Chemical composition and band bending at Al_2O_3/GaAs interface formed via *in situ* Al_2O_3 atomic layer deposition on pristine GaAs

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We report on the x-ray photoelectron spectroscopy (XPS) study of Al_2O_3/GaAs interface obtained by *in situ* atomic layer deposition (ALD) of Al_2O_3 on pristine (001) oriented GaAs. The *in situ* approach enables us to benefit from the contamination-free GaAs surface at the beginning of the Al_2O_3 deposition. We are going beyond the scopes of the previous studies [1] and examine the *in situ* Al_2O_3 ALD process in detail, namely varying sequence and number of precursors' pulses at the deposition beginning, deposition temperature, thickness of the deposited Al_2O_3 layer and also the surface termination of the GaAs. The Al_2O_3/GaAs structures (Fig. 1 (a), inset) are fabricated in a multi-chamber growth system, which includes a Scienta Omicron molecular-beam epitaxy (MBE) chamber and a FlexAL®II ALD system connected via transfer modules. MBE is employed to grow non-intentionally *p*-doped GaAs layer onto a GaAs (001) wafer. We deposit Al_2O_3 using trimethylaluminium (TMA) as a metal precursor, the oxygen source being deionized water. The characterization of the Al_2O_3/GaAs interface is performed *ex situ* by XPS with an Al K α (1486.6 eV) X-ray source.

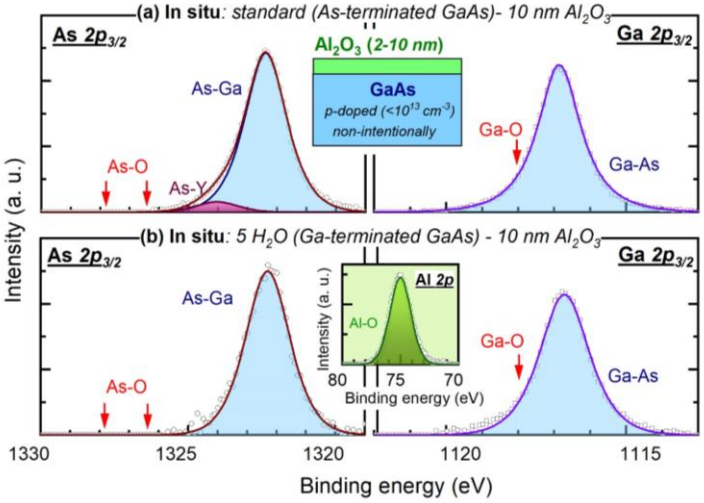

Fig.1. Photoelectron spectra for the As $2p_{3/2}$ (left) and Ga $2p_{3/2}$ (right) core-level features after *in situ* deposition of 10 nm Al_2O_3 on GaAs surface at 300 ˚C. The Al_2O_3 deposition begins with 1 TMA pulse (standard) (a) and 5 H_2O pulses (b). Inset: (a) Al_2O_3/GaAs structure; (b) Photoelectron spectra for the Al $2p_{5/2}$.

High-resolution spectra are taken for arsenic (As 3*d* and As $2p_{3/2}$), gallium (Ga 3*d* and Ga $2p_{3/2}$), aluminium (Al 2*p*) and oxygen (O 1*s*) using a step size of 0.1 eV and pass energy of 23.5 eV. The inset of Fig. 1 (b) represents the Al 2*p* spectrum with only one peak assigned to Al-O bond in Al_2O_3 and this confirms the successful growth of Al_2O_3 on the GaAs surface. The O/Al ratio calculated from the measured Al 2*p* and O 1*s* spectra varies from 1.4 to 1.6 and indicates high stoichiometry of the grown oxide. We show that in the case of 'standard' Al_2O_3 deposition (Fig. 1 (a)) on the As-terminated GaAs surface, which begins with a TMA pulse, followed by a water pulse, the Al_2O_3/GaAs interface is free from high-valence arsenic (As_2O_3 and As_2O_5) and gallium (Ga_2O_3) oxides if the Al_2O_3 layer has a thickness of 5 nm and more. However, we reveal formation of low-valence arsenic oxides (As^{2+} and As^{1+} oxidation states (peak As-Y in Fig. 1 (a))). The Al_2O_3 deposition performed on the Ga-terminated GaAs surface and started with $5H_2O$ pulses leads to the formation of a completely Ga/As-oxide-free Al_2O_3/GaAs interface (Fig. 1(b)). Analysis of the XPS data shows that the band bending in GaAs at the Al_2O_3/GaAs interface is reduced by 0.3 eV compared to the bending in the case of not passivated GaAs surface. This indicates the reduction of the interface states density, i.e. unpinned state of the Fermi level at the *in situ*-Al_2O_3/GaAs interface. Photoluminescence measurements of Al_2O_3/GaAs structures confirm the reduced density of the interface states. Our study delivers criteria for high-quality passivation of GaAs surface.

References

[1] T. W. Pi et al., Nanotechnology **26**, 164001 (2015).