Adsorpion of Gases on β-Ga_2O_3 Surfaces

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β-Ga_2O_3 is a transparent conductive oxide with a fundamental bad gap of $E_G = 4.9$ eV [1]. Its typical *n*-type conductivity is controllable via the growth conditions, intentional doping or post-growth heat treatment [2]. Due to its large band gap, β-Ga_2O_3 is a promising candidate for applications in high power electronics e. g. in field effect transistors with high breakdown voltages [3]. Additionally, since its conductivity is dependent on the ambient conditions, β-Ga_2O_3 can be used in oxygen sensors [4].

In this contribution, we address the question how its surface properties develop under typical ambient conditions, i. e. under H_2O and O exposure, but in a controlled way. Therefore, we used a gas-inlet for H_2O vapor and an atomic O source. The β-Ga_2O_3 single crystals were grown with the Czochralski method [5] and cleaved under UHV-conditions in order to achieve intrinsic surface conditions before gas adsorption. Using Auger electron spectroscopy (AES), low energy electron diffraction (LEED), and scanning tunneling microscopy/spectroscopy (STM/STS), we show how the different adsorbed atoms/molecules change the structure and electronics properties of β-Ga_2O_3(100) and (001) surfaces in comparison to the freshly cleaved surfaces. On the (100) surface, large clusters of H_2O with an undisturbed surface in between were observed. However, STS showed no change in the electronic states. All spectra exhibit a large apparent band gap due to upwards band bending. Negative tunneling voltages gave rise to an accumulation current. Also, an additional exposure to atomic O did not lead to a change in the electronic states, although it lead to a higher surface coverage. On the (001) surface, oxygen covered almost the complete surface. STS showed that O lifts the band bending inherent in clean β-Ga_2O_3 surfaces.

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[1] M. Mohammed *et al.*, Journal of Physics: Conference Series **286**, 012027 (2011)
[2] Z. Galazka *et al*., Journal of Crystal Growth **404**, 184 (2014)
[3] K. Tetzner *et al*., IEEE Eletrcon Device Letters **40**, 1503-1506 (2019)
[4] M. Bartic, physica status solidi (a) **213**, 457-462 (2015)
[5] Z. Galazka, J. Appl. Phys. **131**,031103 (2022)

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Suplementary Pages

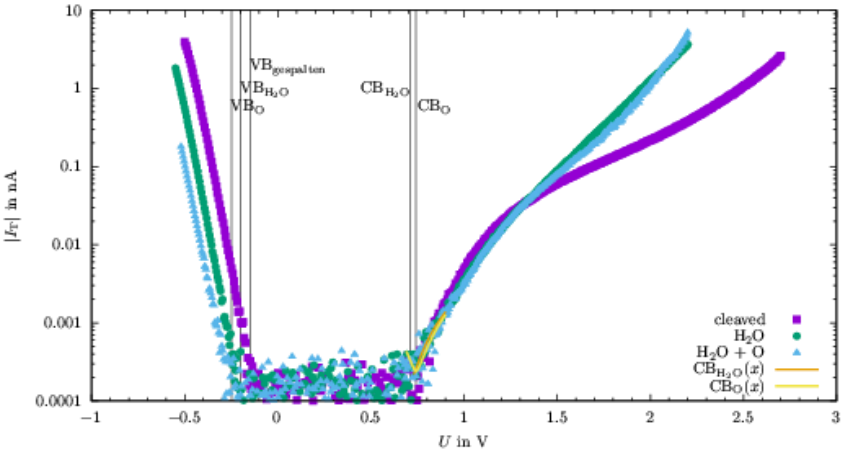

Figure 1: STS on the β-Ga_2O_3 (100) surface at $I_{\mathrm{set}} = 30$ pA and $U = 1.3$ V. The spectra were recorded on the freshly cleaved surface (violet), after an exposure to $D_{\mathrm{H_2O}} = 0.06$ L of H_2O (green) and after an additional exposure to $D_{\mathrm{O}} = 0.36$ L of O (blue). The onset of the conduction band lies at $U = +0.7$ V, due to band bending. Negative tunneling voltages give rise to an accumulation current whose onset shifts slightly to more negative voltages after the adsorption of gases.

