Itinerant metamagnetic transition in the ferromagnet LuCo₃ induced by high field: Instability of the 3*d*-electron subsystem

D. S. Neznakhin [1,*] D. I. Radzivonchik,[2] D. I. Gorbunov,[3] A. V. Andreev,[4] J. Šebek [4]
A. V. Lukoyanov [2,1] and M. I. Bartashevich [1]

[1]*Ural Federal University, 620002 Ekaterinburg, Russia*

[2]*M.N. Miheev Institute of Metal Physics, Ural Branch of the Russian Academy of Sciences, 620108 Ekaterinburg, Russia*

[3]*Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany*

[4]*FZU Institute of Physics, Czech Academy of Sciences, 18221 Prague, Czech Republic*

LuCo₃ is an itinerant ferromagnet whose magnetic properties strongly depend on the position of the 3*d* electronic states relative to the Fermi level. Here, we report on the magnetization of a LuCo₃ single crystal in pulsed magnetic fields up to 58 T. We find a field-induced phase transition just below 50 T from a low-spin to a high-spin state. The transition shows a pronounced anisotropy of the magnetization jump and hysteresis. A series of *ab initio* calculations based on the density functional theory show that the transition is due to a significant change in the occupancies of the Co 3*d* electronic states. At the same time, some features in the majority spin density of the Co 3*d* states are slightly modified and pass through the Fermi level when the spin state is changed, which leads to the instability of the 3*d*-electron subsystem. Thereby, the applied magnetic field causes a significant redistribution in the majority and minority spin states in the Co 3*d* subsystem, which results in the sharp change in the magnetization.

I. INTRODUCTION

Binary intermetallic compounds based on rare-earth (*R*) elements and cobalt combine two principally different types of electrons. The 4*f* electrons are localized, whereas the 3*d* electrons are partly itinerant and participate in conduction. As such, the Co atoms carry different ordered magnetic moments as a function of the stoichiometry due to a variable filling of the 3*d* band [1]. The *R*-rich compounds (*R*₃Co) show a paramagnetic behavior where *R* is a nonmagnetic element, e.g., Y, La or Lu [2]. On the other hand, the Co-rich compounds (*R*₂Co₁₇) with Y and Lu are ferromagnetic with a magnetic moment of $1.6\,\mu_B$/Co (metallic cobalt has $1.7\,\mu_B$/Co). The compounds with an intermediate Co content (*R*Co₂ and *R*Co₃) show the most interesting physics. Here, the Co magnetic moment substantially depends on the *R* sublattice. The *R*Co₂ compounds are paramagnets for *R* = Y, Ce, Lu [3–5], ferromagnets for *R* = Pr, Nd [5], and ferrimagnets for *R* = Gd, Tb, Dy, Ho, Er, Tm [5]. The strong dependence of the Co moment on the *R* sublattice can be observed most clearly for ErCo₂. The ferrimagnetic order of this material abruptly collapses at the Curie temperature, $T_C = 31\,K$, when the Er 4*f* states can no longer sustain the induced magnetic moment of the Co 3*d* electrons [4]. Ferri- or ferromagnetic ordering can also be realized in the *R*Co₃ [6,7] compounds. The magnetic moments of the *f* and *d* elements and *f*-*d* exchange interaction play a major role in the formation of the magnetic state in *R*Co₃ too.

In this respect, the *R*Co₂ and *R*Co₃ compounds are of great interest. It is necessary to know the magnetic properties of the Co sublattice to understand those of the *R* sublattice in *R*Co₃.

The magnetic properties of the Co sublattice can be studied, e.g., on YCo₃ since Y is nonmagnetic. This material crystallizes in a trigonal structure of PuNi₃ type (space group $R\bar{3}m$) in which the Co atoms occupy three inequivalent positions. YCo₃ is a ferromagnet with the Curie temperature of 301–310 K [6,8,9]. Neutron-scattering measurements revealed a strong dependence of the Co moment on local surroundings, with the Co moments varying from about 0.4 to $1.0\,\mu_B$ [8,10]. Magnetization measurements of a polycrystal in fields up to 110 T uncovered two metamagneticlike anomalies at 60 and 82 T [11]. It was suggested that the first-order transitions occur successfully on different Co sites. In Ref. [10] it was shown that for YCo₃, both the ferrimagnetic and ferromagnetic ground states can be realized since their energies have similar values. For ferrimagnetic YCo₃ the magnetic transitions occur in two stages: magnetic moments of Co atoms in one of three inequivalent positions change from antiparallel to nonmagnetic at the first transition and then to ferromagnetic at the second transition. It was also suggested that all cobalt atoms are in a ferromagnetic state and the transitions occur due to a change in the state of cobalt from a low-spin (LS) state to a high-spin (HS) state [9,11]. For example, transitions from the LS to the HS state are observed in the ThCo₅ [12], Y(Co, Ni)₅ [13] and YCo₅ [14] ferromagnets. Magnetostriction measurements of the (Y₁₋ₓNdₓ)Co₃ compounds can be another confirmation of the ferromagnetic state in YCo₃. In the system (Y₁₋ₓNdₓ)Co₃ the critical fields

---

of the metamagnetic transitions are reduced as compared to YCo_3 due to the influence from the exchange field from the magnetic Nd sublattice. It was found that the volume magnetostriction is positive at both transitions [15]. This supports the earlier interpretation that the Co magnetic moment increases at both transitions. In the case of the collapse of the Co moment, as suggested in Ref. [11] for the first metamagnetic transition, one can expect negative volume magnetostriction, as observed in $(Er_{1-x}Lu_x)Co_2$ [16].

