Atomic and electronic structure of transition-metal doped $LaAlO_3/SrTiO_3$ interfaces

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In 2004, the discovery of a two-dimensional electron gas (2DEG) at the interface between two insulating perovskites $LaAlO_3/SrTiO_3(001)$ [1] has motivated a large research effort, which has led to the discovery of new interfacial properties (magnetism, superconductivity, tunable Rashba effect…), offering consequently a new playground to investigate condensed-matter fundamental mechanisms and new opportunities for proposing alternatives concepts for future electronic devices. Among the different possibilities to tune these properties, doping the interface may be considered as an efficient way to modify the electronic properties either directly or via induced modifications in the atomic structure.

The present study participates to this effort by exploring $LaAlO_3/SrTiO_3$ interfaces doped with transition-metal atoms, namely iridium or cobalt atoms. Cobalt was chosen as a dopant because of its role in developing a dilute magnetic semiconductor state in TiO_2 [2], whereas novel properties arising from an interplay between strong spin-orbit interaction and electron correlations could be expected in the case of Ir doping. Besides, the 5d electronic structure of Ir doping could increase the carrier mobility at the interface compared to 3d electrons [3].

High quality nanostructures, typically $LaAlO_3$(5u.c.)/doped-$SrTiO_3$(1u.c.)/$SrTiO_3$ (substrate), were grown by pulsed laser deposition (PLD). Atomically resolved high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) was implemented to probe the local structure at the interface and quantify the level of strain near the interface, whereas the electronic structure was investigated by electron energy loss spectroscopy in a STEM. We will report the evolution of the electronic and atomic structure of the doped $LaAlO_3/SrTiO_3$ interface as a function of the doping level [4], and its consequence on the transport properties. A special emphasis will be put on the location of the dopant atoms (preferred atomic site, cationic inter-diffusion, state of strain…) using a combination of experimental techniques and first-principles calculations.

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[2] Y. Matsumoto *et al*, *Room-temperature ferromagnetism in transparent transition metal-doped titanium dioxide*, Science **291**, 854 (2001).
[3] S. Nazir *et al*, *Nb and Ta layer doping effects on the interfacial energetics and electronic properties of $LaAlO_3/SrTiO_3$ heterostructure: first-principles analysis*, Phys. Chem. Chem. Phys. **18** (2016), 2379–2388.