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EINLADUNG zum IFP-SEMINAR

Hardmagnetic properties of transition metals and rare earths (T - R) compounds

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Host: Josef Fidler

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Ort: Institut für Festkörperphysik, TU Wien
Wiedner Hauptstraße 8-10, 1040 Wien
Seminarraum DC rot 07 (roter Bereich, 7. OG)

Abstract:

This work focuses on the hardmagnetic properties of transition metals and rare earths (T - R) compounds with advanced permanent magnetic properties, which has led to their application in many technologies including automotive and data storage. The focus is on two families of compounds with stoichiometries RCo_5 ($R = Sm, Pr$ and Y), and $R_2Fe_{14}B$ ($R = Pr, Nd, Dy$ and Y). Two important properties, which determine usefulness for permanent magnet application are stored energy in a unit volume $(BH)_{\max}$ and the coercive field H_C. These macroscopic hysteretic properties depend not only the shape and the microstructure of a magnet, but also on the intrinsic properties of the grains, most importantly saturation magnetization M_S and magnetocrystalline anisotropy energy (MAE).

Computational methods can be used to research these intrinsic properties and allow an understanding of the atomistic effects, which in turn influence coercivity and hysteresis. Using numerical methods based on density functional theory, M_S and MAE in the mentioned (R - T) compounds are calculated at 0 K for ideal crystals, utilizing an LAPW code (WIEN2k) and a PAW code (VASP). The results of the calculations are presented and the conclusions that can be drawn from them and their implications are discussed. The presentation covers results on non-substituted phases, changes due to strain effects and substitution, as well as the impact of substitution on the coercive field.