An ELNES study of $LiAlO_2$

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(100)γ-$LiAlO_2$ is considered to be a promising substrate which allows for growth of both c- and m-plane oriented GaN layers [1]. In contrast to conventional substrates like SiC the advantage of (100)γ-$LiAlO_2$ is the very small lattice mismatch of about 1.4%. Also, it allows the growing of non-polar m-plane GaN which shows absence of internal electrostatic fields along the growing direction. This makes it possible to generate new efficient white light-emitting diodes (LEDs) [2]. At certain growth conditions the $LiAlO_2$-single crystals contain a core of inclusions. Also at the GaN/$LiAlO_2$ interface there are inclusions which are partly surrounded by cavities in the $LiAlO_2$-matrix. These inclusions at the interface are suspected to be the cause of a spontaneous separation of thick GaN layers. This effect may be used in the future to generate GaN layers for homoepitaxy which would allow to produce almost defect free GaN wafers.

Preliminary TEM analysis using electron diffraction showed that the inclusions mentioned above consist of $LiAl_5O_8$ [3]. But also the formation of Al_2O_3 can occur. Simulations of Oxygen K-edge ELNES spectra were carried out using the full potential linear augmented plane wave code WIEN97. TEM analysis comprising STEM and EELS was carried out on a 200 kV JEOL JEM2200FS microscope at Humboldt-University Berlin. In Figure 1 the simulated and experimental spectra are compared. Considering the known limitations of the simulation program, the very good agreement of simulation and experimental spectra is remarkable.

The investigations showed that the inclusions in γ-LiAlO2 consist of $LiAl_5O_8$. It was also found that the specimen is damaged due to electron beam irradiation. Comparison of ELNES simulations and experimental spectra did not only show the already known transformation of $LiAlO_2$ into $LiAl_5O_8$ [4] but also an unexpected transition to Al_2O_3 which is shown in Figure 2. At the beginning the two peaks of $LiAlO_2$ can be clearly identified, while the intensity of the first peak is decreasing until the peak is transformed to the shoulder in the rising edge of Al_2O_3. These changes can be attributed to the following reactions:

$5\ LiAlO_2 \rightarrow 2\ Li_2O \uparrow + LiAl_5O_8$

$2\ LiAl_5O_8 \rightarrow Li_2O \uparrow + 5\ Al_2O_3$.

The spectra contain an additional peak at 531 eV which is marked with an arrow in Figure 2. This peak is observed as long as the transformation from $LiAlO_2$ to Al_2O_3 takes place. This suggests that it can be associated with the loss of Li_2O. The peak can be attributed to a π*-resonance which occurs when an electron is excited from a σ-molecular orbital to a π*-orbital [5]. Li_2O has a similar structure as H_2O which means that there are only σ-bondings and no π*-resonance can occur. Thus, the peak at 531 eV can be attributed to molecular oxygen. We conclude that the electron beam sets free O_2 due to heating of the sample. This causes a change in the chemical composition of the sample so that it becomes more Al-rich.

Further investigation of the $LiAlO_2$ transformation will allow an adaption of the production parameters for fabrication of defect-free $LiAlO_2$.

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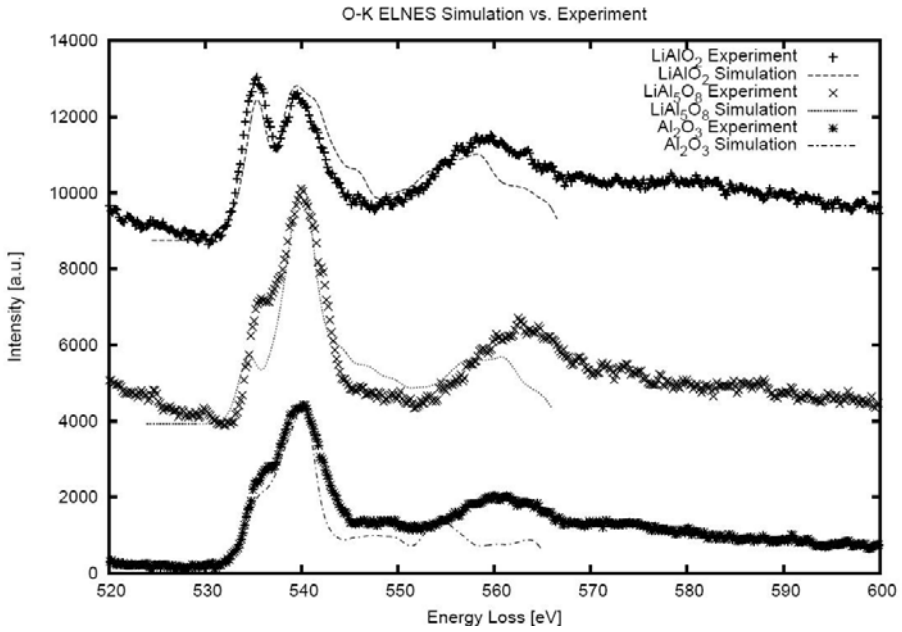

Figure 1. Comparison of simulated and experimental ELNES spectra of oxygen K-edge. From top to bottom $LiAlO_2$, $LiAl_5O_8$ and Al_2O_3.

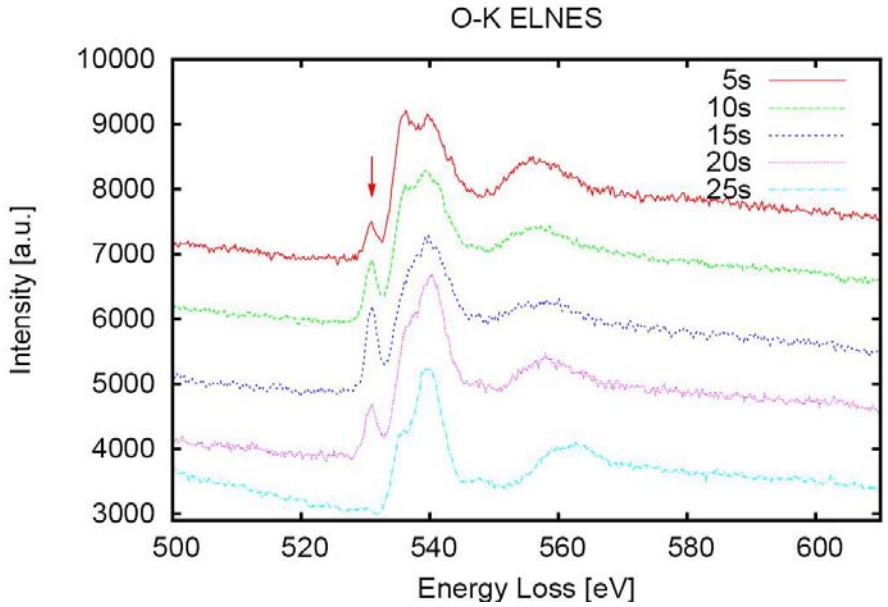

Figure 2. Spectra acquired at intervals of five seconds. The transformation of $LiAlO_2$ to Al_2O_3 is clearly visible. The π^*-resonance peak of molecular oxygen at 531 eV is marked with an arrow.

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