Temperature Dependence of Lattice Parameters for Er_3T (T= Ni, Rh, Ir)

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Problem:
The three compounds Er_3Ni, Er_3Rh and Er_3Ir exhibit an anomalous, anisotropic behavior with temperature:
• The lattice constant c increases with temperature in all of these compounds, which is in contrast to Gd_3T (with T=Ni, Rh, Ir) [2].
• All compounds of Er_3T (with T=transition metals) are expected to crystallize in the orthorhombic Fe_3C-type structure (after [1]) and in the SG Pnma.
•To understand the anomalous behavior of the lattice parameters we studied the structure of Er_3Ir at 150K, 200K and 300K by single crystal X-ray diffraction.

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Experimental Setup :

4-circle HUBER diffractometer

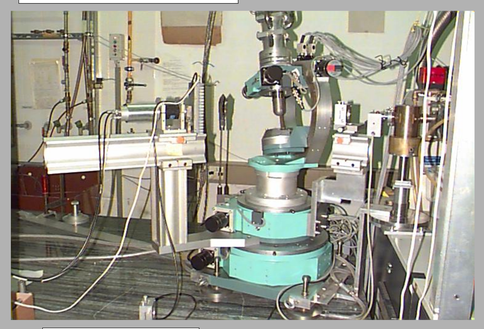
STOE interface controlled by STADI4 software

