Temperature Dependence of Lattice Parameters for Gd_3T (T= Ni, Rh, Ir)

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Problem:

The three compounds Gd_3Ni, Gd_3Rh and Gd_3Ir exhibit an anomalous, anisotropic behavior with temperature:

- The variation of the lattice parameters down to the Neel temperature is anisotropic, below that temperature there is an anomalous variation of these parameters, this must be related to the spontaneous magnetization.
- All compounds of Gd_3T (with T=transition metals) are expected to crystallize in the orthorhombic Fe_3C-type structure (after [1]) and in the SG Pnma. In this investigation we tried to verify this assumption by single crystal X-ray diffraction.

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Experimental Setup :

4-circle HUBER diffractometer

NONIUS rotating anode

Graphite monochromator (bent in one direction): MoKα

CRYOGENICS closed cycle He-cryostat

The 4-circle LT-diffractometer

Diffraction Geometry

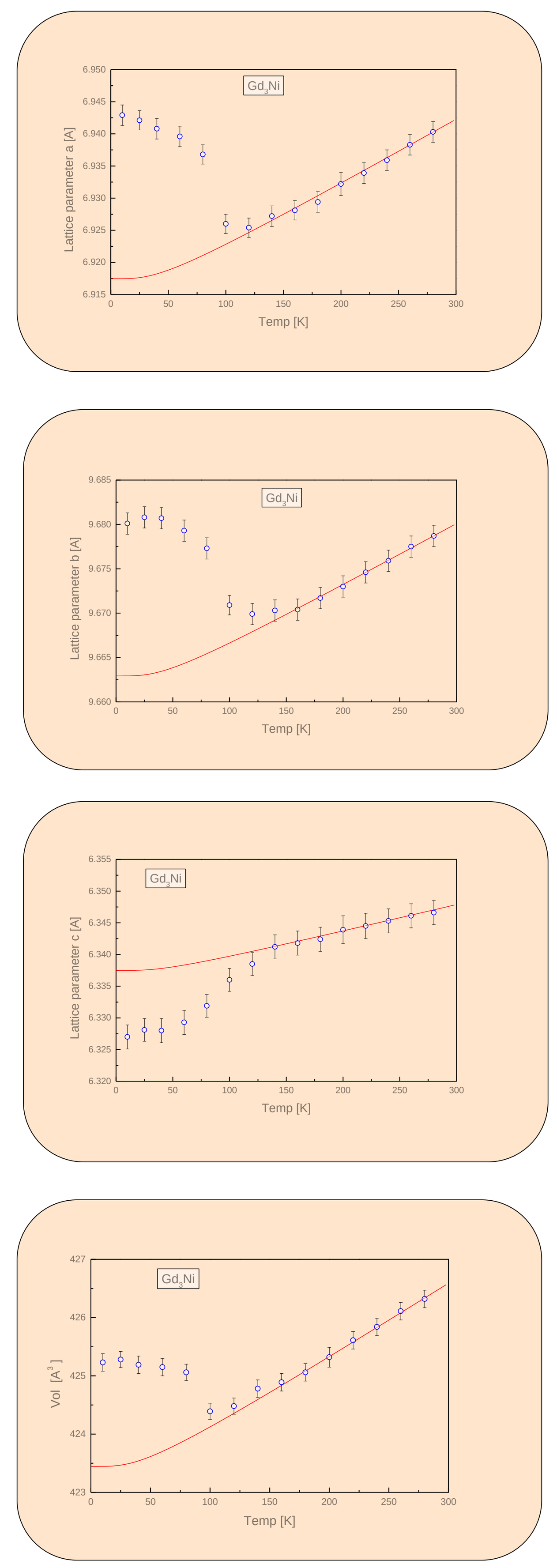
Experimental Method:

The single crystals were obtained by the Czchrochalski method from a levitated melt. The temperature during the diffraction experiment was controlled within 0.1K. The refinement of the cell parameters was carried out by measuring of about 60 reflections with high 2 θ-values and their Friedel pairs at both sides of the primary beam. An ω-scan was carried out at + and - 2 θ and ω. The center of gravity was determined by the difference of the two ω-centers.

