Low Temperature Phase Transitions in GdPdAl

J. Kusz[1], H. Böhm[2], E. Talik[1] and M. Skutecka[1]

[1]*Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland*

[2]*Institut für Geowissenschaften/Mineralogie, Johannes Gutenberg-Universität, D-55099 Mainz, Germany*

Acknowledgment: The work is financially supported by the Materialwissenschaftliches Forschungszentrum der Johannes Gutenberg-Universität Mainz and by a KBN project, Poland.

Experimental

Experimental Setup :

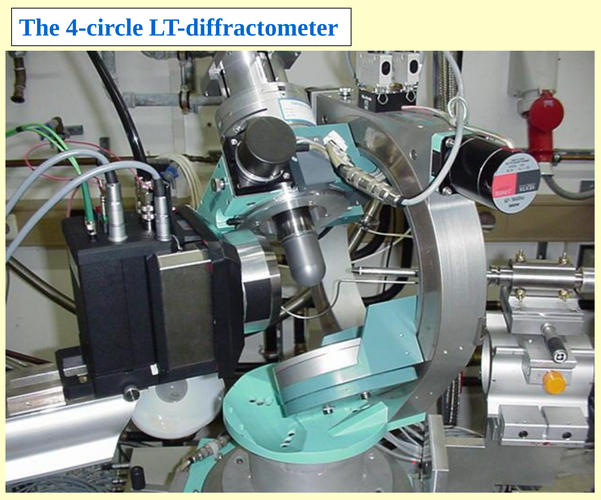
4-circle HUBER diffractometer

SCHNEIDER rotating anode

OSMIC multilayer monochromator: Cu Kα

CRYOGENICS closed cycle He-cryostat

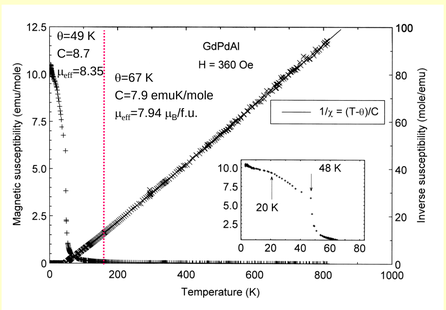
The 4-circle LT-diffractometer



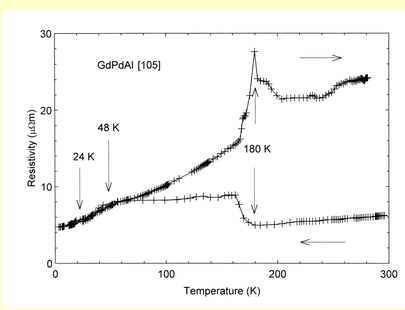
Experimental Method:

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.

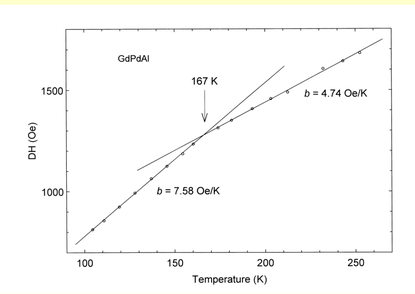
Magnetic, electrical and ESR Measurements



The temperature dependence of the magnetic susceptibility exhibits a change of the slope at about 180 K and a magnetic transition at 48 K and 20 K.

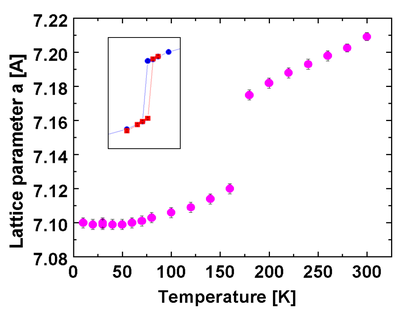


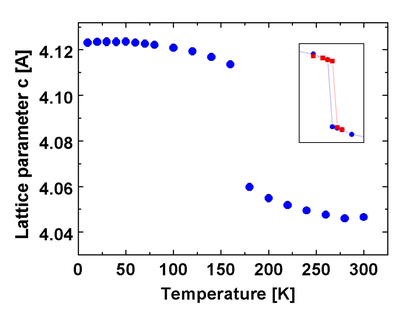
Anomaly in the temperature dependence of the electrical resistivity of GdPdAl. In the cooling heating cycle a thermal hysteresis is observed.

