Cancellation of spin and orbital moments in URhGe under pressure: A density-functional prediction

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The local-spin-density approximation (LSDA) is used to perform density-functional total-energy calculations for the ferromagnetic superconductor URhGe in the magnetic and in the nonmagnetic states under high pressure. Our calculations show that the ferromagnetic ground state is energetically preferred in a wide pressure range, even though the nearest U-U interatomic distance is much below Hill's limit. An intriguing behavior of the total magnetic moment upon application of pressure is observed. Due to a compensation of spin and orbital contributions, the total moment vanishes at a pressure of about 12 GPa. If the pressure is further enhanced, the total moment reappears, before a nonmagnetic ground state is obtained at about 50 GPa.

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I. INTRODUCTION

During the past decades, magnetic properties of the 5*f*-electron compounds have been extensively studied from a fundamental point of view. Their properties are unlike those usually observed in itinerant *d*-electron transition metals but also differ from those of localized 4*f*-electron rare-earth-based systems. In the first case, the *d*-electron magnetism may be explained in terms of the Stoner-Wohlfarth model,[1] whereas in the localized 4*f*-electron system Hund's rules and crystal-field effects are dominating. Due to the dualism between localized and itinerant character of 5*f* electrons, the 5*f*-electron compounds show a variety of intriguing phenomena, as heavy fermion behavior, unconventional superconductivity, quantum critical phase transitions, non-Fermi liquid state or coexistence of superconductivity with magnetic order.

Compounds with the composition U*TM* (where *T* stands for a transition metal and *M* for a *p*-type metalloid) form a large group with similar properties.[2] The magnetism in this group is determined by the hybridization between 5*f* and *spd* states. URhGe, crystallizing in the orthorhombic TiNiSi-type structure (space group *Pnma*), was classified as an itinerant electron ferromagnet with the ordering temperature T_C =9.5 K.[3] The crystal structure is characterized by zigzag uranium chains extending along the *a* crystallographic axis (Fig. 1). In the unit cell, the U, Rh, and Ge atoms occupy the 4*c* Wyckoff positions. Neutron-diffraction studies of URhGe have found a noncollinear structure with uranium magnetic moments oriented in the *a*-*c* plane and tilted from the *c* axis by an angle of about 31°.[4] These latter data are in good agreement with local spin density approximation (LSDA) calculations[5] yielding an antiferromagnetic (AF) component of 0.03 μ_B and a ferromagnetic component of 0.29 μ_B. The existence of AF ordering of pairs of uranium atoms along the *a* axis is allowed by the nonsymmorphic space group.[6] However, the tiny AF component has not been observed experimentally from neutron single-crystal experiments.[7,8] The contradictory experimental results for URhGe were attributed to a relatively small magnetic anisotropy in the *b*-*c* plane.[9] Details of sample preparation could modify the magnetic anisotropy and give rise to different moment orientations.

URhGe exhibits one more interesting feature, a coexistence of *p*-wave superconductivity and ferromagnetic order found below T_{sc}=0.25 K.[7] Re-entrant superconductivity was found in an applied magnetic field.[10] One should emphasize that the superconductivity is observed at ambient pressure. Another related system, UGe_2, was earlier characterized as a superconducting ferromagnet but at enhanced pressure in the range of 1.0–1.6 GPa.[11] It was proposed that in this pressure range, where the Curie temperature of uranium digermanide tends to 0, a ferromagnetic quantum critical point (FQCP) exists.[12] In order to find a FQCP in URhGe, Hardy *et al.*,[13] performed measurements of specific heat and resistivity of polycrystalline samples under high pressure. They reported a shift of the superconducting temperature T_{sc} to lower values with pressure and a final collapse of T_{sc} near 4 GPa.[14] Also, a linear increase of T_C up to 18 K measured at a maximum pressure of 12 GPa was found.[14] Such a behavior is not common for itinerant ferromagnets, for which the transition temperature T_C in most cases decreases with increasing pressure. A related reduction in the total magnetic moment was concluded from specific heat data,[13] but no direct data were published.

