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Magnetovolume effects in RCo_2 compounds ($\text{R} = \text{Gd}, \text{Dy}, \text{Er}$) from *ab initio* calculations

Ilja Turek^{1,2}, Jan Ruzs², Martin Diviš²

¹*Institute of Physics of Materials, Academy of Sciences of the Czech Republic,
Žitkova 22, 61662 Brno, The Czech Republic*

²*Department of Electronic Structures, Faculty of Mathematics and Physics, Charles University,
Ke Karlovu 5, 12116 Praha 2, The Czech Republic*

The Laves phase intermetallic compounds RCo_2 , where R denotes a rare-earth metal, exhibit a number of interesting magnetic properties. The latter include pronounced variations of resistivities and lattice parameters accompanying changes of the magnetic state. The underlying magnetic phase transitions can be caused by temperature changes and/or by an applied magnetic field [1].

A generally accepted explanation of the magnetostriction observed in magnetic RCo_2 compounds with the C15 cubic structure is based on the magnetovolume effect of Co atoms [1]: the magnitude of the local Co-magnetic moment depends on an effective molecular field due to the local R-magnetic moments and the corresponding magnetic pressure contributes to the resulting volume of the compound. Other authors emphasize that the Co-moment is equally sensitive to the molecular field and to the lattice constant itself [2].

A detailed quantitative analysis of these magnetovolume phenomena based on *ab initio* electronic structure calculations has not been given yet. First-principles calculations of RCo_2 are difficult for two reasons: (i) the standard local spin-density approximation (LSDA) fails to describe properly the cohesive properties due to the localized 4f-orbitals of R atoms, and (ii) the paramagnetic phase of the compounds is featured by non-vanishing local R-magnetic moments pointing in random directions, breaking thus the perfect translational symmetry of the solid on microscopic scale.

Here we present results of *ab initio* calculations of equilibrium lattice

parameters of the RCo_2 compounds ($\text{R} = \text{Gd}, \text{Dy}, \text{Er}$) for a few models of their magnetic structure appropriate on both sides of the magnetic phase transition.

The electronic structure calculations were carried out in the all-electron scalar-relativistic tight-binding linear muffin-tin orbital (TB-LMTO) method in the atomic sphere approximation (ASA) [3]. Accuracy of the ASA has been checked by a full-potential technique (FLAPW) [4] where possible. The standard LSDA was complemented by an open-core (OC) treatment of the 4f-orbitals of R atoms by taking these orbitals as a part of the atomic core.

The investigated magnetic structures comprise not only the usual ferrimagnetic (FM) structure observed for the magnetic ground state, but included two states relevant at elevated temperatures as well: the so-called disordered-local-moment (DLM) state with zero Co-moments and non-zero R-moments oriented randomly, and a partial DLM (pDLM) state. The latter is a collinear structure with non-vanishing ordered Co-moments and disordered Ising-like R-moments. The DLM and pDLM states were treated in the coherent potential approximation (CPA). It should be noted that the molecular field acting on Co atoms due to the local R-moments vanishes both in the DLM and the pDLM states.

As expected, standard LSDA results for the lattice parameters were too low as compared to the experimental ones. For example, for the DyCo_2 with the FM structure, the experimental lattice parameter ($a_{\text{exp}} = 7.188 \text{ \AA}$) lies about 5% above the

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calculated ones ($a_{\text{FLAPW}} = 6.805 \text{ \AA}$, $a_{\text{LMTO}} = 6.847 \text{ \AA}$).

Results of the LSDA-OC calculations using the LMTO method are summarized in Table 1. The equilibrium lattice parameters in the FM state are now slightly higher than the experimental ones but the relative deviations are below 1%. Moreover, the well-known lanthanoid contraction (a decrease of a in the sequence Gd-Dy-Er) is reproduced as well.

Table 1. The lattice parameters a of RCo_2 (in \AA ; R = Gd, Dy, Er): experimental and calculated in different magnetic states X (X = FM, DLM, pDLM), relative deviations r_X (X = DLM, pDLM) of the calculated lattice parameters with respect to the FM state, and the calculated local Co-magnetic moments m_X (in μ_B ; X = FM, pDLM).

$< r_{\text{exp}} < 0.002$ for the three compounds considered here [1]. The calculated DLM-FM relative deviations, r_{DLM} , are higher by a factor of 4 (Tab. 1) which indicates that a complete collapse of the local Co-moment above the magnetic transition temperature should cause much bigger magnetovolume effects than observed. It should be noted that the LMTO-ASA magnitudes of the Co-moments in the FM state agree reasonably with previous full-potential results [5].

As mentioned by many authors, spin fluctuations at the Co-sublattice play non-negligible role in these systems [1,2]. To a certain extent, their effect can be simulated in terms of the pDLM state, where non-zero Co-moments coexist with disordered R-moments. As can be seen from Table 1, the Co-moments can be formed even in the pDLM state, i.e., without the molecular field caused by the R-sublattice. The magnitudes of the Co-moments in the pDLM state are only slightly smaller than those in the FM state (Tab. 1) which proves that the Co-Co exchange interaction is stronger than the R-Co coupling. The small reduction of the Co-moment magnitude in the pDLM state with respect to the FM state leads to tiny relative changes of the lattice constant between these states (Tab. 1).

Our results indicate that magnetovolume effects due to a complete collapse of the Co-

	Gd	Dy	Er
a_{exp}	7.256	7.188	7.144
a_{FM}	7.312	7.253	7.203
m_{FM}	1.230	1.192	1.161
a_{DLM}	7.248	7.197	7.151
r_{DLM}	0.0088	0.0078	0.0072
a_{pDLM}	7.301	7.247	7.200
r_{pDLM}	0.0015	0.0009	0.0004
m_{pDLM}	1.098	1.105	1.114

The calculated lattice parameters in the DLM and pDLM states are smaller than in the FM ground state (Tab. 1). The measured relative deviation of the lattice parameter accompanying the magnetic phase transition can be roughly estimated in the range 0.0015

moment in the RCo_2 compounds are appreciably bigger than experimentally observed. Consequently, a full quantitative explanation of these effects will be impossible without taking into account the spin fluctuations on the Co-sublattice. A tendency to the spontaneous polarization of the Co-sublattice even in absence of the molecular exchange field due to the R-sublattice has been proved as well.

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