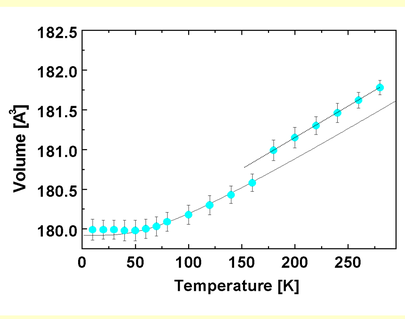


The dependence of the ESR line widths upon temperature of GdPdAl. Obviously there is a change in the slope of the curve at 167 K..

X-ray measurements







Temperature dependence of the lattice parameters *a* and *c* of GdPdAl . The linear thermal expansion coefficients α for the lattice parameters:

	α_a [K^{-1}]	α_c [K^{-1}]	α_V [K^{-1}]
120 – 160 K	$2.5 \cdot 10^{-4}$	$-1.29 \cdot 10^{-4}$	$6.5 \cdot 10^{-4}$
180 – 280 K	$2.6 \cdot 10^{-4}$	$-1.65 \cdot 10^{-4}$	$7.9 \cdot 10^{-4}$

The solid line for the cell volume is calculated from the Grüneisen-Debye theory (θ_D=260 K); it shows a hypothetical non-magnetic behaviour below 50 K..

Bond lengths

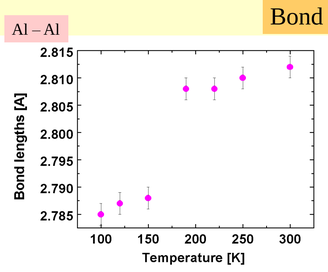
•The single crystal structure was determined at 300 250, 220, 190, 150, 120 and 100K using the SHELX93 program. The obtained R_1-values are 0.028, 0.028, 0.029, 0.028, 0.029, 0.028 and 0.028, respectively.

•The space group P6m2 does not change below the phase transition.

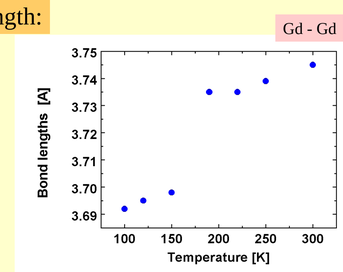
•The main structural difference between the low (LT) and high temperature phase (HT) are differences in the inter–atomic distances.

Bond length:

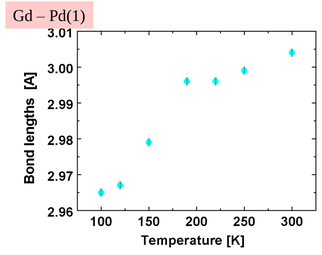
Al – Al



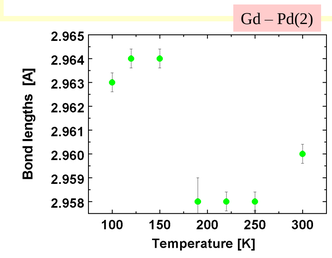
Gd - Gd



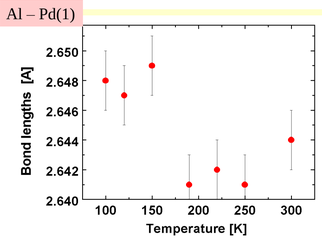
Gd – Pd(1)



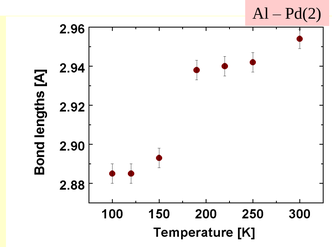
Gd – Pd(2)



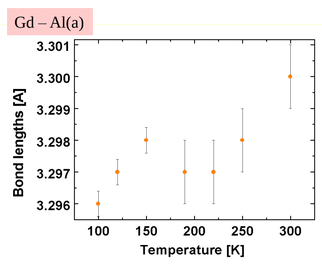
Al – Pd(1)