In contrast to the behavior of URhGe, the magnetism of UGe_2 is already suppressed by application of a moderate

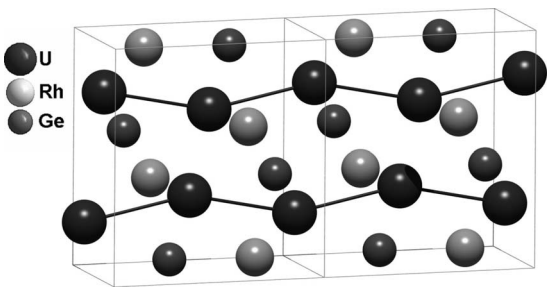

FIG. 1. Structure of URhGe with marked U-U zigzag chains.

pressure of 1.6 GPa.[12] This finding opposes the naive picture that a larger uranium moment (μ_{U-tot}=1.48 μ_B in UGe_2, μ_{U-tot}=0.4 μ_B in URhGe)[4,7,8] would indicate stronger localization of the 5*f* states than a smaller uranium moment and a related insensitivity of the magnetic state to pressure. This picture has indeed to be abandoned, since moment reduction (referred to the atomic moment) does occur both in localized systems (e.g., by crystal or ligand-field interaction) and in itinerant systems (by hybridization or Kondo-like incomplete screening).[15] One also should always bear in mind the antiparallel orbital moment contribution. In any case, the measured pressure sensitivity of the magnetic ordering temperature supports an itinerant picture in both systems.

In previous work it was shown, that density-functional calculations using the LSDA are appropriate to reproduce the magnetic properties of URhGe at ambient pressure.[5,9] Shick[5] also tested the LSDA+*U* method, but found a magnetic moment in worse agreement with experiment than by LSDA. To revise those previous calculations and to investigate the magnetism of URhGe under pressure, we carried out full-potential, full relativistic LSDA total-energy calculations taking into account nonmagnetic (NM) and ferromagnetic (FM) states. The calculations were performed with and without optimization of the structural degrees of freedom. Besides the magnetic ground state, the present paper reports the related electronic structure and an intriguing, unusual pressure dependence of the magnetic moment.

This introduction is followed by computational details (Sec. II), results and discussion (Sec. III), and summary (Sec. IV).

II. COMPUTATIONAL DETAILS

The calculations were performed using the full relativistic version[16] of the all-electron full-potential local-orbital (FPLO) band structure method (FPLO of 5.00–18).[17] The four-component Kohn-Sham-Dirac equation, which takes into account spin-orbit coupling in all orders, is solved self-consistently. The basis set comprised U (5*f*, 6*d*, 7*s*, 7*p*) valence and (5*d*, 6*s*, 6*p*) semicore states, Rh (4*d*, 5*s*, 5*p*) valence and (4*p*, 4*s*) semicore states, and Ge (3*d*, 4*s*, 4*p*) valence and (3*s*, 3*p*) semicore states. Brillouin zone integrations were carried out with the linear tetrahedron method using an irreducible sampling mesh with 452 *k* points for all self-consistent calculations and with 1252 *k* points for the density of states (DOS) calculations. The Perdew-Wang 92 (Ref. 18) parametrization of the exchange correlation potential was used. The quantization axis of magnetic moments was set along the *c* axis.[7,8]

As a starting point of the calculations, structure parameters from single-crystal neutron diffraction experiments at 20 K (Ref. 8) were taken. The experimental volume is defined by the lattice parameters, $V_0^{exp}=abc$, a=6.873 Å, b=4.330 Å, and c=7.506 Å. Further, six internal parameters were reported in Ref. 8: x_U=−0.001, z_U=0.224, x_{Rh}=0.221, z_{Rh}=0.591, x_{Ge}=0.779, and z_{Ge}=0.590.

For both FM and NM states, a first set of total energy vs volume data was evaluated by using the experimental internal parameters and c/b and a/b lattice parameters ratios.

TABLE I. Calculated elastic, magnetic, and electronic properties of URhGe. NR: except the volume, the experimental structural degrees of freedom are kept fixed; R: all structural degrees of freedom are relaxed as described in Sec. II.

