Atomic Structure and Electronic Properties of the Non-Polar In_2O_3 and β-Ga_2O_3(100) surfaces

C. S. Schulze,[1] R. Zielinski,[1] J.K. Hofmann,[1] C. Bruckmann,[1] Z. Galazka,[2] and H. Eisele[1]

[1] *Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany*

[2] *Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany*

In_2O_3 and β-Ga_2O_3 belong to the transparent conducting oxides (TCOs), being promising candidates for a wide field of applications like in solar cells, in detectors, and for high-power devices. In order to achieve high efficiency in electronic and opto-electronic devices a variety of prerequisites are necessary, as e.g., high crystal quality with low defect densities, adjustable conductivity by doping, controllable surfaces and interfaces, etc. Especially the doping mechanisms and the resulting high electron mobility are still under broad discussion for sesquioxide material: Mainly oxygen vacancies are under strong debate about their functionality [1]. We use scanning tunneling microscopy (STM) and spectroscopy (STS) in order to analyze the atomic structure of the non-polar surfaces. Since non-polar surfaces typically show no intrinsic surface states within the fundamental band gap of semiconductor materials, it is furthermore possible to study bulk and doping states using these methods [2].

Both semiconductors, In_2O_3(111) and β-Ga_2O_3(100) show at their respective non-polar surface a 1×1 surface unit cell without reconstruction upon *in situ* cleavage. We found the unreconstructed surface unit cell in the case of In_2O_3(111) in empty state images with atomic resolution. In respective room-temperature STS spectra we can identify the conduction band contribution, the direct and the indirect valence band as well as at least 3 intrinsic states being located within the band gap. Due to the variation of the growth parameter we can assign at least some of these states to charge transfer levels of impurities and vacancies. Since the Fermi level is located within the fundamental band gap, we can exclude an intrinsic electron accumulation for the freshly cleaved surface, while in air aged samples show a strongly different behavior, i.e. metallic appearance as in the case of a surface electron accumulation.

The β-Ga_2O_3(100) surface also shows atomic resolution in empty state images. Even more, we can identify single dopant atoms. In the corresponding STS spectra we can assign the conduction band contribution and again charge transfer levels, originating most likely from vacancies of the three differently coordinated oxygen atom positions within the unit cell. Even more, we can identify a charge transfer level, which we can assign to Si doping. Due to our findings from differently doped samples we conclude that the conductivity from unintentionally doped β-Ga_2O_3(100) can be assigned to background doping by Si.

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[+] Author for correspondence: holger.eisele@physik.tu-berlin.de