

Infrared Spectroscopy Study of Functional Metal Oxides

Rebecca CERVASIO

(Ligne AILES, Synchrotron SOLEIL, Gif-sur-Yvette, France)

Mardi 11 juillet 2023 – 14h00
Amphithéâtre SOLEIL

Functional metal oxides are an integral part of advanced technologies today. Functional properties such as ferroelectricity, piezoelectricity and superconductivity are obtained through different compositions, structures and physical forms. Metal oxides deposited as nanometer thin films may play a key role in microelectronics. The present study aims to couple infrared (IR) spectroscopy and Density Functional Theory (DFT) simulations to probe the various phases in thin layers and to determine the differences with their bulk counterparts. Three families of thin films compounds are studied. (1) $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$: optical measurements are used to characterize the sample in the normal state using a multilayer stacking model and the energy gap is extracted below T_C ; (2) $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$: its tetragonal to cubic phase transition is investigated, together with probing phonon signatures for various thicknesses. Using DFT simulations adapted to reproduce the complexity of solid solutions, the polar modes responsible for the loss of ferroelectricity in the paraelectric cubic phase are identified; (3) $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$, a promising ultra thin lead-free ferroelectric material for which we performed the first optical investigation on films of various thickness and phases. The various phonon structures, assigned using DFT calculations, provide possible IR signatures for ferroelectric and non ferroelectric samples.

Les membres du jury sont :

Maël GUENNOU
Yann GALLAIS
Nita DRAGOE
Sophie DE BRION
Pascale ROY
Jérôme CREUZE
Émilie AMZALLAG

Assistant professor
Professeur
Professeur
Professeure
Directrice de recherche
Professeur
Maître de Conférences

Université du Luxembourg
Université Paris Cité
Université Paris-Saclay
Institut Néel/CNRS/U. Grenoble Alpes
CNRS (SOLEIL)
Université Paris-Saclay
Université Paris-Saclay

Rapporteur & Examineur
Rapporteur & Examineur
Examineur
Examinatrice
Directrice de thèse
Invité
Invitée



Vous êtes cordialement invités au pot qui suivra

THÈSE