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Borderline first-order magnetic phase transition in AlFe₂B₂

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ABSTRACT

The thermal evolution of lattice parameters coupled with heat capacity data provide insight into tailorable magnetism-structure attributes in the orthorhombic compound $AlFe_2B_2$ that was synthesized with and without small additions of gallium. Temperature-dependent X-ray powder diffraction experiments conducted through the magnetic phase transition reveal that the *a*- and *b*-parameters of both samples increase with increasing temperature while the *c*-parameter decreases. While a weak volumetric thermal expansion is noted over a range of temperatures well below and above the magnetic phase transition, anomalous behavior was observed within the phase transition region itself to reveal a magnetostructural phase transition with borderline first-order character in the Ga-modified sample but of more second-order character in the Ga-free sample. It is established that the nearest-neighbor Fe-Fe interatomic distance within the *(ab)*-plane plays a dominant role in influencing the magneto-functional response of these compounds. The magnetocaloric properties are discussed in the context of temperature-induced changes of the interatomic bonding that are influenced by the hypothesized presence of iron antisite defects in the $AlFe_2B_2$ lattice.

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1. Introduction

Correlating magneto-functional response with lattice character provides insight into fundamental drivers that control and fine-tune magnetic properties for applications. One emerging application is room-temperature cooling or thermal management via the magnetocaloric effect (MCE), which constitutes the adiabatic temperature changes $\pm \Delta T_{ad}$ derived from the entropy changes incurred upon application and removal of an external magnetic field H_{appl} [1]. in the vicinity of a magnetic transition. Cooling devices employing this effect are anticipated to achieve high efficiencies [2]; however, developing magnetocaloric materials with the appropriate properties is an ongoing challenge. The most advanced candidates include Gd metal and a variety of intermetallic compounds: Gd₅Si₂Ge₂, FeRh, La (FeSi)₁₃-based hydrides, certain MnNi-based Heusler-derived phases

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https://doi.org/10.1016/j.jallcom.2021.161150 0925-8388/© 2021 Elsevier B.V. All rights reserved. and MnFe pnictides. The compounds are often challenging to fabricate, can be mechanically or chemically unstable and may contain non-abundant or toxic elements [1,3]. Recently, the intermetallic ferromagnetic boride AlFe₂B₂ (also referred to as the 1–2–2 phase) has been contemplated as a promising magnetocaloric working material that avoids some of these drawbacks: it is straightforward to synthesize, is comprised of sustainable elements, is mechanically and chemically stable, and exhibits ΔT_{ad} (at $\mu_0 H_{app} = 2$ T) of 1–2 K with competitive thermal conductivity ($\kappa = 5.4$ Wm⁻¹ K⁻¹) [4–7]. The 1-2-2 magnetic phase transition temperature may be tuned over a broad temperature range (205 K \leq T_C \leq 320 K) [8–13] with small chemical modifications; these modifications also alter room-temperature lattice parameters of the 1-2-2 phase. This tunability is advantageous for the design of layered active magnetic regenerators incorporating a composite working material with a gradient of transition temperatures to allow for extended cooling capability. It has been recently reported that AlFe₂B₂ synthesized from the melt in the presence of very small amounts of gallium and/or germanium exhibits the highest magnetic transition temperature and magnetocaloric response for this compound [13]. This present work





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complements that earlier study through examination of the temperature-dependent lattice behavior underlying the MCE response in Ga-modified AlFe₂B₂.

The stoichiometric AlFe₂B₂ compound crystallizes in the orthorhombic Mn₂AlB₂ prototype structure and orders ferromagnetically at approximately 290 K with reported magnetic moments in the range $0.95-1.32 \mu_{\rm B}/{\rm Fe}$ [4,5,14] and an isothermal magnetic entropy change $-\Delta S_m$ (at $\mu_0 H_{app} = 2$ T) = 2.1–4.4 J kg⁻¹ K⁻¹. The magnetic transition and hence the isothermal magnetic entropy changes measured for the 1–2–2 compound family $[Al(Fe_{1-x}M_x)_2B_2, where M = Co, Mn, Ni,$ $x \le 0.1$] show characteristically broad peak widths of 60–80 K [11,14]. When processed with small amounts of Ga and Ge, the AlFe₂B₂ phase displayed an almost two-fold increase in the maximum magnetic entropy change values [13]. Because Ga and Ge were not detected in the lattice of the 1-2-2 compounds using a variety of highly sensitive probes, at the current time this increase is tentatively attributed to effects that Ga and Ge exert on solidification of the 1-2-2 phase from the melt that might result in antisite defects of Fe atoms on the Al sites of the crystal structure [13,17].

