RESONANT PHOTOEMISSION STUDIES OF Fe DOPED $SrTiO_3$ THIN FILMS

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Doping is one of the methods to control the properties of a model perovskite $SrTiO_3$ (STO) which is an insulator with the band gap of 3.2 eV. One of the interesting cases is Fe doping. Several exciting effects have been reported for Fe doped crystals, especially electrical degradation connected with electrocoloration. Fe doped STO thin films exhibit promising switching properties with possible application in memristive memories [1]. The main feature determining these properties is modification of the electronic structure where the role of the in-gap states is crucial [2]. To get insight into the contribution of Fe and main components to the electronic structure we have performed X-Ray Absorption Spectroscopy and Resonant Photoemission studies.

The epitaxial Fe doped STO films with thickness of about 20 nm were obtained by PLD (Pulsed Laser Deposition) method on the Nb doped $SrTiO_3$ single crystal substrate. Three samples were studied — films doped with 2% Fe, 5% Fe and the undoped $SrTiO_3$ film. The samples were annealed in UHV conditions prior to study at 150°C, 300°C and 630°C.

The XAS spectra on $L_{2,3}$ edge of titanium and iron and K edge of oxygen were obtained with the use of two methods — total electron yield (TEY) measured by the drain current and Auger electron yield (AEY). The methods have different surface sensitivity.

The valence band spectra were obtained for the photon energies corresponding to in- and off- resonance of iron, titanium and oxygen. It enabled to separate the contributions from those elements to valence band and especially to the region of the STO energy gap. It appeared that Fe is present in two oxidation states Fe^{2+} and Fe^{3+} in the films. It turned out from the XAS spectra that the content of Fe ions in two different valence states was the same for both nominal doping levels and it varied with the annealing temperature. The content of 2+ Fe was higher in the surface region what can be related with the concentration of oxygen vacancies.

We were able to distinguish contribution from both Fe oxidation states to the valence band. For Fe^{3+} the electronic states are located mostly above the top of the valence band whereas for Fe^{2+} there are distributed within the gap forming a relatively broad structure.

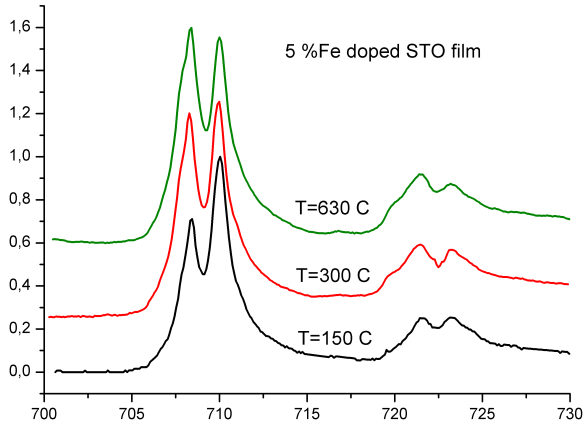

Figure 1: XAS spectra of the 5% Fe doped $SrTiO_3$ film obtained with the use of TEY mode at various temperatures.

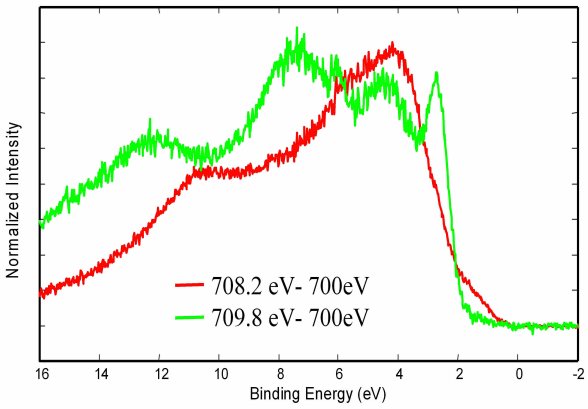

Figure 2: Partial density of Fe 3*d* sates (PDOS) obtained from the on- and off-resonance photoemission spectra for photon energies corresponding to two peaks in the Fe L_3 absorption edge (h = 708.2 eV (on-resonance), h = 709.8 eV (on-resonance) and h = 700 eV (off-resonance)), 2% Fe doped $SrTiO_3$ film.

References

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