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X-Ray diffraction (XRD) applied to Nanoscience.

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X-Ray diffraction is a very well known technique largely used for morphological characterization of condensed matter ranging from minerals to biosystems. The D8 Advance Bruker diffractometer at CNIS operates with the Mo-anode tube, delivering high energy X-ray beam, with high penetration e.g. in metal or heavy elements containing materials. The instrument is designed for delivering ultimate quality diffraction data, combined with ease of use and ample flexibility in order to quickly switch to different operative options: in fact it can operate both in transmission and reflection modes, with the different angular resolution. Results obtained by the XRD can be very well combined with the SEM images to extract complete structural information on complex and nanostructured materials.

Right now the instrument is used to explore the microscopic structure of liquids, powders, films samples. Its high brilliance allows collecting robust data sets in a few minutes, thus opening the way to potential in situ kinetic studies, including phase transitions, in operando devices etc.

We operate with both custom Bruker and homemade experimental setups, extending the performance of the instrument.

In the last few years several research groups in Sapienza University took advantage of the facility and their performed studies can be roughly divided in subgroups.

- Crystal structure determination,
- Phase identification,
- Phase quantification,
- Contaminant detection and analysis,
- Structure of amorphous systems
- Structural changes under specific conditions

We will present and discuss selected studies performed at the XRD-lab demonstrating the capability of the instrument for the structural investigation of solar cells, electrodes, amorphous polymers nanostructured liquids.

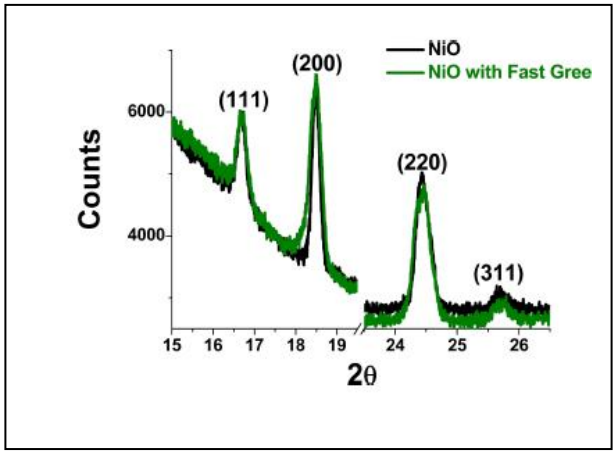

Fig. 1 XRD spectra of NiO prepared by Rapid Discharge Sintering in the pristine (black) and dye-sensitized states (green) [1]

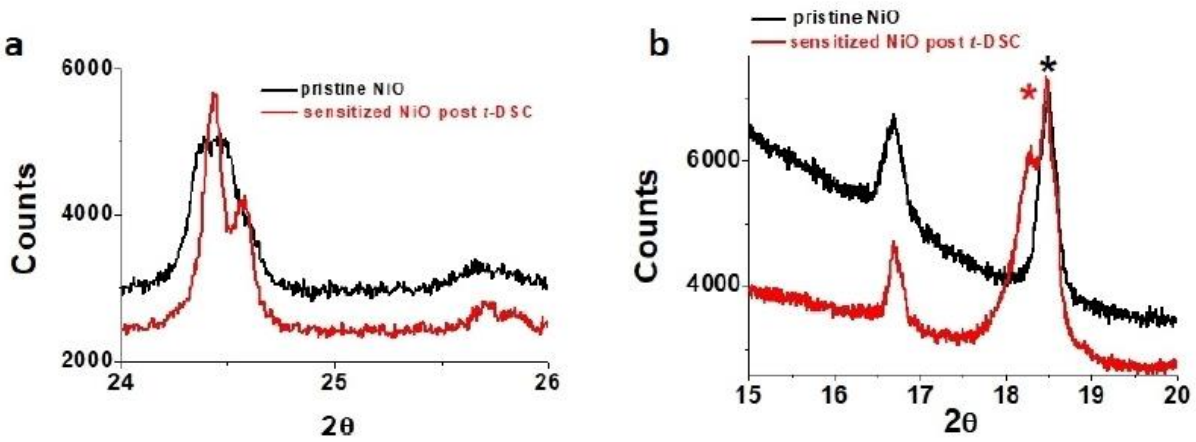

Figure 2. XRD spectra of NiO prepared by Rapid Discharge Sintering before and after employment as Fast Green sensitized photocathode in the t-DSC. [1]

References

[1] Matteo Bonomo, Stephen Sheehan, Denis P. Dowling, Lorenzo Gontrani, and Danilo Dini " First Evidence of Electrode Reconstruction in Mesoporous NiO After Operation as Photocathode of Dye-Sensitized Solar Cells" ChemistrySelect 2018, 3, 6729 – 6736