New insights into design of the metamorphic buffer layers

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Metamorphic technology is one of the techniques used during the epitaxial growth to overcome the lattice mismatch problem and to fabricate active layers of the structures with an acceptable defect density [1]. In the approach, a metamorphic buffer layer (MBL) with a gradually varied composition is grown on a commercial substrate to accommodate most of the strains and accumulate the majority of misfit and threading dislocations. Composition profile of the MBL has a significant impact on the distribution of strains and defect density in metamorphic heterostructures. Usually, MBLs with steplike or linear-graded composition profiles are used due to easier growth process and the possibility to use a Dunstan's relaxation theory. The lack of complete relaxation theory for compositionally nonlinear-graded MBLs and scarce experimental studies restrict their utilization in the device structures. However, several models predict a wider top region free of dislocations for nonlinear-graded buffers as compared to steplike or linear-graded ones.

Recently, we have demonstrated the effectiveness for high lattice mismatch of compositionally convex-graded InAlAs MBL grown on GaAs substrates by molecular beam epitaxy (MBE) both experimentally [2], and theoretically [3]. Such MBL allowed achieving the defect density at its top less than 10^7 cm^{-2} and fabrication on it the In(As,Sb)/In(Ga,Al)As quantum well (QW) active region exhibiting bright mid-IR (2.0-4.5 μm) photoluminescence with IQE value of 5% at 300K [4], as well as two-dimensional InGaAs/InAlAs QW channel with the electron mobility up to 17500 cm^2/Vs at 300K [5].

Here we report on further optimization of $In_xAl_{1-x}As$ MBL composition profile, using a computational approach for determination of the equilibrium misfit dislocation (MD) density and strain along the growth direction of the heterostructures, aimed at achievement of the lowest possible defect density at the MBL top. The simulations were performed using the method based on iteration searching for the minimum total energy of the system and carried out for different MBLs composition profiles of the form $x \sim z^{1/n}$ (z – coordinate along the growth direction). The effectiveness of MBL composition profile with large n as well as growth problems of such MBLs and their possible solutions are discussed. Novel non-linear graded composition profile is proposed, which allows twice reduction of the MD density at the top part of MBL as compared to the convex-graded one. The impact of single highly tensile strained GaAs layers (1-15 nm) embedded into the non-linear graded InAlAs MBLs on distributions of strain and MD density along the growth direction is demonstrated and quantitatively verified. The work was supported in part by Russian Science Foundation (#22-79-00265).

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