Magnetic stripes in the UCoGe superconductor

Pablo de la Mora¹ and O Navarro²

¹Departamento de Física, Facultad de Ciencias, Universidad Nacional Autónoma de México, Apartado Postal 70-542, 04510 México DF, México
and Instituto de Investigación en Materiales, Universidad Nacional Autónoma de México, Campus Morelia.

²Instituto de Investigación en Materiales, Universidad Nacional Autónoma de México, Apartado Postal 70-360, 04510 México DF, México

E-mail: delamora@unam.mx

Abstract. The magnetic superconductor UCoGe is analyzed with an electronic structure package, spin-orbit coupling and intra-atomic repulsion (via Hubbard $U_H$) were included. The possibility of an antiferromagnetic configuration is studied, but it is found to be unstable, also the non-collinear magnetization seems to be ruled out. The magnetization is given mainly by the Co-atoms with $M = 0.6 \mu_B$/f.u. The U-atoms have two magnetic moments; $M = 0.07$ and $0.32 \mu_B$/f.u. arranged in an alternated planes along the $b$-direction forming magnetic stripes.

1. Introduction
Recently UCoGe was found to be both superconducting, $T_c = 0.8$ K, and ferromagnetic, $T_C = 3$ K, with a small magnetic moment, $M = 0.03 \mu_B$/f.u. (Huy et al. 2007). Electronic quantum mechanical calculations have shown that both the U-atoms and the Co-atoms have a magnetic moment much larger than the experimental one, all the atoms are aligned ferromagnetically giving a total value of $M \approx 0.78 \mu_B$/f.u. (de la Mora and Navarro 2008, Diviš 2008). In an attempt to conciliate these two different values various ferro- and antiferromagnetic calculations were performed.

2. Computational details
Electronic quantum mechanical calculations were done with the WIEN2k package (Blaha et al. 2001), which is a Linearized Augmented Plane Wave (FP-LAPW) method based on Density Functional Theory (DFT). Spin-orbit coupling is included in a second-variational way, and the strong correlations in uranium were included via LDA+$U_H$ (SIC) (contributed by Pavel Novák). The Generalized Gradient Approximation of Perdew, Burke and Ernzerhof (1996) was used for the treatment of the exchange-correlation interactions. The energy threshold to separate localized and non-localized electronic states was -6 Ry. The muffin-tin radii were: $2.5a_0$ for uranium, $2.43a_0$ for cobalt, $2.48a_0$ for rhodium, and $2.15a_0$ for germanium ($a_0$ is the Bohr radius). The criterion for the number of plane waves was $R_{MT}^{min} \times K_{max}^{max} = 9$ and the number of k-points was 462 (7×11×6), for the case with all the atoms independent the number of k-points was 225 (5×9×5).
3. Results and discussion

The UCoGe compound has a deformed MgB$_2$ structure; it has undulated Co-Ge graphene-like sheets intercalated by U atoms (figure 1). In contrast to MgB$_2$, the bonds are not covalent but metallic.

The electronic structure calculations were performed using the cell parameters of Huy et al. (2007) and the atomic positions of Canepa et al. (1996). Spin-orbit interaction was included for uranium and cobalt, the intra-Coulombic repulsion $U_{II}$ was also included for uranium 5d, with a $U_{II} = 0.362$ eV (de la Mora and Navarro 2008).

In our previous work (de la Mora and Navarro 2008), in order to have a better description of the system, all the atoms in the unit cell (which contains four formula units) were treated as independent atoms, that is, they could have different values in their electronic properties.

![Figure 1. Crystal structure of UCoGe. Co and Ge form undulated horizontal planes, U form vertical zigzag chains.](image)

**Table 1.** Energies, in meV/f.u., of the different magnetic configurations. The most stable, the ‘all spins up’ $c$-direction configuration, is taken as reference.

| Magnetization direction | Magnetic moment ordering | Energy | $\Delta E$ relative to ‘all spins up’ |
|-------------------------|--------------------------|--------|-------------------------------------|
| $b$                     | All spins up             | 10.8   | 0                                   |
|                         | U1 and U2 up             | 35.3   | 24.5                                |
|                         | U1 and U3 up             | 23.4   | 12.6                                |
|                         | U1 and U4 up             | 85.2   | 74.4                                |
|                         | All spins up             | 0      | 0                                   |
| $c$                     | U1 and U2 up             | 27.6   | 27.6                                |
|                         | U1 and U3 up             | 39.8   | 39.8                                |
|                         | U1 and U4 up             | 61.2   | 61.2                                |
In the present paper the magnetic moments of the unit cell were arranged in all the possible antiferromagnetic orders; a) all spins up (ferromagnetic), b) U1 and U2 spins up (U3 and U4 spins down), c) U1 and U3 spins up and d) U1 and U4 spins up. These calculations were done for the \( b \)- and \( c \)- magnetic moment directions which are the most stable orientations. The magnetic moments are given in table 1, the antiferromagnetic configurations have higher energy than the corresponding ferromagnetic one. The ferromagnetic configuration in the \( c \)-direction is the most stable, the experimental results on single crystals (Huy et al. 2008) find that the magnetization is in this direction, but the experimental magnetic moment is smaller.

