Pis'ma v ZhETF, vol. 117, iss. 11, pp. 863 – 864

Electron correlation effects in paramagnetic cobalt

A. S. Belozerov[+1)], *V. I. Anisimov*[*×]

[+]*Department of Physics, University of Hamburg, 20355 Hamburg, Germany*

[*]*M. N. Mikheev Institute of Metal Physics, Russian Academy of Sciences, 620108 Yekaterinburg, Russia*

[×]*Ural Federal University, 620002 Yekaterinburg, Russia*

Submitted 19 April 2023
Resubmitted 2 May 2023
Accepted 3 May 2023

DOI: 10.31857/S1234567823110095, EDN: djrpkp

Metallic cobalt is a canonical ferromagnet with an extremely high Curie temperature of 1418 K, which is significantly larger than that in iron (1043 K) and nickel (631 K). The experimental magnetic moment of ferromagnetic cobalt is also high ($1.7\,\mu_B$) and exceeded only by iron ($2.2\,\mu_B$) among all $3d$ metals.

At low temperatures, cobalt is ferromagnetic with the hexagonal close packed (hcp) lattice, which upon heating to 720 K transforms into the face-centred cubic (fcc) one. Further heating to 1418 K leads to a transition to the paramagnetic phase, which is stable up to a melting point of 1770 K.

The electronic structure of cobalt has been theoretically studied using density functional theory (DFT) within local density and generalized gradient approximations. These studies addressed electronic, structural and magnetic properties of both phases [1–6], but neglected the dynamic electron correlations, which were shown to be significant in other $3d$ metals [7–11]. Moreover, the DFT alone corresponds to zero temperature and cannot be applied directly to the paramagnetic state.

To obtain an accurate treatment of local many-body effects at finite temperatures, the DFT can be combined with model approaches, such as the dynamical mean-field theory (DMFT) [12]. This combination is called DFT + DMFT [13] and can be applied to both magnetically ordered and paramagnetic states at any ratio of Hubbard parameter U to bandwidth.

In this paper, we study the influence of Coulomb correlations on spectral and magnetic properties of paramagnetic fcc cobalt by the DFT + DMFT approach.

In contrast to the bcc iron, the obtained electronic self-energies exhibit a quasiparticle shape with the quasiparticle mass enhancement factor $m^*/m \sim 1.8$. These value corresponds to a moderately correlated metal and is greater than those for chromium (1.17) [9], nickel (1.25) [10], and vanadium (1.7) [11].

The calculated uniform magnetic susceptibility follows the Curie–Weiss law with the Curie–Weiss temperature $\Theta = 1240$ K, which is 13 % less than the experimental Curie temperature of 1418 K.

To clarify the underlying cause of the Curie–Weiss behaviour, we calculate the local magnetic susceptibility $\chi_{\rm loc} = 4\mu_B^2 \int_0^\beta \langle S_z(\tau) S_z(0)\rangle d\tau$, where S_z is the z-component of the local spin operator, β is the inverse temperature, τ is the imaginary time. The inverse of $\chi_{\rm loc}$ also depends linearly on temperature. This finding indicates that the Curie–Weiss behaviour of uniform magnetic susceptibility is caused by formation of local magnetic moments.

To investigate the degree of magnetic moment localization, we examine the local spin-spin correlation function $\chi_{\rm spin}(\tau) = \langle S_z(\tau) S_z(0)\rangle$ and its real-frequency counterpart $\chi_{\rm spin}(\omega)$. The latter is obtained by Fourier transforming $\chi_{\rm spin}(\tau)$ to imaginary frequency and then analytically continuing to real frequency ω. In the top panel of Fig. 1, we present the obtained $\chi_{\rm spin}(\tau)$ and the real part of $\chi_{\rm spin}(\omega)$ in comparison with those of paramagnetic chromium [9], which is a canonical itinerant antiferromagnet, and bcc iron [14] known as a system with well-defined local magnetic moments. One can see that $\chi_{\rm spin}(\tau)$ for cobalt has an instantaneous average $\langle S_z^2\rangle = 0.75$, which is lower than iron's value of 1.6 and close to that of chromium. However, in contrast to Cr, $\chi_{\rm spin}(\tau)$ for cobalt saturates to a finite value at $\tau \to \beta/2$, indicating some localization of magnetic moments.