It is more appropriate to study the $LuCo_3$ compound to elucidate the magnetic properties of the Co sublattice in RCo_3 materials with magnetic heavy rare-earth elements. The reason is the atomic radius of Lu (1.75 Å), being closer to those of Er and Tm (1.75–1.76 Å), as compared to the atomic radius of Y (1.81 Å). Such a small difference could be important for the exchange interactions. The magnetic properties of $LuCo_3$ were studied rather briefly on polycrystals. It has a spontaneous magnetic moment of about $M_s = 1.8 \mu_B$, an uniaxial magnetic anisotropy with anisotropy field $\mu_0 H_a = 10$ T at 20 K and Curie temperature $T_C = 362$ K [17]. Indeed, the significantly higher Curie temperature of $LuCo_3$ as compared to YCo_3 shows how sensitive cobalt is to the local coordination.

Investigations of strongly anisotropic materials require single crystalline samples. We grew a $LuCo_3$ single crystal and performed magnetization measurements in pulsed magnetic fields up to 58 T. We found field-induced phase transitions for field applied along the easy and hard magnetization directions just below 50 T. Our density functional theory calculations suggest that the transitions are due to feature in the majority density of the Co $3d$ states near Fermi level.

II. EXPERIMENTAL AND CALCULATION DETAILS

A $LuCo_3$ single crystal was grown by a modified Czochralski method in a three-arc furnace from the high-purity elements Lu (99.9%) and Co (99.99%). The pulling of the crystal was done under argon protecting atmosphere at a speed of 15 mm/h, a tungsten rod was used as a seed. The result was a single crystal with a diameter of 5 and a length of 15 mm. X-ray powder diffraction analysis and energy-dispersive x-ray spectroscopy showed that the synthesized compound has less than 0.5 wt. % of the impurity phase $LuCo_2$. $LuCo_3$ has a trigonal crystal structure of $PuNi_3$ type (space group $R\bar{3}m$) with the lattice parameters $a = 4.956$ Å and $c = 24.126$ Å. The Lu and Co atoms occupy two and three crystallographically nonequivalent sites, respectively [Fig. 1(a)]. A backscattered Laue diffraction pattern along the [001] axis of the crystal is shown in Fig. 1(b). The [001] axis is a threefold axis (identical directions are shown by arrows), which confirms the trigonal structure of $LuCo_3$.

Magnetization measurements in static magnetic fields up to 7 T between 2 and 380 K were performed using MPMS-XL7 EC. Magnetization in pulsed fields up to 58 T was measured at the Dresden High Magnetic Field Laboratory by the induction method using a coaxial pickup coil system. Absolute values of the magnetization were calibrated using static-field data. The high-field magnetometer is described in detail in Ref. [18].

To investigate the electronic and magnetic properties of $LuCo_3$, the QUANTUM ESPRESSO software package [19,20]

was used. The Perdew-Burke-Ernzerhof generalized gradient approximation for the exchange-correlation potential with spin polarization and projector augmented wave method were employed. The energy limit of 60 Ry for plane waves was used for achieving sufficient convergence in the self-consistency cycle in our calculation. The integration in reciprocal space was performed by tetrahedron method of the Bloechl's version over an $8 \times 8 \times 8$ $\boldsymbol{k}$-point grid.

III. RESULTS AND DISCUSSION

A. Magnetic measurements

$LuCo_3$ displays a uniaxial magnetic anisotropy. The spontaneous magnetic moment along the easy [001] axis is $M_s = 1.77 \mu_B$ [Fig. 2]. This gives $0.59 \mu_B$ for the average Co magnetic moment. For comparison, the spontaneous magnetic moment is $1.8 \mu_B$ for polycrystalline YCo_3 [11], for a single crystal this value is lower, $M_s = 1.50 \mu_B$ [9]. However, given the strong sensitivity of the ordered magnetic moments to the local surroundings, Co atoms in different crystallographic positions of $LuCo_3$ likely carry different moments, similar as

FIG. 1. Crystal structure of $LuCo_3$ (a) and backscattered Laue diffraction pattern of the $LuCo_3$ single crystal along the [001] axis (b).
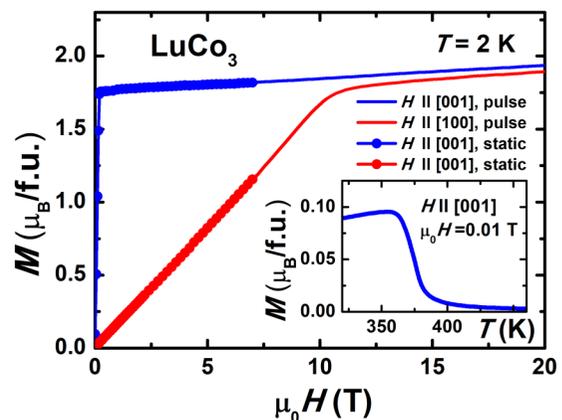
FIG. 2. Magnetization for field applied along the [100] and [001] axes of $LuCo_3$ at 2 K. The inset shows temperature dependence of magnetization of $LuCo_3$ for field applied along the [001] axis at $\mu_0 H = 0.01$ T.

was found for YCo$_3$ [8,10]. The [100] axis is the hard magnetization direction. At 2 K, the anisotropy field is $\mu_0 H_a = 10.5$ T, which is larger than that of YCo$_3$, $\mu_0 H_a = 8.2$ T [11].