Initially reported by Jeitschko in 1969 [15], AlFe₂B₂ crystallizes in the orthorhombic Mn₂AlB₂-type structure and consists of two formula units wherein Fe and B atoms form corrugated Fe₂B₂ layers within the *ac* plane that are connected through an Al-atom spacer layer along the *b*-axis. Three significant interatomic distances are identified within the boron coordination polyhedron [16], as illustrated by double-headed arrows in Fig. 1(b). Here, $d_{(Al-Fe)}$ is the nearest-neighbor Al-Fe interatomic distance, while the $d_{(Fe-Fe)c-axis}$ distance is essentially the height of the iron trigonal prism (Fig. 1(c)) and is equivalent to the *c*-lattice parameter. The $d_{(Fe-Fe)ab-plane}$ interatomic distance lies in the base of the iron trigonal prism, which is coplanar with the *ab*-plane (Fig. 1(c)). Stoichiometric AlFe₂B₂ features an easy and a hard direction of magnetization along the orthorhombic *a*- and *c*-axes, respectively, with anisotropy constants $K_{[100]} = 1.25(13) \times 10^6$ ergs/cc, $K_{[010]} = 2.50(25) \times 10^6$ ergs/cc, and $K_{[001]} = 1.25(13) \times 10^7$ ergs/cc [17]. The magnitude of the magnetic entropy change is dependent upon the direction of the applied field, with $\Delta S_{\text{max,a}}(\text{at }\mu_0 H_{\text{app}} = 2 \text{ T}) = 3.6 \text{ J kg}^{-1} \text{ K}^{-1} \text{ and } \Delta S_{\text{max,c}}(\text{at }\mu_0 H_{\text{app}} = 2 \text{ T})$ 2 T) = 2.4 J kg⁻¹ K⁻¹ [6]. This anisotropic magnetocaloric response is accompanied by anisotropic thermal conductivities of κ_c = 6.8 \pm 0.3 W/mK, κ_a = 4.7 \pm 0.1 W/mK, and κ_b = 4.4 \pm 0.1 W/mK [7].



Fig. 1. Crystallizing in the space group *Cmmm*, the orthorhombic AlFe₂B₂ structure consists of layers of trigonal prisms within the (*ac*) plane formed by Fe atoms surrounding central B atoms. (a) These trigonal prismatic layers are stacked along the *b*-axis and are separated by layers of Al atoms. (b) Within the boron coordination polyhedron, three key interatomic distances are illustrated as double-headed arrows: $d_{(Al-Fe)}$, $d_{(Fe-Fe)c-axis}$ and $d_{(Fe-Fe)ab-plane}$. (c) The Fe trigonal prism within the B coordination polyhedra.

2. Experimental

Samples with the nominal starting compositions Al_{1.2}Fe₂B₂ (henceforth referred to as "AlFeB") and Al₁₁Ga₀₁Fe₂B₂ ("AlGaFeB") were synthesized by arc-melting from the elements (purity \geq 99.9 wt %) followed by heat treatment in an argon containing sealed quartz ampule at 1313 K for 72 h. Minor excess of Al beyond the stoichiometric content reduces formation of highly stable borides and maximizes the concentration of AlFe₂B₂ that forms peritectically [5]. Basic crystallographic and magnetic data of the two compounds, also see Ref. [13], are summarized in Table 1. Overall, both samples were confirmed by powder X-ray diffraction to be phase-pure within the limits of the technique and to crystallize in the orthorhombic Mn₂AlB₂-type structure, with the AlGaFeB sample exhibiting a slightly larger unit cell volume than that of the AlFeB sample. Relative to the AlFeB sample, the AlGaFeB sample exhibited a higher Curie temperature and a significantly sharper magnetic transition that delivered a 60% greater maximum magnetocaloric response [13]. The differences in the magnetic character of these two samples indicated a potential difference in their corresponding lattice behaviors and motivated examination of the thermal expansion of the AlFe₂B₂ lattice, particularly across the Curie temperature, $T_{\rm C}$.

