Computer simulation of GaAs/GaAs(001) epitaxial growth considering V/III flux ratio

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The kinetic Monte Carlo method is used to investigate V/III flux ratio effect on the submonolayer growth processes during molecular beam epitaxy of GaAs on the GaAs(001) substrate. The crystal is represented as a two-dimensional lattice having the physically adequate zinc blende structure of GaAs. The starting surface is prepared in the $\beta 2(2\times4)$ reconstruction of GaAs(001) with two top layer As dimers per unit cell. We take into account the alteration of activation energy of each included microscopic process depending on the location and top-layer environment of a particle.

We observe that at temperature (T) of 580°C and growth rate (v) of 0.1 monolayer (ML) per second the island density (N) is saturated after deposition of 0.06 ML GaAs in the range of V(As_2)/III flux ratio $J_{As/Ga}$ from 3 to 40. The simulation yields $N = 2\cdot10^{12}$ cm^{-2} at these technological parameters. Islands preferentially form in the trenches and favor elongation along the $[1\bar{1}0]$ direction (Fig. 1). These results give good agreement with experiments [1,2].

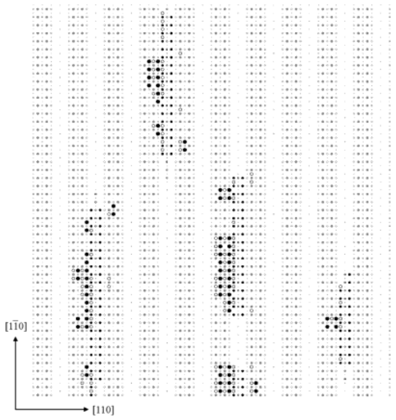

Fig. 1. Island morphology in a simulation area of 160 Å × 200 Å after deposition of 0.06 ML GaAs at T = 580°C, v = 0.1 ML/s, $J_{As/Ga}$ = 10

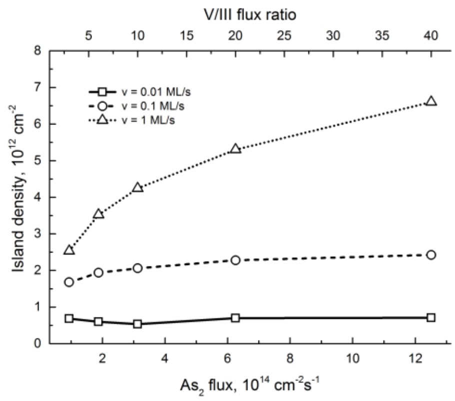

Fig. 2. Island density as a function of V/III flux ratio after deposition of 0.06 ML GaAs at different growth rates (T = 580°C)

We reveal the V/III flux ratio dependence of the island density. It rises nearly two times with the increase of $J_{As/Ga}$ from 3 to 40 at 550°C (v = 0.1 ML/s) and nearly three times at a growth rate of 1 ML/s (T = 580°C) (Fig. 2). The calculated fraction of arsenic atoms in the growing film made it clear that As_2 desorption is low under these conditions whereas at lower growth rates and higher temperatures arsenic atomic fraction is less. Moreover, at a rate of 0.01 ML/s larger flux ratios are needed to provide stoichiometric GaAs growth since arsenic atomic fraction exceeds 0.5 at $J_{As/Ga}\geq10$. Otherwise, surplus Ga adatoms form uncovered strings in the trenches.

The fraction of arsenic atoms rises with the increase of V/III flux ratio, but after deposition of 0.2 ML GaAs and more it exceeds 0.5 over the wide range of $J_{As/Ga}$ from 3 to 40 and doesn't change significantly. Thereby, V/III flux ratio influences the island characteristics but doesn't break compound stoichiometry. It enables enhanced control of GaAs epitaxial film morphology.

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