

# Anisotropy of resistivity in hexagonal late transition metals and their alloys

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## Abstract

Transport properties of hexagonal transition metals Co, Ru, and Os at finite temperatures are studied by means of *ab initio* electronic structure techniques and the Kubo linear response theory. An alloy analogy model for a quantitative treatment of the electrical conductivities due to temperature-induced lattice vibrations (phonons) and spin fluctuations is applied with focus on anisotropy induced by the hexagonal structure. The resistivity anisotropy in Co is found opposite to that in Ru and Os, in agreement with existing experimental data. This result is ascribed to the strong itinerant ferromagnetism of Co which leads to profound differences in the electronic structure and conductivities in the majority and minority spin channels. A similar sensitivity to spin polarization is predicted for the anisotropy of residual resistivity in random hexagonal Co-rich Co–Ni and Co–Ni–Fe alloys.

Keywords: electrical resistivity, spin polarization, hexagonal systems, random alloys

(Some figures may appear in colour only in the online journal)

## 1. Introduction

Anisotropy of physical properties represents a general feature of crystalline solids. Examples are given by the well-known elastic behavior of materials or the magneto-crystalline anisotropy of ferromagnets. A notable exception to this rule are, e.g. transport properties of cubic systems without spontaneous magnetic order, where the corresponding transport coefficients (comprised in the conductivity tensor) exhibit the same symmetry as in a homogeneous isotropic continuum.

The anisotropy of transport properties of transition-metal based systems attracted lots of attention during the last several decades especially for magnetically ordered alloys and compounds. This interest is due to relevance of the accompanying phenomena for magnetic memory devices. The anisotropic magnetoresistance reflects primarily sensitivity of longitudinal electric resistivities to the mutual orientation of the electric current and magnetization. In single crystals, however,

also the direction of magnetization with respect to crystallographic axes plays an important role [1]. Similar sensitivity has also been reported for the transverse transport quantities, such as the anisotropic anomalous Hall effect in ferromagnetic hcp cobalt [2]. The most recent development in this area includes investigation of these phenomena in antiferromagnets, both collinear [3] and non-collinear [4].

Since materials prospective for spintronic applications are often multicomponent, with several sublattices and layered structures [5, 6], the anisotropy of their transport properties can originate not only in their magnetic structure, but also in their crystalline structure. Assessment of a separate effect of magnetism and geometry on the resulting anisotropy of transport properties is a difficult problem, partly due to the fact that spin polarization can strongly influence the stability of crystal structures. The ground-state crystal structure of ferromagnetic 3d transition elements Fe (bcc) and Co (hcp) differs from that of their nonmagnetic 4d and 5d isoelectronic counterparts which form hcp (Ru, Os) and fcc (Rh, Ir) lattices; this difference is a consequence of ferromagnetism of Fe and Co [7]. Similarly, the presence or absence of spin polarization

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in binary transition-metal alloys is often responsible for the observed atomic ordering phenomena [8].

The late transition metals Co, Ru, and Os belong all to the same group VIII of the periodic system of elements and they crystallize in the same hcp structure. However, their longitudinal resistivities  $\rho_{xx} = \rho_{yy}$  for currents in the basal  $ab$  plane and  $\rho_{zz}$  for currents along the three-fold  $c$  axis exhibit different anisotropies, namely,  $\rho_{xx} < \rho_{zz}$  for Co [9], whereas  $\rho_{xx} > \rho_{zz}$  for Ru and Os [10]. This fact can be ascribed to a number of potential sources, such as a different number of valence electrons, a slightly different hexagonal  $c/a$  ratio ( $c/a = 1.62$  for Co,  $c/a = 1.58$  for Ru and Os), the ferromagnetism of Co, or the increasing strength of spin-orbit interaction in sequence Co, Ru, and Os. The simple crystal structure and the chemical similarity of these three pure metals call for detailed explanation of their transport properties.

The purpose of this paper is to identify the mechanism responsible for the observed resistivity anisotropy in hcp Co, Ru, and Os by means of up-to-date first-principles techniques. Moreover, anisotropy of residual resistivities in random hcp alloys based on these elements is studied as well. This allows us to treat all basic origins of electron scattering in transition-metal systems, namely, the scattering on phonons and magnons at finite temperatures, which is relevant for pure metals, and the scattering on impurities, which dominates for substitutionally disordered alloys.