	NR	R
V_0 (Å^3)	217.8	215.8
B_0 (GPa)	161	139
B'	5.0	4.6
ΔE (meV)	−25	−25
μ_{U-spin} (μ_B)	0.98	1.04
μ_{U-orb} (μ_B)	−1.22	−1.12
$\lvert\mu_{U-tot}\rvert$ (μ_B)	0.23	0.08
$\lvert\mu_{U-orb}/\mu_{U-spin}\rvert$	1.27	1.07
$N(E_F^{NM})$ (states/eV f.u.)	9.4	9.2
$N(E_F^{FM})$ (states/eV f.u.)	6.0	5.6

Related results will be indicated below as "not relaxed" (NR). For example, the lowest energy is obtained at V_0^{NR}. Subsequently, all eight parameters were evaluated at eight different volumes for the FM state in the following way: (i) a/b was optimized using experimental internal parameters and c/b; (ii) c/b was optimized using experimental internal parameters and a/b; (iii) one internal parameter was optimized using optimized c/b and a/b, and the five other experimental internal parameters; this procedure was repeated for all six internal parameters. Related results will be indicated below as "relaxed" (R). Finally, using the eight relaxed parameters, the total energy is recalculated at several volumes in order to obtain V_0^R.

Due to the limitations of the used code, which does not allow yet to perform noncollinear spin-orbital structure calculations we assumed that all spin and orbital moments are collinear in our calculations for the ordered state. Future calculations for other spin configurations under pressure, e.g., with allowing an AF component,[5] would be interesting. The results of such calculations would be helpful for understanding magnetic properties of URhGe under pressure, especially for checking any influence of possible noncollinear structure on the cancellation of spin and orbital moments in this compound.

III. RESULTS AND DISCUSSION

A. Ambient pressure

Table I displays calculated properties of URhGe both with and without relaxation of the internal parameters and axis ratios. The equilibrium volume V_0^{NR} is about 2.4% smaller than the experimental value of 223.4 Å^3, while after complete relaxation the difference increased to about 3.4%. These values represent a reasonable amount of overbinding, compared with data available for different actinide compounds.[19] The bulk modulus B_0 and its derivative B' will be discussed in the next section.

The U-U interatomic distance d_{U-U} was found to decrease from the experimental value 3.45 Å to about 3.35 Å in the

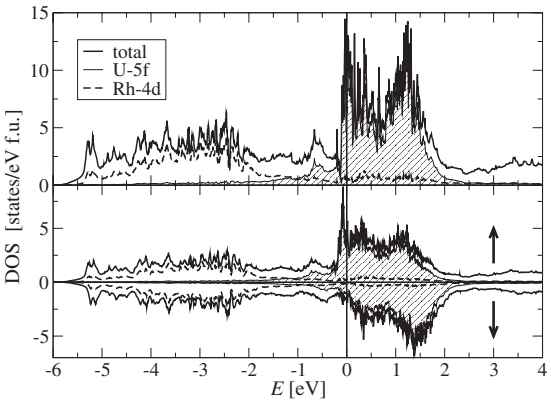

FIG. 2. DOS and PDOS of URhGe after relaxation of structural parameters ($V=V_0^R$). Upper and lower panels display results of a NM and of a FM calculation, respectively. The spin channels are indicated by arrows. The Fermi level is situated at energy zero.

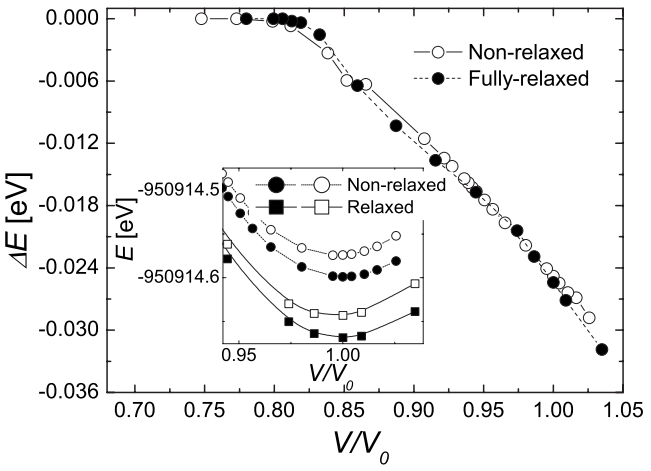

FIG. 3. Stabilization energy of the FM state as a function of volume reduction. The inset shows the total energy vs the reduced volume. In the inset, full symbols denote the FM ground state and empty symbols denote the NM state. All energies are given per formula unit.

case with relaxation. Full optimization also resulted in a reduction in the total energy by 80 meV, referred to the energy minimum of the NR calculation. In comparison, the stabilization energy of the FM ground state amounts to $\Delta E(V_0) = E_{\mathrm{FM}} - E_{\mathrm{NM}} = -25$ meV in both cases. Thus, the energy gain by magnetic order does not depend on details of the structural parameters.

