

MAP-fis Essay Proposal, 2015-2016

(please write in English)

Supervisor

Name: Joaquim Agostinho Gomes Moreira

e-mail: jamoreir@fc.up.pt

Title

Manipulating the metal-insulator transition and emergence of new functionalities in nickelate-based superlattices

Area

(Materials, Optics, Condensed Theory, High Energy Theory,....);

Condensed Matter Physics

Summary of Proposal

Rare-earth nickelates $RNiO_3$ are fascinating compounds, known for their bandwidth controlled metal-insulator transition (MIT) [1-3]. Bulk $LaNiO_3$ does not display a MIT, remaining paramagnetic metal at all temperatures [2,3]. The other $RNiO_3$ are paramagnetic metals at high temperatures but between 100 and 600K they are semiconducting, exhibiting charge disproportionation and a unique antiferromagnetic ordering [2-4].

It is possible to engineer interfaces between $RNiO_3$ and other transition-metal-oxides at atomic scale precision [3,5-8], tailoring the coupling between electronic/orbital degrees of freedom with structure[5-8]. Efforts have been focused on the understanding and controlling MIT in $RNiO_3$ by strain. Moreover, new interface phenomena in $RNiO_3$ based superlattices have been emerged.

$LaNiO_3$ is the most studied in ultrathin film form or incorporated in superlattices, mainly due to theoretical predictions of orbital ordering and high T_c superconductivity [9]. As the thickness is reduced to only few unit cells, the transport evolves from a metallic to a strongly localized character and the sheet resistance reaches a value close to the quantum of resistance in 2D [10]. Hall measurements and electric field effect experiments have revealed p-type conduction, with a carrier density electrostatically tuned [6,11]. Recently, it was demonstrated that transport in $LaNiO_3$ can be manipulated through changes in its surface termination [7].

The studied $LaNiO_3$ -based superlattices concerns the $(LaNiO_3)_n/(LaAlO_3)_m$ and $(LaNiO_3)_n/(LaMnO_3)_m$, with n,m ranging from 4 up to 10 [12,13]. Work has concentrated on the $LaNiO_3$ bilayer sandwiched between $LaAlO_3$. Broken-symmetry 2D ground-states in (111)-oriented



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(LaNiO₃)_n/(LaAlO₃)_m superlattice is foreseen, and an unexpected Jahn-Teller distortion with d_z^2 orbital polarization and a ferromagnetic/ferroelectric Mott insulating phase in the double perovskite (1/1) suggests strain orbital control [12]. The LaNiO₃ bilayer has a switchable multiferroic insulating ground-state. In (LaNiO₃)_n/(LaMnO₃)_m superlattices, unexpected exchange-bias in (111)-oriented superlattices involving LaNiO₃ and LaMnO₃ layers was reported, due to a complex magnetic structure induced in the nonmagnetic LaNiO₃ [13]. Magnetic reconstructions at the interfaces of the (LaNiO₃)_n/(LaMnO₃)_n superlattices have been studied via a hybrid microscopic model.

Other RNiO₃ compounds are scarcer studied in the form of thin films and superlattices. The most current are SmNiO₃ and NdNiO₃ [14,15]. The experimental studies concern the effect of the epitaxial strain on the MIT temperature. It was found that for compressive strain the MIT temperature is reduced about 200K, while for tensile strain the MIT temperature is weakly changed [15]. Much smaller changes are observed in the Néel temperature [15,16]. Very recently, calculations have proposed that PbNiO₃ is antiferromagnetic and ferroelectric, with a very large electric polarization of $\sim 100\mu\text{C}/\text{cm}^2$, exhibiting LiNbO₃-type structure [17].

A systematic and deeply study of both ultrathin films and RNiO₃-based superlattices (R=Nd,Sm,Pb) is still missing and the origin of the MIT in these RNiO₃ is also under debate [18,19]. An investigation of the transport and magnetic properties of SmNiO₃ and NdNiO₃ as a function of compressive/tensile strain using different substrates and crystallographic orientations, as well as the possible existence of 2-dimensional electronic gas (2DEG), at the interface between suitable terminated substrate and RNiO₃ films has not yet been studied.

To date, RNiO₃-based superlattices involving high ferroelectrics and multiferroics have not been reported, yet. In such superlattices, the RNiO₃ layers can deform via piezoelectric effect, tuning MIT, and the magnetic properties. The transition into the insulator state of the RNiO₃ layers modify internal depolarizing electric fields, determining domain dynamics in ferroelectric layers. Outstanding is to achieve polarization reversal by magnetic fields, using multiferroics.

It is expected that the outcomes of this proposal can yield novel functionalities and open a new field of fundamental and applied research.

The essay aims are:

- a) to develop a critical literature reading in order to write a state-of-art of the proposed topic, highlighting the current outstanding problems.
- b) based on the critical assessment of the published research, to write a thesis proposal, presenting the main objectives to be reached, a research plan and the methodology to be follow.

References

(to allow students first look at topic)

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