

Supplementary Materials: Tuning the Electrical Properties of NiO Thin Films by Stoichiometry and Microstructure

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Figure S1 shows the oxygen partial pressure as a function of oxygen flow rate, while the other parameters (like current on the Ni target and pumping speed) are fixed the same with the NiO thin films deposition process. The hysteresis curve of oxygen partial pressure demonstrates that the reactive sputtering process with 4 sccm O₂ locates at the transition mode and is quite near the metallic mode. Thus, an oxygen sub-stoichiometry is expected. In the case of 11 sccm O₂, the target is fully poisoned and oxygen over-stoichiometric NiO thin films are expected.

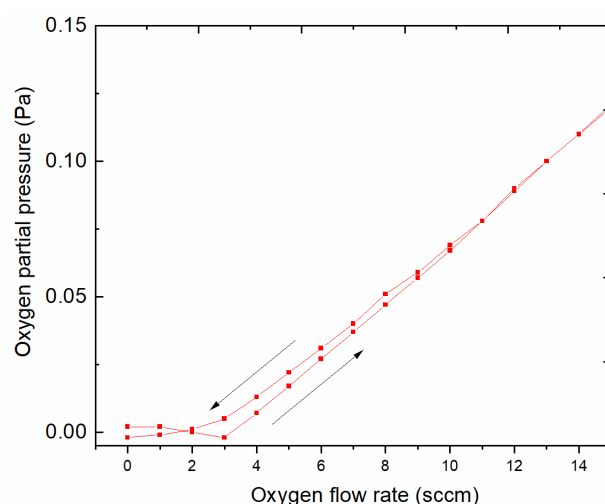


Figure S1. Evolution of the oxygen partial pressure as a function of the oxygen flow rate.

The general procedures to do the quantification by XPS. O1s XPS spectra are shown in Figure S2. The Advantage software is used to determine the compositions. First, the charge shift is performed via the C1s peak. Then background is subtracted. Following, quantification is done by selecting O and Ni XPS spectra. In order to verify the quantification analyses by XPS, the NiO thin film grown with 11 sccm O₂ has also been characterized by Rutherford-Backscattering Spectrometry (RBS) at Helmholtz Zentrum Dresden Rossendorf (HZDR), as shown in Figure S3. The RBS simulation software is SimNRA. Chu & Young model is used for the straggling. Rutherford (including Anderson screening) is used cross-sections. NiO_{1.13} determined by RBS is close to that of NiO_{1.12} by XPS. Then, the same procedures are used to analyze the compositions of NiO thin films grown by 4 and 7 sccm O₂.

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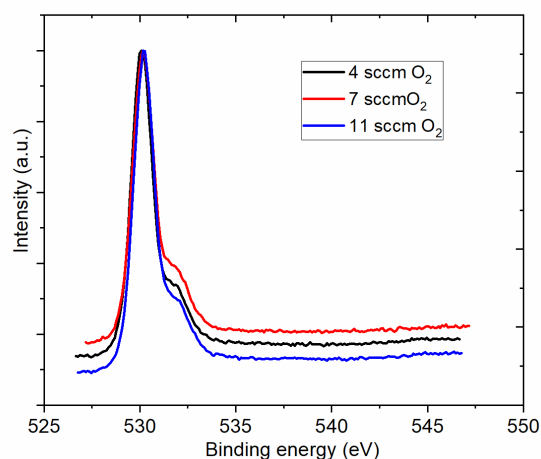


Figure S2. O1s XPS spectra of various NiO thin films deposited with different oxygen flow rates.

