ESRF	**Experiment title:** Critical phenomena under Verwey transition in $REBaFe_2O_{5+w}$	**Experiment number:** 01-01-226
Beamline: BM01B	**Date of experiment:** from: 05.07.2000 to: 11.07.2000	**Date of report:** 9.2.2001
Shifts: 18	**Local contact(s):** Mr. Hermann Emmerich	*Received at ESRF:*

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Report:

Synchrotron x-ray powder diffraction data were collected for six compositions of $GdBaFe_2O_{5+w}$ across the oxygen non-stoichiometry range of $-0.10 < w < 0.40$, as a function of temperature between 100 and 310 K. Up to the non-stoichiometry level of $w = 0.24$, an abrupt structural and volume change is monitored manifesting a Verwey-type transition of the first order. The evolution the unit-cell parameters as a function of temperature across the transition is shown in Fig. 1 and the atomic parameters of the low-temperature charge-ordered phase and the high-temperature mixed-valence phase are refined for several non-stoichiometry levels. The values of ΔV, combined with differential scanning calorimetry (DSC) data allow evaluation of the thermodynamics of the transition. It is seen that ΔS, ΔV and T_V decrease with increased oxygen loading (w), in line with increasing destabilization of the charge-ordered state due to the non-stoichiometry.
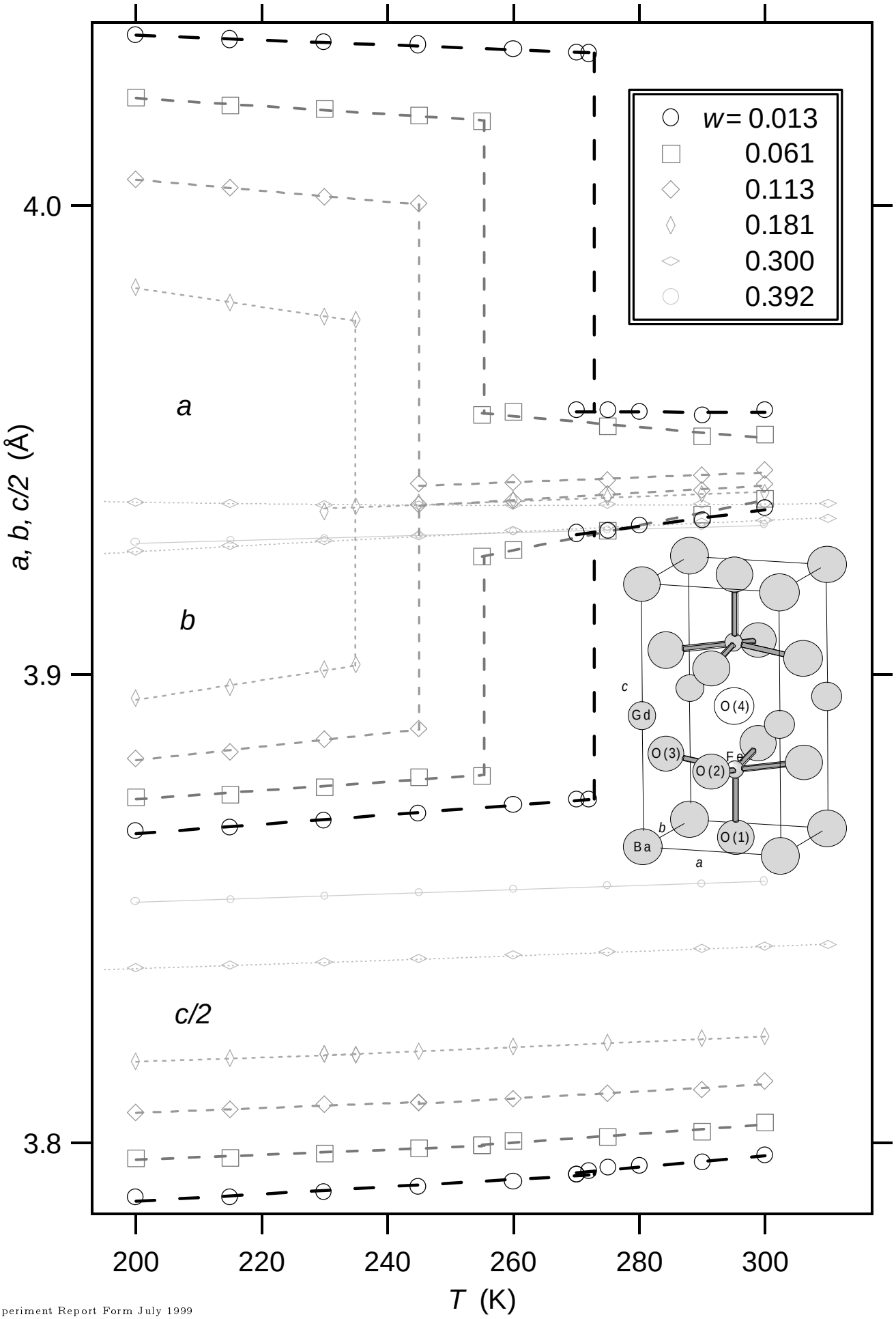
Fig. 1: Unit-cell parameters of $GdBaFe_2O_{5+w}$ as a function of temperature T and non-stoichiometry w, referring to the double (volume) perovskite cell drawn in inset. Estimated standard deviations do not exceed the size of the symbols.