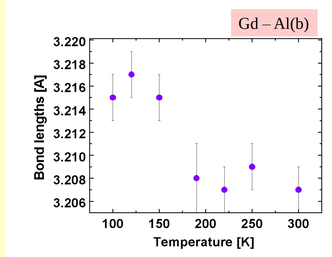
Al – Pd(2)



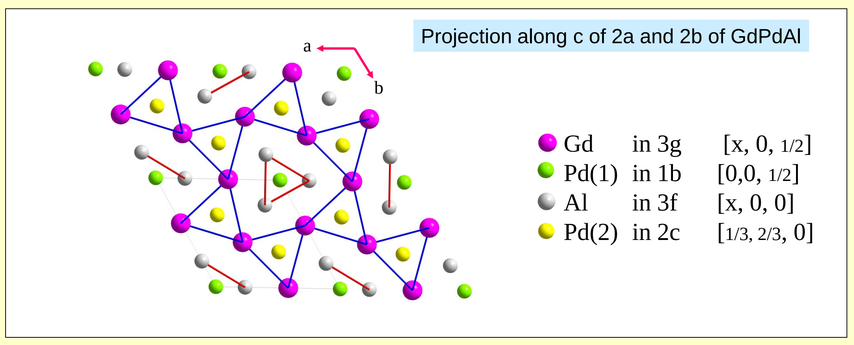
Gd – Al(a)



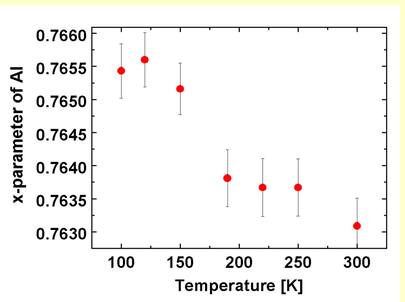
Gd – Al(b)

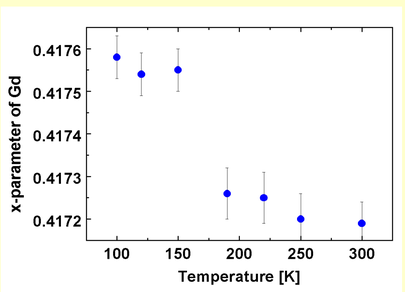


Structure



Gd forms edge sharing trigonal prisms with Pd(2) in the centre; Al forms isolated trigonal prisms with Pd(1) in the centre. Both prisms are shifted by ½ with respect to each other along **c**. Two different kinds of layers are formed within the structure: One layer at z = 0 with Al-Pd(2) and another layer at z = ½ with Gd-Pd(1) When the temperature is lowered into the LT phase there is a sudden decrease in the bond lengths (increase of x) within the equilateral triangles and an increase along the edges of each prism.





Conclusion

•Between 10 K and 300 K single crystals exhibit a hexagonal ZrNiAl – type structure with a space group *P6m2*.

•A pronounced contraction of the lattice parameter *a* (decrease of 0.7 %) and an expansion of the lattice parameter *c* (increase of 1.3 %) were observed at 180 K on cooling.

•A hysteresis of 5K between heating and cooling is indicative for a first order phase transition.

•Magnetic susceptibility, electrical and ESR measurements give evidence for a phase transition at 180 K.

•A magnetic phase transition is observed at 48 K. Below this ordering temperature a magneto-volume effect occurs in the unit cell volume (magnetostriction at 10 K $\omega_V=(V_{exp}-V_{calc})/V_{calc}=4.5 \cdot 10^{-3}$).

•At 180 K the phase transition appears to be isostructural; the same kind of phase transition has been observed at another ZrNiAl-type structure, at GdNiAl.

•The main differences between the LT and the HT phase are differences in the inter-atomic distances: On decreasing the temperature both Gd and Al atoms within each layer get closer to each other and also closer to the Pd atoms whereas the distance between the layers is increased. This leads to a decrease of the *a* lattice parameter and to an increase of the *c* lattice parameter.