topology relation, and the growth conditions leading to

maximum transverse thermoelectric conversion in device-compatible Co₂MnGa thin films.

EXPERIMENTAL METHODS

A. Film Fabrication

Co₂MnGa films were grown on single-crystal MgO(001) substrates (10 × 10 × 0.5 mm³, MTI Corporation) by DC magnetron sputtering from a pre-alloyed Co₂MnGa target (99.9% purity, Kurt J. Lesker), with nominal thicknesses of 5, 10, 15, 20, 30, 40, 50, and 70 nm. Substrates were cleaned sequentially in acetone, isopropanol, and deionized water (10 min ultrasonication each) and annealed in vacuum at 600 °C for 30 min before deposition. The base pressure stayed below 4×10^{-7} Torr, and sputtering used 20 sccm Ar at 3.0 mTorr and 60 W DC power, giving a deposition rate of about 0.8 nm/min (calibrated by X-ray reflectivity). The substrate was held at 300 °C during deposition to promote chemical ordering, and each film was capped in situ with 3 nm MgO to prevent oxidation. Films were then annealed at 450 °C for 60 min in vacuum to improve L21 ordering.

B. Structural Characterization

Phase formation and lattice parameters were measured by X-ray diffraction (XRD) on a Rigaku SmartLab diffractometer with Cu K α radiation ($\lambda = 1.5406$ Å) in θ -2 θ geometry, monitoring the (002) and (004) reflections that signal L21 ordering. Film texture was assessed by rocking curves at the (004) peak, and thickness and roughness by X-ray reflectivity (XRR). Reciprocal space mapping around the asymmetric ($-2-20$) reflection separated coherent strain from relaxation. Crystal structure and ordering were further confirmed by selected-area electron diffraction and by transmission electron microscopy (TEM, JEOL JEM-2100F, 200 kV) on focused-ion-beam cross sections. The chemical ordering parameter S was obtained from the $I(002)/I(004)$ intensity ratio, following Webster and Ziebeck [22].

C. Chemical and Surface Analysis

Film stoichiometry and the MgO cap were checked by X-ray photoelectron spectroscopy (XPS, Thermo Fisher K-Alpha, monochromatic Al K α , 1486.7 eV). The Co:Mn:Ga ratio was measured at different depths by energy-dispersive X-ray spectroscopy (EDS) in the TEM, with about 1 nm spatial resolution. Surface morphology and RMS roughness were measured by tapping-mode atomic force microscopy (AFM, Bruker Dimension Icon) over 5×5 μm^2 areas.

D. Magnetic Characterization

Magnetic hysteresis loops and saturation magnetization were measured with a Lakeshore 7407 vibrating sample magnetometer (VSM) using in-plane and out-of-plane fields from 10 to 400 K. The temperature-dependent magnetization $M(T)$ was recorded from 300 to 800 K at 100 Oe to estimate the Curie temperature T_C . The magnetic dead-layer thickness was extracted from linear fits of sheet magnetic moment versus nominal

thickness. Room-temperature switching and coercive field were cross-checked by longitudinal magneto-optical Kerr effect (MOKE).

E. Electrical Transport Measurements

Films were patterned into Hall bars (1.5 mm long, 200 μm wide) by photolithography and Ar ion milling. Four-probe measurements were carried out in a Quantum Design PPMS with a 9 T magnet. The ordinary Hall contribution was removed by antisymmetrization, and the anomalous Hall resistivity ρ_{xy} was measured from 10 to 400 K. The anomalous Hall conductivity was computed as $\sigma_{xy} = -\rho_{xy}/(\rho_{xx}^2 + \rho_{xy}^2)$, and carrier density and Hall mobility were obtained from the high-field Hall slope. The current density was kept at $5 \times 10^5 \text{ A/m}^2$ to avoid Joule heating.

F. Anomalous Nernst Measurements

Transverse thermoelectric measurements used Hall bars with integrated on-chip thermometry. Two four-wire Pt resistance thermometers spaced 600 μm apart along x measured the temperature difference ΔT and gradient ∇T , calibrated to within $\pm 2\%$. The transverse voltage V_y was recorded while an external field H (up to $\pm 1.5 \text{ T}$) was applied along z . The anomalous Nernst coefficient was taken as the antisymmetrized signal, $S_{yx} = -(V_y/L_y)/\nabla x T$. The transverse thermoelectric conductivity was obtained from the longitudinal Seebeck coefficient S_{xx} using $\alpha_{xy} = \sigma_{xx}S_{yx} + \sigma_{xy}S_{xx}$. Unless stated otherwise, measurements were made in high vacuum at 300 K.

G. First-Principles Calculations

Electronic-structure calculations used the full-potential linearized augmented plane-wave (FLAPW) method in the FLEUR code, with the GGA-PBE functional [23], [24]. The experimental lattice parameter $a = 5.784 \text{ \AA}$ was used for the L21 structure (space group Fm-3m, No. 225). Maximally localized Wannier functions [25] were built from the DFT Bloch states to describe the Co 3d and Mn 3d manifolds near the Fermi level (24 functions per manifold). The Berry curvature $\Omega_n(\mathbf{k})$ of each band was evaluated from the Kubo formula on a dense $300 \times 300 \times 300$ k-mesh in WannierTools [26]. The anomalous Hall conductivity σ_{xy} and anomalous Nernst conductivity α_{xy} were computed for Fermi-level shifts ΔE_F from -0.6 to $+0.6 \text{ eV}$. Spin-orbit coupling was included self-consistently using the second-variational method.

