

STUDY OF THE ELECTRONIC STRUCTURE OF CE-BASED HEAVY-FERMION SYSTEMS EXPOSED TO THE LOW-ENERGY NEUTRINO DENSE FLUX

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Abstract.

The class of compounds based on f-elements (Ce) attracts great attention because of their unusual properties. They are characterized by a heavy-fermion state, which occurs in them under certain external actions. Heavy-fermion materials have unique properties. The objective of the work is the investigation of a change in the electronic structure in a number of Ce-based systems under the action of a dense neutrino flux in order to develop the technology for the essential change of material properties. To increase the density of the neutrino flux by several orders of magnitude, the phenomenon of diffraction is used. The investigation of the electronic structure of Ce-based systems on the electron magnetic spectrometer using the x-ray electron method and the calculations of the density of states at different temperatures has shown the decrease in the intensity of the localized resonance maximum near Fermi level with increasing temperature.

Introduction

The class of compounds based on f-elements (Ce) attracts great attention because of their unusual properties. They are characterized by a heavy-fermion state, which occurs in them under certain external actions. A heavy fermion is a mixed formation from strongly localized f-states and Fermi spd-electrons, which is characterized by a sharp increase in the weight of sd electrons and in their effective mass by 2 – 3 orders of magnitude, a sharp growth in the density of states and the appearance of the resonance maximum near Fermi level; the latter is responsible for the unique properties, which are important for the usage of metal parts made from these materials at certain conditions. For example, coating metal parts of machines and machinery with these materials leads to an increase in their breaking strength by several orders of magnitude and provides much better protection of them.

Results and discussion

The objective of the work is the investigation of a change in the electronic structure of a number of Ce-based heavy-fermion systems under the action of a dense neutrino flux upon them in order to develop a technology for essential change of mechanical, magnetic, electrical and other physical properties of heavy-fermion materials.

In order to increase the neutrino flux density by several orders of magnitude, it is offered to use the phenomenon of diffraction. This can be achieved in the following manner: the device containing the source emitting neutrinos is equipped with several diffraction elements; the diffraction elements are either crystals or diffraction gratings; they are placed outside the line of the neutrino incidence on the target and bent in the direction of the indicated line. The diffraction elements can be displaced in a plane, which goes through the element and the line of the neutrino incidence on the target and the line of focusing in a specified direction.

The introduction into the neutrino-emitting device of the diffraction elements in the form of bent crystals (for example, in accordance with Johann's method [1] using an inverted scheme [2]) or diffraction gratings allows to increase the neutrino flux density because on every diffraction element an increase of many times (by 8 orders of magnitude, for 100 elements – by 10 orders) in the density of low-energy electronic neutrinos takes place.

It is offered to expose metal parts made from heavy-fermion materials to a powerful neutrino beam in order to change the physical properties of said materials by heating them by the

neutrino beam (due to kT). The advantage of such use of neutrino beams lies in the fact that the distances between a target and a neutrino source can be unlimited.

Since the diffraction device can turn relative to the parts of the world, it is possible to orient it in the direction of a supposed target. The change of heating temperature for the target is achieved by the change of the focus size and the bending of the gratings.

It is known that the properties of numerous heavy-fermion materials change at certain temperatures, which influence the range of their application. For example, the $CeCu_2Si_2$ system is a superconductor but when heated above 20 K it loses its superconducting property; the $CeCu_6$ system, which has an effective magnetic moment about $2.7 \mu B$ and a magnetic susceptibility 0.2, is a paramagnetic at a low temperature and when heated it acquires a magnetic order. The change of the properties of heavy-fermion materials due to phase transitions caused by the neutrino flux heating is associated with the change in their electronic structure.

The investigation of the electronic structure of the cerium-based compounds was conducted on an electron magnetic spectrometer using the x-ray photoelectron spectroscopy method [3] and the calculations of the density of states at various temperatures. Since the adequate potentials of interactions for the systems under study are absent, a more simplified approach is used. It is believed that the distributions of the deviations of atoms from the equilibrium positions in the lattice at final temperatures can be described by a random function of Gauss distribution [4]. A model system consisted of 8 unit cells. The coordinates of atoms at final temperatures were calculated using a pickup of random numbers [4] for the calculation of root-mean-square deviation from equilibrium positions.

The calculation of the electronic structure was carried out with the use of the linear method of muffin-tin orbitals in the approximation of atomic sphere (TB-LMTO-ASA) [5]. This method allows taking into account the covalent character of binding and the nonspherical distribution of the electron density. At present, the TB-LMTO-ASA method is the most quick and economic method for the electronic structure calculation. Its effectiveness and accuracy have been checked on numerous objects.

Let us consider the $CePd_3$ heavy-fermion system as an example. In $CePd_3$, the 4f level is close to Fermi level and to 5d6sp orbits of Ce, which leads to their hybridization and the appearance of intermediate valence in this system. Such systems have unique properties, which depend on temperature, namely, the magnetic-paramagnetic transition, abnormal compressibility, heat capacity, electrical conduction, etc.

Fig. 1 shows total and partial densities of states for $CePd_3$ calculated with the band calculation method TB-LMTO-ASA.

It is shown that the positions of the maxima of the density of states in the valence band and the valence band width vary insignificantly relative to Fermi level with the temperature increasing to 10 K. The largest changes take place in the 4f density of states; the d,p,s partial densities of states of Ce and Pd change weakly. The intensity of the localized maximum near Fermi level decreases with the temperature growth by 15% - 20% and shifts from Fermi level by 0.05 eV. At low temperatures, the resonance maximum has splitting due to the hybridization of localized (f) and nonlocalized (s,p,d) electrons [6]. With increasing temperature the splitting decreases (Fig. 2).

