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Application of X-ray absorption and resonant photoemission spectroscopy to study electronic states of iron through 3p-3d transition for SrTiO₃:Fe epitaxial film

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The strontium titanate STO is promising material for electronic application. The electrical properties of this material can be tuned by iron doping.

The synchrotron radiation was used to study of SrTiO₃ doped by 2% of iron thin film. As was shown in our earlier work the oxidation states of iron in the STO:Fe thin films is in a mixture of Fe²⁺ and Fe³⁺ states [1]. In order to confirmation and distinguish oxidation states of iron at sub-surface layer of the film we performed X-ray absorption study in range of the Fe M-edge threshold.

The pure SrTiO₃ is an isolator with a energy gap of 3.6 eV. The valence band of SrTiO₃ contains mainly O2p-Ti3d hybridized states. The influence of Fe3d electrons on the density of states in the energy gap was study by resonant photoemission in range Fe3p-3d resonance. Measured spectra are compared with the results obtained for Fe2p-3d resonance [2].

The X-ray absorption spectra obtained for the Fe M-edge contains two main peaks at 53 eV and 59.6 eV of photon energy. In order to analysis of the shape obtained curve we performed atomic multiplet calculation of Fe3p absorption spectra using the CTM4XAS program [3]. To verify obtained result also photoemission Fe3p spectra was measured and compared with calculation.

In figure 1a only a shape of the first peak of absorption was showed.

The valence band spectra, presented in figure 1b, were measured in the binding energy range from -3 to 13 eV. We explored the photon energy range across the Fe3p-3d photoionization threshold (47 eV – 54 eV). Two features A and B are clearly visible at energy of about 4 eV and 6 eV, respectively. The relative intensity of observed maxima is changed with energy of photon. The intensity of B feature increases for the energy of photon higher than $h\nu=53$ eV.

The valence band spectra measured -in and -off resonance was presented in figure 2. Small changes at localization of B feature are visible.

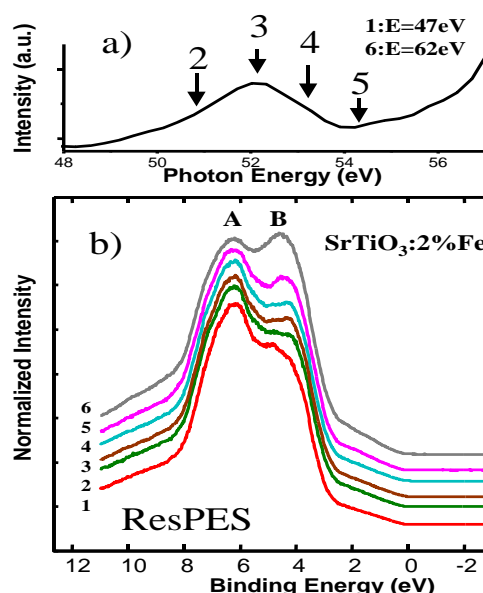


Figure 1. a) Fe M-edge XAS spectra recorded for Fe doped STO films obtained in AEY mode. b) Photoemission spectra of the valence band region measured in range of photon energy corresponding to Fe3p-3d photoionization threshold.

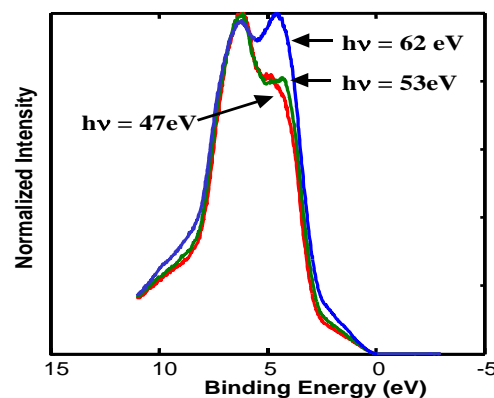


Figure 2. The details of valence band spectra measured at energy of photon -in and -off resonance.

The mixed valence of iron was discussed based on the X-ray absorption spectroscopy and atomic multiplet calculation. The influence of Fe 3d state on valence band STO:Fe film was study by resonant photoemission. Small difference in shape of valence band was detected in resonance.

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- [1] A. Koehl, *Phys. Chem. Chem. Phys.* **15** (2014) 8311.
[2] J. Szade *et. al.*, *in preparation*
[3] E. Stavitski, F. M. F. de Groot, *Micron* **41** (2010) 687.