The magnetic moments displayed in Table I show a weak, but not negligible dependence on the relaxation of the structural parameters. While the spin moment increases by 6% upon relaxation, the absolute value of the orbital moment is reduced by 9% compared to the case without relaxation. These points to a stronger sensitivity of orbital magnetism to structural details in comparison with spin magnetism. In general, the magnetism of $5f$ and $4f$ intermetallics is quite sensitive to changes in structural parameters or alloying. The opposite sign of spin and orbital moment is due to spin-orbit coupling in a less than half-filled shell (third Hund's rule). It results in an almost complete compensation between spin and orbital moment and in a total uranium moment of about 0.1 μ_B (relaxed case). The magnetic moments induced on the Rh and Ge sites are very small, about 0.03–0.05 μ_B. The total moments per chemical unit cell amount to 0.18 μ_B (NR) and 0.35 μ_B (R), respectively. Shick[5] and Diviš *et al.*[9] reported a similar value of 0.3 μ_B at experimental lattice geometry. All calculated total moments are slightly smaller than the accepted experimental value for the total moment, about 0.4 μ_B. A possible reason lies in the fact that the LSDA approach tends to underestimate the orbital moment.[19]

Figure 2 displays densities of states obtained in the relaxed case. These data are consistent with results from both previous studies.[5,9] The occupied valence band is about 6 eV broad. It is dominated by Rh $4d$ states between −5.5 eV and −2.0 eV. Between −2.0 eV and the Fermi level, a significant degree of hybridization between Rh $4d$ and U $5f$ states is visible. U $5f$ states are predominat in the proximity of the Fermi level and up to +2.0 eV. The two-peak character of the uranium $5f$ contributions (nonmagnetic case) is caused by spin-orbit coupling. The Fermi level cuts the U $5f$ peak with angular momentum $j=5/2$, whereas U $5f_{7/2}$ states form the maximum about 1.25 eV above E_F.[9] The high DOS at the Fermi level gives raise to a ferromagnetic instability. Spin splitting (lower panel of Fig. 2) provides additional structure to the U $5f$ DOS and reduces its magnitude (see Table I). Another (slight) reduction in the DOS at the Fermi level is obtained by the complete structure relaxation. Our value of about 6 states per eV and formula unit can be compared with the similar value of 17.5 states per eV and 4 f.u. published in Ref. 5.

B. High pressure

The effect of pressure is investigated for both NR and R cases, in order to check the influence of the relaxation on the magnetic properties. The results of related total-energy calculations for both NM and FM states are displayed in the inset of the Fig. 3. To obtain the bulk modulus and its derivative, the FM data are fitted with the Murnaghan equation of state,[20]

$$E(V) = E(V_0) + \frac{B_0 V}{B'}\left[\frac{(V_0/V)^{B'}}{B'-1} + 1\right] - \frac{B_0 V_0}{B'-1}. \qquad (1)$$

The results are displayed in Table I. It should be noted that the obtained bulk modulus, $B_0 \approx 140$ GPa, is comparable with that observed in another UTM compound, namely in URhAl where $B=175$ GPa.[21]

The variation in the stabilization energy of the ferromagnetic ground state, $\Delta E(V/V_0)$, is shown in the Fig. 3. Both NR and R curves are very similar. This confirms that the spin magnetism, which is mainly responsible for the energy difference, is only influenced by the volume but not by the other structural degrees of freedom. It is interesting to note that the magnetic state is stable in a wide volume range, down to a critical volume $V_c \sim 0.8\ V_0$. In comparison, LSDA calculations on UGe_2 show, that in uranium digermanide ferromagnetism vanishes, when the hydrostatic compression of the unit cell reaches $V_c/V_0 \sim 0.94$.[22] The pressure needed to suppress magnetism in URhGe can be estimated via $P(V)$