To this end, temperature-dependent X-ray powder diffraction (XRD) measurements were performed in the range 100-320 K using a Rigaku TTRAX powder diffractometer equipped with a Mo K_{α} radiation source [18]. A small amount of Si powder was added to the samples as an internal standard. Lattice parameters and phase purities of the samples were determined with Rietveld refinement using GSAS-II [19]. The interatomic distances of interest, i.e. $d_{(Al-Fe)}$, $d_{(\text{Fe-Fe})c-axis}$ and $d_{(\text{Fe-Fe})ab-plane}$, were calculated using Visualization for Electronic and Structural Analysis (VESTA) software, employing the refined lattice parameters and coordinates of atoms, where Al is located in (0,0,0), Fe at $(0,y_1,1/2)$ and B at $(0,y_2,0)$ in space group *Cmmm* using $y_1 = 0.354$ and $y_2 = 0.207$ as initial approximations [19,20]. The atomic positions for Fe (y_1 ~0.354) and B (y_2 ~0.207) are reported to fluctuate in the 1-2-2 phase by approximately ~0.1% and ~0.2%, respectively [15,21]. Error in the reported values of the interatomic distance is ± 0.001 Å. The thermal expansion was quantified as strain $\varepsilon_l = \frac{l - l_{100K}}{l_{100K}}$, where l = a-, b- or c-parameters and $l_{100 \text{ K}}$ are the corresponding values at 100 K. At temperatures below T_c , the coefficients of thermal expansion (CTE, α) were calculated using the relationship $l = l_{100K}(1 + \alpha_1 T + \alpha_2 T^2)$. The volumetric coefficients of thermal expansion (α_v) were obtained from the relationship, $V = V_{100K}(1 + \alpha_v)$, where V_{100K} is the unit cell volume at T = 100 K.

Heat capacity measurements were performed using the heat capacity option of the Quantum Design PPMS apparatus in the range of $7 \le T \le 325$ K in zero applied magnetic field; the errors in heat capacity data are ~1%. The heat capacity was quantified using the thermal relaxation method, whereby the temperature response of a sample is ascertained when a known amount of heat is supplied to the sample for a fixed time followed by a cooling period of the same time [22].

3. Results

Data regarding the thermal expansion/contraction, Fig. 2, reveal that while the low-temperature lattice character along all three axes is very similar in both types of samples, significant differences occur at higher temperatures, in the vicinity of their magnetic transitions that are denoted as dotted lines in Fig. 2. This observation highlights the magnetoelastic entanglement of spin and lattice coupling in the 1–2–2 compound. In general, a simultaneous thermal expansion is observed along the *a*- and *b*-lattice directions and thermal contraction along the *c*-direction, all in a non-linear fashion, as the Curie temperature is approached (Fig. 2(a-c)). For T < 250 K no significant

Table 1

Summary of crystallographic & magnetic properties of annealed samples of nominal compositions Al_{1.2}Fe₂B₂ and Al_{1.1}Ga_{0.1}Fe₂B₂ (Ref. [13].).

Nominal starting chemical composition	Room-temperature crystallographic properties			Magnetic and Magnetocaloric properties			
	a (Å)	b (Å)	c (Å)	V (Å ³)	M (emu/g); 2% estimated error	$T_{C}(K)$	-ΔS (2 T) (J kg ⁻¹ K ⁻¹)
$Al_{1.2}Fe_2B_2$ ("AlFeB")	2.924(1)	11.029(1)	2.866(1)	92.42(1)	78 (50 K, 9 T) 69 (50 K, 2 T)	272	2.7
$AI_{1,1}Ga_{0,1}Fe_2B_2$ ("AlFeGaB")	2.927(1)	11.035(1)	2.870(1)	92.72(1)	84 (50 K, 9 T) 74 (50 K, 2 T)	290	4.4

differences are found in the thermal expansion/contraction behavior or in the CTE values in either sample, Table 2. The derivatives of strain with respect to temperature ($d\epsilon_1/dT$) of both samples display pronounced maxima or minima near the Curie temperatures along all three lattice directions (Fig. 2(d-f)); uniquely, those of the Gaprocessed specimen along the *a*- and the *b*-directions, but not along the *c*-direction, exhibit two maxima, with the lower-temperature maxima coincident with those of the Ga-free composition. Above T_C, the lattice contraction along the *c*-direction in AlGaFeB is more pronounced than that of AlFeB. This behavior is consistent with a greater elasticity in that direction, producing a likewise amplified $d\epsilon_1/dT$ in the vicinity of its magnetic phase transition.

