

# Laboratori Nazionali di Frascati

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## SURFACE XANES AT OXYGEN K-EDGE OF OXIDE GROWN ON NICKEL

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The surface oxidation of Ni has been studied by oxygen K-edge surface X-ray absorption near edge structure (XANES) at the Grasshopper line of Frascati synchrotron radiation facility. Surface X-ray absorption spectra were detected by partial electron yield in the range of energy from 500 to 600 eV. We have measured the O K-edge XANES of clean nickel single crystal surface exposed to oxygen at low pressure. The data have been compared with the spectra of stoichiometric NiO sample and defective Ni<sub>1-x</sub>O oxide grown under controlled conditions.

The XANES spectrum of stoichiometric NiO above the O K-edge is compared with the calculated spectrum by one-electron full multiple scattering theory in the real space<sup>(1)</sup>. We show that the full-multiple scattering calculation including several shells of neighbouring atoms gives full account of the main spectra features as shown in Fig. 1.

The spectrum of stoichiometric NiO shows extra features b and f due to many body final state configurations. The ground state of NiO is described as an interatomic intermediate valent system<sup>(2)</sup> where there is configuration interaction between  $|3d^8\rangle$  and  $|\underline{L}3d^9\rangle$  configurations. The first sharp peak at oxygen threshold is assigned to the transition to the ligand hole of the  $|\underline{L}3d^9\rangle$  configuration and therefore its intensity is a measure of probability of this configuration<sup>(3)</sup>.

The surface oxygen K-XANES of the surface oxide grown on Ni surface at room temperature in the ultra high vacuum has been measured. The analysis of the high energy multiple scattering peaks indicates a contraction of the Ni-O distance.

This spectrum has been compared with the bulk spectrum of defective Ni<sub>(1-0.03)</sub>O prepared at 1200°C with an oxygen partial pressure of  $10^{-8}$

torr<sup>(4)</sup>. The comparison shows that the oxide grown on nickel surface at room temperature is non stoichiometric and we show that very small values of non stoichiometry can be detected by O K-edge XANES.

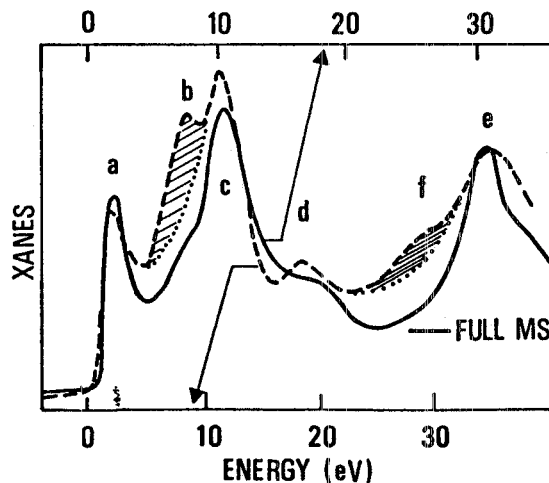


Fig. 1 - Oxygen K XANES of NiO measured by electron partial yield (dashed line). The theoretical full multiple scattering calculation in the real space is plotted after having expanded the scale to take account of the energy dependent exchange energy. The dashed areas indicate the peaks b and f which are due to multielectron final state configurations.

We have found that a drastic reduction of the intensity of the peak a at threshold in the oxide grown at low oxygen pressure. This result gives evidence of reduction of probability for the  $13d_{\underline{L}}$  configuration in the surface oxide.

In conclusion the XANES spectra of non stoichiometric oxide grown on nickel surface give unique information both on the oxygen site structure and on the ionicity of the Ni-O bond.

#### References:

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