

GDR HOWDI 2022 MEETING: GAP(111)B-SE SURFACE FOR TMD EPITAXIAL GROWTH

Niels Chapuis, Christophe Coinon, Dominique Deresmes and Xavier Wallart

Univ. Lille, CNRS, Centrale Lille, Junia, Univ. Polytechnique Hauts-de-France, UMR 8520 - IEMN - Institut d'Electronique de Microélectronique et de Nanotechnologie, F-59000 Lille, France

Over the past few years, 2D-Transition Metal Dichalcogenides (TMDs) have revealed great potential for optoelectronics and nanoelectronics devices, thanks to their exceptional properties, not encountered in other materials. They can be grown by van der Waals epitaxy allowing the use of materials with significant mismatch. Van der Waals epitaxy is usually performed on 2D substrates such as graphene, hBN or mica but 3D substrates can also be used after a proper surface passivation treatment, which for III-V semiconductor substrates has been applied successfully on GaAs(111)B surfaces. Since rather high growth temperatures are needed in order to get high quality-TMD layers [1], GaP might represent an interesting alternative to GaAs considering its higher thermal stability. In this study, we present results relative to the preparation of n and p-type GaP(111)B surfaces and to their Selenium passivation.

The substrate is first deoxidized in a III-V MBE reactor under PH_3 and H_{at} fluxes to prepare a clean GaP(111)B surface before being transferred in a TMD epitaxial chamber where the surface is annealed under a Selenium flux with a Beam Equivalent Pressure in the 10^{-6} - 10^{-5} T range. Samples are characterized *in-situ* by Reflexion High Energy Diffraction (RHEED), X-Ray and UV photoemission spectroscopies (XPS/UPS) and *ex-situ* by Atomic Force Microscopy (AFM).

After deoxidization, the GaP(111)B surface exhibits a (2x2) reconstruction before turning immediately to a (1x1) one under Selenium exposure, revealing the impact of Se on the atomic structure of the GaP surface. On the clean GaP(111)B surface, XPS reveals one main bulk component for the *Ga3d* and *P2p* core level lines (CL) and one surface component for the *P2p* one. After Selenium exposure, this surface component vanishes whereas a second component appears on the *Ga3d* spectrum evidencing the presence of Ga-Se bonds. The position of Selenium atoms in the atomic mesh compared to the initial GaP(111)B surface has been investigated using XPS photodiffraction. The evolution of the Ga3d and P2p XPS intensities with polar angle (Figure 1) are characteristics of a GaP(111)B surface whereas the lack of any intensity modulation for *Se3d* demonstrates that Se atoms stay in the outermost atomic plane. On p-type substrates, UPS measurements reveal a slight change in work function (from 5.05eV to 5.3eV) and an increase of the surface band bending of 0.15 eV after Selenium treatment. Contrarily, this latter has no influence on the surface morphology and roughness as evidenced in the AFM images of figures 2a and 2b where atomic steps, mean terrace length (280 nm) and mean RMS roughness (0.3 nm) remain unchanged.

References

[1] C. Vergnaud et al., Nanotechnology 31, 255602 (2020)

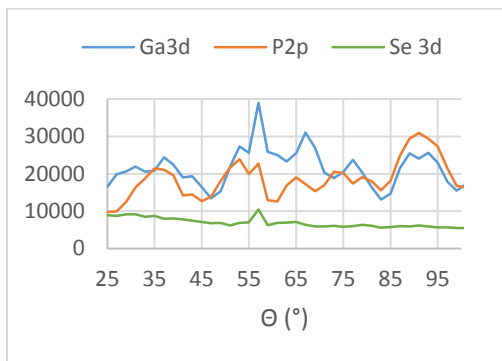


Figure 1: XPS photodiffracted intensities for polar angle variations along the $\langle 112 \rangle$ direction recorded on a GaP(111)B sample annealed at 700°C under Se flux

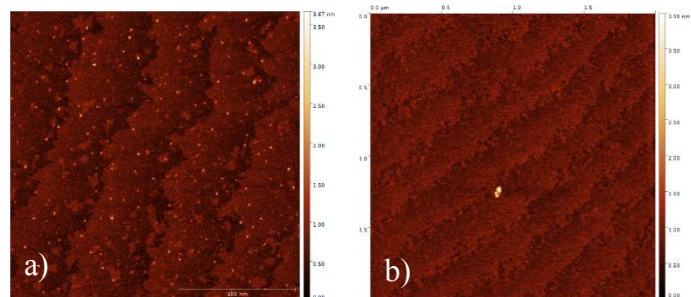


Figure 1: AFM images ($2\mu\text{m} \times 2\mu\text{m}$) of GaP(111)B surfaces
a) after deoxidization
b) after annealing at 700°C under Se flux