

ELECTRONIC AND MAGNETIC PROPERTIES OF $\text{La}_{1-x}\text{Pr}_x\text{Pb}_3$ ALLOYS

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The low-temperature properties of $\text{La}_{1-x}\text{Pr}_x\text{Pb}_3$ alloys were studied experimentally in the last years [1-2]. For low concentration of Pr the quadrupolar Kondo effect was observed [2-3]. These systems have AuCu_3 type cubic crystal structure. In this work we have studied the electronic and magnetic properties of $\text{La}_{1-x}\text{Pr}_x\text{Pb}_3$ alloys for $0 < x < 1.0$. The band structure was calculated by ab-initio FPLO-CPA [4-5] method in the local spin density approximation. The spin polarised band calculations were performed for the experimental lattice parameters. We have applied the full relativistic mode for LaPb_3 and PrPb_3 alloys, however in the case of the disordered systems we used the coherent potential approximation in the scalar-relativistic mode. The exchange correlation potential was assumed in the form of [6]. The spin polarised band calculations give the spin magnetic moment on Pr $m_{spin}=2.33\mu_B$ and the orbital magnetic moment $m_{orb}=-3.11\mu_B$.

[1] T.Kawae et al. *Phys.Rev B* **65**, 012409 (2001).

[2] T.Kawae et al. *Phys.Rev.Lett.* **96**, 027210 (2006).

[3] T.Onimaru et al. *Phys.Rev.Lett* **94** 197201 (2005).

[4] K. Koepernik and H. Eschrig, *Phys.Rev.B* **59**, 1743 (1999).

[5] K. Koepernik, B. Velicky, R. Hayn, and H. Eschrig, *Phys.Rev.B* **55**, 5717 (1997).

[6] J.P.Perdew and Y.Wang, *Phys.Rev.B* **45**, 13244 (1992).