| | | |
|---|---|---|
| ESRF | **Experiment title:**<br>**THE STRUCTURE OF THE RECONSTRUCTION(S) OF MGO(111) BY GRAZING INCIDENCE -RAY DIFFRACTION (GIXD)** | **Experiment number**:<br>SI-709 |
| **Beamline**:<br>ID03 | **Date of experiment**:<br>from: 23.11.2001 to: 01.12.2001 | **Date of report**:<br>10 March 2004 |
| **Shifts:**<br>18 | **Local contact(s)**:<br>Christopher Walker | *Received at ESRF:* |

**Names and affiliations of applicants** (* indicates experimentalists):

Antoine BARBIER[*1], Jacques JUPILLE[*2], , Fabio FINOCCHI[3], Claudine NOGUERA[3], Odile ROBACH[4]

CEA Grenoble, DRFMC/SP2M, 17, rue des Martyrs, 38054 Grenoble Cedex, France, (2) Laboratoire CNRS/St-Gobain, "Surface du Verre et Interfaces", B.P.135, 93303 Aubervilliers Cedex, (3) Laboratoire de Physique des Solides, Batiment 510 – Université Paris-Sud 91405 Orsay CEDEX, (4) E.S.R.F.

**Report:**

The present experiments aimed at completing previous measurements on the MgO(111)-p(2x2) reconstructed surface in the low temperature range. As expected the reconstruction signal has been found sensitive to temperature and partial oxygen pressure (figure 1).

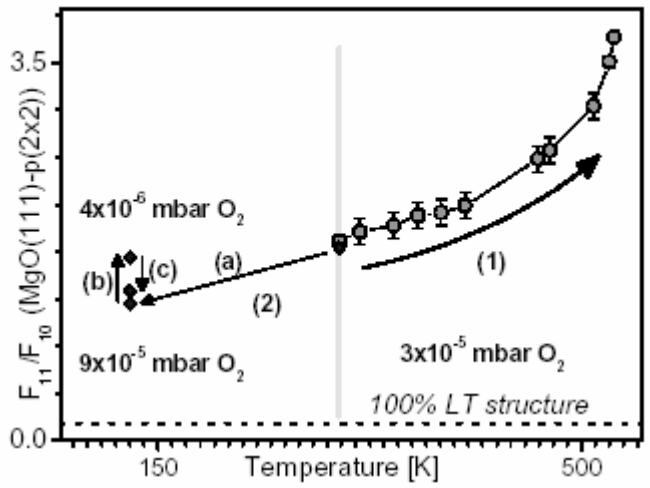


FIG. 1: Ratio between the in surface plane (11) and (10) $p(2 \times 2)$ reconstruction structure factors as a function of temperature $T$ and oxygen partial pressure $P_{O_2}$. (1) $T$ increases and $P_{O_2}=3\times10^{-5}$ mbar. (2a) $T$ decreases and $P_{O_2}=9\times10^{-5}$ mbar. At low $T$, $P_{O_2}$ is first decreased (2b) to $4\times10^{-6}$ mbar and then increased again (2c) to $9\times10^{-5}$ mbar. The horizontal dotted line indicates the expected ratio for the $LT$ pure structure, while a ratio of 11.6 corresponds to the $HT$ structure (see text). The $LT$ and $HT$ experiments were performed on two different samples.

The complete data set for several temperatures and oxygen partial pressure has been investigated in a cooperative approach with theoretical models evaluated in the DFT formalism. This approach allowed to exclude the ozone like reconstruction and showed that the spinel configuration was only a metastable surface state. The final model, that satisfies both the theoretical approach and the GIXD data consists of a mixture of two reconstructions (i) the predicted O-terminated octopole configuration and (ii) an epitaxial Mg layer that adopts a configuration close to the spinel structure proposed for NiO(111) for high temperatures and reducing conditions.

These results are currently under publication in Physical Revue Letter where all details about the analysis are reported.

This study may have cleared the question of the surface structure of polar rock-salt oxides as was proposed. The interpretation of GIXD data based on numerically relaxed structural models probably is also one of the major achievements of the present study.

## Stability of rocksalt (111) polar surfaces: beyond the octopole

Fabio Finocchi,[1] Antoine Barbier,[2] Jacques Jupille,[1] and Claudine Noguera[1]
[1] *Groupe de Physique des Solides, UMR 7588 CNRS and Universités Paris 6 - Paris 7 Campus de Boucicaut, 140 rue de Lourmel, 75015 Paris, France*
[2] *CEA/Saclay, DRECAM-SPCSI, 91191 Gif-Sur-Yvette, France*

(Dated: November 26, 2003)

Stable polar oxide surfaces must be simultaneously electrostatically compensated and in thermodynamic equilibrium with the environment. As a paradigm, the MgO(111)-$p(2 \times 2)$ reconstructed surface is shown to involve combinations of Mg-covered terminations with peculiar insulating electronic structure, favored in O-poor conditions, and the O-terminated octopole, stabler in more O-rich environments. Such a picture, which could not have been foreseen by either experiments or simulations separately, goes beyond the Wolf model and reconciles the theory with the experimental data taken in variable thermodynamic conditions.

PACS numbers: 68.35.Bs; 68.47.Gh; 68.35.Dv; 61.10.Nz; 71.15.Nc

To be published during spring 2004 in Physical Review Letters.

[1] A.Barbier and G.Renaud, Surface Science Letters 392 (1997) L15
[2] A. Barbier, C.Mocuta, H.Kuhlenbeck, K.F.Peters, B.Richter and G.Renaud, Phys. Rev. Lett. **84**, 2897-2900 (2000).
[3] A. Barbier, C.Mocuta and G.Renaud, Phys. Rev. B **62**, 16056-16062 (2000).
[4] D.Wolf, Phys. Rev. Let. **68** (1992) 3315
[5] R.Plass, J.Feller, M.Gajdardziska-Josifouska et al., Surf. Sci. 414 (1998) 26
[6] R.Plass, K.Egan, C.Collazo- et al. Phys. Rev. Lett. 81 (1998) 4891