INSTITUT NEEL Grenoble

PhD grant

Title

MAGNETIC AND ELECTRONIC PROPERTIES OF DOPED TETRAGONAL CUO FILMS

Context :

Tenorite CuO phase is unique amongst the monoxides of the 3d transition elements in having a monoclinic unit cell, rather than the cubic rock salt structure and octahedral coordination. CuO is antiferromagnetic with a Néel temperature of 230 K. This value is at odd with the trend of increasing T_N with atomic number observed for 3d transition metal monoxides, and is explained with its structure. The magnetic properties are function of the super-exchange interaction between copper ions. This interaction increases with Metal-O-Metal bond angle and is maximum for a linear configuration (bond angle of 180°) [1]. This condition is realized for most of members of the 3d transition metal monoxides series (MnO, FeO, CoO, NiO). In monoclinic CuO this angle is either 109° or 146°. The aim of our research project is the growth and study doped CuO films exhibiting peculiar properties by making use of the recent advancements associated with the epitaxial growth of a new tetragonal CuO phase, in which the Cu-O-Cu bond angle is of 180° [2].

Objectives and means available :

We will develop films for two different kind of applications. The first objective is the growth of magnetic semiconductor films which are critical in spintronic applications [3]. More challenging, a second class of films will be studied with possibly superconducting properties, which will be also elaborated starting from the tetragonal CuO phase. The motivation comes from the fact that CuO can be regarded as the model parent compound of the high temperature cuprate superconductors [4].

A joint computational and experimental approach will be adopted. Ab initio calculations will be performed in synergy with experiments for the choice of the most appropriate dopant element. For growing ferromagnetic semiconductors, Fe and Co dopants will be firstly considered. Changing the nature of dopant, we expect also to be able to grow metallic films hopefully with superconducting properties. For that, the films need to be doped with elements which can provide extra electrons, in analogy with the case of n-type semiconductors. Remembering that CuO is a charge transfer insulator with divalent Cu, we will try to replace copper with trivalent metals. Copper substitution with Al and Ti will be first studied by DFT calculations.

In terms of methodologies, this project will have three axes that will work in synergy: (1) the ab initio calculation of the electronic properties, (2) the growth, (3) the structural determination and measurement of the electronic and magnetic properties.

Tetragonal CuO was grown in epitaxy on $SrTiO_3$(100) by different techniques: pulsed laser deposition, magnetron sputtering, and electron beam evaporation (MBE). In this project, the sample growth will be performed by reactive MBE. The growth of the doped films will be realized by co-evaporation of Cu and of the dopant element on the substrate in atomic oxygen atmosphere.

The structure of the most promising samples will be determined by grazing incidence x-ray diffraction (GIXRD), which is a particularly appropriated method for the study of the growth and the structure of ultrathin TMOs [5]. These studies require a synchrotron radiation source and proposals will be submitted to suitable beamlines.

The transport and magnetic properties as a function of the applied magnetic field (up to 8 Tesla) and temperature (in the range 1.6-300 K), will be measured *ex situ* using the techniques available at the Néel Institute.
The electronic structure calculations will be performed by employing the DFT+U scheme. The Hubbard U correction is necessary to restore the correct hybridization of the d states near the Fermi level which is a manifestation of the strong electron correlation [6,7].

References

[1] T. Kimura et al., Nature Mater 7, 291–294 (2008). https://doi.org/10.1038/nmat2125
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[3] S. M. Yakout, J. of Superconductivity and Novel Magnetism (2020) 33, 2557.
[4] A Junod et al 1989 J. Phys.: Condens. Matter 1 8021
[5] A. D. Lamirand, S. Grenier, V. Langlais, A. Y. Ramos, H. C. N. Tolentino, X. Torrelles, M. De Santis, Surface Science 647, 33 (2016). http://dx.doi.org/10.1016/j.susc.2015.12.005
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Possible collaboration and networking :

The thesis will be carried out at the Néel Institute, where methods of elaboration, and study of structure and properties are available. The theoretical calculations will be carried out at SIMAP.

Required profile :

We look for a highly motivated student with a good background in condensed matter and solid-state physics and a strong interest in experimental activity.

Foreseen start for the grant : 01/10/2024

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