Electronic Structure of the $CeCu_9In_2$ Compound

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Abstract. Intermetallic compounds of cerium exhibit many unusual properties due to a presence of unpaired electron in the 4f Ce shell. Coupling between carriers from conduction band and local 4f moments leads to the Kondo effect, which is manifested by formation of a variety of physical states like e.g. Kondo lattices, Kondo insulators, fluctuating valency or quantum criticality. The ground state which is realized in a dense Kondo system is a result of competition between on-site Kondo screening and intra-site Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. The first interaction leads to a quenching of local moments, while the second one favors magnetic ordering. The instability which emerges between magnetic and non-magnetic Kondo lattice is responsible for the occurence of quantum critical point.

Riveting physics of Kondo effect can be conveniently studied by photoelectron spectroscopy as well as by measurements of transport and thermodynamic properties such as electrical resistivity and specific heat. In this work we would like to present results obtained for polycrystalline samples of the $CeCu_9In_2$ compound synthesized by arc melting technique. Studied compound crystallizes [1] in the YNi_9In_2-type tetragonal structure, which is characterized by large coordination numbers. Electrical resistivity of $CeCu_9In_2$, measured down to 2 K, varies with temperature in a way typical of Kondo lattice systems. One can observe minimum of electrical resistivity at temperature equal to 150 K and pronounced maximum at temperature equal to 45 K. In the temperature range from 45 K to about 100 K, electrical resistivity obeys logarithmic law. At low temperatures (below 12 K) Landau-Baber-Pomeranchuk law is obeyed, which testifies the Fermi liquid ground state in the system. Specific heat reveals pronounced anomaly at temperature equal to 1.8 K, which arises most probably due to the crystal field excitations. X-ray photoemission spectra of the 3d Ce levels, measured with MgK_α radiation ($h\nu$=1253.6 eV) at temperature equal to 12.5 K, have got satellite structure, which testifies coupling between 4f states and conduction band. Spectra of valence band, collected with application of ultraviolet photoelectron spectroscopy at temperature equal to 12.5 K, do not show so called Kondo peak at the Fermi level. However, there is a visible structure related to the $4f^1_{7/2}$ final state in the He-II ($h\nu$=40.8 eV) spectra. We have performed theoretical calculations in order to provide comparison with experimental results. Band structure has been calculated with application of full potential local orbital (FPLO) code in scalar relativistic version. Local spin density approximation has been used. Calculated Fermi surface reveals pair of some nearly flat parallel sheets, which can suggest existence of nesting in the $CeCu_9In_2$ compound. We also provide data for the isostructural compound $LaCu_9In_2$, in order to elucidate the influence of 4f electrons on electronic structure and physical properties.

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References

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