## 2. Methods and models

The calculated results were obtained by means of the fully relativistic tight-binding linear muffin-tin orbital (TB-LMTO) method in the atomic sphere approximation [11]. Both non-magnetic and spin-polarized versions were used in combination with the coherent potential approximation (CPA) for an efficient treatment of substitutionally disordered systems [12]. Selfconsistency of the effective one-electron potentials was achieved in the local spin-density approximation (LSDA) with the exchange-correlation potential parametrized according to [13]. The valence basis comprised  $s$ -,  $p$ -,  $d$ -, and  $f$ -type orbitals; other numerical details for the studied hexagonal systems were similar to those employed in a previous study of tetragonal alloys [14]. Optionally, the scalar-relativistic version of the TB-LMTO technique (neglecting spin-orbit interaction) was applied as well.

The electronic transport properties were studied in the framework of the static Kubo linear response theory. The central quantity, namely, the electrical conductivity tensor  $\sigma_{\mu\nu}$  ( $\mu, \nu = x, y, z$ ) was formulated with a systematic neglect of intraatomic electron motion; the interatomic electron hoppings were then described in the TB-LMTO technique [15, 16]. This formalism was worked out in detail for electron scattering on random static fluctuations of the one-electron potential in substitutional solid solutions; the configuration averaging is done in the CPA including the vertex corrections to  $\sigma_{\mu\nu}$  [17]. The so-called Fermi-sea contribution to  $\sigma_{\mu\nu}$  [18], relevant only for the antisymmetric part of the conductivity tensor, i.e. for the anomalous Hall effect, has been omitted in this work focused on the longitudinal transport properties.

For the numerical implementation, a tiny imaginary part of magnitude  $\varepsilon = 10^{-5}$  Ry has been added to the real Fermi

energy  $E_F$ , so that the CPA-selfconsistency condition and all Green's functions are evaluated at complex energies  $E_F \pm i\varepsilon$ . The averages over the first Brillouin zone (BZ) were performed on a uniform mesh of reciprocal-space vectors equivalent to  $128 \times 10^6$  sampling points in the full BZ.

The above-described techniques are directly applicable to residual resistivities of random crystalline alloys. The study of phonon-induced finite-temperature electronic transport properties of pure metals was done within the alloy analogy model [19]. In this approach, the displacements of atoms from their equilibrium positions induce random shifts of the frozen one-electron atomic potentials obtained from the selfconsistent LSDA calculations at zero temperature. The displaced atom represents an analogy to a particular chemical component in a multicomponent substitutionally disordered alloy with the ideal (undistorted) crystal structure. The system is then treated in the CPA as an effective  $N$ -component random alloy where  $N$  denotes the finite number of quasi-random displacement vectors  $\mathbf{u}_i$  of a single atom and their probabilities (concentrations)  $c_i$ ,  $i = 1, 2, \dots, N$ , see [19] for more details. In this work, the root-mean-square (r.m.s.) displacement  $\bar{u}$  (average magnitude of the single-atom displacements), defined by  $\bar{u}^2 = \sum_{i=1}^N c_i \mathbf{u}_i^2$ , was related to a finite temperature  $T$  by means of the simple Debye theory employing experimental values of the Debye temperature  $\theta_D$ .

The alloy analogy model was originally formulated in the Korringa-Kohn-Rostoker (KKR) multiple-scattering theory [19]; the present work employs its recently developed TB-LMTO version [20, 21]. The alloy analogy model was used to a number of cubic systems while its application to hexagonal Gd [22] represents rather an exception. In this study, the experimental low-temperature lattice parameters of Co ( $a = 0.25030$  nm,  $c = 0.40574$  nm) [23], Ru ( $a = 0.27028$  nm,  $c = 0.42742$  nm) [24], and Os ( $a = 0.27315$  nm,  $c = 0.43148$  nm) [25] were used. The random atomic displacements were represented by  $N = 8$  quasi-random vectors of the same magnitude  $\bar{u}$  with directions and probabilities respecting hexagonal symmetry of the lattice. The Debye temperatures  $\theta_D$  were chosen as 445 K for Co [26], 550 K for Ru, and 467 K for Os [27].