The Curie temperature is determined from $M(T)$ measurements in a field of 0.01 T. It is equal to 376 ± 5 K [inset in Fig. 2], which is close to the value obtained for a polycrystalline LuCo$_3$ sample, 362 K [17]. As pointed out in Ref. [21], the Curie temperature of LuCo$_3$ decreases with increasing pressure at a rate of $dT_C/dP = -2.3$ K/0.1 GPa due to a weakening of the exchange interactions with decreasing volume of the unit cell. Since the unit cell volume of LuCo$_3$ is smaller than that of YCo$_3$, it is logical to expect that T_C of the latter compound should be higher, which is not observed in experiment. In R-Co compounds, T_C is approximately proportional to the square of the Co moment [22]. According to a molecular field theory, $T_C \sim S_{Co}(S_{Co} + 1)$, where S_{Co} is the quasispin of a 3d ion, which is proportional to the average Co magnetic moment [5]. Therefore, $T_C \sim M_s^2$. Since $M_s(\text{LuCo}_3) > M_s(\text{YCo}_3)$, then $T_C(\text{LuCo}_3) > T_C(\text{YCo}_3)$, as confirmed in experiment.

LuCo$_3$ shows a field-induced magnetic transition centered at about 47 T for field applied along both, the easy and hard directions [Fig. 3(a)]. The transition displays hysteresis and is of first order. Although the critical fields are very close for both field directions, one observes a pronounced anisotropy of the transition. The anomaly for field applied along the easy [001] axis is more pronounced. For this direction, the magnetization jump is from 2.22 to 3.90 μ_B, whereas for the hard [100] direction the magnetization changes from 2.25 to 3.57 μ_B. The transition for the easy axis shows a broader hysteresis as well.

The high-field magnetization of LuCo$_3$ contrasts strongly with that of YCo$_3$ [11]. The former shows a single transition, whereas two transitions were found for the latter. Given that both compounds have close magnetization values above the transitions, 3.57–3.90 μ_B for LuCo$_3$ and 3.69 μ_B for YCo$_3$, one may assume that LuCo$_3$ will show no additional anomalies above 58 T. Alternatively, the difference in the high-field magnetization is due to the magnetic anisotropy related to the existence of nonquenched orbital moments [23–25].

With increasing temperature, the transition becomes less pronounced [Figs. 3(a)–3(e)]. The critical field (H_{cr}) of the phase transition for field applied along the [100] axis increases from 45.2 to 48.5 T between 2 and 120 K [Fig. 4]. H_{cr} for a field applied along the [001] axis is almost temperature independent. The H_{cr} values were determined as the middle point between the ascending and descending branches of the transition [inset in Fig. 4]. The hysteresis (ΔH_{cr}) at the transition gradually decreases for both directions and goes to zero above 80 K [Fig. 4].

