

# “L+1 rule” for continuous electron-hole excitations in photoemission spectra

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Low-energy excitations in valence bands are studied by means of XPS spectroscopy. The analysis of a form of core levels spectra gives the size of effects of electron-hole interactions on atoms of different chemical elements in the compound  $\text{Ni}_{0.5}\text{TiTe}_2$ . The rule for many-electron excitations in solids under action of core-level photo holes is offered.

Ti2*p* and Te3*d* XPS spectra in the intercalated compound  $\text{Ni}_{0.5}\text{TiTe}_2$  are shown in fig. 1. The lines of the Ti2*p* spin-orbital doublet are broadened asymmetrically due to many-body excitations of valence-band electrons generated by sudden creation of the 2*p* photo holes [1]. At the same time such effects on the Te3*d* lines are much smaller. To extract the quantitative information the experimental spectra were approximated by a sum of two spin-orbital lines and an inelastic background  $I_{bg}$ :  $I(E) = I_1(E) + I_2(E) + I_{bg}(E)$ . The form of each line  $I_j(E) = A_j \text{Im} g(E - E_j - i\Gamma_j)$  is determined by an imaginary part of the power function [2]

$$g(z) = \frac{1}{(1-\alpha)b} [1 - (1-b/z)^{1-\alpha}] \quad (1)$$

Here  $A_j$  is line weights;  $\alpha$  is the asymmetry coefficient, shown intensity of the valence electron excitations accompanying creation of the photo hole;  $b$  is their maximal energy;  $E_j$  and  $\Gamma_j$  stand for binding energy and decay of the lines. The power of electron-hole interaction for different XPS lines in  $\text{Ni}_{0.5}\text{TiTe}_2$  has the following magnitudes:

Line	Ti2 <i>p</i>	Te3 <i>d</i>	Ti 3 <i>s</i>	Te4 <i>d</i>
$\alpha$	0.33	0.06	0.23	0.08

The asymmetry of a spectrum (dynamic screening of the photo hole) in titanium is much more, than in other components of compound. It is characterized by  $\alpha = 0.33$  (the values of  $\alpha$  in nickel and tellurium are small, see table and spectra). The important conclusion follows. Despite of a collective character of the valence band electrons in solids, their reactions on photo holes, arising on core levels of various elements, are completely different. Exaggerating, it is possible to tell, that in this case there is no common band excitations, each atom in itself.

Analyses of XPS spectra of  $\text{Ni}_{0.5}\text{TiTe}_2$  and other compounds allow us to conclude that the many-body excitations in solids are followed by the “ $l + 1$  rule”: photo-hole with the moment  $l$  shakes up the band electrons of  $l + 1$  states, mainly. So, for example, 3*d*-electrons react basically on 2*p*-hole, therefore the many-electron effects are strongest on titanium atoms.

These effects are smaller on nickel atoms because of the almost filled Ni 3*d*-shell does not respond on external perturbations. The Te 3*d*- and 4*d*-spectra are narrow symmetric lines like in an isolated atom because of *f*-electrons absence.

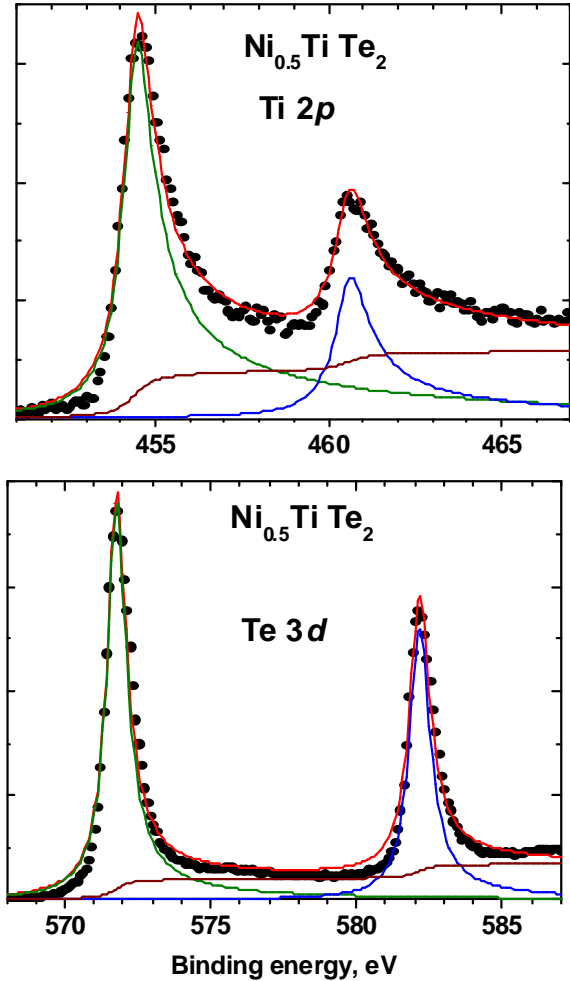


Fig. 1. Ti2*p* and Te3*d* XPS spectra in the compound  $\text{Ni}_{0.5}\text{TiTe}_2$  and their decomposition on sum of two standard lines (1) and a background.

The origin of the rule is connected to prevalence of the dipole matrix elements in coulomb interaction  $l' = l \pm 1$ . However the probability of a transition with reduction of the orbital moment in solids is much less than that in free atoms because of strong delocalization of electron states with the moment  $l - 1$ . In result the  $l + 1$  transition dominate, as it is clearly visible in experimental spectra.

[1] S. Doniach, M. Sundjic, J. Phys. C **3** (1970) 285.

[2] V. I. Grebennikov, J. Electr. Spectr. Rel. Phenom. **137-140** (2004) 741.