The effect of spin polarization of ferromagnetic Co was included by means of the one-electron Kohn-Sham-Dirac Hamiltonian incorporating an effective (exchange-correlation) magnetic field coupled to electron spin [28, 29]. The direction of Co magnetization was chosen along  $c$  axis (the magnetic easy axis); tilting the magnetization direction into the basal  $ab$  plane induces relative changes in electrical resistivities less than 0.5% which is at least an order of magnitude smaller than the resistivity anisotropies owing to different directions of the electric current [9]. For this reason, the present work was confined to the bulk Co magnetization parallel to  $c$  axis.

In ferromagnetic systems at finite temperatures, fluctuating directions of local magnetic moments can be considered as another source of electron scattering besides the atomic displacements [19]. In this study, we employed for ferromagnetic Co a simple model of tilted moments [30, 31] with  $M$  directions  $\mathbf{n}_j = (\sin \vartheta \cos \varphi_j, \sin \vartheta \sin \varphi_j, \cos \vartheta)$ ,  $j = 1, 2, \dots, M$ , given by a fixed angle  $\vartheta$  and quasi-random

angles  $\varphi_j$  uniformly distributed over interval  $[0, 2\pi]$ . We chose  $M = 12$  and  $\varphi_j = j\pi/6$ , which results in  $MN = 96$  components occupying all sites of the hcp lattice. The temperature-dependent values of  $\vartheta$  were estimated from identification of  $\cos \vartheta$  with reduced magnetization and from an existing parametrization of the experimental temperature dependence of Co magnetization [32].

### 3. Results and discussion

In this study, we considered four hcp systems: Co, Ru, and Os, whereby Co was treated both in a ferromagnetic (FM) and a nonmagnetic (NM) state. The calculated resistivities  $\rho_{xx}$  and  $\rho_{zz}$  in the fully relativistic theory as functions of the r.m.s. displacement  $\bar{u}$  are displayed in figure 1 together with available experimental data [9, 10]. The displacements  $\bar{u}$  are given in units of the Bohr radius  $a_B = 52.92$  pm. One can see that the calculated results for Ru (figure 1(c)) and Os (figure 1(d)) reproduce semiquantitatively the experimental trends including the resistivity anisotropy,  $\rho_{xx} > \rho_{zz}$ . The results for Co depend strongly on its magnetic state: the calculated and measured resistivities for FM Co (figure 1(a)) exhibit the same anisotropy,  $\rho_{xx} < \rho_{zz}$ , which is opposite to that encountered in Ru and Os. However, the calculated anisotropy for NM Co (figure 1(b)) is in line with that for other NM metals (Ru and Os), which contradicts the room-temperature experiment performed with FM Co [9]. These facts indicate that the difference of resistivity anisotropy between Co and Ru or Os is due to the spontaneous FM order of Co, whereas the role of different number of valence electrons is of minor importance.