In Refs. [26–28] it was shown that the critical field of itinerant system with a field induced metamagnetic transition from the paramagnetic ground state to the ferromagnetic state depends on the lattice parameters. H_{cr} increases if the lattice parameters reduce. However, in the case of LuCo$_3$ and YCo$_3$, the atomic size of the rare-earth element plays a key role, since the lattice parameters of LuCo$_3$ are smaller than those of YCo$_3$, but $H_{cr}(\text{LuCo}_3) < H_{cr}(\text{YCo}_3)$. The critical field of a metamagnetic transition from para- to ferromagnetic state should be proportional to T^2 according to the theory of
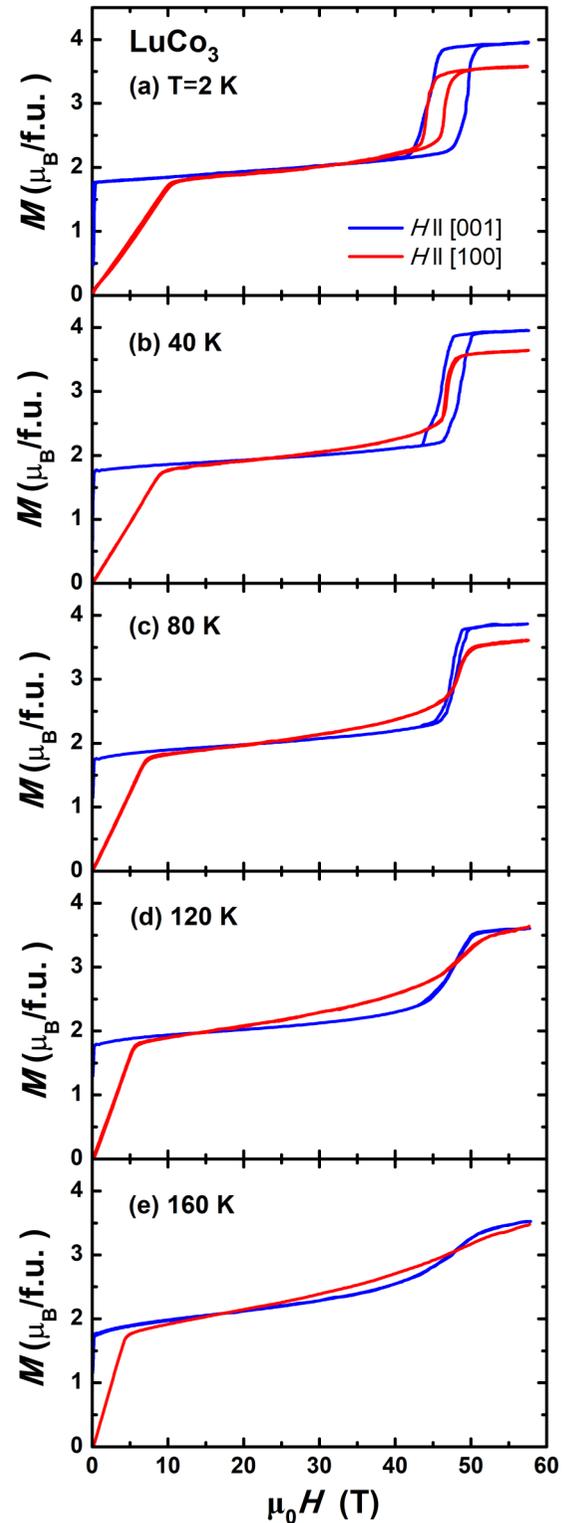
FIG. 3. High-field magnetization for field applied along the [100] and [001] axes of LuCo$_3$ at (a) 2, (b) 40, (c) 80, (d) 120, and (e) 160 K.

thermal fluctuations [29]. However, only a linear growth of H_{cr} is observed for LuCo$_3$ along the [100] direction [Fig. 4]. Such feature of the $H_{cr}(T)$ dependence can be attributed to the effect of exchange field of the Co sublattice in LuCo$_3$, that
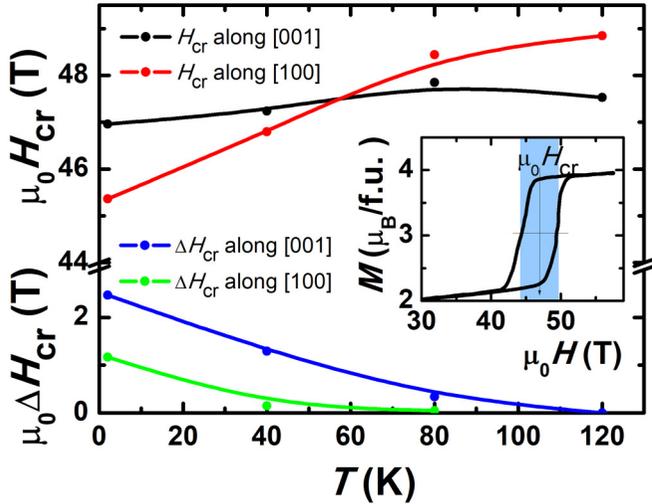
FIG. 4. Temperature dependences of the critical field, H_{cr}, and hysteresis, ΔH_{cr}, of the field-induced transition for field applied along the [001] and [100] axes of LuCo$_3$.

FIG. 5. Calculated averaged and partial magnetic moment of cobalt atoms as a function of the relative volume $v = V/V_0$. To facilitate visualization, we give only a few points for Co(3b) and Co(18h) sublattices. The arrows indicate the Co(6c)-Co(18h) inter-atomic distances (d) for the corresponding relative volumes.

changes with temperature. Thus, it can be concluded that the theories developed for classical metamagnetic transitions are not fully applicable to LuCo$_3$.

B. Theoretical studies of the electronic structure

As already shown above, for a LuCo$_3$ single crystal, an abrupt increase in the magnetic moment occurs when a magnetic field $\mu_0 H = 47$ T [Fig. 3(a)] is applied. In terms of the electronic subsystem, such a transition in a ferromagnet can be considered as a manifestation of a spin phase transition from the LS to the HS of electrons. To understand the nature of this transition, we performed a series of *ab initio* calculations based on the density functional theory (DFT) for different unit cell volumes obtained by isotropic changes of the crystal cell parameters. In previous studies of the related RCo$_5$ compounds [30], it was concluded that a change in the unit cell volume and an increase in the magnetic field effectively impact the electronic subsystem in a very similar way and should generally lead to qualitatively similar results. The main effect of these external influences on the electronic structure is expected to be the broadening of the electronic bands with some shift electronic states with respect to the Fermi energy, while the general structure of the electronic states is not significantly changed.