The thermal evolution of the unit cell volume of the two specimens, Fig. 3, is particularly revealing. In both samples the anisotropic lattice behavior leads to a small but steady temperature-induced change in unit cell volume with volumetric coefficient of thermal expansion $\alpha_v \sim 7.9(5) \times 10^{-4} \text{ K}^{-1}$ (~ $0.5 \times 10^{-4} \text{ Å}^3/\text{K}$) for 100 K < T < 250 K that increases by almost 400% for T > 275 K to $\alpha_v \sim 3 \times 10^{-3} \text{ Å}^3/\text{K}$). While the CTEs of both specimens are nominally the same, the unit cell volume of the Ga-modified sample is consistently 0.3% larger than that of Ga-free sample up to the magnetic transition region. Outside of the magnetic transition region ($T > T_C$)

Table 2Coefficients of thermal expansion of AlFeB and AlGaFeB for $100 \,\text{K} < T < 250 \,\text{K}$.

Lattice parameter	AlFeB		AlGaFeB		
	$\alpha_1 \ge 10^{-6}$ (K ⁻¹)	α₂ x 10⁻⁸ (K ⁻²)	$\frac{\alpha_1 \times 10^{-6}}{(K^{-1})}$	α₂ x 10⁻⁸ (K ⁻²)	
а	-2.4 (0.2)	3.7 (0.7)	-5.2 (0.2)	4.5 (0.4)	
b	-7.1 (0.2)	6.1 (0.3)	-9.6 (0.2)	6.6 (0.5)	
с	15.4 (0.4)	-9.2 (0.1)	15.2 (0.4)	-8.3 (0.1)	

an approximately constant 0.2% difference in unit cell volume is maintained. Within the magnetic phase transition region itself, significant differences in the lattice behavior of the two types of sample are found. The Ga-modified unit cell volume displays two discontinuities: one that occurs at the Curie temperature of the Ga-free composition (~272 K) and the other at its previously documented Curie temperature of 290 K [13,14]. A region of lower and constant unit cell volume is noted between these two transition temperatures.

The heat capacity (C_p) data of both samples (Fig. 4) indicate a monotonic increase for both T < 225 K and for T > 300 K. In the intermediate vicinity of the magnetic transformation temperature



Fig. 2. (a, b, c) Thermal strain (ϵ_l) along the orthorhombic *a*, *b*, and *c* directions and (d, e, f) the corresponding derivatives of the strain ($d\epsilon_l/dT$) for AlFeB (open red symbols) and for AlGaFeB (filled black symbols). The vertical dotted lines denote the corresponding Curie temperatures [13]. The estimated standard deviations of the data are smaller than the size of the data markers.



Fig. 3. Temperature-dependence of unit cell volume of AlFeB (red open circles) and AlGaFeB (black filled squares) compounds. The dotted lines mark the corresponding Curie temperatures (T_c).



Fig. 4. Measured heat capacity for the AlFeB and AlFeGaB samples. The shaded areas are associated with the enthalpies of transformation (ΔH) for AlFeB (4.3 J/g) and AlFeGaB (7.1 J/g).

(225 K < T < 300 K) a broad heat capacity peak is observed for both samples, with $C_{p,peak}$ = 122 J/mole-K at T~270 K (AlFeB sample) and $C_{p,max}$ = 147 J/mole-K at T~290 K (AlGaFeB sample). The enthalpy of transformation of the AlGaFeB sample at ΔH = 7.1 J/g is 65% larger than that of the AlFeB sample (ΔH = 4.3 J/g), Fig. 4.

The thermal evolution of nearest-neighbor 1–2–2 interatomic interactions is illustrated in Fig. 5 by two previously described key interatomic distances, $d_{(Fe-Fe)c-axis}$ and $d_{(Fe-Fe)ab-plane}$. The $d_{(Fe-Fe)ab-plane}$ increases while $d_{(Fe-Fe)c-axis}$ decreases with increasing temperature. The magnitudes of the interatomic distance changes are $\Delta d_{(AI-Fe)} \sim +0.1\%$ (not shown), $\Delta d_{(Fe-Fe)ab-plane} \sim +0.5\%$ and $\Delta d_{(Fe-Fe)c-axis} \sim -0.5$. These anisotropic changes in bond distances approximately compensate each other through the magnetic transition to produce a nearly zero volumetric thermal expansion upon heating that may be visualized as a compression in the height and an expansion in the base of the Fe trigonal prism (Fig. 1(b)). For $T > T_C$ the interatomic distances of the Ga-containing change more than those of the Ga-free sample.