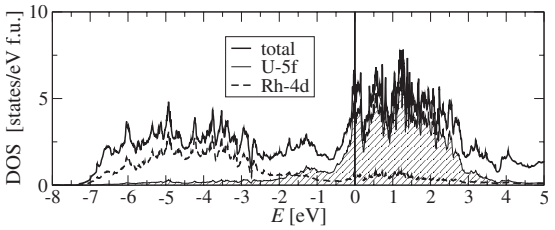

FIG. 4. DOS and PDOS of URhGe for $V=0.77\ V_0$ (R case). The Fermi level is situated at energy zero.

$=[(V_0/V)^{B'}-1]B_0/B'$, yielding $P(V_c)\approx 50$ GPa. At such a pressure, the uranium-uranium interatomic distance would be reduced from about 3.4 Å (at V_0) to 2.9 Å (at $V_c/V_0\sim 0.8$). This value is much lower than the Hill limit ($d_{\text{U-U,Hill}}=3.4-3.6$ Å) which earlier was considered as a lower limit for the occurrence of magnetic order in uranium compounds.[23] It should be noted that hydrostatic pressure leads to a quite anisotropic response of the lattice: the strain along the a axis is much larger than along the other axes. Thus, the U-U distance is about two times more reduced than one would expect in the case of an isotropic compression.

Figure 4 displays the DOS obtained for $V/V_0^R=0.77$, where only the NM solution is stable. The occupied band width is enhanced from 6 eV at ambient pressure to about 7 eV, and the 5f band width is enhanced from 2 eV at ambient pressure to about 3.5 eV. This strong band broadening more or less completely hides the spin-orbit splitting which amounts to about 1 eV and the 5f PDOS loses its two-peak character. The 5f-dominated DOS at the Fermi level is accordingly reduced and magnetism is suppressed.

Figure 5 displays the variation of the uranium-projected local-orbital moment, $\mu_{\text{U}-orb}$, and spin moment, $\mu_{\text{U}-spin}$, as a function of the reduced volume. As already discussed, the spin magnetism is mainly affected by the volume change and less by the complete structural relaxation. Gradual decrease in the volume leads to an approximately linear reduction in

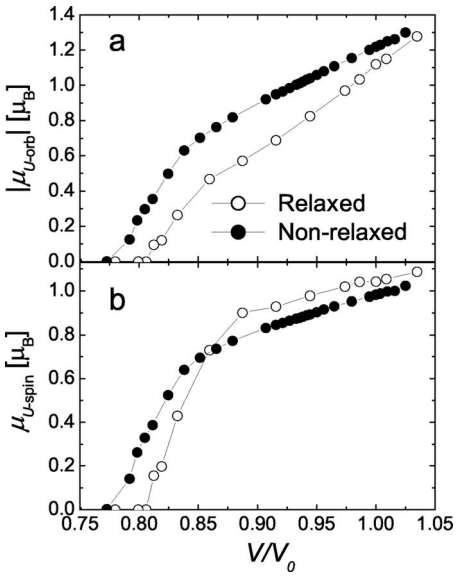

FIG. 5. Volume dependence of uranium-projected orbital (a) and spin (b) magnetic moments for both NR and R cases.

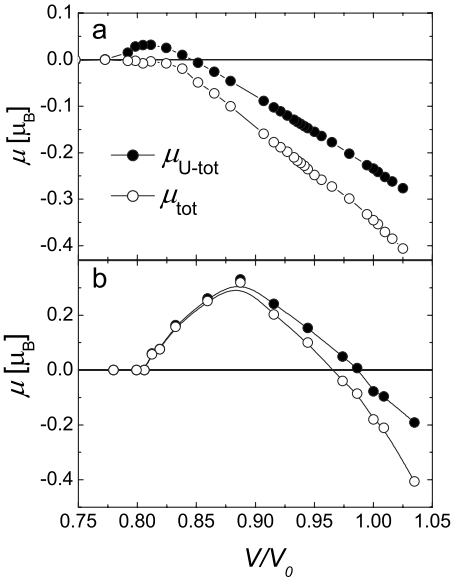

FIG. 6. Volume dependence of the total uranium-projected moment (filled circles) and of the total moment per formula unit (open circles). Panels (a) and (b) show results of NR and R calculations, respectively.