The results of the calculated averaged (over the sublattices) magnetic moment of the cobalt atoms depending on the relative volume $v = V/V_0$, where V and V_0 are the current and experimental (with zero compression) cell volumes of the LuCo$_3$ single crystal, respectively, are shown in Fig. 5. In fact, from the *ab initio* calculations we obtained two distinctive HS and LS states in LuCo$_3$ with a drastic change between them. It can be seen that there is only one abrupt transition with a significant change in the Co magnetic moment by approximately 0.5 μ_B, which corresponds to the average experimental value of 0.56 μ_B. Excluding hysteresis, the calculated dependence generally corresponds to the shape of the high-field part of the $M(H)$ curve, shown in Fig. 3(a). Note that the hysteresis is
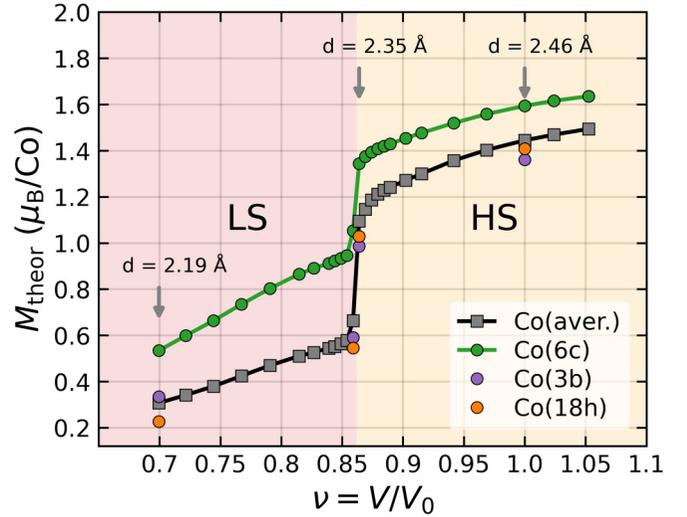
not realized in the calculation, since there is an unambiguous determination of the global minimum total energy at the given parameters in DFT. The calculated averaged magnetic moments for the two relative volumes $v = 0.85$ and 0.87, which are closely located in the transition region, see Table I, have values of 0.58 and 1.15 μ_B, respectively, and have a good correlation with the experimental values of 0.74 and 1.30 μ_B. Thus, the modeled HS and LS states in LuCo$_3$ and the character of the spin transition are found in a very good agreement with experimental data. Additionally, in our calculations we found that the calculated equilibrium cell volume for LuCo$_3$ is only 3% less than the one corresponding to the experimental crystal structure parameters.

Figure 5 also provides insight of the behavior of the magnetic moments in the cobalt atoms sublattices. For the experimental volume ($v = 1$), the Co(6c) atom has the largest magnetic moment, which is 1.6 μ_B. In our calculations, the averaged magnetic moment of the Lu atoms is -0.50 μ_B for this volume ($v = 1$) mostly due to the 5d contribution equal to -0.34 μ_B, whereas in the LS state ($v = 0.85$) the corresponding Lu moments are -0.19 and -0.12 μ_B, respectively. Because the 5d states are very extended in energy and hybridize with both the majority and minority spin electronic 3d states of the Co atoms almost equally. The small magnetic moment of Lu is aligned in the opposite direction to the Co magnetic moments. Directions of magnetic moments

TABLE I. Averaged Co magnetic moments, M_{theor}, in LuCo$_3$ calculated at the relative unit cell volumes near the spin transition and experimentally determined moments, M_{exp}, for the [001] direction.

Spin state	V/V_0	M_{theor}, μ_B/Co	M_{exp}, μ_B/Co ($T = 2$ K)
LS	0.85	0.58	0.74
HS	0.87	1.15	1.30

