

USE OF ACCURATE STRUCTURE DATA FROM X-RAY POWDER DIFFRACTION TO SIMULATE THE MAGNETIC PROPERTIES OF RARE EARTHS

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The possibility to predict the physical as well as chemical properties of solid state compounds just by computerized simulation using structural data only and employing as simple models as possible can be in a way considered as the ultimate goal of materials science. Among the physical properties of interest in rare earth solid state compounds, the magnetic properties are important since one of the main fields of application of selected rare earths are the permanent magnets. However, the simulations using sophisticated models require sophisticated input data, too.

In this report, the average paramagnetic susceptibility of the RE³⁺ ions in RE oxybromide powders, REOBr (RE = Ce - Nd, Sm, Eu, Tb - Yb), were simulated between 2 and 298 K by calculations based on the modified point charge (PCEM) and the simple overlap (SOM) models. Both methods used the structural data determined from the Rietveld analyses of the X-ray powder patterns measured with an ordinary laboratory set-up consisting of an Enraf-Nonius PDS120 X-ray powder diffractometer equipped with an INEL CPS120 position sensitive detector. The results show that the Curie-Weiss behaviour of the temperature evolution of the paramagnetic susceptibility of most REOBr materials could be simulated with high reliability down to low temperatures. Even the anomalous low temperature behaviour was reproduced rather correctly. It is thus possible to obtain coherent structural data reliable enough with ordinary laboratory X-ray diffractometer set-up to be used in simulating the magnetic properties of rare earths in solid state compounds.