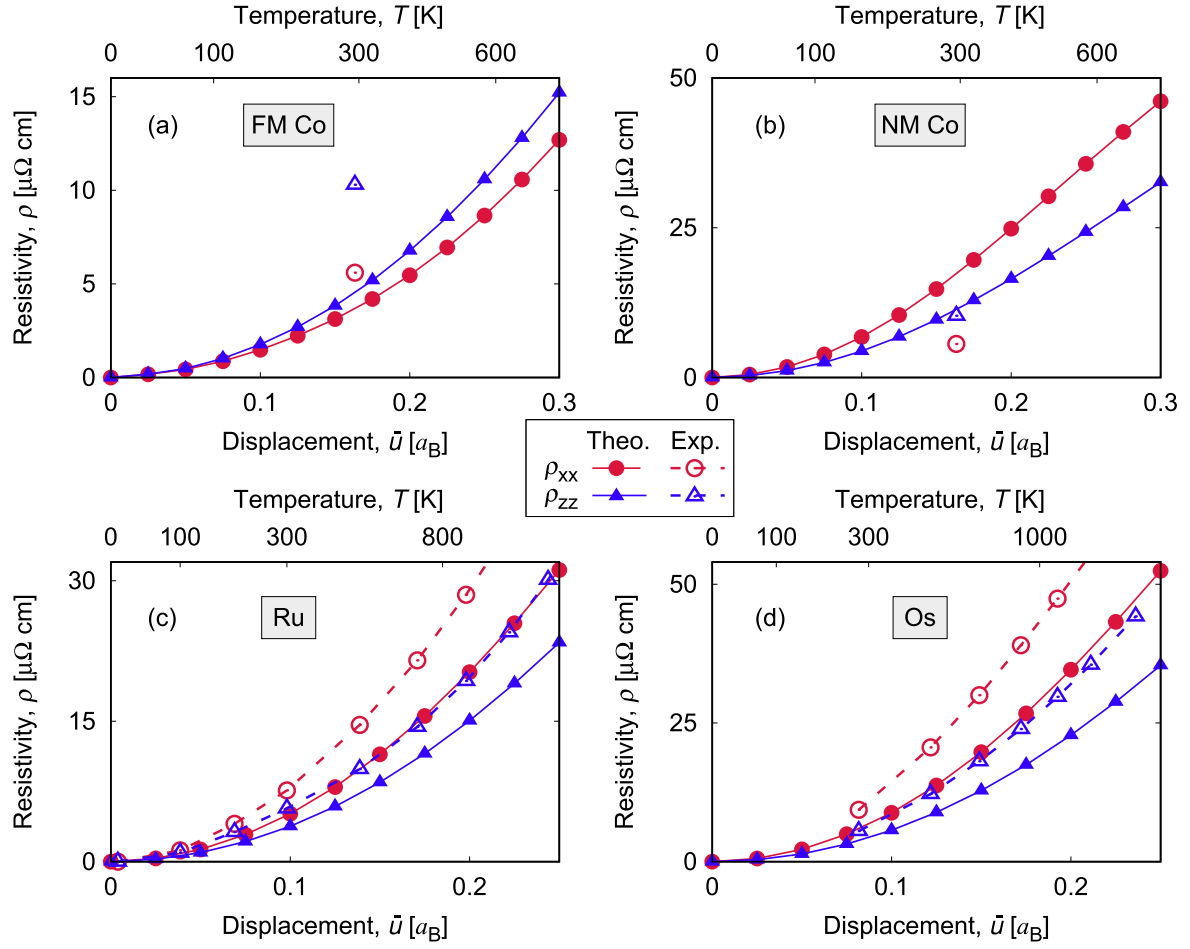
In order to estimate the effect of spin-orbit interaction, we studied the resistivities of Co (FM and NM), Ru, and Os in the scalar-relativistic approximation. The obtained values and trends of dependences on  $\bar{u}$  (not shown here) are close to those in the fully relativistic theory (figure 1). Table 1 summarizes all resistivities (both in the scalar-relativistic and the fully relativistic approach) for a particular r.m.s. displacement  $\bar{u} = 0.2 a_B$ . One can clearly see that spin-orbit interaction has a small effect on the resistivities ( $\lesssim 10\%$ ) and on their anisotropy in all four cases studied.

The scalar-relativistic approximation applied to electron transport in FM Co with perfectly collinear spin structure is equivalent to the well-known two-current model [33] in which the total conductivity equals a sum of conductivities in the majority (spin  $\uparrow$ ) and minority (spin  $\downarrow$ ) channels. These spin-resolved conductivities are given in table 1 in terms of the corresponding resistivities (reciprocal values of the conductivities). Two facts should be mentioned. First, the majority-channel conductivities are an order of magnitude larger than their minority-channel counterparts, so that the electrical current is carried mainly by the spin- $\uparrow$  electrons. Second, the anisotropy of the spin- $\downarrow$  resistivities is qualitatively the same as that in all NM cases, whereas the anisotropy of the spin- $\uparrow$  resistivities resembles that of the total resistivities in the Co FM case. One can thus conclude that the sensitivity of the anisotropy to the spin polarization of hcp Co is due to the strong spin dependence of transport in FM Co. This feature

can be explained by the well-known difference between the majority and minority electronic structures in FM Co [34]. The exchange splitting in this strong itinerant ferromagnet shifts the majority valence  $d$ -band below the Fermi energy, so that  $E_F$  lies in a region of  $sp$ -like states, whereas the minority  $d$ -band is only partially occupied, containing holes above the Fermi level. The broad  $sp$ -band corresponds to high electron velocities, in contrast to the narrow  $d$ -band related to small velocities. This results in much higher majority conductivities as compared to the little conductive minority channel (table 1).