in $4f$-$3d$ intermetallics are determined by a number of factors including the type of R and $3d$ atoms, values of moments, hybridization, and various types of exchange interactions in the $4f$-$3d$ compounds [5,31,32]. The Co($3b$) and Co($18h$) atoms have the similar magnetic moments equal to $1.4\,\mu_B$. and have the same shape as the averaged Co moment, for this reason, in Fig. 5 only a few values for these two types of Co are given. Figure 5 shows that all sublattices undergo a large jump in the transition region. The main contribution to magnetization in the HS state is given by the Co($18h$) atoms, as is easy to see, owing to the small difference between the magnetic moments of the sublattices. The dominant contribution to the LuCo$_3$ magnetism is determined by the atoms of the Co($6c$) and Co($18h$) sublattices. Co($6c$) atoms are located between two pure Co($18h$) layers. The Co($6c$)-Co($18h$) interatomic
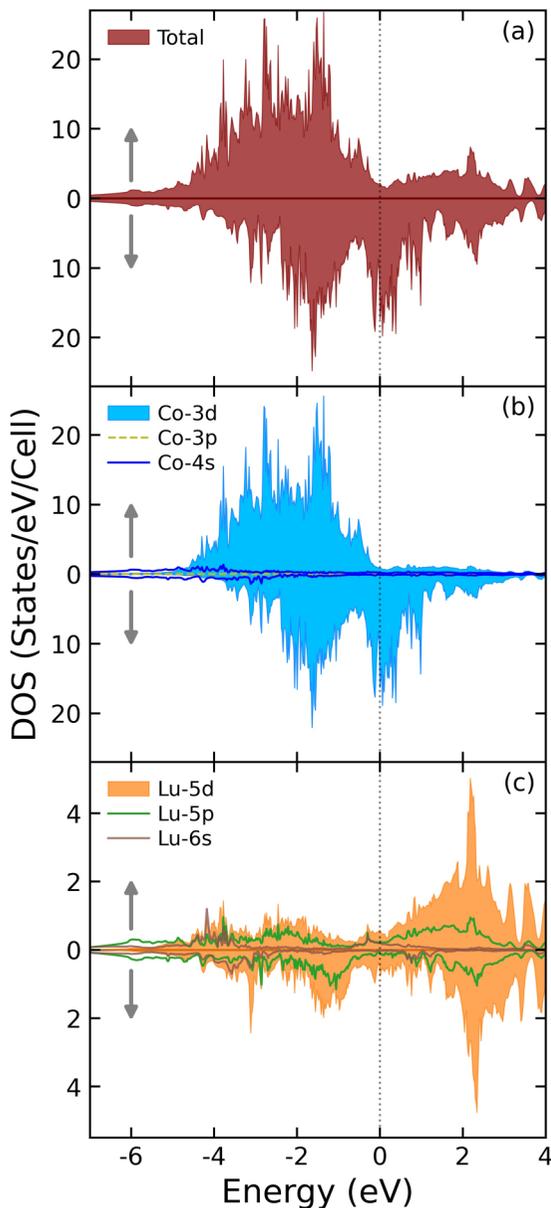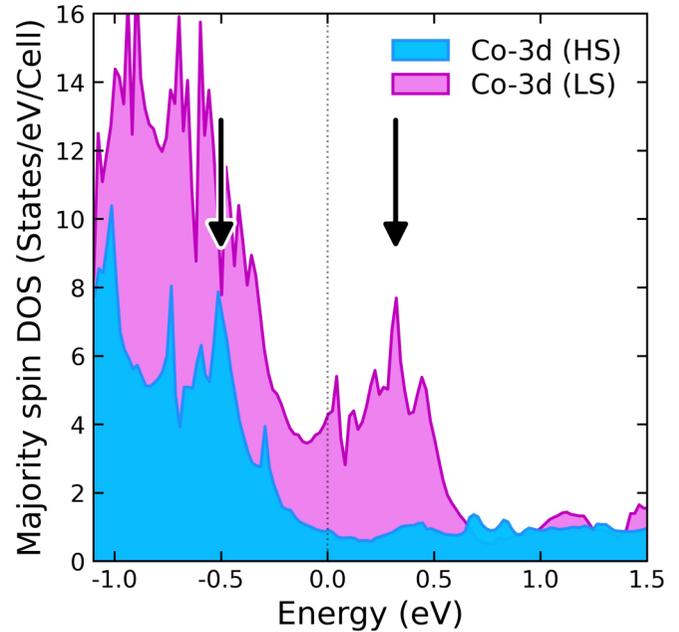
FIG. 7. The majority density of states of the Co atoms for the relative unit cell volumes $\upsilon = 1$ (HS) and $\upsilon = 0.85$ (LS).

distance is minimal in LuCo$_3$ and is $d = 2.46\,\text{Å}$ at $\upsilon = 1$ (the distances for other υ are indicated in the Fig. 5). This distance defines the characteristic interatomic scale in LuCo$_3$, since the Co($18h$)-Co($18h$) and Co($3b$)-Co($18h$) distances, are only slightly (about 0.01 Å) larger than the Co($6c$)-Co($18h$) one. Note that in LuCo$_2$, the minimum distance of Co-Co atoms is 2.54 Å (based on data [33]), which is greater than the one in LuCo$_3$.

The behavior of the magnetic characteristics of LuCo$_3$ can be understood through its electronic structure analysis for different volumes. Since we have not found calculations of the electronic structure for LuCo$_3$ in the literature, we first present its general structure. The spin-polarized total and partial density of states of the Lu and Co atoms in the energy range from -7 to 4 eV for the experimental lattice parameters ($\upsilon = 1$) are shown in Fig. 6. The main contribution to the filled d band and, consequently, the total filled density of electronic states [Fig. 6(a)] is formed by the $3d$ states of the Co atoms [Fig. 6(b)], which are approximately located in the energy range from -5 eV to 0 eV. The second largest contribution to the total density of states is formed by the $5d$ states of the Lu atoms [Fig. 6(c)]. Other states contribute less to this energy range.

Let us now compare the majority ($\uparrow$) density of states of the Co atoms for the relative unit cell volumes $\upsilon = 1$ (HS) and $\upsilon = 0.85$ (LS) [Fig. 7]. Both densities of states near the Fermi level have a sharp peak, namely, about -0.5 eV for $\upsilon = 1$ and 0.35 eV for $\upsilon = 0.85$. The main contribution to this peak is formed by the electrons with the symmetry $d_{xz,yz}$. A sharp decrease of the Co magnetic moment is equivalent to the peak in the $3d$ band passing through the Fermi level [Fig. 5].