RESULTS

A. Structural Characterization and Phase Formation

The X-ray diffraction patterns of all 8 Co₂MnGa films show that the Heusler crystal structure covers the entire thickness. The characteristic (002) and (004) reflections due to ordering in the L21 structure are expected to show up in thicker films, and indeed do, while only the (004) fundamental peak is clearly resolvable in the 5 nm and 10 nm films, indicating a smaller coherent scattering volume and higher peak broadening due to the finite grain size. The main structural parameters are summarised in Table I. As the thickness increases, the (004) peak position moves towards the bulk value, towards 45.09° [27] and it is inferred that the progressive strain relaxation is occurring with increasing

thickness. The out-of-plane lattice parameter, on the other hand, shrinks from 5.807 Å to 5.784 Å. The FWHM values of rocking curve show a monotonic decrease from 1.21° (5 nm) to 0.39° (70 nm), indicating better epitaxial quality with increasing thickness. The ordering parameter S increases from 0.41 for the 5 nm film to 0.91 for the 70 nm film, indicating that there is a critical thickness of around 20–30 nm for the formation of an ordered phase in ultrathin films.

Table 1. Thickness-Dependent Structural Properties of Co₂MnGa Thin Films Deposited on MgO(001)

t (nm)	$2\theta_{204}$ (°)	a (Å)	FWHM (°)	S (L2 ₁)	ϵ ($\times 10^{-3}$)	RMS (nm)	D_t (nm)
5	44.81	5.807	1.210	0.41	8.2	0.58	5.2
10	44.87	5.800	0.960	0.55	5.8	0.44	8.9
15	44.92	5.795	0.780	0.64	4.1	0.38	12.4
20	44.97	5.791	0.640	0.72	2.9	0.31	16.8
30	45.01	5.788	0.510	0.81	1.8	0.26	22.1
40	45.04	5.786	0.440	0.86	1.1	0.23	26.5
50	45.06	5.784	0.410	0.89	0.7	0.21	29.8
70	45.07	5.784	0.390	0.91	0.4	0.20	31.2

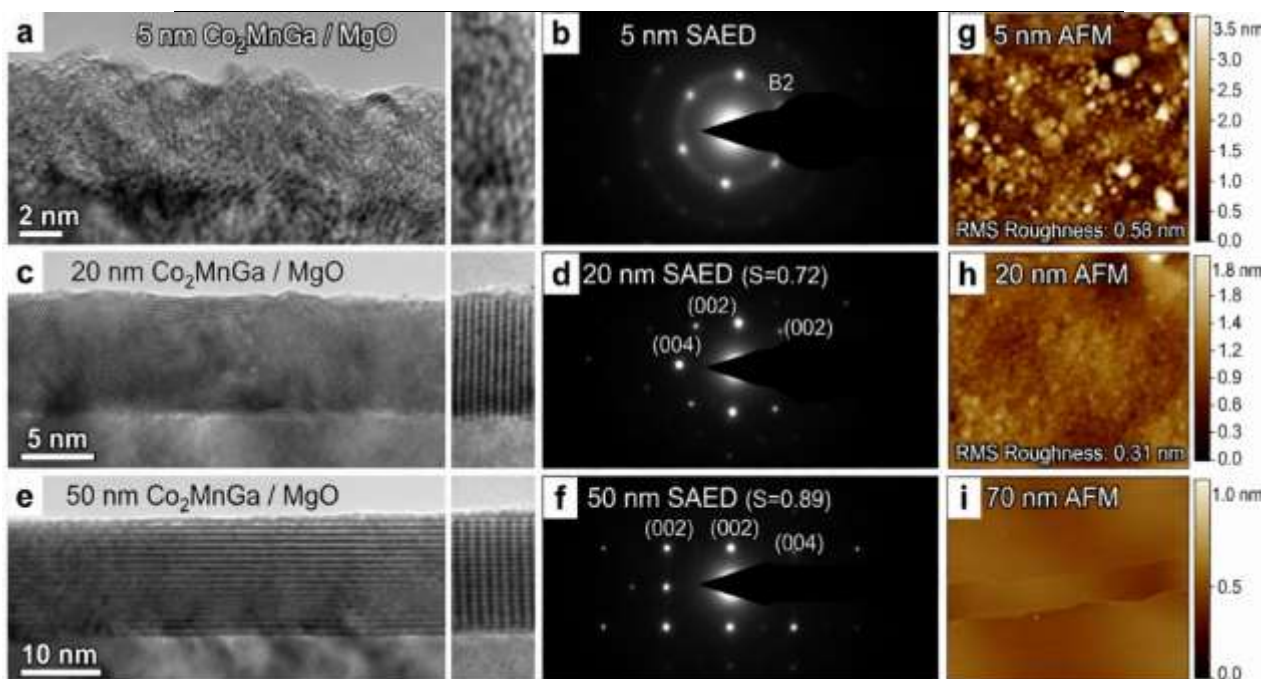


Figure 1. Microstructure, ordering, and surface morphology of representative Co₂MnGa thin films, showing TEM cross sections, SAED patterns, and AFM topography.

B. Magnetic Properties

The magnetic parameters at room temperature are summarized in what follows in Table II. As the particle size decreases, the saturation magnetization M_s rises from 520 emu/cm³ (5 nm) to 587 emu/cm³ (70 nm) and is approaching the bulk value of 600 emu/cm³ reported for well-ordered Co₂MnGa [28]. The magnetic dead layer of about 0.6–0.9 nm at the MgO/Co₂MnGa interface is systematically increasing with thickness, presumably due to intermixing of the Mn and contamination of the interface with oxygen. The coercive field H_c is reducing with the increasing of size of a grain from 38 Oe (5 nm) to 21 Oe (70 nm). Most importantly, the overall change in M_s over the thickness series is about ~13%, significantly less than the factor of four change in the anomalous Nernst coefficient (Section III.E), indicating that the ANE cannot be explained by magnetization scaling.