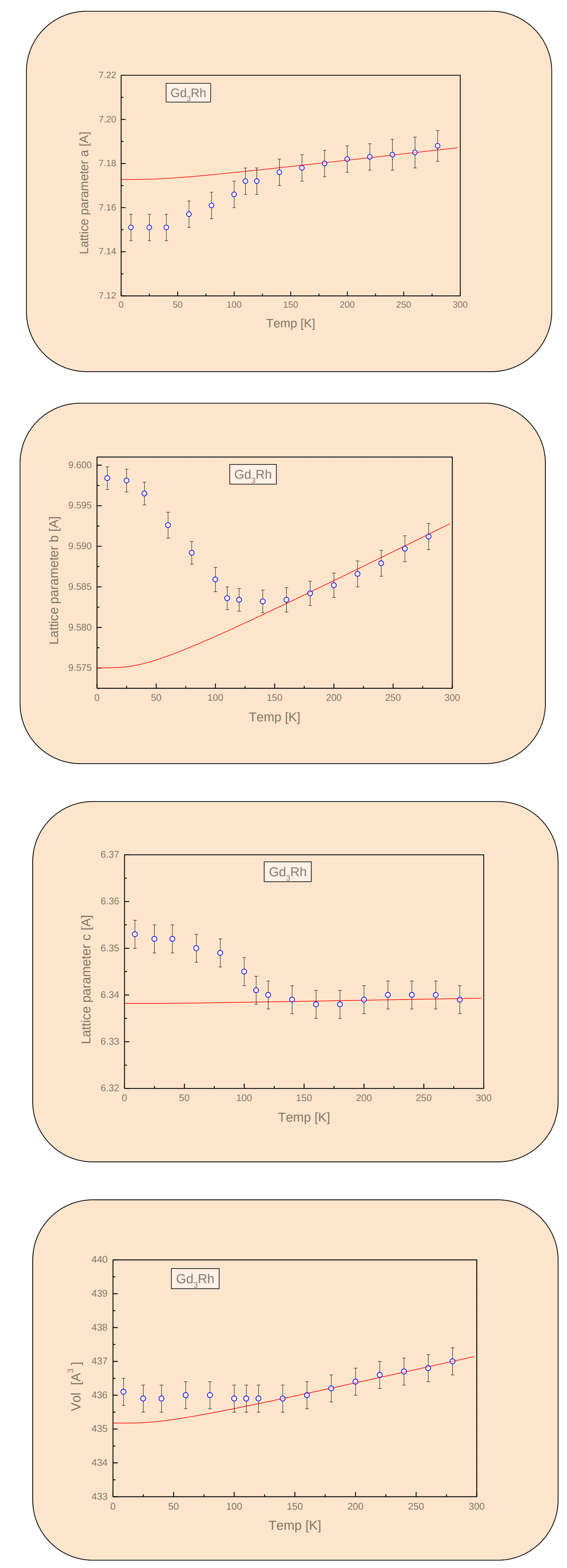
Experimental results:

The variation of the lattice parameters with temperature

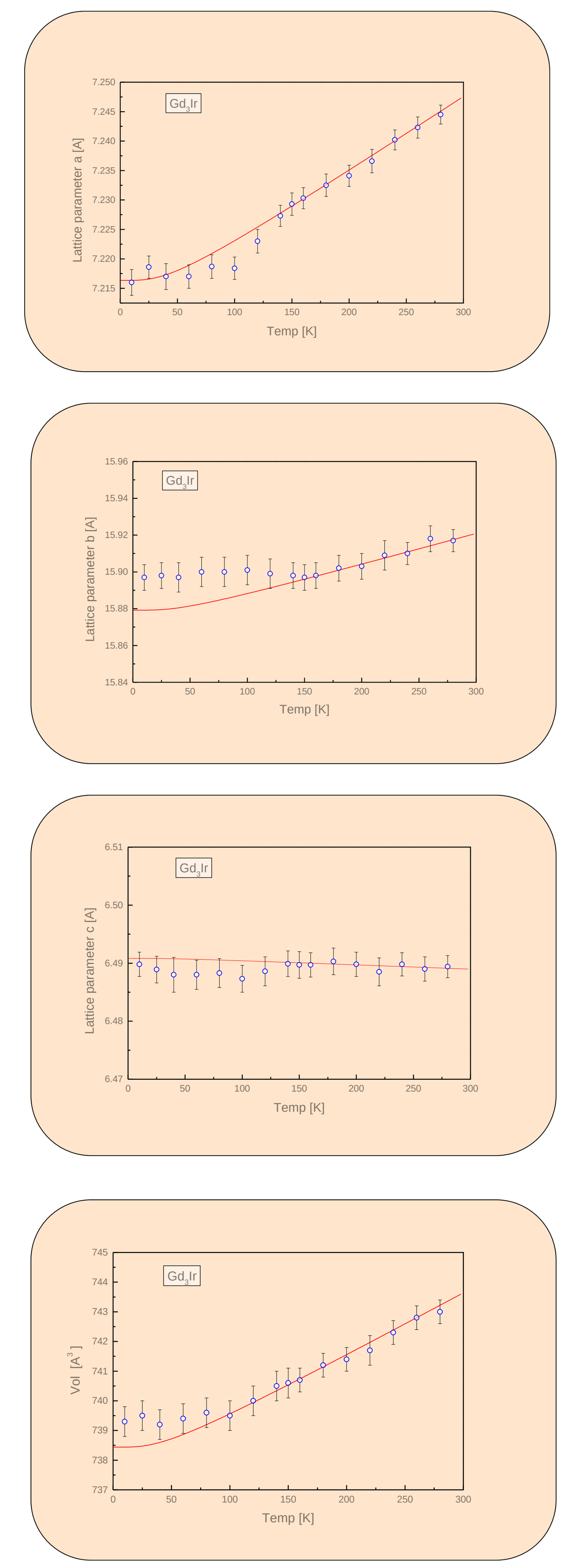
Gd_3Ni



Gd_3Rh



Gd_3Ir



Analysis:

The various curves have been fitted assuming a Debye Temperature of 157K (as for Gd_3Co): The transition to the forced ferromagnetic state is accompanied by a large strain :

Sign of the **extra strain** at the transition:

	Gd_3Ni	Gd_3Rh	Gd_3Ir
along **a**	+	-	-
along **b**	+	+	+
along **c**	-	+	-
volume	+	+	+

Thermal expansion coefficients at 300K.:

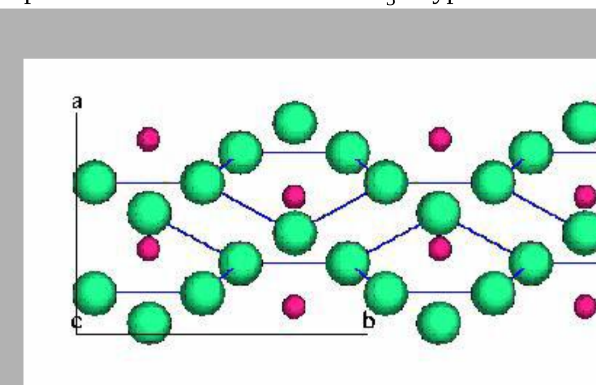
	Gd_3Ni	Gd_3Rh	Gd_3Ir
α_a 10^5 [K]$^{-1}$	10.03	5.84	12.59
α_b 10^5 [K]$^{-1}$	6.92	7.21	16.80
α_c 10^5 [K]$^{-1}$	4.19	0.457	-0.74

Neel temperature [3,4]:

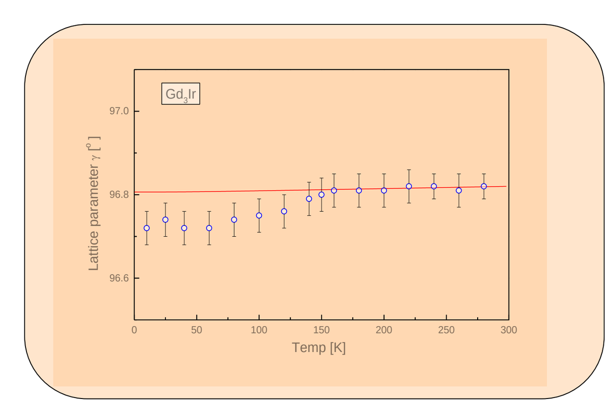
	Gd_3Ni	Gd_3Rh	Gd_3Ir
T_N **[K]**	100	112	155

Discussion and Results:

The compound exhibits a deviation from the orthorhombic Fe_3C-type structure: The SG of Gd_3Ir is found to be monoclinic C2/c. The lattice constants appear to be a_o = 15.929 Å, b_o = 6.488 Å, c_o = 7. 250 Å, β = 96.93 °. This means that one lattice constant is doubled (because of the C-centering) as compared with the orthorhombic Fe_3C-type structure.



The basic Fe_3C-type structure (two cells along **b**).



The variation of the monoclinic angle ß with temperature.

Literature

[1] Landolt-Börnstein, Vol.III, 26 (Springer 1989)
[2] N.V. Baranov et al. *J. Alloys and Compounds* **202**, (1993) 215-224
[3] E. Talik et al. , *J. Alloys and Compounds*, **223** (1995), 87
[4] E. Talik et al., *J. Magn Magn Mater*. **140-144** (1995) 795