**Table 2.** Magnetic moments (\( \mu_0 \)), with the magnetization in the \( b \)- and \( c \)-direction for the ferromagnetic case.

| Atom | \( b \) | \( c \) | \( a \)-direction |
|------|--------|--------|-----------------|
| U    | 0.094  | 0.073  | 0.070           |
|      | 0.116  | 0.319  | -0.124          |
|      | 0.108  | 0.073  | -0.069          |
|      | 0.103  | 0.322  | 0.122           |
| Tot/f.u. | 0.105  | 0.179  |                 |
| Co   | 0.625  | 0.610  | 0.033           |
|      | 0.608  | 0.589  | -0.041          |
|      | 0.613  | 0.609  | -0.033          |
|      | 0.621  | 0.589  | 0.042           |
| Tot/f.u. | 0.615  | 0.586  |                 |
| Tot/f.u. | 0.722  | 0.764  |                 |

**Figure 2.** Density of States for the ferromagnetic configuration with the magnetization in the \( c \)-direction. Up-spin: upward, down-spin: downward.
In our previous work (de la Mora and Navarro 2008) the most stable configuration for the magnetic moment was in the \( b \)-direction. In the present work we found that the system is quite unstable and the convergence conditions should be quite strict, giving as a result that the \( c \)-direction is the most stable configuration.

The total magnetic moments (spin plus orbital) of the atoms for the \( b \)- and \( c \)-direction are given in table 2. U has large spin and orbital moments but in opposite directions which almost cancel. Cobalt has moderate spin and small orbital moments, both in the same direction. Therefore the main contribution comes from cobalt.

For the \( c \)-direction there is a deviation (canting) of the magnetic moments in the \( a \)-direction, while for the \( b \)-direction there is no canting. This canting is large for the total moments, the spin and orbital moments have opposite signs in their main component and the individual canting is relatively small (< 6°). This small value probably rules out a fully non-collinear magnetic order.

An interesting result, for the ferromagnetic configuration with the magnetization in the \( c \)-direction, is that there is a clear differentiation of the magnetic moment values into two groups, and these are grouped around the U-chains, see figure 1. The U-atoms in the A-chain have a small magnetic moment, \( \approx 0.07 \mu_B \), while in the B-chain the value is considerably larger, \( \approx 0.32 \mu_B \). The Co-atoms contiguous to these chains follow the same trend, although the magnetic moment difference is much smaller; the Co-atoms contiguous to the A-chains have \( \approx 0.59 \mu_B \) while for the B-chain it is \( \approx 0.61 \mu_B \). Therefore there is a modulation of the magnetic moment, or stripes, along the \( b \)-direction.

For the \( b \)-direction there is no magnetic moment differentiation, probably due to the fact that there is no canting.

The Density of States (DOS) is shown in figure 2. At the Fermi energy there is a narrow and deep drop, for the up-spin. For the down-spin the drop is larger by a factor of 3.5, and it is not so narrow, as if the material wanted to have a half-metal character.

### 4. Conclusions

In an attempt to conciliate with the small experimental magnetic moment, electronic structure calculations were done on UCoGe with different ferro- and antiferromagnetic configurations. The latter ones were found to have higher energy than the corresponding ferromagnetic one, being the ferromagnetic configuration in the \( c \)-direction the most stable, as a consequence it was not possible to find the small magnetic moment. The small deviations of the different components of the magnetic moments from the principal direction seem to rule out a non-collinear magnetic arrangement. There is a narrow partial gap at the Fermi energy which is deeper for the down-spin-DOS. The Co-atoms have a magnetic moment due mainly to the spin \( M = 0.6 \mu_B/f.u. \). The U-atoms have large spin and orbital contributions in opposite directions giving a small total moment. The value of this total moment has two values, \( M = 0.07 \) and \( 0.32 \mu_B/f.u. \), alternating in the \( b \)-direction forming magnetic stripes.

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