The calculated resistivities  $\rho_{xx}$  and  $\rho_{zz}$  for FM Co agree with available experimental data only semiquantitatively, see figure 1. However, the observed relation  $\rho_{xx} < \rho_{zz}$  is reproduced correctly and one should thus examine the robustness of the resistivity anisotropy with respect to spin fluctuations neglected in the results displayed in figure 1(a). We have chosen particular values of  $\bar{u} = 0.175 a_B$  for the displacements and  $\vartheta = 0.045\pi$  for the tilted moments; these values seem realistic (see section 2) for temperatures around room temperature of the resistivity measurement [9]. The resulting resistivities due to a separate effect of phonons ( $\rho_{\mu\mu}^{\text{ph}}$ ) and spin fluctuations ( $\rho_{\mu\mu}^{\text{sf}}$ ), and due to the simultaneous effect of both scattering mechanisms ( $\rho_{\mu\mu}^{\text{ph,sf}}$ ) are summarized in table 2. One can see that the net effect of spin fluctuations yields opposite anisotropy ( $\rho_{xx}^{\text{sf}} > \rho_{zz}^{\text{sf}}$ ) than that of the displacements ( $\rho_{xx}^{\text{ph}} < \rho_{zz}^{\text{ph}}$ ). The same anisotropy due to the spin fluctuations ( $\rho_{xx}^{\text{sf}} > \rho_{zz}^{\text{sf}}$ ) has also been obtained in a recent theoretical study of hcp Gd [22]. Nevertheless, the combination of both mechanisms yields the Co anisotropy in line with experiment, i.e.  $\rho_{xx}^{\text{ph,sf}} < \rho_{zz}^{\text{ph,sf}}$ . This can be explained by significantly smaller values of  $\rho_{\mu\mu}^{\text{sf}}$  as compared to  $\rho_{\mu\mu}^{\text{ph}}$ . Note, however, that the effects of phonons and spin fluctuations on the resistivity are not simply additive, as can be documented by non-negligible difference between the sum of both resistivities ( $\rho_{\mu\mu}^{\text{ph}} + \rho_{\mu\mu}^{\text{sf}}$ ) and the resulting  $\rho_{\mu\mu}^{\text{ph,sf}}$ . This non-additivity is equivalent to a violation of the Matthiessen's rule, which in the present case underestimates the values of  $\rho_{\mu\mu}^{\text{ph,sf}}$  by about 29% for  $\rho_{xx}$  and 27% for  $\rho_{zz}$ . A similar non-additive behavior of resistivities due to both scattering mechanisms has been observed in recent theoretical studies of Fe and Gd [22, 35, 36], which contrasts the results for Ni where the Matthiessen's rule is practically satisfied [20].

The calculated resistivities differ from the measured values (figure 1) for several reasons. First, the correlations between displacements of neighboring atoms are completely neglected in the alloy analogy model. For FM systems, similar correlations between fluctuating directions of local magnetic moments (magnetic short-range order) are neglected as well. Second, the relaxation of one-electron potentials accompanying the displacements should also be taken into account in a true adiabatic approach going beyond the frozen-potential approximation adopted here. Third, the harmonic approximation and the simple Debye model for phonon spectra represent further points to be improved in the future. Finally, the CPA neglects certain correlations between the random single-site  $t$ -matrices describing scattering with respect to the



**Figure 1.** Calculated resistivities  $\rho_{xx}$  (full circles) and  $\rho_{zz}$  (full triangles) in the fully relativistic alloy analogy model as functions of the r.m.s. displacement  $\bar{u}$ : (a) for FM Co, (b) for NM Co, (c) for Ru, and (d) for Os. The approximate temperature scale according to the Debye theory is marked on the upper horizontal axis. The experimental values of  $\rho_{xx}$  (open circles) and  $\rho_{zz}$  (open triangles) are taken from [9] for Co and from [10] for Ru and Os.

**Table 1.** Calculated resistivities  $\rho_{xx}$  and  $\rho_{zz}$  for the r.m.s. displacement  $\bar{u} = 0.2 a_B$ . The results refer to the scalar-relativistic approximation; the values in parentheses are obtained in the fully relativistic approach. The data shown for Co FM  $\uparrow$  and Co FM  $\downarrow$  correspond respectively to majority and minority spin channel in the two-current model.

