Theoretical study of the As surfactant effect on the nitridation of GaAs (001) surfaces

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Abstract – Density Functional calculations were employed, together with kinetic Monte Carlo simulations, to study the kinetic involved in the nitridation of GaAs (100) surfaces. From the obtained results, we have found that N prefers to be absorbed at the unoccupied sites of the surfaces. At the As-rich GaAs substrates, they push the As-dimer out of the surface, inducing the As surfactant effect observed in the III-Nitride growth. Finally, due to the low mobility of N, the kinetic of the N island formation follows the Vollmer-Weber mode, increasing both the surface roughness and the extended defects found in these systems.

Group III-nitrides (AlN, GaN, InN) and the corresponding alloys have attracted great interest due to their successful applications in the electronic and optoelectronic device technology. For their growth, via epitaxy techniques, in the zincblende structure, which is the best structure for the electronic devices, a lot of substrates have been proposed and the nitridation of Si, SiC, or GaAs surfaces seems to be the most efficient ones.

In order to understand the mechanisms for III-Nitride growth in the zinc-blende structure, we present, in this work, a systematic theoretical study of the adsorption of N over As-rich GaAs (100) (2×1) surfaces based both on accurate, parameter-free, self-consistent total energy and force calculations using the density functional theory, the local-density approximation for the exchange-correlation term, within the plane-wave pseudopotential method (abinit code [1]), together with a kinetic Monte Carlo simulation of the epitaxial growth, based on the solid-on-solid approach [2]. We have used the Troullier-Martins pseudopotentials and, in the calculations, supercells build up of 5 atomic layers and a vacuum region equivalent of 5 atomic layers. The calculated total energies were used as transition rates for the kinetic processes in our Monte Carlo simulation.

We have analyzed the changes in the bond-lengths and in the bond-angles before and after deposition as well as the total energy behaviour with the adsorbate chemical potential variation. Our results agree well with the available experimental data, whenever the comparison is possible. From our results, we have found that the N-atoms prefer to be adsorbed at the unoccupied sites of the surface. At the As-rich GaAs substrate, they push the As atoms out of the surface as shown in Fig. 1, inducing the observed surfactant behaviour during the growth [3]. Based on our results, the kinetic of the N island formation (Fig. 2), due to the low mobility of N at the surface, follows the Vollmer-Weber mode, increasing the surface roughness as well the experimental observed extended defects at the substrate surface, such as screw dislocations or inversion domains.
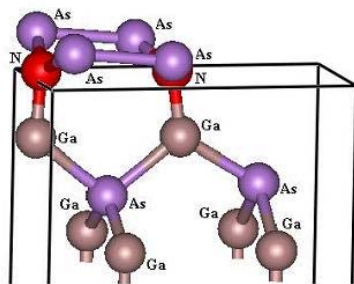

Figure 1: Relaxed atomic positions after the adsorption of two N atoms over the GaAs (100) (2×1) surface.
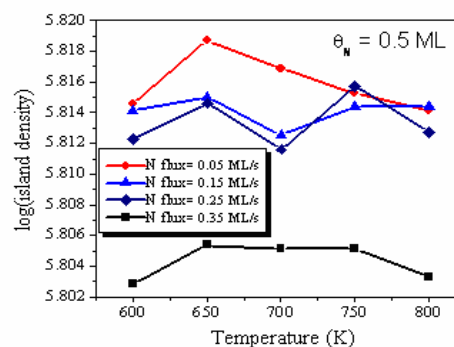

Figure 2: Temperature dependence of the logarithm of island density obtained by our Monte Carlo simulations.

References

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