Crystal growth and electronic structure of R_7Pd_3 (R=Gd, Tb, Dy, Ho, Er)

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Gd_7Pd_3 exhibit interesting magnetocaloric properties for magnetic refrigeration devices. It belongs to the R_7Pd_3 intermetallics (R - rare earth) which crystallize in the hexagonal Th_7Fe_3-type of crystal structure which belongs to the space group P6-3mc [1]. The lattice parameters of the Gd_7Pd_3 single crystal are a= 10.008Å, c= 6.287Å, while for the polycrystalline sample they were a= 9.985 Å and c=6.272 Å [1]. In this structure, the Pd atoms are situated in 6c position in Wyckoff notation, the Gd atoms are in 2b and 6c positions.

The thermal variation of the magnetic susceptibility of Gd_7Pd_3 exhibits a ferromagnetic transition at T_c = 323 K. The effective magnetic moment calculated per gadolinium ion is μ_{eff} = 7.98 μ_B [1]. The aim of this work is to obtain a good quality single crystals of these group of intermetallic componds for XPS and magnetic measurements. Fig. 1 shows the X-ray Berg-Barrett topography of the Gd_7Pd_3 single crystal, grown by the Czochralski method from a levitated melt, which confirms the good quality of the obtained crystal.

Fig. 1. Berg-Barrett topography of Gd_7Pd_3 single crystal.

The measured XPS valence band of Gd_7Pd_3 exhibits a narrowing and moving away from the Fermi level to higher binding energy of the Pd 4d (Fig. 2). X-ray - photoemission spectrum of Gd 4d core level shows a wide spread structure over 30 eV (Fig. 3).

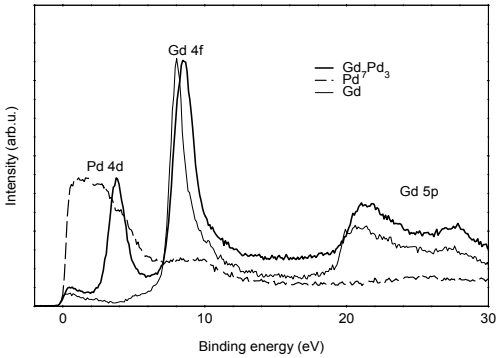

Fig. 2. XPS valence band, Gd 4f and 5p of Gd_3Pd and pure Pd.

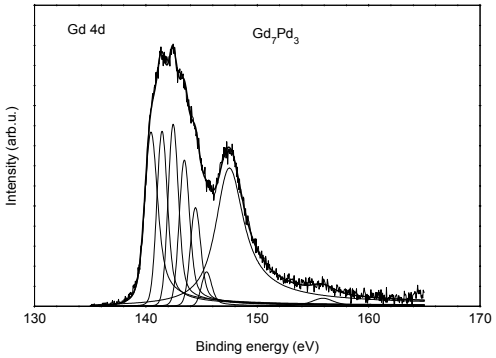

Fig. 3. The multiplet structure of Gd 4d in the compound.

This shape is caused by the strong 4d - 4f Coulomb, exchange and spin–orbit interations. The main part, in low binding energy region, is is splited into to peaks separated above 5 eV by 4d core spin - orbit interaction. The first peak corresponds to mainly ^9D final states while the furher peaks of the spectrum have mainly ^7D character. The first peak exhibit additional multiplet structure. The 4d-4f 4f (super - Coster - Kronig) decay process in the final states is mainly responsible for the broadening and a shape of the spectrum. This process is very sensitive to the direction of the spin. For the spin parallel states (^9D) the lifetime broadening is small while for the spin antiparallel states (^7D), at higher binding energy, the term dependent lifetime effect is large.

[1] F. Canepa, M. Napoletano, S. Cirafici, Intermetallics 10 (2002) 731.

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