The positions of the majority and minority spin states with respect to the Fermi level is controlled by external magnetic

FIG. 6. Spin-polarized total and partial density of states of the Lu and Co atoms for the experimental lattice parameters ($\upsilon = 1$, HS).

field. If the system is in the LS state, the sharp peak in the majority density of the Co states moves upward in energy with magnetic field, approaching to the Fermi level. At the same time, the minority density of the Co states remains high near the Fermi level. According to the generalized Stoner criterion [34,35], the high density for both spin states, $(n_\uparrow(E_F))^{-1} + (n_\downarrow(E_F))^{-1} > 4I$, where $n_{\uparrow,\downarrow}(E_F)$ is the spin density of states at the Fermi level and I is the Stoner parameter, leads to an instability of the system. In fact, the instability causes the peak to instantly pass ("overjump") through vicinity of the Fermi level in order to realize a stable HS state. This leads in turn to an abrupt increase (decrease) in the number of electrons in the majority (minority) spin state and, as a consequence, to an abrupt increase in the magnetic moment, which is observed in experiment.

distinctive HS and LS states of the Co atoms in LuCo$_3$ for different Co-Co distances are found with a drastic change between them of approximately $0.5\,\mu_B$, which is in a good agreement with the average experimental value of $0.56\,\mu_B$ for this jump. The reason for this drastic change we relate to the presence of instability in the Co 3d density of states. The magnetization jump reflects a transition from a LS to a HS state as a sharp peak in the majority density of the Co 3d states passes through the Fermi level. It was also found that the magnetic moments of all three types of the Co atoms have a similar type of behavior during the spin transition. The magnetic moments of the Co(3b) and Co(18h) atoms are very close to the average value of the Co magnetic moment, the magnetic moment of the Co(6c) has the higher value but also shows the characteristic spin transition change.

IV. CONCLUSION

LuCo$_3$ is an itinerant ferromagnet (Curie temperature 376 ± 5 K) with a large uniaxial magnetic anisotropy. We found a magnetic field-induced phase transition just below 50 T for magnetic field applied along the easy and hard magnetization directions. The transition shows a pronounced anisotropy of the magnetization jump and hysteresis. Our *ab initio* calculations based on the DFT reveal that a strong sensitivity of magnetic subsystem of LuCo$_3$ to magnetic field is due to the significant change of the occupancies of the Co 3d electronic states. In the theoretical calculations, two

[1] A. S. Markosyan, Magnetism 3d of Alloys of 4f (R) and Elements (T), in *Encyclopedia of Materials: Science and Technology* (Elsevier, Amsterdam, 2001).

[2] K. H. J. Buschow, Intermetallic compounds of rare-earth and 3d transition metals, Rep. Prog. Phys. **40**, 1179 (1977).

[3] Z. Śniadecki, N. Pierunek, B. Idzikowski, B. Wasilewski, M. Werwiński, U. K. Rößler, and Yu. Ivanisenko, Influence of structural disorder on the magnetic properties and electronic structure of YCo$_2$, Phys. Rev. B **98**, 094418 (2018).

[4] E. Gratz and A. S. Markosyan, Physical properties of RCo$_2$ Laves phases, J. Phys.: Condens. Matter **13**, R385 (2001).

[5] J. J. M. Franse and R. Radwanski, Magnetic properties of binary rare-earth 3d-transition-metal intermetallic compounds, in *Handbook of Magnetic Materials*, edited by K. H. J. Buschow, Vol. 7 (Elsevier, Amsterdam, 1993).

[6] Q. He and Y. Guo, Magnetic phase relations of RCo$_3$, IEEE Trans. Magn. **51**, 1 (2015).

[7] I. Y. Gaidukova and A. S. Markosyan, d-magnetism instability in R-Co intermetallic compounds, J. Sci. Adv. Mater. Devices **1**, 105 (2016).

[8] E. Kren, J. Schweizer, and F. Tasset, Polarized-neutron-diffraction study of magnetic moments in yttrium-cobalt alloys, Phys. Rev. **186**, 479 (1969).

[9] M. I. Bartashevich, T. Goto, M. Yamaguchi, I. Yamamoto, and A. V. Andreev, Thermal expansion and high field magnetization of a single crystal γ-phase hydride YCo$_3$H$_{3.9}$, Solid State Commun. **82**, 201 (1992).

[10] X. Y. Cui, J. Liu, P. A. Georgiev, I. Morrison, D. K. Ross, M. A. Roberts, K. A. Andersen, M. Telling, and D. Fort, Effect of H on the crystalline and magnetic structures of the YCo$_3$-H(D) system. I. YCo$_3$ from neutron powder diffraction and first-principles calculations, Phys. Rev. B **76**, 184443 (2007).

[11] T. Goto, H. A. Katori, T. Sakakibara, and M. Yamaguchi, Successive phase transitions in ferromagnetic YCo$_3$, Phys. B **177**, 255 (1992).

[12] D. Givord, J. Laforest, and R. Lemaire, Polarized neutron study of the itinerant electron metamagnetism in ThCo$_5$, J. Appl. Phys. **50**, 7489 (1979).

[13] H. Yamada, K. Terao, F. Ishikawa, M. Yamaguchi, H. Mitamura, and T. Goto, Itinerant-electron metamagnetism of Y(Co, Ni)$_5$, J. Phys.: Condens. Matter **11**, 483 (1999).

