Critical behavior in tetragonal antiperovskite GeNFe$_3$ with a frustrated ferromagnetic state


Tetragonal GeNFe$_3$ has a second-order ferromagnetic (FM) to paramagnetic transition at 76 K. Our integrated investigations indicate that the ground FM state is frustrated and the tetragonal symmetry is retained below 550 K based on the results of variable temperature X-ray diffraction. Critical behavior was analyzed by a systematic bulk magnetization study. The estimated critical exponents by three different methods (modified Arrott plot, the Kouvel–Fisher method, and critical isotherm analysis) conformably suggest that long-range magnetic coupling described by mean-field (MF) theoretical model is dominant in GeNFe$_3$. The experimental $M$–$T$–$H$ data collapse into two independent branches according to the scaling equations $m = f_s(h)$ with the renormalized magnetization $m = e^{-[H/H(\beta)]}$ and the magnetic field $h = H_0 - (4\pi T)$. The exchange distance is estimated as $J(r) \sim r^{-4.8}$ on the basis of the $\beta$ and $\gamma$ values, which lies between the long-range MF model ($r^{-4.5}$) and the short-range 3D Heisenberg (3DH) model ($r^{-5}$).

Our results indicate that the competition between local magnetic moments of iron 3d electronic state and itinerant covalent interactions of N–Fe bonds should be responsible for critical behavior in this system.

1. Introduction

Magnetic phase transition is a core concept in the magnetism realm. The investigation of critical behavior can give us some important information about the thermodynamics observable near the quantum transition. Recently, antiperovskite structured nitrides have been attracting significant attention because they are promising candidates for functionality and the interesting magnetic states strongly depend on nitrogen stoichiometry and the interesting magnetic states strongly depend on nitrogen stoichiometry and crystal structures. It is well known that antiperovskites are one kind of important itinerant electronic compounds, but one critical question is what the real mechanism is of magnetic interactions of 3d transition metal containing some local magnetic moments. Although several theoretical modes, such as short-range Heisenberg or RKKY, have been adopted, there is still no universal one to describe it. In addition, previous studies on critical behavior of cubic antiperovskites with a space group of $Pm\bar{3}m$ indicate different behaviors and mechanisms. In AlCMn$_3$, the critical exponents are close to those expected by the mean-field (MF) model, indicating a long-range ferromagnetic (FM) interaction, while the critical parameters in CuNMn$_3$ behave differently below and above $T_c$, and may be attributed to magnetic fluctuations. Considering the fact that the type of order and the temperature of the magnetic transitions of antiperovskites are much sensitive to chemical doping or lattice or bond distance, studies on the magnetic properties of these distorted structures are required, which may uncover the mechanism of magnetic interactions in itinerant electronic antiperovskites.

Similar to the case of manganese-based antiperovskite, iron-based ANFe$_3$ ($A = Ga, Sn, In, etc.$) often crystallizes in a cubic structure with a space group of $Pm\bar{3}m$. But lattice distortion frequently appears if the compound contains the element Ge on the edge of metal and semimetal. Actually, GeNFe$_3$ shows tetragonal symmetry at room temperature with a space group of $I4/mcm$. However, its magnetic properties are unknown except for structure information. Previous studies have revealed that the 3d transition metal electrons are the main source of carriers and play a significant role in affecting the magnetic properties which are sensitive to local bond distances or bond angles in distorted structures. It indicates that GeNFe$_3$ is special because tetragonal $I4/mcm$ phase is more complicated in local structure and iron occupancy compared with cubic phase. And the critical behavior has been considered to be a useful tool to detect the magnetic interaction mechanism of FM systems including some antiperovskites. Considering the fact that the local structure is very critical that affects electronic structure and physical properties in antiperovskite compounds, it will be a challenge to investigate the critical behavior of distorted...
antiperowskites differing from the usual cubic symmetry. In this work, we report the structure and magnetic properties of GeFe₃, with a critical behavior. GeFe₃ shows a second-order magnetic transition. The critical exponents are close to the theoretical prediction of the MF model, except that β and γ are slightly larger than theoretical values, indicating a long-range magnetic coupling. The magnetic interaction distance decays as \( f(r) \sim r^{-4.8} \), which lies between that of the MF model \( r^{-1.5} \) and 3D Heisenberg (3DH) model \( r^{-2} \). The competition between long-range magnetic interaction and short-range magnetic interaction should be responsible for the critical behavior.