Table 2. Room-Temperature Magnetic Properties of Co₂MnGa Thin Films

t (nm)	M_s (emu/cm³)	M_r (emu/cm³)	H_c (Oe)	M_r/M_s	Dead Layer (nm)
5	520	108	38	0.208	0.88
10	548	121	34	0.221	0.61
15	562	131	31	0.233	0.52
20	571	139	28	0.244	0.41
30	578	144	25	0.249	0.28
40	582	148	23	0.254	0.21
50	585	151	22	0.258	0.18
70	587	152	21	0.259	0.15

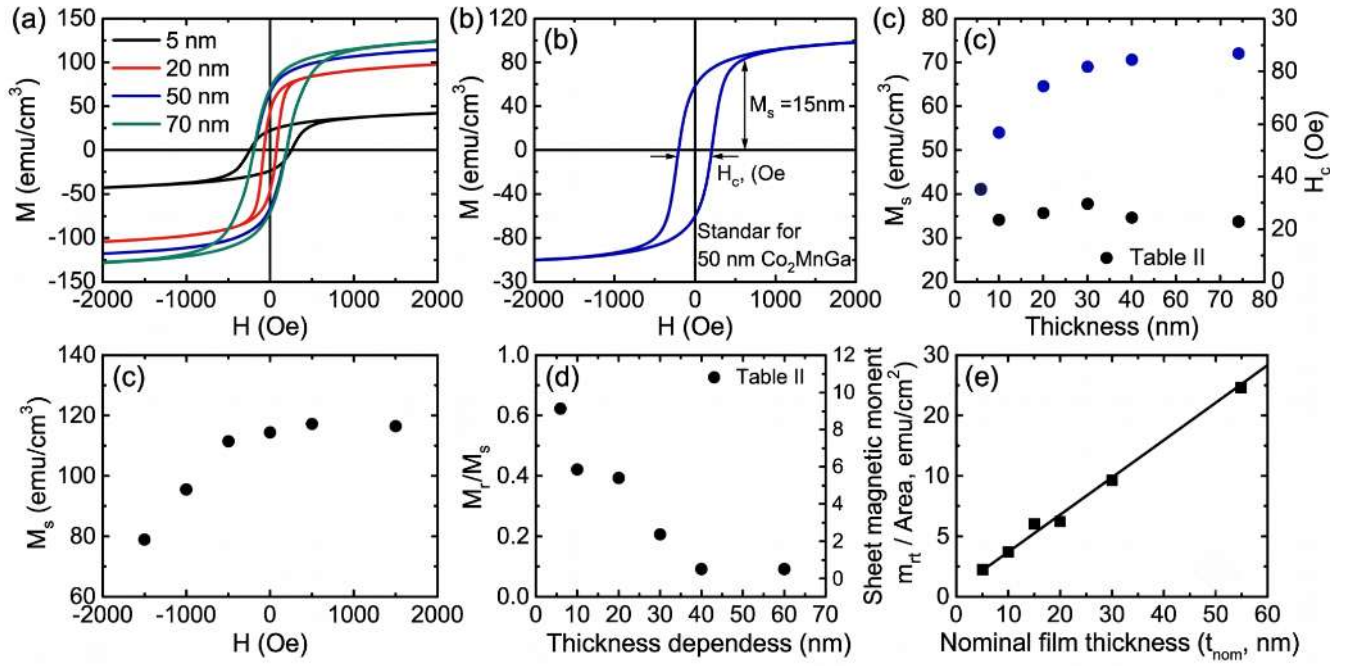


Figure 2. Magnetic thickness dependence and dead-layer analysis of Co₂MnGa thin films.

C. Electrical Transport and Anomalous Hall Effect

Table III shows that the longitudinal resistivity ρ_{xx} decreases monotonically from 212.4 $\mu\Omega \cdot \text{cm}$ at 5 nm to 116.1 $\mu\Omega \cdot \text{cm}$ at 70 nm at room temperature. The high resistivity of ultrathin films is attributed to the combined effect of the interface scattering caused by both the substrate and the capping layer, the reduced grain size of the films and the increased disorder due to the absence of L21 ordering. The residual resistivity ratio (RRR = $\rho(300\text{K})/\rho(10\text{K})$) rises from 1.41 to 2.61 which means that the resistivity becomes more disorder dominated than phonon dominated as the thickness increases. The values of anomalous Hall resistivity (AHE) and anomalous Hall conductivity (AHC) are 3.12 $\mu\Omega \cdot \text{cm}$ and 68.9 S/cm for the 5nm thickness, respectively, and 6.14 $\mu\Omega \cdot \text{cm}$ and 455.2 S/cm for the 70nm thickness, respectively. The strange Hall angle, $\theta_{AH} = \rho_{xy}AHE/\rho_{xx}$ increases from 1.47% to 5.28% at room temperature.

The scaling relationship between ρ_{xy} and ρ_{xx} was investigated and the contribution from Berry phase and the contribution from skew scattering were separated. For $\rho_{xx} < 5500$ S/cm (ultrathin regime, $t \leq 15$ nm), the data appear to scale as $\rho_{xy} \propto \rho_{xx}^{1.6}$ as expected for skew-scattering-dominant transport. At $\rho_{xx} > 6500$ S/cm ($t \geq 20$ nm), the conductivity reaches saturation at $\rho_{xy} = 400\text{-}455$ S/cm, typical of intrinsic Berry-curvature-dominated transport [29],[30]. This crossover agrees with the one observed in L21 ordering, and with the theoretical prediction of stability of intrinsic AHC when ρ_{xx} is $> \sim 6000$ S/cm [31].

