Unveiling the mechanisms of hydrogen induced phase transitions in nickelate films

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An increasing number of studies are showing the possibility of tuning the electronic properties of functional materials via an unconventional dopant: hydrogen. In correlated oxide interfaces, and especially in rare-earth nickelates, hydrogen-induced reversible electronic and structural phase transitions have been uncovered [1-2]. Neutron and x-ray scattering methods are without doubt one of the best way to characterize in a non-destructive and non-local way these systems. Here we will show the multi-stage phase transformation observed at room temperature for $LaNiO_3$ upon exposure to hydrogen gas. Electrical transport shows a subsequent metal-insulator-metal transition. We will present the results of in situ neutron reflectometry (NR), which allowed us to distinguish and quantify oxygen depletion, hydrogen incorporation, and lattice expansion (Figure 1). These are all different mechanisms that can explain the electronic modification of the host layer. In addition to the neutron measurements, we will present results from in situ synchrotron x-ray diffraction and x-ray absorption, which helped to understand the reaction with hydrogen and its effects on the Ni valence. This work highlights the need of combining appropriate complementary techniques to correctly identify the source of modifications induced by hydrogen exposure in complex systems such as transition metal oxides.

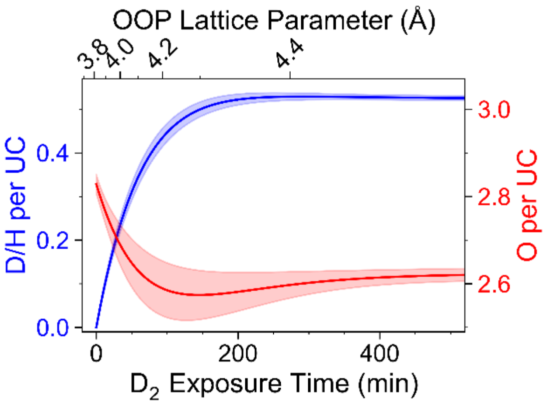

Fig.1 Hydrogen and oxygen stoichiometry and lattice expansion of the $LaNiO_3$ thin film upon exposure to deuterium gas at RT determined by in situ NR.

[1] J. Shi, Y. Zhou, S. Ramanathan, *Nat. Commun.* **5**, 4860, (2014).
[2] Haowen Chen, et al. *Nano Letters* **22**, 8983-8990, (2022).

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