ENRAF-NONIUS rotating anode

Bent graphite monochromator: CuKα

CRYOGENICS closed cycle He-cryostat

The 4-circle LT-diffractometer

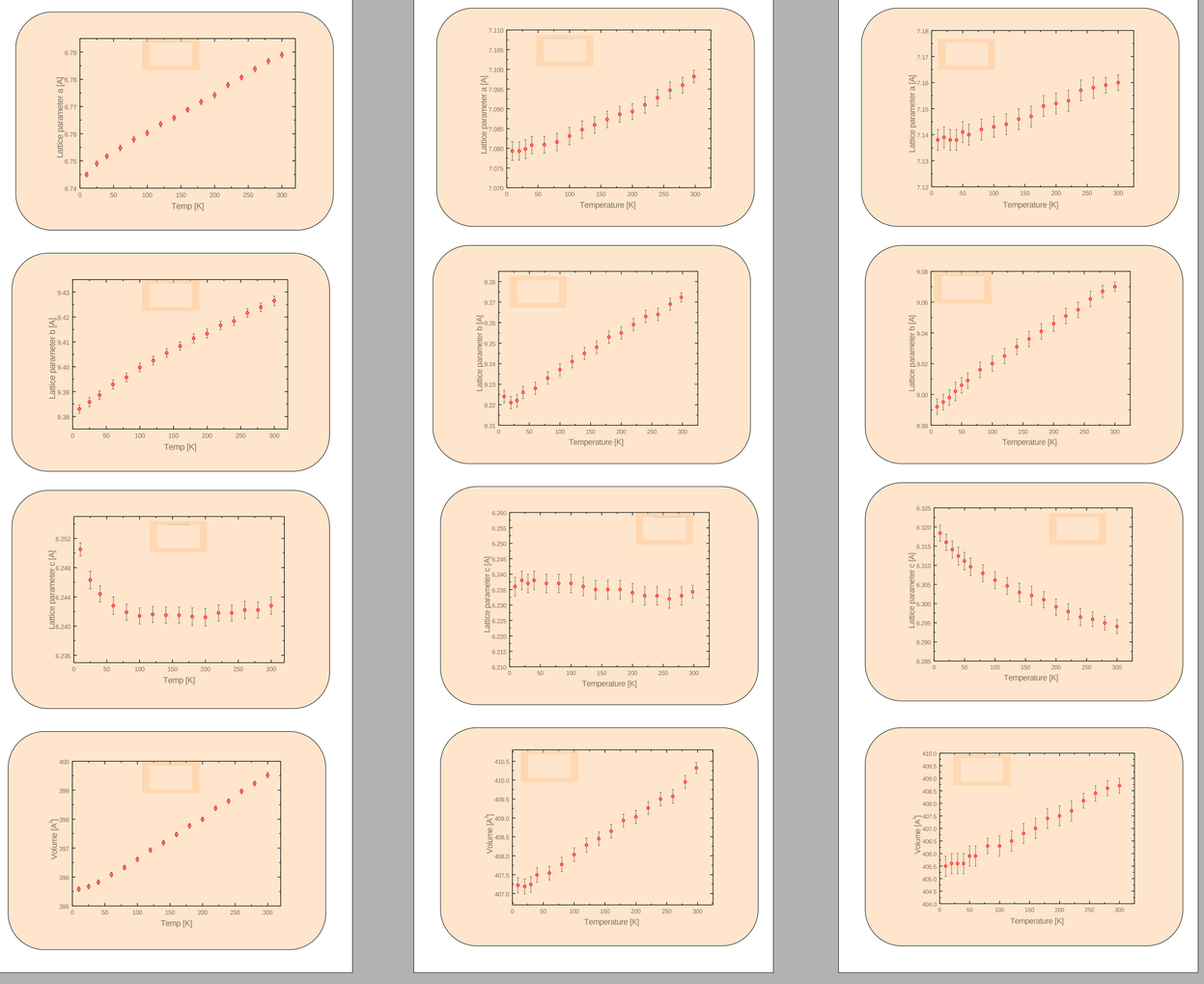


Diffraction Geometry

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 on 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.
The data collection for Er_3Ir was carried out on a CAD4 diffractometer (MoKα, graphite monochromator) at 150 K, 200 K and 300 K in the range $2\theta < 70°$ (ω-2θ scan).

Er_3Ni | Er_3Rh | Er_3Ir



Analysis:

The thermal expansion coefficients have been determined at two different temperatures :

Thermal expansion coefficients at 10K.:

	Er_3Ni	Er_3Rh	Er_3Ir
α_a 10^5 $[K]^{-1}$	22.3	3.7	5.0
α_b 10^5 $[K]^{-1}$	18.7	11.1	35.0
α_c 10^5 $[K]^{-1}$	-20.7	1.3	-18.2

Thermal expansion coefficients at 300K.:

	Er_3Ni	Er_3Rh	Er_3Ir
α_a 10^5 $[K]^{-1}$	15.4	8.1	5.0
α_b 10^5 $[K]^{-1}$	13.1	15.2	29.7
α_c 10^5 $[K]^{-1}$	1.2	5.0	-4.1

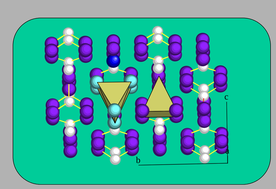
Neel temperature [3,4]:

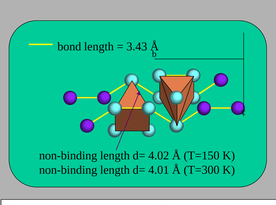
	Er_3Ni	Er_3Rh	Er_3Ir
T_N **[K]**	10 [4]	26 [3]	?

Discussion and Results:

The compound Er_3Ir exhibits the Fe_3C-type structure with the orthorhombic SG Pnma :
The lattice constants (at 150 K) are a_o = 7.1427 Å, b_o = 9.0344 Å, c_o = 6.2926 Å.
The structural refinement was carried out by the program SHELX93.
No. of measured reflections 2045 No. of unique reflections 945
No. of variables 23 Absorption correction :ψ-scan
R1 5.4% (150 K) 5.4% (200 K) 4.5% (300 K)

In the three compounds the transition metal has been replaced, which influences the sign of the change in the thermal expansion coefficient α_c . The strongest negative change is observed in the Ir-compound. This behavior can be understood by comparing the bond distances within the coordination polyhedron of Ir and between the neighboring polyhedra. The bulk change in the lattice constants between 150 K and 300 K is 0.014 Å for **a** 0.036 Å for **b** and -0.009 Å for **c**.





The refined structure of Er_3Ir : (b,c)-plane and the shortest bond length of Er-Er

		150 K	200 K	300 K
Er - Ir		2.821(1)	2.821(1)	2.825(1)
		2.728(1)	2.731(2)	2.731(1)
		2.834(2)	2.833(2)	2.833(1)
		2.911(1)	2.911(1)	2.908(1)
Er - Er		3.432(2)	3.436(2)	3.443(1)
		3.435(2)	3.436(2)	3.442(2)
		3.456(2)	3.458(2)	3.464(1)
		3.489(1)	3.489(1)	3.490(1)
		3.496(2)	3.501(2)	3.507(1)
		3.526(2)	3.525(2)	3.525(1)
		3.587(1)	3.590(1)	3.596(1)

Bond lengths at 3 different temperatures

Literature

[1] Landolt-Börnstein, **Vol.III, 26** (Springer 1989)
[2] J. Kusz et al., J. Appl. Cryst. in press. (2000)
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[4] E. Talik et al., *J. Magn Magn Mater*. **157/158** (1996) 405-406