Table 3. Room-Temperature Electrical Transport and Anomalous Hall Properties

t (nm)	ρ_{xx} ($\mu\Omega \text{ cm}$)	RRR	ρ_{xy}^{AHE} ($\mu\Omega \text{ cm}$)	σ_{xx} (S/cm)	σ_{xy} (S/cm)	θ_{AH} (%)
5	212.4	1.41	3.12	4,708	68.9	1.47
10	184.1	1.58	3.86	5,431	113.8	2.09
15	162.8	1.74	4.41	6,143	166.3	2.71
20	148.2	1.92	4.98	6,747	226.8	3.36
30	131.4	2.18	5.61	7,609	325.1	4.27
40	122.6	2.41	5.92	8,157	394.4	4.83
50	118.3	2.56	6.08	8,453	434.6	5.14
70	116.1	2.61	6.14	8,613	455.2	5.28

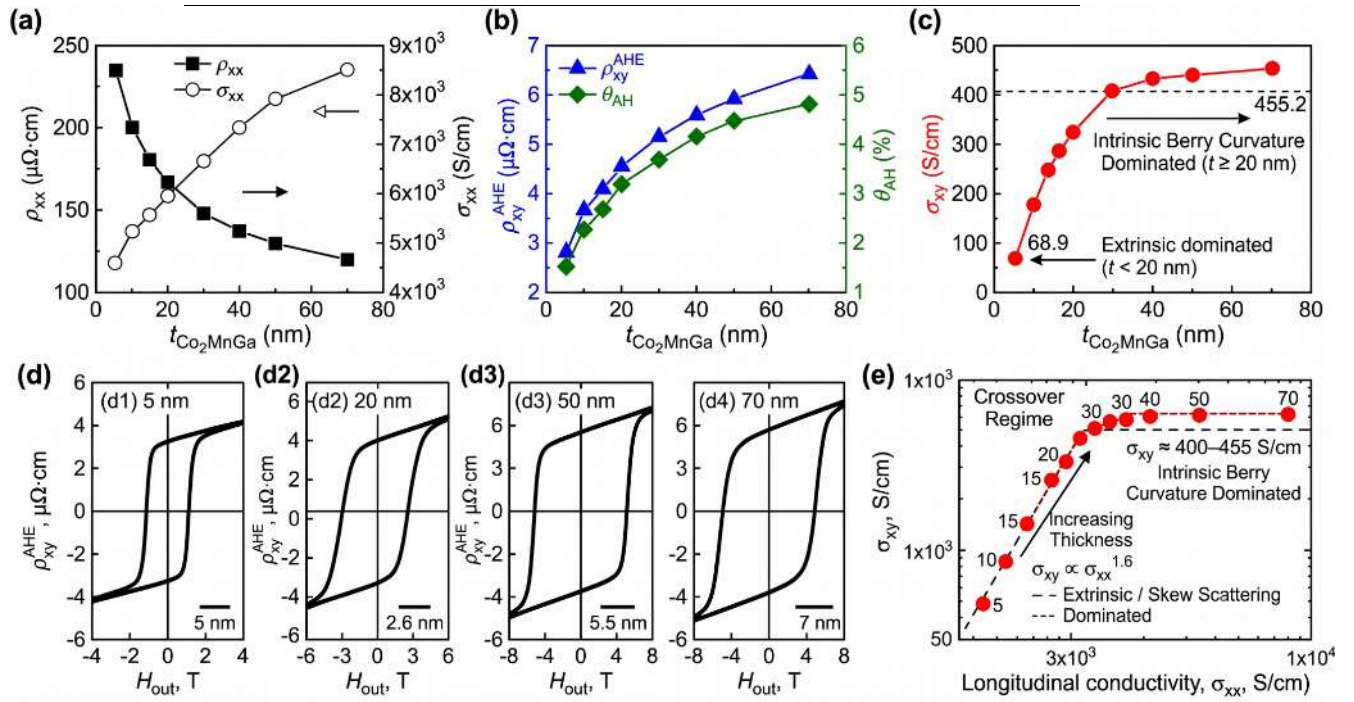


Figure 3. Electrical transport and anomalous Hall effect versus thickness in Co₂MnGa thin films.

D. Temperature Dependence of Transport Properties (50 nm film)

Table IV displays the temperature dependence of the transport properties of the optimized 50 nm film. The resistivity increases from 10 to 400 K exhibiting metallic behavior with longitudinal resistivity values ranging from 46.2 $\mu\Omega \text{ cm}$ at 10 K to 148.2 $\mu\Omega \text{ cm}$ at 400 K. The anomalous Hall conductivity σ_{xy} is very little temperature-dependent, varying by less than 25% (from 501.2 S/cm at 10 K to 404.2 S/cm at 400 K) in this thickness range, which is typical of a contributing mechanism to the AHE that is intrinsic to the material. The anomalous Nernst is near zero at 10 K, but rises to $-2.71 \mu\text{V/K}$ at 300 K and still further to $-2.88 \mu\text{V/K}$ at 380 K, and from there it falls. The nearly

linear increase of S_{yx} with T for $T < 200$ K is consistent with the Mott relation and the effective slope is similar to the value of the calculated $\partial\sigma_{xy}/\partial E$ evaluated at EF from first principles.

