DOUBLE 4f-COLLAPSE AT PHASE ISOMORPHIC TRANSITION IN $Ce_{0.9-x}Yb_xTh_{0.1}$

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Dependence of the macroscopic characteristics of the phase isomorphic Ce_γ—Ce_α transition (temperature, pressure, transition type, critical point coordinates, volume effect, etc.) on metallic impurities input in the crystal lattice has been studied in detail /1/. The influence of the impurities on the Ce microscopic properties (4f-shell population, 4f-electron removal degree at transition, etc.) is less known and practically nothing is known about the electronic structure (its evolution) of the impurity atom put into the lattice.

In this work the X-ray K-lines shift method /2/ was used to study the electronic structure of Ce and Yb in $Ce_{0.9-x}Yb_xTh_{0.1}$ in range $0 \leqslant x \leqslant 0.2$ at T=77 and 300 K. (The addition in the Ce-Yb-system of 10% Th prevents β—Ce formation at low temperature).

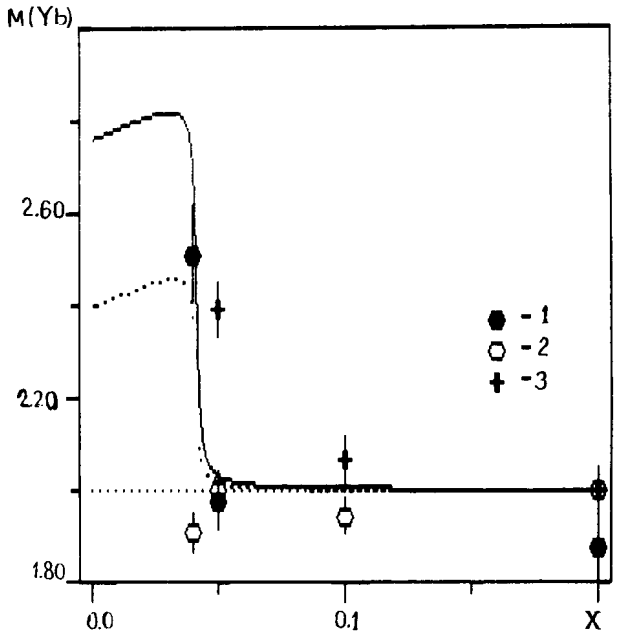

Fig. 1. Dependence of Ce valence m(Ce) in $Ce_{0.9-x}Yb_xTh_{0.1}$ on composition:
1 — T=77K, *2* — T=300K, *3* — T=77K after cooling of sample to T=4.2K. At insertion above — dependence of lattice constant in $Ce_{0.9-x}Yb_xTh_{0.1}$ on x

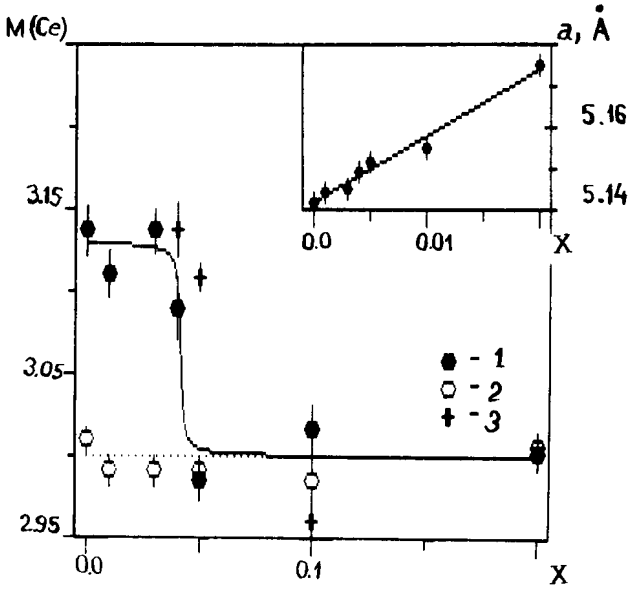

Fig. 2. Dependence of Yb valence m(Yb) in $Ce_{0.9-x}Yb_xTh_{0.1}$ on composition:
1 — T=77K, *2* — T=300K, *3* — T=77K after cooling of sample to 4.2K. Solid and dashed lines — computer calculation for $n_{cr.}(Ce)=n_{cr.}(Yb)=1$ and $n_{cr.}(Ce)=2$, $n_{cr.}(Yb)=1$ respectively

The results of our investigations are given in fig. 1 and 2. It is seen from fig. 1 that the cooling of the $Ce_{0.9-x}Yb_xTh_{0.1}$ samples from the $x\leqslant 0.05$ range initiate the electronic transition from the Ce threevalent state (open circles) to the IV-state (dark circles and crosses) similar to the Ce_γ—Ce_α transition in pure Ce /3/.

Simultaneously with the 4f-collapse in the Ce-atom at low temperature the 4f-collapse in the Yb-atom is observed (fig. 2): the Yb-valence increases abruptly at $x\leqslant 0.05$ from the value $m_{Yb}=1.99\pm\pm 0.02$ ($x>0.05$) to $m_{Yb}=2.42\pm 0.05$ (the simultaneous Ce and Yb valence change in $Ce_{0.9-x}Yb_xTh_{0.1}$ is reversible with temperature).

The electronic Yb^{2+}—Yb^{3+} transition is connected apparently with local contraction of the Yb-atoms generated by the Ce_γ—Ce_α transition in this alloy because the Ce_α metallic radius is less than Yb^{2+} and Yb^{3+} radiuses ($r_{Ce\alpha}=1.715$A, $r_{Yb^{2+}}=1.904$A, $r_{Yb^{3+}}=1.704$A). At such assumption the «birth» probability of the Yb^{3+}-atom will first of all depend on the surrounding Ge^{4+} «presses».

The process of the Yb^{3+} «birth» in $Ce_{0.9-x}Yb_xTh_{0.1}$ alloy has been modelled for a face-centered cubic lattice with a random distribution of the Ce^{3+}, Ce^{4+}, Yb and Th-atoms and assuming that initially divalent atoms Yb turn into threevalent ones if: 1) the number of Ce^{4+}-atoms in the first coordination sphere is more then or equal to some critical number $n_{cr.}(Ce)$; 2) the Yb threevalent atoms, having appeared as a result of the Yb^{2+}—Yb^{3+} transition, stimulate, in their turn, the transition of all the remaining neighboured Yb^{2+} atoms in the threevalent state.

The calculation results are shown in fig. 2 by a solid line for $n_{cr.}(Ce)=1$ and $n_{cr.}(Yb)=1$ and by a dashed line for $n_{cr.}(Ce)=2$, $n_{cr.}(Yb)=2$. It is seen from fig. 2 that these results correspond well to experimental data.

Therefore, in this work the Ce and Yb simultaneous valence increase in $Ce_{0.9-x}Yb_xTh_{0.1}$ at phase isomorphic transition was found experimentally for the first time.

REFERENCES

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