To obtain a more quantitative estimate of moments localization, we consider the real part of $\chi_{\rm spin}(\omega)$ shown in the right panels of Fig. 1. Specifically, the half-width of the peak in $\mathrm{Re}[\chi_{\rm spin}(\omega)]$ at its half-height is nearly equal to the inverse lifetime of local magnetic moments [8]. The obtained results indicate that the lifetime of magnetic moments in cobalt is about 10 times

[1)]e-mail: alexander.s.belozerov@gmail.com

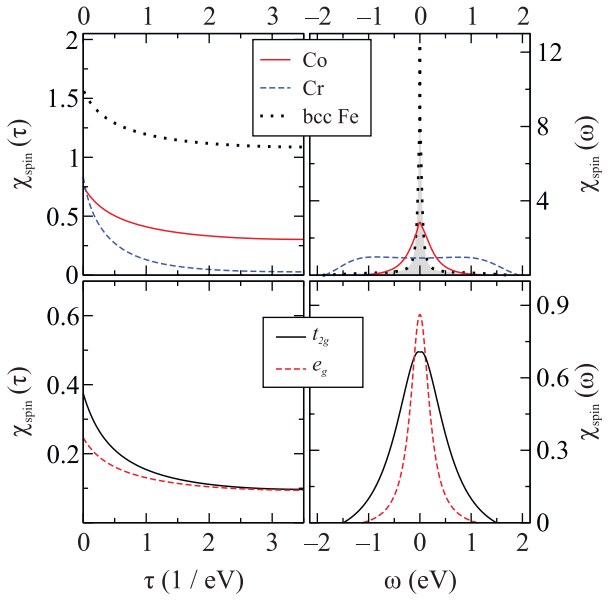

Fig. 1. (Color online) Local spin-spin correlation functions in the imaginary time τ (left panels) and real frequency ω (right panels) domains calculated by DFT + DMFT method for cobalt in comparison with those of paramagnetic chromium [9] and bcc iron [14] (top panels). Bottom panels: orbital-resolved spin-spin correlation functions for cobalt

lower than in bcc iron, but about 8 times larger than in chromium.

To identify the dominant wave-vector of magnetic response, we calculate the momentum dependence of the static magnetic susceptibility. The obtained results reveal the dominance of ferromagnetic correlations.

To summarize, we have investigated the electronic and magnetic properties of fcc cobalt by DFT + DMFT approach. The computed uniform and local magnetic susceptibilities follow the Curie–Weiss law, which has been shown to occur due to the partial formation of local magnetic moments. We found that the lifetime of these moments in cobalt is significantly less than in bcc iron, implying that the magnetism of cobalt is more itinerant. Furthermore, contrary to previous reports for bcc iron [7], we have not observed substantial orbital selectivity in cobalt. In particular, all obtained electronic self-energies in cobalt exhibit a quasiparticle shape with the quasiparticle mass enhancement factor $m^*/m \sim 1.8$, corresponding to moderately correlated metal. Analyzing the momentum dependence of static magnetic susceptibility, we found a strong tendency to ferromagnetic ordering.

We thank A. A. Katanin for the valuable discussions. The DFT + DMFT calculations were supported by the Russian Science Foundation (project # 19-12-00012). A. S. Belozerov was supported by the Alexander von Humboldt Foundation.

This is an excerpt of the article “Electron correlation effects in paramagnetic cobalt”. Full text of the paper is published in JETP Letters journal. DOI: 10.1134/S0021364023601379

1. E. G. Moroni, G. Kresse, J. Hafner, and J. Furthmüller, Phys. Rev. B **56**, 15629 (1997).
2. T. C. Leung, C. T. Chan, and B. N. Harmon, Phys. Rev. B **44**, 2923 (1991).
3. M. Körling and J. Häglund, Phys. Rev. B **45**, 13293 (1992).
4. J.-H. Cho and M. Scheffler, Phys. Rev. B **53**, 10685 (1996).
5. S. F. Matar, A. Houari, and M. A. Belkhir, Phys. Rev. B **75**, 245109 (2007).
6. V. A. de la Peña O’Shea, I. de P. R. Moreira, A. Roldán, and F. Illas, J. Chem. Phys. **133**, 024701 (2010).
7. A. A. Katanin, A. I. Poteryaev, A. V. Efremov, A. O. Shorikov, S. L. Skornyakov, M. A. Korotin, and V. I. Anisimov, Phys. Rev. B **81**, 045117 (2010).
8. P. A. Igoshev, A. V. Efremov, A. I. Poteryaev, A. A. Katanin, and V. I. Anisimov, Phys. Rev. B **88**, 155120 (2013).
9. A. S. Belozerov, A. A. Katanin, and V. I. Anisimov, J. Phys.: Condens. Matter **33**, 385601 (2021).
10. A. Hausoel, M. Karolak, E. Şaşıoğlu, A. Lichtenstein, K. Held, A. Katanin, A. Toschi, and G. Sangiovanni, Nat. Commun. **8**, 16062 (2017).
11. A. S. Belozerov, A. A. Katanin, and V. I. Anisimov, Phys. Rev. B **107**, 035116 (2023).
12. A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
13. V. I. Anisimov, A. I. Poteryaev, M. A. Korotin, A. O. Anokhin, and G. Kotliar, J. Phys.: Condens. Matter **9**, 7359 (1997).
14. A. S. Belozerov, A. A. Katanin, and V. I. Anisimov, Phys. Rev. B **96**, 075108 (2017).