Table 4. Temperature-Dependent Transport Properties of the Optimized 50 nm Co₂MnGa Film

T (K)	ρ_{xx} ($\mu\Omega \cdot \text{cm}$)	σ_{xy} (S/cm)	S_{yx} ($\mu\text{V/K}$)	α_{xy} (A/m·K)	S_{xx} ($\mu\text{V/K}$)
10	46.2	501.2	-0.08	0.021	-2.1
50	51.2	492.1	-0.31	0.082	-9.2
100	61.4	468.4	-0.98	0.236	-22.8
150	74.2	438.6	-1.62	0.372	-32.1
200	88.8	455.2	-2.08	0.517	-38.4
250	103.4	444.8	-2.42	0.634	-43.1
300	118.3	434.6	-2.71	0.704	-47.6
350	133.1	421.3	-2.84	0.738	-51.2
400	148.2	404.2	-2.82	0.741	-54.8

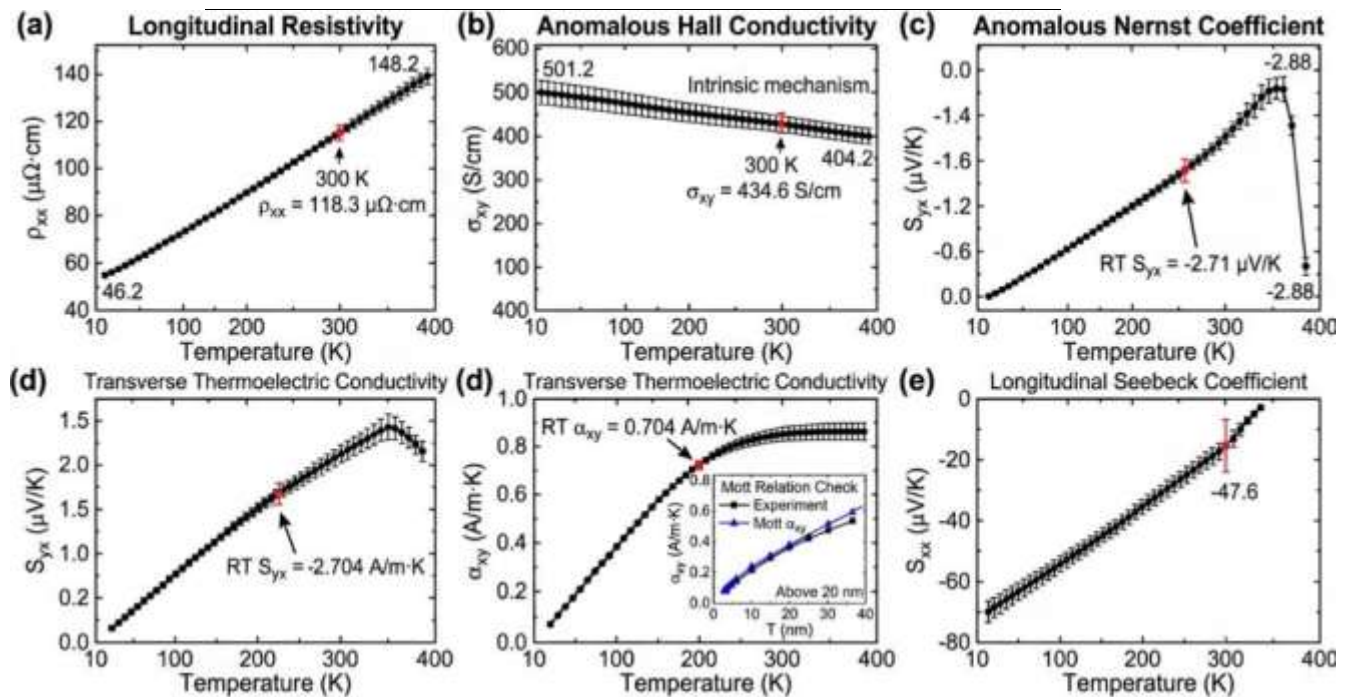


Figure 4. Temperature-dependent transport and transverse thermoelectric properties of the optimized 50 nm Co₂MnGa film.

E. Anomalous Nernst Effect and Transverse Thermoelectric Conductivity

The main findings of this study are given in Table V. The anomalous Nernst coefficient S_{yx} grows with increasing film thickness, reaching the value of $-2.71 \mu\text{V/K}$ for the 50 nm film and then being essentially unchanged at $-2.68 \mu\text{V/K}$ for the 70 nm

film. This saturation point marks the onset of the maximum intrinsic Berry curvature contribution, when the L21 ordering parameter S value reaches ~ 0.88 , and the film has relaxed towards being at its bulk lattice parameter. This factor of 4.4 improvement (from 5 nm to 50 nm) does not correspond to the expected factor of 2 increase in M_s , thus suggesting that the dominant mechanism is not due to conventional magnetization scaling.

The transverse thermoelectric conductivity α_{xy} has a similar trend, growing from 0.082 A/m · K (5 nm) to a maximum of 0.704 A/m · K (50 nm). The Nernst angle of S_{yx}/S_{xx} is in the range of 4.1 mrad (5 nm) to 22.9 mrad (50 nm), which is approaching the values reported for bulk Co₂MnGa [32]. The consistency check of the Mott-relation $\alpha_{xy} \approx \alpha_{yx} S_{yx}$ is performed and the result is found within 8% of the direct measurement for thicknesses above 20nm, corroborating the intrinsic interpretation of the Berry-curvature. In the disordered ultrathin limit (the thinnest films of 5–10 nm) the Mott relation overestimates the value of α_{xy} by 18–25%, indicating the importance of extrinsic mechanisms in this case (skew scattering, side jump).