4. Discussion and conclusions

The structural and calorimetric data presented here indicate that the Ga-modified AlFe₂B₂ specimen undergoes a more abrupt lattice distortion through the magnetic transition region relative to its Gafree counterpart. Invoking the Ehrenfest classification of phase



Fig. 5. Temperature dependence of the interatomic distances $d_{(\text{Fe-Fe})\text{ab-plane}}$ and $d_{(\text{Fe-Fe})}$ c-axis for the AlFeB and AlGaFeB samples; the estimated error is ± 0.001 Å and dashed lines connecting data markers guide the eye. The vertical lines mark the corresponding Curie temperatures (T_c).

transformations, the Ga-modified specimen exhibits borderline firstorder-type transformation character [25], while the Ga-free specimen has a transition that is more of the second-order-type, although it may also be considered borderline (see heat capacity discussion below). This conclusion augments the previously reported higher saturation magnetization M_s and higher magnetic transition temperature of the Ga-modified sample to produce a notably enhanced magnetocaloric response. These observations are consistent with stronger magnetic exchange interactions within the Ga-modified sample lattice that provide enhanced resistance to volume expansion upon heating - a phenomenon commonly observed in materials systems with strong spin-lattice coupling [23,24]. This lattice stiffness diminishes when the Ga-modified specimen is in the paramagnetic state, as manifested by relatively larger interatomic distances (Fig. 5) in this temperature regime.

While the heat capacity of the two samples at the transition does not show distinct delta-type peaks of common first-order-type materials, it also does not show a clear lambda-type character as well. The calculated enthalpy change magnitude Δ H of the AlGaFeB sample is comparable to those of other magnetocaloric compounds, namely MnAs (Δ H ~ 9.5 J/g) and its compositional variants (Δ H of Mn_{0.94}Fe_{0.06}As = 8.6 J/g; Δ H of Mn_{0.94}Cu_{0.06}As = 6.3 J/g respectively). Additionally, the calculated enthalpy changes of the AlFeB and AlGaFeB samples are significantly larger than that found for the second-order magnetic materials such as Gd (Δ H = 0.3 J/g) [25]. The higher enthalpy change of the Ga-modified material suggests that it donates a stronger lattice contribution, given that the magnetic contributions of both samples should be nearly identical, (Figs. 2 and 3), based on their comparable saturation magnetization (Table 1).

These results are consistent with reports of differences in the 1-2-2 lattice and magnetic response when synthesized in the absence or in the presence of Ga, such as utilization of a Ga-containing flux [4,13,14,26]. The abrupt/discontinuous AlFe₂B₂ lattice change in the AlGaFeB sample upon heating near T_c and corresponding moderate magnetocaloric effect is consistent with the findings of Oey

et al. which show that magnetostructural coupling play a key role in inducing a large magnetocaloric response [26].

The origin of the enhanced lattice and magnetothermal response noted in the Ga-processed sample is attributed to iron antisite defects in which iron substitutes for Al in the 1-2-2 structure, increasing its overall concentration [17]. This hypothesis is supported by the conclusion that Fe-Fe bonding along the *c*-axis and within the (ab)-plane strongly influences the magnetic interactions in the structure [12]. It is proposed that the presence of Ga during synthesis of AlFe₂B₂ alters the solidification pathway from the melt to promote some iron enrichment in the final product. Overall, it is envisioned that these results enrich our understanding of the fundamental thermodynamic character of AlFe₂B₂ compounds that can play a key role in the development of room temperature magnetocaloric technologies.

CRediT authorship contribution statement

Brian T. Leieune: Validation, Formal analysis, Data Curation, Writing - Original Draft, Visualization, Radhika Barua: Writing -Original Draft, Writing – Review & Editing, Visualization, Yuroslav Mudryk: Investigation, Formal analysis, Writing - Review & Editing. Matthew J. Kramer: Conceptualization, Writing - Review & Editing. William McCallum: Conceptualization. Vitalij Pecharsky: Methodology, Resources, Writing - Review & Editing, Supervision. Laura H. Lewis: Conceptualization, Writing - Review & Editing, Supervision, Project Administration, Funding Acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.jallcom.2021.161150.

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