Theoretical calculations of resonant Auger electron spectroscopy for impurity Ni doped SrTiO3

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$SrTiO_3$(STO) has a band gap of 3.25 eV, which results in an absorption edge at UV wavelengths. It has been suggested that the band gap can be reduced by doping Ni at the Ti position, shifting the absorption edge into the visible range. In a previous study [1], Ni was doped in STO thin films and resonant photoemission spectroscopy was performed at the Ni L_3-edge resonance to study the local electronic structure changes induced by Ni doping. Resonant Auger electron spectroscopy (RAES) has been performed to analyze the electronic states of Ni, which occupies an in-gap level. However, direct theoretical calculations of the electronic correlations formed by Ni and the ligand field have not been performed.

Therefore, this study aimed to analyze the electronic states of impurities and perform theoretical calculations of RAES spectra for Ni-doped STO. The research methodology employed DFT+U calculations using the density functional theory DFT-based calculation software VASP, and multiplet code.

Calculated spectra using the density of states obtained from VASP calculations included hybridization with ligands and the overall system state, but no resonances corresponding to multi-term effects were observed. Consequently, an extended nearest-neighbor cluster model multi-term calculation was performed, incorporating hybridization with ligands into the atomic multiplet calculation. For the hybridization with the ligand, parameters obtained from a tight-binding approximation calculation using the results from the VASP calculation were performed. From the results, resonances, not only from valence electron states and multipole effects but also from charge transfer transitions from the ligand, which do not appear in atomic multipole calculations, were obtained.

These results demonstrate that cluster model multiplet calculations can show resonances in experimental spectra not captured by multiplet effects or charge transfer transitions in previous calculations. Furthermore, they confirm that multiplet effects and ligand hybridization significantly influence the analysis of the electronic states of impurity Ni measured by RAES.

References

[1] Fatima Alarab,et al . Phys. Rev. B, Vol. 104, p.165129 (2021)