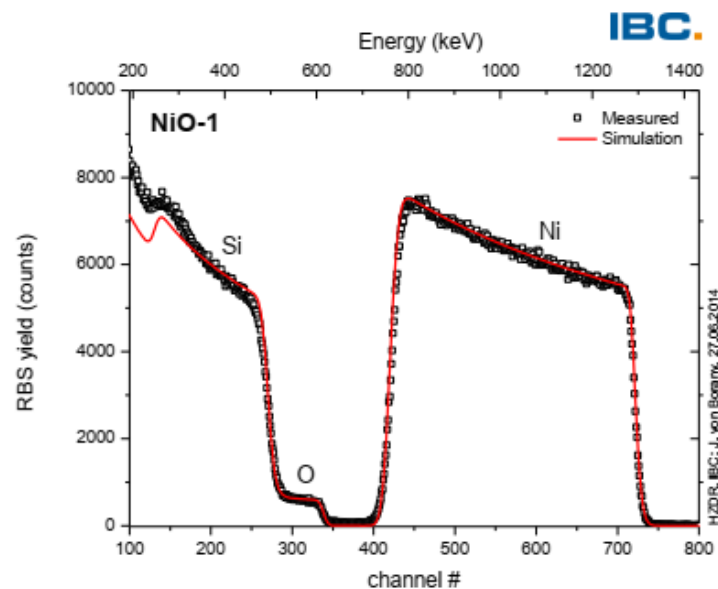


Figure S3. RBS spectra of NiO thin film grown with 11 sccm O₂.

The Ni $2p_{3/2}$ XPS spectra of NiO thin films with different resistivity or stoichiometry are present in Figure S4. However, these spectra look quite similar with each other.

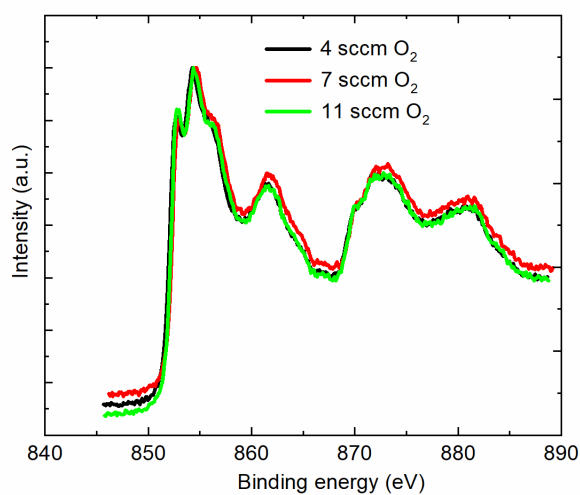


Figure S4. Ni $2p_{3/2}$ XPS spectra of NiO thin films deposited with different oxygen flow rates (4, 7 and 11 sccm O_2).

Figure S5 shows the O K edge ELNES spectra of NiO thin films deposited with different oxygen flow rates (4, 7 and 11 sccm). Although these thin films exhibit significant discrepancy on resistivity, quite a little difference is observed in their O K edges, as seen in Figure S4.

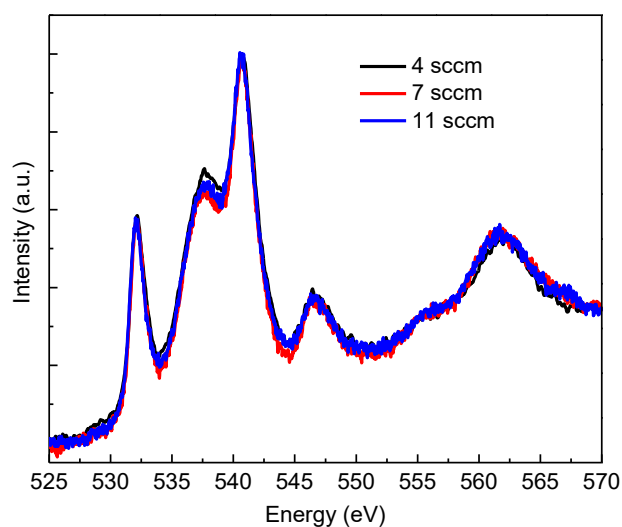


Figure S5. O K edge ELNES spectra of various NiO thin films deposited with different oxygen flow rates.