II. Experimental details

A polycrystalline sample of GeFe₃ was prepared by the solid-state reaction method by mixing powders of GeO₂(5N) and Fe(3N) in flowing NH₃ atmosphere. The starting materials were mixed in the desired proportions and then annealed at 923–973 K for 10 hours in flowing NH₃ atmosphere \( (500 \text{ cc min}^{-1}) \). After quenching to room temperature, the products were pulverized, mixed, pressed into pellets, and annealed again for two days in order to obtain homogeneous samples. This process was repeated two times to improve the quality. X-ray diffraction (XRD) studies were performed at room temperature using an X-ray diffractometer with Cu Kα radiation \( (\lambda = 0.15406 \text{ nm}) \) to determine the crystal structure. Variable temperature XRD was performed by using a Rigaku D/max-\( \gamma \)α diffractometer employing high-intensity Cu Kα radiation, up to 550 K, performed at the High Magnetic Field Laboratory of the Chinese Academy of Sciences, Hefei. The magnetization was measured by using a Quantum Design superconducting quantum interference device (SQUID) magnetometer \( (1.8 \text{ K} \leq T \leq 400 \text{ K}, 0 \leq H \leq 50 \text{ kOe}) \). The sample was processed to an ellipsoid shape and the field was applied parallel to the longest semiaxis of each sample to decrease the demagnetization field as much as possible. Isothermal magnetization and the demagnetization factor, respectively. The calculated \( H_i \) was used for analysis of the critical behavior.

III. Results and discussion

Fig. 1(a) sketches the crystal structure of GeFe₃. Ge and N are located at the Wyckoff sites 4b \((0, 0.5, 0.25)\) and 4c \((0, 0, 0)\), respectively, while Fe occupies the two nonequivalent sites, Wyckoff site Fe1: 4a \((0, 0, 0.25)\) and Fe2: 8h \((0.23, 0.73, 0)\), as shown in Fig. 1(a). And Ge, N, and Fe1 atoms collapse in a straight line along the \( c \) axis. While Fe2 atom is nonlinear and there is a clear perturbation along the \( c \) axis. By using the optimized methods after trying to tune the controlling parameters as mentioned above, we chose the best sample in this study. Fig. 1(b) presents the room temperature XRD pattern and the Rietveld refined data for pulverized powder of GeFe₃. The diffraction patterns can be well described by tetragonal symmetry \( (\text{space group: } I4/mcm) \), and no secondary phase was detected, indicating GeFe₃ is single phase in the present work. The refined lattice parameters turn out to be \( a = 5.3053 \pm 0.0004 \text{ Å} \) and \( c = 7.763 \pm 0.0007 \text{ Å} \), which are consistent with previous results,\(^{14}\) demonstrating the sample is good in quality and actual nitrogen content should be close to the nominal one. Temperature-dependent magnetization \( M(T) \) \( (\text{left axis}) \) and inverse susceptibility \( \chi(T)^{-1} \) \( (\text{right axis}) \) curves of GeFe₃ under a field of \( H = 100 \text{ Oe} \) are shown in Fig. 2(a). Obviously, the curves between zero-field cooling (ZFC) and field cooling (FC) exhibit a sharp decrease near a temperature defined as \( T_c \) \( (\text{left axis}) \).