System	$\rho_{xx}$ ( $\mu\Omega$ cm)	$\rho_{zz}$ ( $\mu\Omega$ cm)
Co FM	5.33 (5.46)	6.02 (6.77)
Co FM $\uparrow$	5.71 (—)	6.87 (—)
Co FM $\downarrow$	80.1 (—)	49.0 (—)
Co NM	24.2 (24.8)	15.9 (16.5)
Ru	19.8 (20.2)	14.8 (15.1)
Os	30.5 (34.6)	20.5 (22.8)

effective medium. Removal of some of these approximations can be done, e.g. within a supercell TB-LMTO technique [30]. However, application of real-space supercell techniques goes beyond the scope of this work. Let us note that the relative difference between the present calculated resistivities and the experimental resistivities is comparable to that obtained in a recent KKR study of hcp Gd [22].

**Table 2.** Calculated resistivities in hcp Co due to a separate effect of phonons,  $\rho_{\mu\mu}^{\text{ph}}$  (for  $\bar{u} = 0.175 a_B$ ), and of spin fluctuations,  $\rho_{\mu\mu}^{\text{sf}}$  (for  $\vartheta = 0.045\pi$ ), and due to the simultaneous effect of both scattering mechanisms,  $\rho_{\mu\mu}^{\text{ph,sf}}$ . The sum of both separate contributions is shown by  $\rho_{\mu\mu}^{\text{ph}} + \rho_{\mu\mu}^{\text{sf}}$ .

	$\rho_{xx}$ ( $\mu\Omega$ cm)	$\rho_{zz}$ ( $\mu\Omega$ cm)
$\rho_{\mu\mu}^{\text{ph}}$	4.19	5.19
$\rho_{\mu\mu}^{\text{sf}}$	0.948	0.721
$\rho_{\mu\mu}^{\text{ph,sf}}$	7.20	8.06
$\rho_{\mu\mu}^{\text{ph}} + \rho_{\mu\mu}^{\text{sf}}$	5.14	5.91

Electron transport in random alloys (substitutional solid solutions) is often dominated by scattering on impurities, which raises a question about the anisotropy of the residual resistivities in hcp alloys and its possible relation to the spin polarization. In this work, we chose three random hcp systems as case studies, namely, a binary  $\text{Co}_{85}\text{Ni}_{15}$  alloy, a ternary  $\text{Co}_{84}\text{Fe}_8\text{Ni}_8$  alloy, and a binary  $\text{Os}_{50}\text{Ru}_{50}$  alloy. The first one represents a stable phase of the binary Co–Ni system for temperatures around room temperature [37], the second one



**Table 3.** Calculated residual resistivities of random hcp alloys.

Alloy	$\rho_{xx}$ ( $\mu\Omega$ cm)	$\rho_{zz}$ ( $\mu\Omega$ cm)
Co <sub>85</sub> Ni <sub>15</sub> FM	0.668	0.851
Co <sub>85</sub> Ni <sub>15</sub> NM	12.0	9.53
Co <sub>84</sub> Fe <sub>8</sub> Ni <sub>8</sub> FM	1.91	2.18
Co <sub>84</sub> Fe <sub>8</sub> Ni <sub>8</sub> NM	11.6	8.95
Os <sub>50</sub> Ru <sub>50</sub>	3.98	2.86

is a hypothetical alloy isoelectronic with pure Co, and the last one is a stable phase at high temperatures [37]. The calculated residual resistivities of these alloys, including the FM and NM states of both Co-based systems, are presented in table 3. The results witness that the resistivity anisotropy is qualitatively the same as in pure elements Co, Ru, and Os (figure 1). This finding proves that the particular scattering mechanism is less relevant for the anisotropy of resistivities in hcp systems based on late transition metals and that the most important factor is the presence or absence of a spontaneous FM order.

#### 4. Conclusions

Employing *ab initio* electronic structure calculations, we have investigated electrical resistivities of hcp systems containing Co, Ru, and Os, with particular attention paid to the resistivity anisotropy. We have simulated electron scattering on phonons, magnons, and impurities on equal footing within the alloy analogy model and the coherent potential approximation. The optional inclusion of spin polarization and of spin-orbit interaction allows us to conclude that the observed resistivity anisotropies in pure elements reflect the strong itinerant ferromagnetism of Co and the absence of spin polarization in Ru and Os, whereas other differences between these elements (number of valence electrons, hexagonal *c/a* ratio, strength of spin-orbit interaction) play only a minor role. This conclusion is not confined to pure metals; the same behavior can also be expected in random hcp alloys based on late transition metals.

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