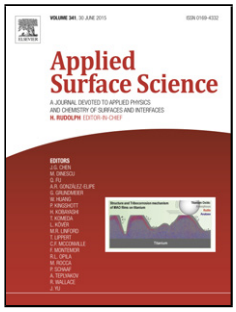

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Combined angle-resolved X-ray photoelectron spectroscopy, density functional theory and kinetic study of nitridation of gallium arsenide

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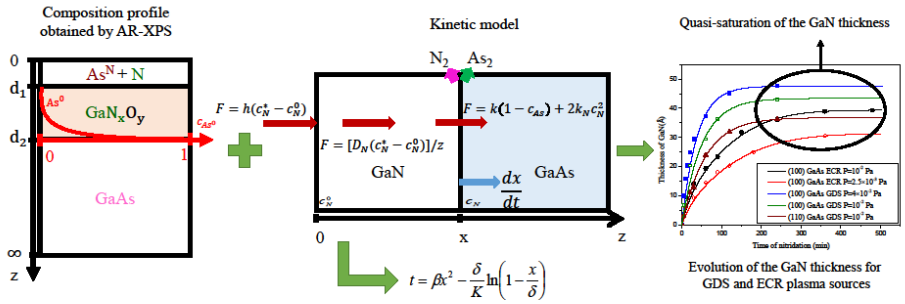
Graphical abstract



Highlights

- Determination of chemical environments and composition of GaN thin film by AR-XPS
- DFT calculations supporting the three-step nitridation process
- Exchange mechanism of As with N at the GaN/GaAs interface leading to quasi-saturation
- Kinetic model describing well the GaN growth on GaAs versus nitridation time

Abstract:

The high density of interface and surface states that cause the strong Fermi pinning observed on GaAs surfaces can be reduced by depositing GaN ultra-thin films on GaAs. To further improve this passivation, it is necessary to investigate the nitridation phenomena by identifying the distinct steps occurring during the process and to understand and quantify the growth kinetics of GaAs nitridation under different conditions. Nitridation of the cleaned GaAs substrate was performed using N_2 plasma source. Two approaches have been combined. Firstly, an AR-XPS (Angle Resolved X-ray Photoelectron Spectroscopy) study is carried out to determine the chemical environments of the Ga, As and N atoms and the composition depth profile of the GaN thin film which allow us to summarize the nitridation process in three steps. Moreover, the temperature and time treatment have been investigated and show a significant impact on the formation of the GaN layer. The second approach is a refined growth kinetic model which better describes the GaN growth as a function of the nitridation time. This model clarifies the exchange mechanism of arsenic with nitrogen atoms at the GaN/GaAs interface and the phenomenon of quasi-saturation of the process observed experimentally.