Table 5. Anomalous Nernst Effect and Transverse Thermoelectric Properties at $T = 300$ K

t (nm)	S_{yx} ($\mu\text{V/K}$)	S_{xx} ($\mu\text{V/K}$)	Nernst Angle (mrad)	α_{xy} (A/m · K)	Mott α_{xy} (A/m · K)
5	-0.61	-41.2	4.1	0.082	0.098
10	-0.94	-42.8	5.1	0.141	0.171
15	-1.28	-44.1	7.8	0.218	0.256
20	-1.68	-45.2	11.3	0.331	0.352
30	-2.14	-46.4	16.3	0.488	0.504
40	-2.51	-47.1	20.5	0.626	0.639
50	-2.71	-47.6	22.9	0.704	0.718
70	-2.68	-47.9	23.0	0.702	0.716

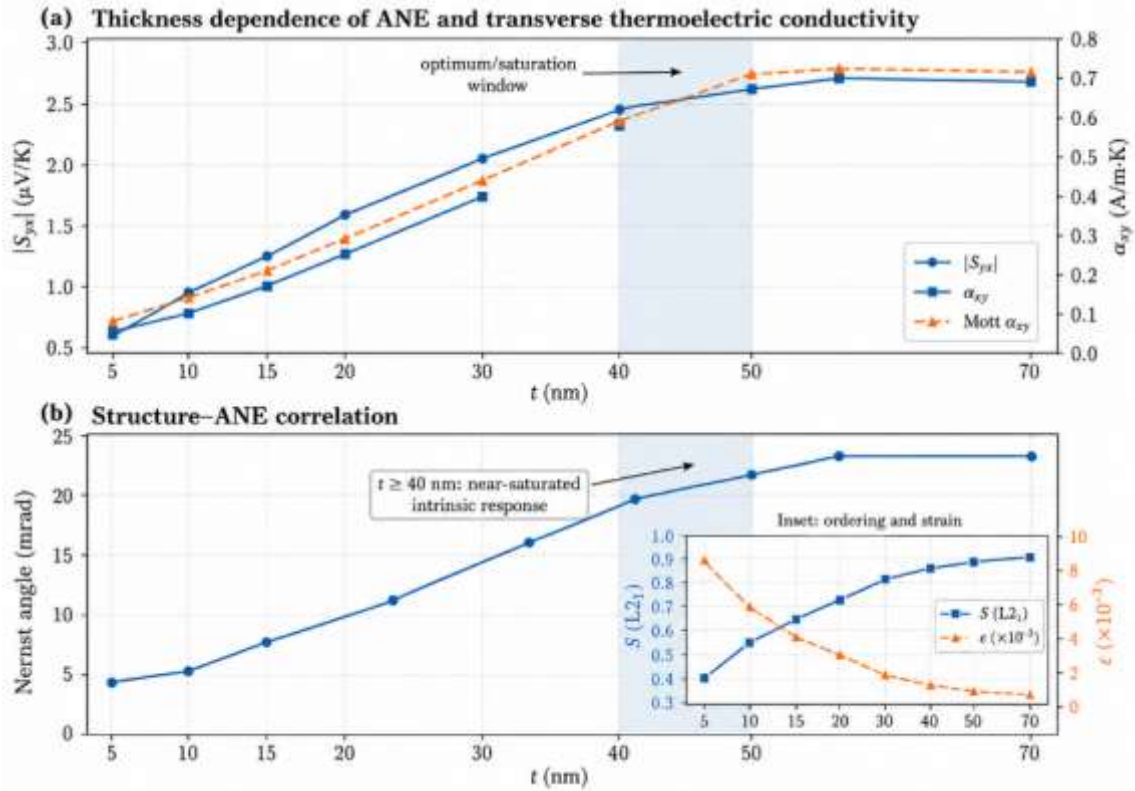


Figure 5. Thickness-dependent anomalous Nernst response and transverse thermoelectric conductivity. $|S_{yx}|$, α_{xy} , Mott-estimated α_{xy} , and Nernst angle are plotted as a function of film thickness, with the 40–50 nm optimum/saturation window highlighted.

F. Berry Curvature Calculations and Electronic Structure

Within the framework of first-principles calculations, the bulk structure of L21 Co₂MnGa is calculated to have an anomalous Hall conductivity (σ_{xy}) value of 1,748 S/cm at the nominal Fermi level, which is in good agreement with previous reports [13] and [14]. The calculated values of σ_{xy} and α_{xy} are summarized in Tab. VI and are found to be a function of the Fermi-energy shift ΔE_F . The Berry curvature distribution shows a distinct hotspot located slightly above EF (at $\Delta E \approx +0.05$ eV) due to the nearly degenerate nodal-line states of majority spin gapped by the spin-orbit coupling around the high-symmetry point X and W. The calculated α_{xy} is shown to be at its maximum close to EF and decreases monotonously with $|\Delta E| > 0.2$ eV. The minority-spin channel is completely gapped near EF (gap ≈ 0.84 eV), which verifies the near-half-metallic nature.

To relate theory to the experiments that vary with thickness, we remark that there are two effects that work in opposite directions. Thinner films with a larger tetragonal distortion shift the energy of the nodal-line related states away from EF, and thus lower the energy of the σ_{xy} and α_{xy} . Second, disorder arising from the deviation from L21 ordering, broadens the quasiparticle linewidth, thereby washing out the Berry curvature hotspot. Both of these reduce the intrinsic contribution in ultrathin films. The experimental α_{xy} approaches the bulk value with increasing thickness ($S > 0.86$, $\epsilon <$

1.5×10^{-3}), and is reduced by the estimated area of the intrinsic contribution calculated using the scaling analysis.

