DFT-based modeling of the point defects migration at the InN/GaN and InGaN/GaN interfaces

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The nitride semiconductors GaN, InN and AlN and their alloys are very attractive for a wide application in optoelectronics. Light emitting diodes (LEDs) and laser diodes (LDs) utilize InGaN/GaN quantum wells as active materials grown by MOVPE or MBE methods. Efficiency of the light emitting diode is still a big technological issue especially in the green region of spectrum. Point defects can drastically affect the optical properties of the devices, especially diffusion of point defects can lead even to the decomposition of quantum wells at high temperatures during the p-type layers growth.

Herein, we present theoretical *ab initio* DFT-based calculations of energy barriers encountered at the migration of neutral and charged point defects V_N, V_{Ga}, V_{In}, V_{Al} in nitride heterostructures. In particular, we model six types of interfaces $In_{1-x}Ga_xN$/GaN (x=0.75, x=0.25, x=0), where the $In_{x-1}Ga_xN$ material is strained to GaN, or the $In_{1-x}Ga_xN$/GaN heterostructure is fully relaxed. We consider defect migration in the growth direction of heterostructure (*c*-direction), as well as in lateral directions. The results of modeling enable tracing of the preferred directions for migration and accumulation of vacancies.

The obtained so far results show that (i) in the case of $In_{0.25}Ga_{0.75}N$/GaN strained with respect to GaN, charged V_N^{3+} diffuse with smaller energy barrier than the neutral ones, (ii) it is possible for V_N^{3+} to accumulate near the $In_{0.25}Ga_{0.75}N$/GaN interface, in the $In_{0.25}Ga_{0.75}N$ material, (iii) neutral V_{Ga} vacancies can be created easier in the bulk part of $In_{0.25}Ga_{0.75}N$ and GaN materials than at the $In_{0.25}Ga_{0.75}N$/GaN interface, (iv) the diffusion of neutral V_{Ga} both from the bulk GaN material and from the bulk $In_{0.25}Ga_{0.75}N$ material towards the $In_{0.25}Ga_{0.75}N$/GaN interface proceeds with decreasing energy barrier. Hence, an accumulation of neutral V_{Ga} vacancies can be observed near the $In_{0.25}Ga_{0.75}N$/GaN interface.

Our results are in a good agreement with experimental data concerning the decomposition of InGaN/GaN quantum wells.

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