[14] D. Koudela, U. Schwarz, H. Rosner, U. Burkhardt, A. Handstein, M. Hanfland, M. D. Kuz'min, I. Opahle, K. Koepernik, K. H. Müller, and M. Richter, Magnetic and elastic properties of YCo$_5$ and LaCo$_5$ under pressure, Phys. Rev. B **77**, 024411 (2008).

[15] K. Koui, M. I. Bartashevich, T. Goto, H. A. Katori, and M. Yamaguchi, Co metamagnetism in Y$_{1-x}$Nd$_x$Co$_3$ under ultra-high magnetic field, Physica B **201**, 143 (1994).

[16] M. I. Bartashevich, H. A. Katori, T. Goto, H. Wada, T. Maeda, T. Mori, and M. Shiga, Collapse of the itenerant Co moment in Er$_{1-x}$Lu$_x$Co$_2$ by the application of high magnetic fields, Physica B **229**, 315 (1997).

[17] F. Givord and R. Lemaire, Proprietes cristallographiques et magnetiques des composes entre le cobalt et le lutecium, Solid State Commun. **9**, 341 (1971).

[18] Y. Skourski, M. D. Kuz'min, K. P. Skokov, A. V. Andreev, and J. Wosnitza, High-field magnetization of Ho_2Fe_{17}, Phys. Rev. B **83**, 214420 (2011).

[19] P. Giannozzi *et al.*, QUANTUM ESPRESSO: A modular and open-source software project for quantum simulations of materials, J. Phys.: Condens. Matter **21**, 395502 (2009).

[20] P. Giannozzi *et al.*, Advanced capabilities for materials modelling with QUANTUM ESPRESSO, J. Phys.: Condens. Matter **29**, 465901 (2017).

[21] D. Bloch and F. Chaisse, Effect of the hydrostatic pressure on Curie temperature in compounds $T\mathrm{Co}_3$ and $T_2\mathrm{Co}_7$ where T-rare earth metal and yttrium, Compt. Rend. Acad. Sci., Series B **274**, 221 (1972) (in French).

[22] D. Givord and R. Lemaire, Magnetic transition and anomalous thermal expansion in R_2Fe_{17} compounds, IEEE Trans. Magn. **10**, 109 (1974).

[23] E. V. Rozenfel'd and A. V. Korolev, Low-temperature magnetization anisotropy in ferromagnetic materials with quenched orbital angular momentum, Zh. Eksp. Teor. Fiz. **108**, 862 (1995) [JETP **81**, 471 (1995)].

[24] A. S. Bolyachkin, D. S. Neznakhin, and M. I. Bartashevich, Effect of magnetization anisotropy and paramagnetic susceptibility on magnetization process, J. Appl. Phys. **118**, 213902 (2015).

[25] A. S. Bolyachkin, D.S. Neznakhin, T. V. Garaeva, A. V. Andreev, and M. I. Bartashevich, Magnetic anisotropy of YFe_3 compound, J. Magn. Magn. Mater. **426**, 740 (2017).

[26] K. Murata, K. Fukamichi, T. Goto, H. A. Katori, T. Sakakibara, and K. Suzuki, Metamagnetic transition in $LuCo_2$ and its pseudo-binary compounds, Physica B **201**, 147 (1994).

[27] N. V. Mushnikov and T. Goto, Itinerant electron metamagnetism of $Y(Co_{1-x}Al_x)_2$ under high pressure and high magnetic fields, J. Phys.: Condens. Matter **11**, 8095 (1999).

[28] N. V. Mushnikov, T. Goto, K. Kamishima, H. Yamada, A. V. Andreev, Y. Shiokawa, A. Iwao, and V. Sechovsky, Magnetic properties of the 5f itinerant electron metamagnet UCoAl under high pressure, Phys. Rev. B **59**, 6877 (1999).

[29] H. Yamada, Metamagnetic transition and susceptibility maximum in an itinerant-electron system, Phys. Rev. B **47**, 11211 (1993).

[30] R. Ballou, M. Shimizu, and J. Voiron, Pressure effects on the metamagnetic transition of $ThCo_5$, J. Magn. Magn. Mater. **84**, 23 (1990).

[31] M. Richter, Band structure theory of magnetism in $3d$-$4f$ compounds, J. Phys. D **31**, 1017 (1998).

[32] A. V. Lukoyanov, Yu. V. Knyazev, Yu. I. Kuz'min, and A. G. Kuchin, Cobalt-related features of spectral and magnetic properties of RNi_4Co ($R =$ Ho, Er), J. Magn. Magn. Mater. **368**, 87 (2014).

[33] P. Villars (Ed.), LuCo Crystal Structure, in *Inorganic Solid Phases, SpringerMaterials (online database)* (Springer, Heidelberg, 2016).

[34] J. Kübler, *Theory of Itinerant Electron Magnetism*, International Series of Monographs on Physics Vol. 106 (Oxford University Press, Oxford, 2017).

[35] M. Cyrot and M. Lavagna, Density of states and magnetic properties of the rare-earth compounds RFe_2, RCo_2 and RNi_2, J. de Phys. **40**, 763 (1979).