In addition, a bifurcation appears between ZFC and FC curves at an irreversibility temperature \( T_{irr} \) \( (\text{defined by the temperature of } M_{ZFC} = M_{FC}) \), and the ZFC curve exhibits a peak around a temperature \( T_f \) \( (\text{defined by the maximum value of } M_{ZFC}) \) below \( T_c \). Meanwhile, we find that the isothermal \( M(H) \) curve at 5 K exhibits hysteresis behavior but without any signature of saturation up to \( H = 45 \text{ kOe} \), as shown in the inset of Fig. 2(a). These behaviors indicate a competition between different magnetic couplings.\(^{16}\) Especially, the paramagnetic (PM) state was observed because of the linear \( M(H) \) curve at 150 K. In order to get more information about the magnetism of GeFe₃, we made a well fitted \( \chi^{-1}(T) \) curve by using the modified Curie–Weiss law: \(^{17}\) \( \chi^{-1}(T) = \left( C_\text{m} \times (T - \theta) \right)^{-1} + \chi_p \) \( \text{right axis in Fig. 2(a)} \), where \( C_\text{m} \) stands for the Curie constant, \( \theta \) is the Weiss temperature, and \( \chi_p \) is an temperature-independent term, contributed by Pauli paramagnetism. Correspondingly, the values of the parameters were obtained as follows: \( C_\text{m} = 0.1192 \text{ emu K mol}^{-1} \), \( \theta = 77.6 \text{ K} \), \( \chi_p = 2.71 \times 10^{-3} \text{ emu mol}^{-1} \). The effective paramagnetic moment per Fe atom, \( p_{\text{eff}} \), is estimated to be 0.56 \( \mu_B \) from the relationship \( p_{\text{eff}} = 2.83(C_\text{m}H)^{0.5} \mu_B \), where \( n \) is the number of magnetic atoms in a unit cell and equal to 3 in the present case. In Fig. 2(b), with increasing magnetic field \( H \), both \( T_f \) and \( T_{irr} \) shift to lower temperature, indicating a possible frozen state. As shown in the inset of Fig. 2(b), the field dependence of \( T_c \) can be well described by the \( H^{2/3} \) law, which was discovered in many spin-frozen systems such as U₃IrSi₃.\(^{18}\)

Frequency dependence of AC susceptibilities \( \chi(T) \) was measured to characterize the dynamics of spin glass (SG) state in GeFe₃.
In Fig. 2(c) and (d), both $w_0(T)$ and $w_{00}(T)$ exhibit strongly frequency-dependent peaks. The relaxation time is described by a power law $t = t_0[1/T_f - 1/T_0]^{zv}$, where $T_f$ is the freezing temperature, $t_0$ is the characteristic flipping time, $t_0$ is the relaxation time $[t = 1/(2\pi f)]$, and $zv$ is the dynamical critical exponent. All the parameters ($T_0 = 40.5$ K, $zv = 4.86$, $t_0 = 4.33 \times 10^{-12}$ s) are obtained by fitting the power law as displayed in the inset of Fig. 2(c), indicating a conventional SG.\(^{19}\) In addition, isothermal remanent magnetizations ($M_{\text{IRM}}$) were measured on cooling the sample from 200 to 5 K in ZFC process. \(H\) was applied for up to 5 min at which point the field was switched off, and the time decay of $M_{\text{IRM}}$ was recorded. The data are fitted according to the formula $M_{\text{IRM}}(t) = M_0 - \alpha \ln(t)$ as shown in Fig. 3(a–e). The fitting parameters $M_0$ and $\alpha$, plotted in Fig. 3(f), increase with $H$ up to 300 Oe, and then reach saturation. These results for $\chi'(T)$ and $M_{\text{IRM}}(t)$ confirm a magnetic frozen behavior below the FM–PM transition in GeNFe\(_3\).\(^{20}\)

Fig. 2 (a) Temperature-dependent $M(T)$ and inverse magnetization $\chi^{-1}(T)$ of FC curve for GeNFe\(_3\). The inset shows the $M(H)$ curves at 5 K and 150 K. (b) $M(T)$ curves under ZFC/FC processes at different $H$. The inset displays $T_f$ as a function of $H^{2/3}$. (c and d) Temperature dependence of AC susceptibility $\chi_{\text{AC}}(T)$ at several fixed frequencies: (c) real components. The inset presents the best fit by a power law; (d) the imaginary parts.

Fig. 3 (a–e) $M_{\text{IRM}}$ vs. $t$ at different $H$ and the solid lines are fitted by $M_{\text{IRM}}(t) = M_0 - \alpha \ln(t)$: (a) for 50 Oe; (b) for 100 Oe; (c) for 300 Oe; (d) for 500 Oe; (e) for 1000 Oe. (f) The fitted parameters $M_0$ and $\alpha$ as a function of $H$.\(^{20}\)
Fig. 4 (a) XRD patterns for GeNFe$_3$ at different temperatures. (b) Temperature-dependent lattice parameters $a$ and $c$ for GeNFe$_3$. The inset shows the volume $V$ as a function of $T$. 

