

# **Database Development for Rare Earths and Rare-earth/transition-metal Compounds**

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**Abstract:** Taking advantage of a home-designed combination of equipments so called as “oxygen-free” in-situ synthesis system, we prepared the nanoscale rare-earth (RE) metals and nanocrystalline rare-earth/transition-metal (RE/TM) compounds. Based on the systematic characterizations we have accumulated basically complete fundamental data for RE metals on the nanoscale. Then the database containing fundamental data of REs and RE/TM (for the time being Sm-Co) compounds has been constructed for both the conventional polycrystalline and nanocrystalline systems. The data include crystallographical information (e.g. crystal structure, lattice parameters, atom occupancy), physical properties (e.g. electrical resistance, thermal conductivity, thermal expansion coefficient), thermodynamic features (e.g. specific heat capacity, enthalpy, entropy, Gibbs energy), phase transformation characteristics (e.g. type, transformation temperature), mechanical properties (e.g. hardness, elastic modulus), functional properties (e.g. intrinsic coercivity, saturation magnetization, remanence, Curie temperature), and etc. Particularly, the database provides a number of data for the nanoscale effects on the mechanical and functional properties. The database may be used as the fundamental references and criteria for the design and development of the RE functional and RE-doping structural materials.

**Keywords:** rare earth, nanoscale, functional properties, mechanical properties, crystallographical information