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Ru 4p → 4d Fano resonance in the $SrRuO_3$ valence band

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The photoemission spectroscopy (PES) is a powerful tool for studying electron correlation effects in solids since the valence band (VB) spectra can directly reveal many body effects. However, experimentally measured VB spectra represent a superposition of both Ru *4d* and O *2p* states, making it difficult to interpret the results. Furthermore, the published PES on $SrRuO_3$ VB also was not totally consistent with each other and interpretations of spectroscopic data are often controversial [1,2]. The electronic structure of thin epitaxial $SrRuO_3$ films has been investigated using resonant photoemission spectroscopy (RPES).

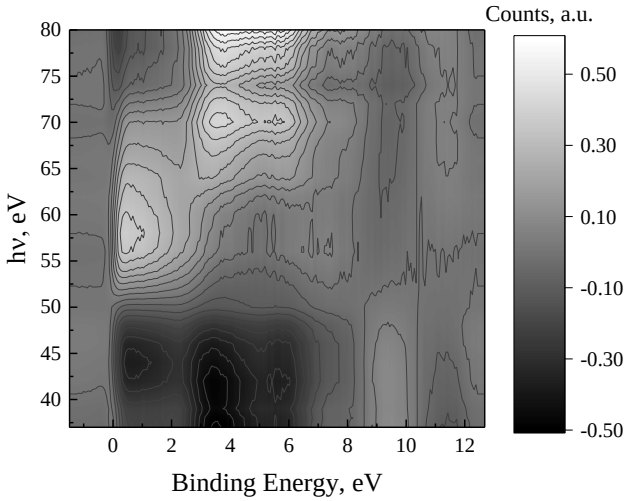

Figure 1. Countur plot of RPES spectra for $SrRuO_3$ thin film. For illustration purposes the difference between measured and the averaged over all *hν* spectra were shown.

Valence band data were collected at photon energies corresponding to *Ru 4p → 4d* threshold and analyzed using Fano expression:

$$F(h\nu) \approx (qw + h\nu - E_{\mathrm{Res}})^2 / [w^2 + (h\nu - E_{\mathrm{Res}})^2] \quad (1)$$

The values of resonance energy E_R, width w, and asymmetry factor q were obtained by PES spectra fitting assuming the Fano behavior of *Ru 4p → 4d* resonance with a linear background corresponding to the monotonic decrease of the Ru 4d and O 2p photoionization cross-sections.

The evident resonant features were observed in the constant-initial-state mode of photoemission in the entire VB binding energy (BE) range ~ 0÷8 eV(see Fig. 1). And may be divided into two regions: Region A (BE ≤ 2.5 eV) – with resonance energy ~ 43÷45 eV and Region B (BE ≥ 5 eV) with resonance energy > 80 eV. Such separation of the valence band is clearly manifested in the distribution of the Fano parameters (see Fig. 2).

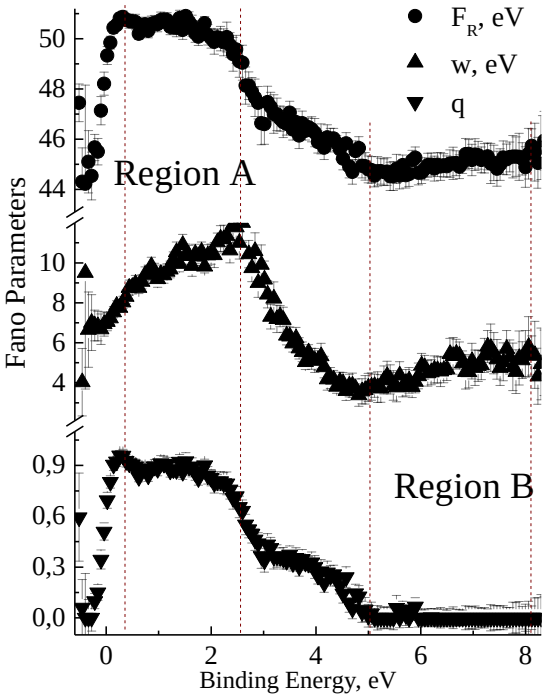

Figure 2. Parameters describing Ru 4d states Fano resonance in $SrRuO_3$ thin epitaxial film. Error bars corresponds to the standard deviation of fitting.

In accordance with theoretical models [3,4] *Ru 4d* states in Reg. A may be attributed to coherent and incoherent states of ruthenium, while states dominating at higher energies to bonding (around 5–7 eV) and nonbonding (around 3 eV) hybridized *Ru 4d – O 2p* states.

Another important result is that in the case of Fano-parameters varying along the valence band, the difference spectrum is no longer directly reflects the density of states and CIS spectra fitting procedure becomes necessary.

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