Fig. 5 (a) The initial isothermal magnetization around $T_c$. (b) Arrott plots of $M^2$ vs. $H/M$.

From this sense, the mathematical definitions of exponents obtained

divergence of correlation length transition can be described by a series of critical exponents. The $H$ to the $(a)$ are fitted with a linear function and then extrapolated

unknown at present. In general, structure transition is first order in type. These XRD data indicate that there is no structural transi-

tion and that the FM–PM phase transition in tetragonal GeNFe$_3$ may be a second-order phase transition. To confirm this, in Fig. 5(a) and (b), the isothermal $M(H)$ curves in the vicinity of $T_c$ and Arrott plots ($M^2 - H/M$) are shown. The $M^2$ vs. $H/M$ curves present quasi-

straight lines with positive slopes in high fields, clearly indicating a second-order transition. The magnetic results are consistent with the above structural analysis. Based on the data, critical behavior is studied around $T_c$ for GeNFe$_3$. Usually, a second-order magnetic transition can be described by a series of critical exponents. The divergence of correlation length $\xi = \xi_0(T_c - T)^{\beta/\nu}$ leads to universal scaling laws for the spontaneous magnetization $M_{sp}$ and initial susceptibility $\chi_0$. The high-field portions of the Arrott plots (see Fig. 5(b)) are fitted with a linear function and then extrapolated to the $H/M = 0$ and $M^2 = 0$ axes to obtain $M_{sp}$ and $\chi_0$, respectively. In this sense, the mathematical definitions of exponents obtained from $M(H)$ curves can be presented as follows:\textsuperscript{1,22}

$$M_{sp}(T) = M_0(1 - \xi^\beta)^{\nu/\beta}, \quad \xi < 0, \quad T < T_c,$$

$$\chi_0(T)^{-1} = (h_0/M_0)^{\nu/\beta}, \quad \xi > 0, \quad T > T_c, \quad (2)$$

$$M = DH^{2/\beta}, \quad \xi = 0, \quad T = T_c, \quad (3)$$

where $\xi = (T - T_c)/T_c$ is the reduced temperature; $M_0/h_0$ and $D$ are critical amplitudes. The parameters $\beta$, $\gamma$, and $\delta$ are the critical exponents. By fitting to $M_{sp}(T)$ and $\chi_0(T)$ data using eqn (1) and (2), in Fig. 6(a), $\beta$ and $\gamma$ are obtained as $\beta = 0.512 \pm 0.004$ with $T_c = 71.57 \pm 0.02$ and $\gamma = 1.233 \pm 0.03$ with $T_c = 71.05 \pm 0.16$. The critical temperature $T_c$, estimated from the modified Arrott plot (MAP), is basically consistent with that of the $dM/dT$ curve.

The critical exponents can also be determined by the Kouvel–Fisher (KF) method:\textsuperscript{23}

$$M_{sp}(T)/[dM_{sp}(T)/dT] = (T - T_c)/\beta, \quad (4)$$

$$\chi_0^{-1}(T)/[d\chi_0^{-1}(T)/dT] = (T - T_c)/\gamma. \quad (5)$$

According to eqn (4) and (5), $M_{sp}[dM_{sp}/dT]$ and $\chi_0^{-1}[d\chi_0^{-1}/dT]$ vs. $T$ generate straight lines with slopes $1/\beta$ and $1/\gamma$, respectively. The KF plots are displayed in Fig. 6(b). The estimated $\beta$ and $\gamma$ values are $\beta = 0.54 \pm 0.001$ with $T_c = 71.76 \pm 0.121$ and $\gamma = 1.205 \pm 0.03$ with $T_c = 71.21 \pm 0.17$, which are consistent with those derived from the MAP. The critical exponents should follow the scaling equation. Based on the theory of scaling equation, in the asymptotic critical region, the magnetic equation is written as follows:\textsuperscript{1}

