Magnetostructural properties of RCo$_2$ (R = rare earth) compounds

DURGA PAUDYAL, YA. MUDRYK, Ames Laboratory of the USDOE, Iowa State University, Ames, IA-50011, V. K. PECHARSKY, K. A. GSCHNEIDNER, JR., Ames Laboratory of the USDOE and Department of Materials Science and Engineering, Iowa State University, Ames, IA-50011 — First principles electronic structure calculations show that the cubic Laves phase (C15) is stable for GdCo$_2$ and TbCo$_2$, while the ground state structures of DyCo$_2$, HoCo$_2$, and ErCo$_2$ are tetragonal distortions of the cubic C15, orthorhombic, and rhombohedral structures, respectively. The R and Co moments exhibit antiparallel coupling, forming a ferrimagnetic state in every ground state structure of RCo$_2$. The predicted magnetostructural properties of RCo$_2$ are in good agreement with x-ray powder diffraction and magnetic measurements. The spin splitting of the conduction electrons due to the indirect R-R exchange plays a crucial role in the magnetostructural transformations in the R = Dy, Ho, and Er RCo$_2$ phases, and accounts for its absence in the monomorphic GdCo$_2$ and TbCo$_2$ compounds.

1This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under contract No. DE-AC02-07CH11358 with Iowa State University of Science and Technology.

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Date submitted: 20 Nov 2008
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