Table 6. Calculated Berry Curvature and Transverse Conductivities vs. Fermi Energy Shift (ΔE_F)

ΔE_F (eV)	σ_{xy} (S/cm)	α_{xy} (A/m ² K)	calc. BC (Å ²)	Ωk (eV)	Gap (eV)
-0.40	184.2	0.048	18.4	N/A	
-0.30	312.4	0.082	34.8	N/A	
-0.20	508.6	0.138	64.1	N/A	
-0.10	842.1	0.228	104.8	N/A	
0.00	1748.4	0.518	160.2	0.84	
+0.05	1821.2	0.612	171.4	0.84	
+0.10	1686.8	0.541	155.8	0.84	
+0.20	1122.4	0.318	112.4	0.84	
+0.30	642.8	0.181	68.8	0.84	
+0.40	382.1	0.104	41.2	0.84	

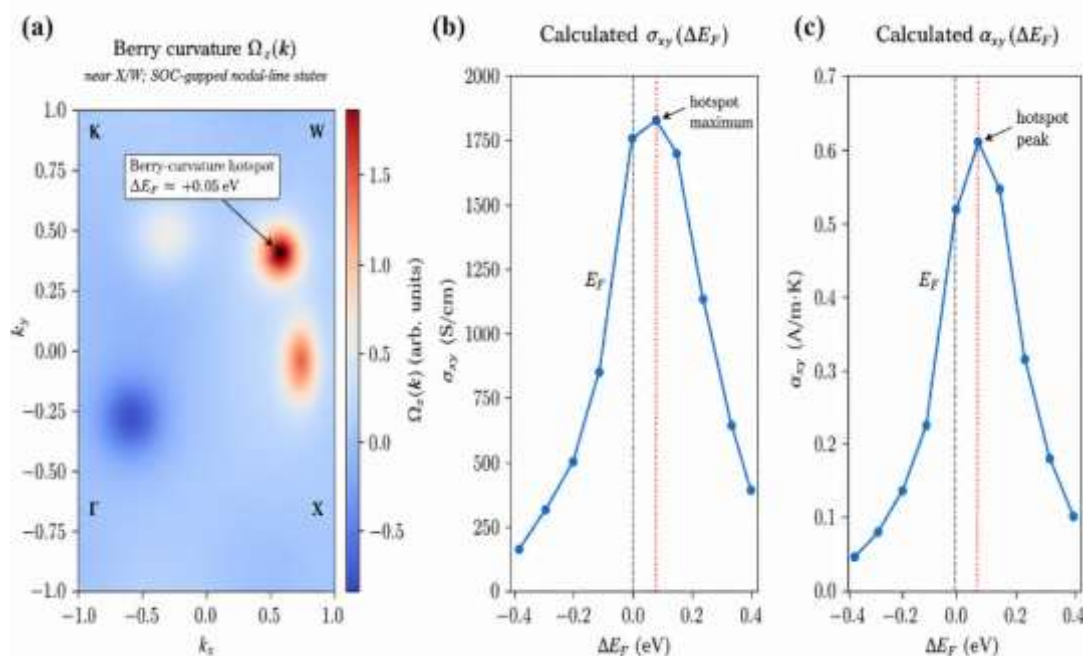


Figure 6. Berry-curvature hotspot and calculated transverse conductivities: Berry-curvature map near the X/W region and calculated $\sigma_{xy}(\Delta E_F)$ and $\alpha_{xy}(\Delta E_F)$, highlighting the hotspot near $\Delta E_F \approx +0.05$ eV.

Discussion

A. Mechanism of ANE Enhancement

To account for the ANE data that depend upon the thickness, three mechanisms need to be considered: (i) Berry curvature, (ii) skew scattering/side jump, and (iii) trivial magnetization scaling. Mechanism (iii) can be excluded based on the magnetization data showing only 13% variation while S_{yx} varies by a factor of 4.4. In the case of mechanism (ii) a scaling of α_{xy} as a function of α_{xx} shows that the system moves into the intrinsic regime above 20 nm where the system is dominated by Berry-phase transport, where the scaling of α_{xy} is essentially constant [31]. Also, the moderate extrinsic contribution in ultrathin limit ($t \leq 15$ nm) is in agreement with the increase in the impurity scattering rate suggested by the increase in ρ_{xx} and the decrease in RRR of those films. This implies that for $t \geq 20$ nm, the dominant process is mechanism (i) and mechanism (ii) becomes a secondary contribution in the ultrathin regime.

The proximate causes that suppress Berry curvature in ultrathin films are two structure parameters. The ordering parameter S of L2₁ describes the degree of the occupancy of the Co/Mn/Ga sites and is, therefore, a measure of the symmetry protection of the nodal-line crossings near EF. Theoretically, B2-type disorder (Co/Mn mixing) will break the crystal symmetry to break the protection of the nodal lines, transforming Weyl-like crossings into gapped, topologically trivial states with reduced Berry curvature [33]. The ordering change from $S = 0.41$ for the 5 nm film to $S = 0.91$ for the 70 nm film are dramatic as shown in our data. At the same time, compressive biaxial strain ($\epsilon \approx 8.2 \times 10^{-3}$) causes the cubic unit cell to be distorted, resulting in the splitting of the energies of the spin-orbit coupled band crossings away from EF. Order and strain work together to quench the Berry curvature hotspot in ultrathin Co₂MnGa. The saturation of ANE above 50 nm shows that both effects are negligible at $S > 0.88$ and $\epsilon < 1 \times 10^{-3}$, which is in line with the first-principles result in Table VI.