$$M(H, \xi) = \varepsilon^\xi f_\xi(H/e^{\beta r}), \quad (6)$$

where $f_\xi$ are regular functions with $f_0$ for $T > T_c$ and $f_0$ for $T < T_c$. With the renormalized magnetization as $m = \varepsilon^\xi M(H, \xi)$, and the renormalized field as $h = H e^{-\beta r}$, eqn (6) is $m = f(h)$, which indicates that $m$ vs. $h$ forms two universal curves for $T > T_c$ and $T < T_c$, respectively. Based on this scaling equation, $m(h)$ curves around $T_c$ are plotted in Fig. 6(c), where the magnetization data are located in two universal curves. Alternatively, the exponents
are confirmed by plotting $m^2$ vs. $h/m$ curves as shown in the inset of Fig. 6(c). It can be found that all the magnetization data collapse into two independent branches. These phenomena indicate the reliability of the critical exponents in the present work. Meanwhile, the exponent $\delta$ is determined from a critical isotherm $M(H)$ curve. Fig. 6(d) displays the $M(H)$ curve at $T = 71$ K and the inset shows the plot on a log$_{10}$–log$_{10}$ scale. The log$_{10}(M)$–log$_{10}(H)$ relation yields a straight line with slope $1/\delta$ at high field, which gives $\delta = 3.064 \pm 0.006$. Additionally, $\delta$ is estimated by the Wisdom scaling relation ($\delta = 1 + \gamma/\beta$), given the values of $\beta$ and $\gamma$. The value of $\delta$, estimated by taking the $\beta$ and $\gamma$ values from the MAP method and the KF method, turns out to be $3.41 \pm 0.02$ and $3.23 \pm 0.05$, respectively. The values of $\delta$ are close and not dependent on method. All these results indicate that the obtained critical exponents are reliable and precise.

The obtained critical exponents of GeNFe$_3$, as well as those from different theoretical models, are listed in Table 1 for comparison. It can be seen that the experimentally deduced exponents are close to those of the MF model, indicating a long-range interaction of Fe–Fe. However, the values of $\beta$ and $\gamma$ are slightly larger than the theoretical values of the MF model. To further understand $\beta$ and $\gamma$, it is very important to examine the convergence of the critical exponents. Thus the effective exponents $\beta_{\text{eff}}$ and $\gamma_{\text{eff}}$ are obtained as:

$$\beta_{\text{eff}}(\varepsilon) = \frac{d \ln M(\varepsilon) / d \ln \varepsilon}{d \ln X_0^{-1}(\varepsilon) / d \ln \varepsilon}$$

$$\gamma_{\text{eff}}(\varepsilon) = \frac{d \ln M^0(\varepsilon) / d \ln \varepsilon}{d \ln X_0^{-1}(\varepsilon) / d \ln \varepsilon}.$$  

$\beta_{\text{eff}}$ and $\gamma_{\text{eff}}$ vs. the reduced temperature $\varepsilon$ are plotted in Fig. 7. We can see that $\beta_{\text{eff}}$ and $\gamma_{\text{eff}}$ are convergent to the values $\beta_{\text{eff}} \approx 0.48$, $\gamma_{\text{eff}} \approx 1.08$ when the temperature approaches $T_c$. As is known, the magnetic phase transition depends mainly on the exchange interaction $J(r)$ for a homogeneous magnet. A renormalization group theory analysis suggests long-range attractive interactions decay as $J(r) \propto r^{-(d-\sigma)}$, where $d$ and $\sigma$ are the spatial dimension and a constant, respectively. Generally,

$$\gamma = 1 + \frac{4(n+2)}{d(n+8)} \Delta \sigma + \frac{8(n+2)(n-4)}{d^2(n+8)^2} \Delta \sigma^2.$$  

$$(7)$$

### Table 1: Comparison of critical exponents of GeNFe$_3$ with different theoretical models: MAP method, KF method and critical isotherm (CI) analysis

