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Anomalous thermal behaviour of YbNiGa and YbPdGa

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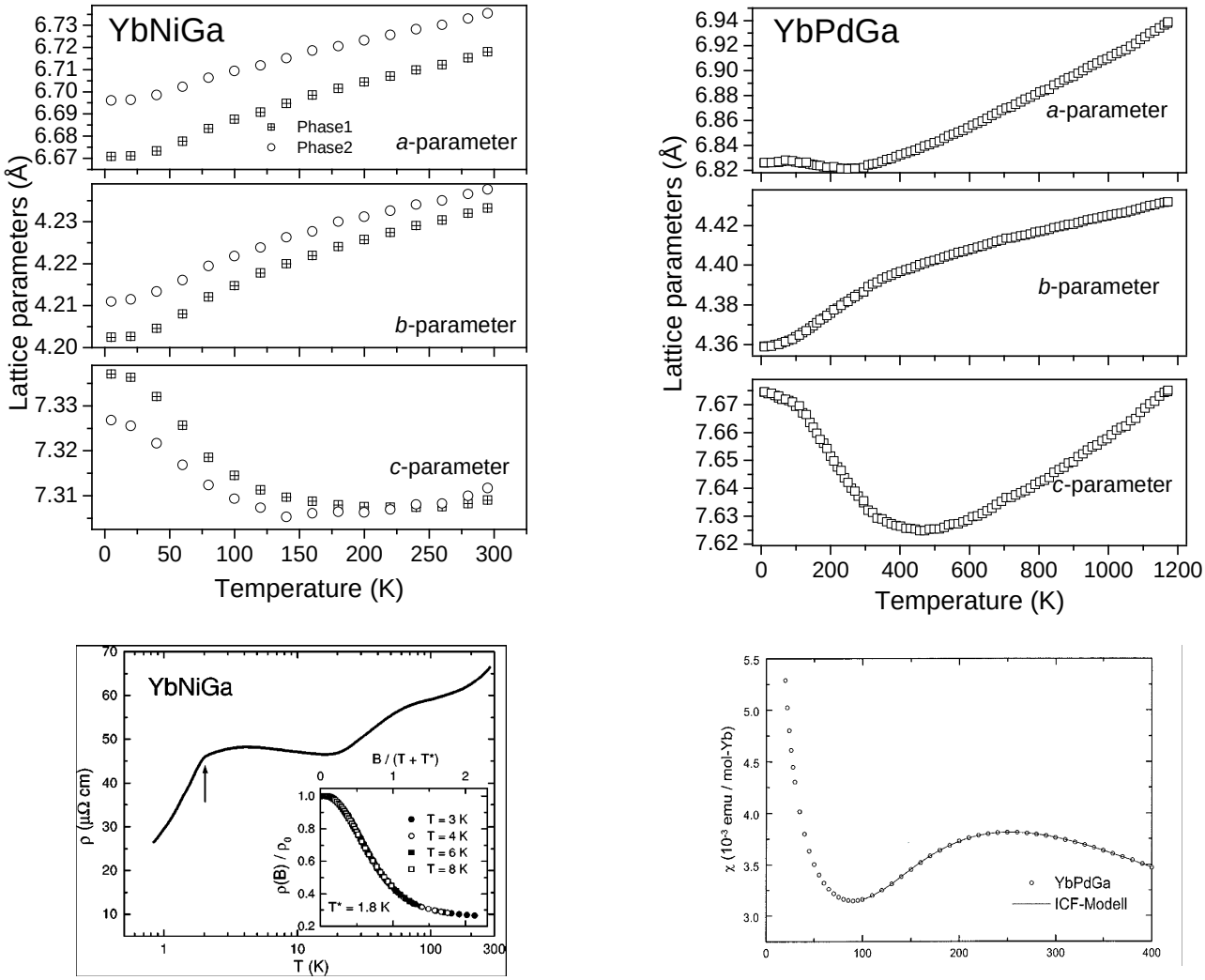
The ternary Yb–*T*–Ga compounds reveal a wealth of anomalous physical phenomena caused by the intricate electronic structure of ytterbium. These phenomena are sensitive to the chemical environment as well as to external conditions. At ambient conditions the ternary equiatomic compounds YbNiGa and YbPdGa adopt an orthorhombic TiNiSi type of structure (sp. group *Pnma*) with only one equivalent crystallographic site for the ytterbium atom (a = 6.728 Å, b = 4.234 Å, c = 7.212 Å for YbNiGa and a = 6.818 Å, b = 4.386 Å, c = 7.634 Å for YbPdGa). The Yb atoms are located within cavities of the covalently bonded 3D framework formed by the respective transition element (*T*) and gallium.

The thermal behaviour of YbNiGa and YbPdGa structures has been studied by *in situ* high-resolution powder diffraction at ID31 beamline of ESRF. Both compounds remain orthorhombic in the whole temperature range investigated.

The diffraction patterns of YbNiGa were collected in the temperature range of 5–300 K. The compounds exhibit a negative expansion in [001] direction in 5–170 K region.

The anomalies observed for YbPdGa (investigated region 5–1173 K) are much more pronounced: clear maxima and minima for [100] direction at 70 K and 220 K, a change of slop for [010] direction at 350 K and unusual U-shape behaviour for [001] direction with the deep minima located at around 480 K. These extrema coincide well with the turning points observed in the magnetic susceptibility curve of YbPdGa which were interpreted as valence fluctuation of Yb^{2+}/Yb^{3+} states. The almost linear decrease of the lattice parameter c could associated with the corrugation of the [PdGa] framework within (010) plane. Starting from 480 K a "normal" thermal expansion is observed.

The quantum chemical analysis on the basis of the obtained structural data are in progress. The previous results of the experiment are submitted as abstract contribution to 17th Conference on Solid Compounds of Transition Elements (Annecy, September 5–10, 2010).



Thermal behaviour of the lattice parameters of YbNiGa (5K–298K) and YbPdGa (5K–1173 K) in comparision with the electrical resistivity and magnetic susceptibilty data