As is seen, in the conduction region the maxima of the partial d-p densities of states of Ce and Pd sharply grows due to a decrease in the hybridization with the Ce 4f electrons.

Conclusion

Thus, when the external conditions (temperature) are changed, phase transitions take place in the heavy-fermion systems, which are of mere electronic nature and relate to the change in filling of the electronic levels.

The decrease of the resonance maximum at increasing temperature is characteristic of the heavy-fermion systems, the physical properties of which change. Due to a decrease in the hybridization of localized 4f states with d,p,s electrons in the CePd₃ system, the strength properties deteriorate.

References

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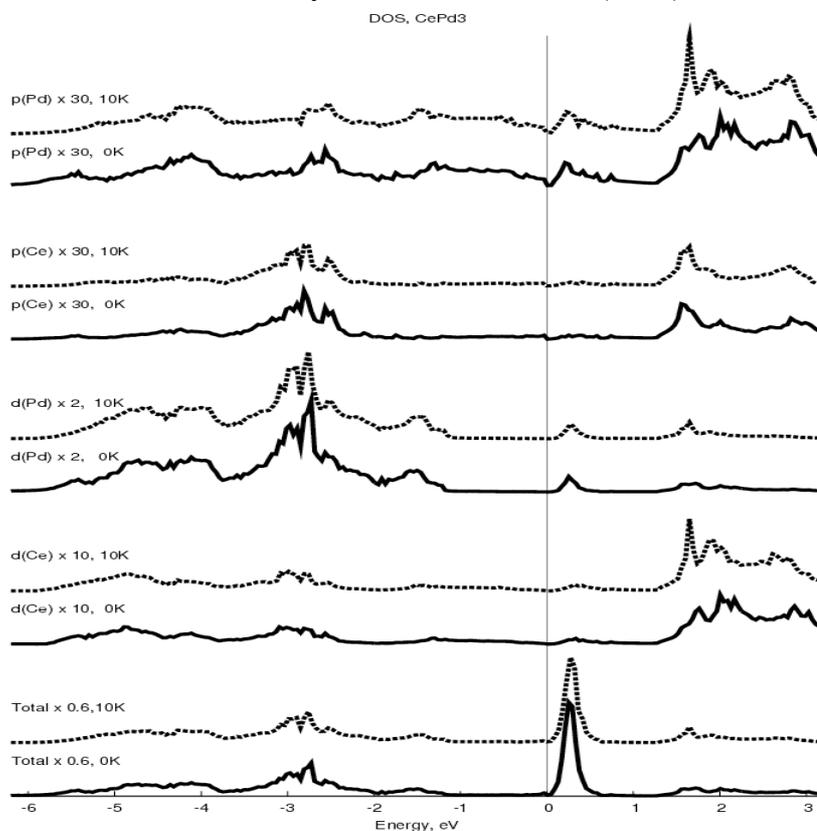


Fig.1 Total and partial densities of states for CePd₃.

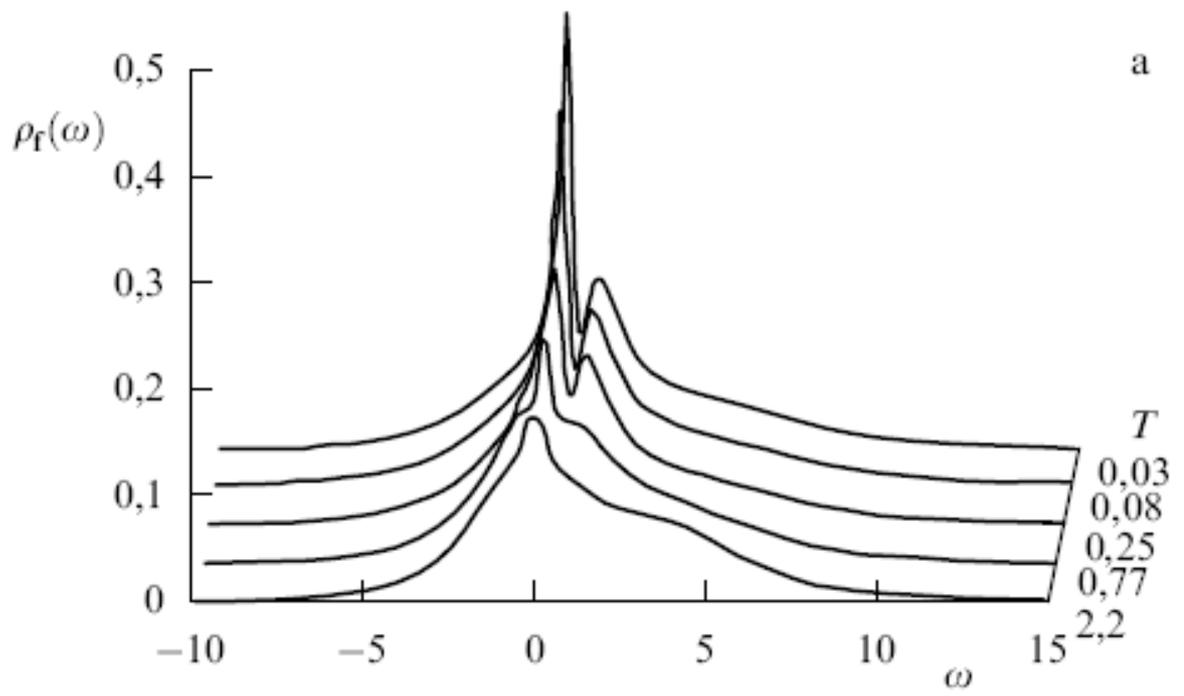


Fig.2. The change of splitting in the resonance maximum at increasing temperature.