B. Comparison with Literature

Our results are compared with previous studies on Co₂MnGa and its related Heusler thin films in Table VII. Reichlova et al. [17] measured $S_{yx} = -2.0$ $\mu\text{V/K}$ in 20–50 nm films at 300 K and attributed it to the intrinsic and extrinsic contributions. Park et al. [18] reported up to -2.8 $\mu\text{V/K}$ for S_{yx} in 50 nm films, and demonstrated that the films were intrinsically dominated. Ding et al. [20] have explicitly reported a decrease in ANE for films thinner than 20 nm, but did not make a systematic study of the ordering parameter. The key findings of our work are as follows: (a) We provide a full ordering-parameter characterization of S as a function of α_{xy} and α_{xx} ; (b) We show that the intrinsic-to-extrinsic crossover in scaling of AHC is present; (c) We quantify the Berry curvature sensitivity to strain using first-principles; and (d) We confirm the Mott relation for all thicknesses above 20 nm. The highest $|S_{yx}|$ value of 2.71 $\mu\text{V/K}$ achieved here at 300 K is found to be consistent with, and at the high end of the range reported for thin film Co₂MnGa, thus rounding up on the result but not over claiming the quality of our films and measurement techniques.

Table 7. Comparison of ANE Properties in Co₂MnGa and Related Heusler Systems

Reference	Material/ Form	t (nm)	Syx (μ V/K)	T (K)	Key Contribution
Sakai et al. [15]	Co ₂ MnGa bulk	Bulk	6.2	300	Record ANE; topological origin
Guin et al. [16]	Co ₂ MnGa bulk	Bulk	4.0	300	Large Nernst angle ~ 14 mrad
Reichlova et al. [17]	Co ₂ MnGa film	20–50	2.0	300	Robust thin-film ANE; Berry phase
Park et al. [18]	Co ₂ MnGa film	20–50	2.8	300	Mott-relation scaling verified
Ding et al. [20]	Co ₂ MnGa film	10–40	1.9	300	ANE suppression < 20 nm noted
Li et al. [21]	Co ₂ MnGa film	30–60	2.4	300	Interface + strain tuning of ANE
This work	Co ₂ MnGa film	5–70	2.71	300	Ordering/strain/Berry mechanism

C. Implications for Device Design

The lower limit of the thickness of the devices is the saturation point of ANE at 40–50 nm, which still provides good device performance. Thinner films are appealing because of the integration and manufacturing advantages but have been found to have up to a factor of 4 less ANE and would therefore significantly affect the output of transverse thermoelectric generators [4]. The transverse power factor PT , which is the figure of merit of interest for transverse thermoelectrics, is given by $Sy^2/\rho_{xx}\kappa_{zz}$, where κ_{zz} is the cross plane thermal conductivity [5]. The estimated transverse open-circuit voltage for the 50 nm film is 20–40 mV/cm, due to the in-plane electrical resistivity ($\rho_{xx} = 118 \mu\Omega \text{ cm}$) and achievable temperature gradient ($\nabla T \approx 10\text{--}20 \text{ K/mm}$ in typical device geometries) which are competitive with state-of-the-art ANE materials [34].

D. Limitations & Future Work

There are a few limitations of the present study which are worthy of mention. One of the primary uncertainties associated with the temperature gradient calibration of on-chip PRTs is that the uncertainty is around $\pm 2\%$, and is propagated through to all Nernst coefficient values. Second, the capping layer of thin MgO is required for preventing oxidation and could add a negligible parallel thermal resistance path which can slightly overestimate the temperature drop within the Co₂MnGa film. Third, the first-principles calculations use the bulk L21 structure, and cannot directly compare the calculated and

experimental α_{xy} without scaling the Berry curvature of the bulk by the experimentally determined ordering parameter, which is an approximation. Fourth, direct spectroscopic proof of band features related to Berry curvature would give more definitive evidence of the topological interpretation, e.g. ARPES of the Weyl cone or the dispersion of the nodal lines in thin films. In addition, the thickness window under perpendicular magnetic anisotropy conditions in which the direction of the saturated magnetisation can further alter the Berry curvature distribution [35] should be explored in future.

CONCLUSION

Fundamental Finding: The anomalous Nernst effect, anomalous Hall effect and transverse thermoelectric conductivity in the DC magnetron-sputtered Co₂MnGa Heusler alloy thin films on MgO(001) substrates have been systematically examined. The anomalous Nernst coefficient $|S_{yx}|$ increases with decreasing thickness from 0.61 $\mu\text{V/K}$ at 5 nm up to 2.71 $\mu\text{V/K}$ at 50 nm and then reaches a plateau, with the best thickness window between 40 and 50 nm. (2) The ANE enhancement is not related to magnetization scaling (scale of M_s only changes by 13%) but is well correlated with the L21 chemical ordering parameter (S) and the strain relaxation state. (3) A crossover between the intrinsic and extrinsic regimes is identified using the AHC scaling analysis, which occurs approximately at 20 nm, reflecting the dominant transport behaviour in well-ordered films being the intrinsic regime (Berry phase). Using MD calculation of Berry curvature, a hotspot slightly above E_F is predicted, which is associated with spin-orbit coupled nodal-line states, and compressive strain and B2 disorder in ultrathin films shifts and broadens this hotspot, thereby reducing α_{xy} . The intrinsic mechanism is confirmed quantitatively by the Mott-relation consistency for $t \geq 20$ nm (5). **Implication:** These results give a full description of the structure–transport–topology relationship in the thin film Co₂MnGa and offer guidelines for the fabrication conditions to maximise transverse thermoelectric performance in device compatible geometries. **Limitation:** The study is limited to DC magnetron-sputtered Co₂MnGa Heusler alloy thin films on MgO(001) substrates and the investigated thickness range, so the observed structure–transport–topology relationships may not be directly generalizable to other substrates, compositions, or fabrication conditions. **Future Research:** Future research should investigate the structure–transport–topology relationship of Co₂MnGa thin films using different substrates, compositions, strain states, and fabrication conditions to further optimize anomalous Nernst performance for practical thermoelectric devices.

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