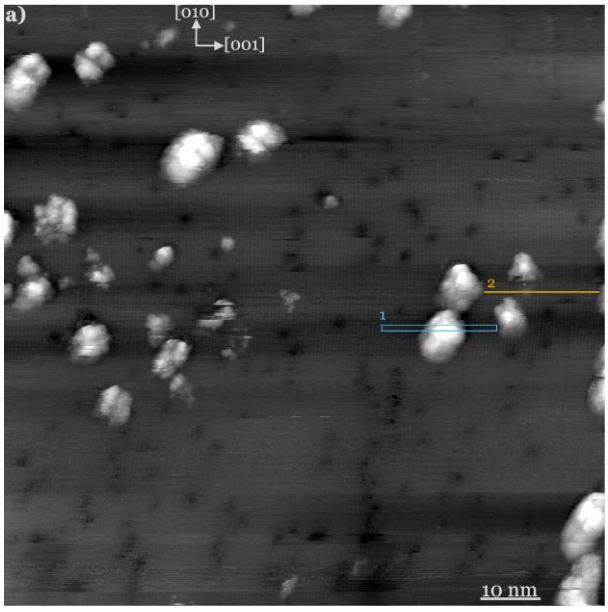

Figure 2: a) Empty states STM Image of the β-Ga_2O_3 (100) surface at $U_S = +3$ V and $I_{\mathrm{T}} = 30$ pA after the exposure to $D_{\mathrm{H_2O}} = 0.06$ L of H2O. The image show multiple large bright contrasts, which are due to water clusters on the surface. In between, the undisturbed surface with atomic resolution and dark contrasts typical for this surface are visible.

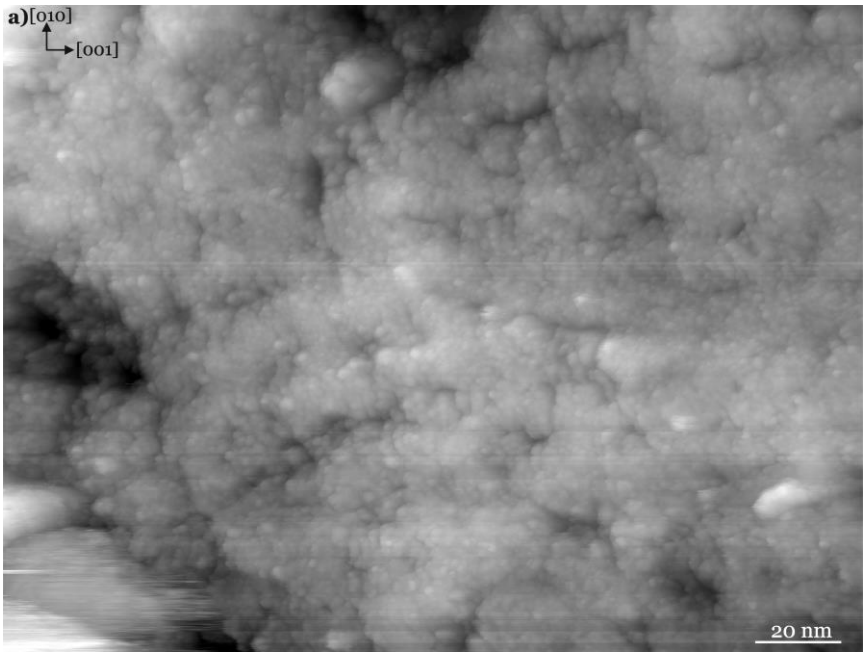

Figure 3: Empty states STM image of the β-Ga_2O_3 (001) surface at $U_S = +3$ V and $I_T = 30$ pA after the exposure to D=0.87 L of O. The complete surface is covered by diffuse, cloudy, irregular structures.

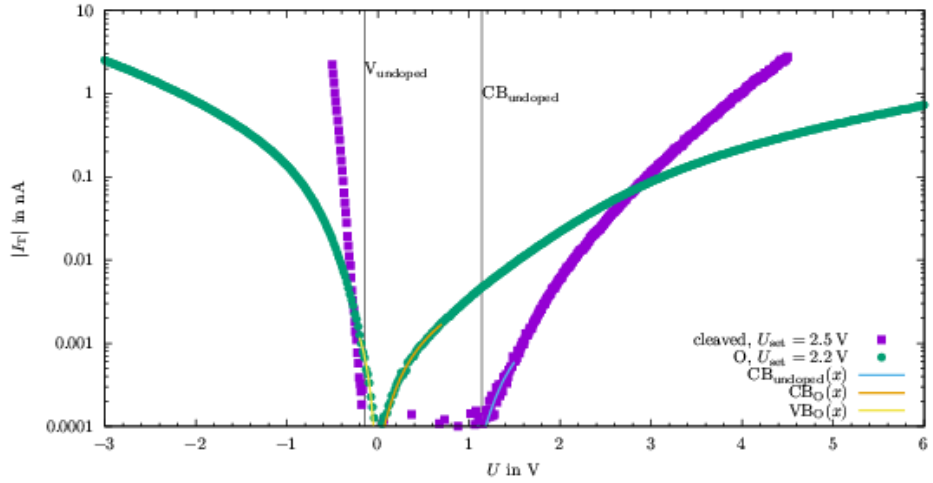

Figure 4: STS on the β-Ga_2O_3 (001) surface at $I_{set} = 30$ pA. The violet spectrum was recorded on the freshly cleaved surface. It shows an accumulation current at negative tunneling voltages. The conduction band onset lies at $U = +1.1$ V due to upwards band bending. The green spectrum was recorded after the exposure to $D_O = 0.87$ L of O. The oxygen lifts the band bending.