the spin moment. At about $V/V_0=0.85$, the slope changes and the spin moment rapidly vanishes. We suppose that this behavior is due to a specific feature of the very structured DOS, e.g., due to a van Hove singularity crossing the Fermi level. At lower pressure, the orbital moment is more sensitive to the structural relaxation than the spin moment. This can be understood from the very nature of orbital magnetism, being related to the direction and strength of atomic bonds. Close to the transition to the NM state, however, the volume dependence of the orbital moment resembles that of the spin moment.

An interesting point to note is a stronger volume dependence of the orbital moment compared with the spin moment as long as $V\gtrsim 0.85\ V_0$. Thus, while the orbital moment predominates at ambient pressure, its relative weight is reduced under high pressure. Figure 6 shows, that there is even a compensation point found for the uranium-projected total moment (full circles). Also, the total moment of the chemical unit cell is displayed in Fig. 6 (open circles). It does not show a compensation point in the NR calculation. In the case of a full lattice relaxation, however, the total moment vanishes at a volume reduction in about 7%, corresponding to a pressure of about 12 GPa. The uranium moment should vanish at an even lower pressure. We predict that further enhancement of the pressure will first lead to a linear increase of the total moment. After passing a pronounced maximum at $V\approx 0.88\ V_0$ ($P\approx 24$ GPa), the total moment decreases linearly till the magnetic state becomes unstable. We would like to stress, that the total moment compensation happens *within the ferromagnetic state*. Thus, our finding does not contradict but rather confirm the observation of a ferromagnetic transition, probed by heat capacity measurements on URhGe up to 13 GPa.[13] The related reduction in the peak-height in the heat capacity vs. temperature by application of pressure corresponds to the reduction in stabilization energy, shown in Fig. 3.

A final comment should be made on the cancellation of different contributions to the total magnetic moment, observed in our calculations. An early prediction of such a situation was made for UN under pressure.[24] Related experimental evidence has been found in a few other 4*f*- and 5*f*-electron systems. Let us consider three examples. It is well known, that for the free Sm^{3+} ion Hund's rules predict a state with an almost complete compensation between spin and orbital magnetic moments. Indeed, a complete cancellation of both contributions was observed in $SmAl_2$ doped with Gd (Ref. 25) due to the interplay of crystal-field splitting and exchange interactions at a particular temperature. Considering 5*f* intermetallics, the itinerant ferromagnet UFe_2 (Ref. 26) was found to be a system with almost zero total magnetic moment on the uranium site at ambient pressure. There, the total moment of the unit cell is nonzero, however. $UFe_{1-x}Ni_xAl$, a pseudoternary system of the U*TM* family, has been studied by Tran *et al.*[27] They have shown, that the saturation moment shows a maximum at $x=0.5$ and goes down to zero close to $x=0.8$. It might be that the moment reduction in this case is also due to a cancellation between spin and orbital components. This situation is however different from our case, since in $UFe_{1-x}Ni_xAl$ the ferromagnetic ordering temperature vanishes together with the moment.[27]

IV. SUMMARY

URhGe, known to show coexistence of ferromagnetism and superconductivity, is predicted to exhibit yet another intriguing feature. We demonstrate by LSDA calculations, that spin and orbital moments on the uranium site compensate, if a high enough pressure is applied. For a pressure of about 12 GPa, a compensation of spin and orbital moments of the whole elementary cell is predicted. Such a situation of zero-moment ferromagnetism is a rare case and has been observed in only a few systems, hitherto. It is in agreement with existing experimental data showing a ferromagnetic transition up to 13 GPa.[13] If pressure is enhanced above about 50 GPa we predict that ferromagnetic order will vanish. This prediction does not exclude the occurrence of other types of magnetic order. The mentioned pressure range is available for experimental techniques like resistivity measurements and structural analysis. Further experimental research in pressures higher than those applied in Ref. 13 is required to verify our theoretical predictions.

Finally, we show that the relaxation of all structural degrees of freedom has a considerable influence on the results of electronic structure calculations for systems with magnetic instabilities and subtle compensation phenomena.

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