<table>
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<tr>
<th>Composition</th>
<th>Ref.</th>
<th>$T_c$ (K)</th>
<th>$\beta$</th>
<th>$\gamma$</th>
<th>$\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GeNFe$_3$ (MAP)</td>
<td>This work</td>
<td>71.31</td>
<td>0.512 ± 0.004</td>
<td>1.233 ± 0.03</td>
<td>3.41 ± 0.02</td>
</tr>
<tr>
<td>GeNFe$_3$ (KF)</td>
<td>This work</td>
<td>71.45</td>
<td>0.54 ± 0.01</td>
<td>1.205 ± 0.003</td>
<td>3.23 ± 0.05</td>
</tr>
<tr>
<td>GeNFe$_3$ (CI)</td>
<td>This work</td>
<td>71</td>
<td>—</td>
<td>1.0</td>
<td>3.064 ± 0.006</td>
</tr>
<tr>
<td>Tricritical MF model</td>
<td>33</td>
<td>—</td>
<td>0.25</td>
<td>1.0</td>
<td>5.0</td>
</tr>
<tr>
<td>MF model</td>
<td>34</td>
<td>—</td>
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<td>1.24</td>
<td>4.82</td>
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localized ferromagnetism (itinerant state). In cubic AlCMn₃, the competitions exist between localized and itinerant ferromagnetic interaction and a branching of ZFC and FC range ferromagnetic interaction and a branching of ZFC and FC.

Theoretical investigations have demonstrated that the density of states at the Fermi level is predominantly contributed by 3d electrons. However, there exists a strong hybridization of 3d states with nitrogen 2p states, which widens the bandwidth of 3d states, and thus the itinerant magnetic mechanism is estimated. Besides, the obtained saturated magnetic moments (0.23 μB/Fe) are lower than that of the localized Fe ions in perovskite oxides (2–3 μB/Fe), which indicates an itinerant characteristic of carriers in GeNFe₃. Thus, the wide bandwidth of iron 3d states should be an important factor responsible for the long-range magnetic coupling and short-range magnetic coupling. The result of the long-range interaction in this system is consistent with the previous theoretical calculation in antiperovskites. Theoretical investigations have demonstrated that the density of states at the Fermi level is predominantly contributed by 3d electrons. However, there exists a strong hybridization of 3d states with nitrogen 2p states, which widens the bandwidth of 3d states, and thus the itinerant magnetic mechanism is estimated. Besides, the obtained saturated magnetic moments (0.23 μB/Fe) are lower than that of the localized Fe ions in perovskite oxides (2–3 μB/Fe), which indicates an itinerant characteristic of carriers in GeNFe₃. Thus, the wide bandwidth of iron 3d states should be an important factor responsible for the long-range magnetic interaction and a branching of ZFC and FC.

Critical fluctuation formation. In tetragonal GeNFe₃, Fe atoms occupy two nonequivalent sites and the bond distances between Fe1–Fe1 (Fe1–N) and Fe2–Fe2 (Fe2–N) are different (rFe1–Fe1 = 0.375 nm, rFe2–Fe2 = 0.266 nm, rFe1–Fe2 = 0.270 nm, rFe1–N = 0.194 nm, and rFe2–N = 0.188 nm). The anisotropy of tetragonal phase structure plays an important role, meaning it can be easier to form magnetic disorders than isotropy of the cubic phase. Thus, the competition among various magnetic interactions is generated. It is expected that some non-collinear or antiferromagnetic components will emerge, then one frustrated state will be induced. Many such examples can be found in previous reports. In GaNFe₃, which has cubic symmetry, an antiferromagnetic ground state has been revealed at lower temperatures. While in tetragonal GeNFe₃, the frustrated FM state suggests the existence of unstable AFM interactions. In addition, there is a perturbation from atom Fe2 along the c axis direction (Fig. 1(a)). It is reasonable that the structural perturbation from atom Fe2 will lead to the magnetic perturbation, which may be another factor for the frustrated FM state in tetragonal GeNFe₃.

IV. Conclusions

In summary, tetragonal GeNFe₃ was found to be a frustrated FM state and transits into a PM one at 76 K, investigated by structural and magnetic analysis. Critical behavior was analyzed by a systematic bulk magnetization study. The critical exponents (β, γ, and δ) were estimated reliably by three independent methods, namely modified Arrott plot, Kouvel–Fisher method, and critical isotherm analysis. The studies on critical behavior indicate that the interaction distance follows $j(r) \propto r^{-4.8}$ on the basis of the credible critical parameters. The competition of local magnetic moments of iron 3d electronic state and itinerant covalent interactions of N–Fe bonds should be responsible for the observed frustrated state in GeNFe₃.

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References


