Evolution of InAs islands in the Stranski-Krastanow mode of InAs/GaAs(001) fabricated using molecular beam epitaxy

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Abstract Based on step-by-step observation using atomic force microscope, two distinctive successive phases were distinguished in accordance with evolution of the three-dimensional InAs islands during the Stranski-Krastanow mode of the InAs/GaAs(001) system fabricated using molecular-beam epitaxy. The initial phase is consistent with a power law, and the latter phase is a comparatively gradual one.

Keywords InAs/GaAs dots, SK mode

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1 Introduction

The two- to three-dimensional (2D-3D) growth mode transition, or Stranski-Krastanow (SK) mode, is a basic phenomenon for heteroepitaxial growth. Generally, in the SK mode for a heterostructure, the epitaxial growth is two-dimensional at the outset. After a deposition of a few monolayers (ML) on the substrate, the growth mode is transformed into a three-dimensional growth mode. The InAs/GaAs(001) fabricated using molecular beam epitaxy (MBE) is a model system in which the self-assembled quantum dots are fabricated via the SK mode, and there have been many experiments as well as theoretical studies on the subject. In spite of much effort to investigate the SK mode for MBE InAs/GaAs(001), its detailed nature still remains poorly understood.

In an early time, it was established that under conventional MBE growth conditions, the critical InAs coverage \( \theta_c \) for the 2D-3D transition is \( \sim 1.6 \) ML, beyond which the 3D InAs islands nucleate and the growth mode is transformed from two- to three-dimensional [1, 2]. After nucleation, the number density of the 3D InAs islands \( N \) increase sharply from quite few to a magnitude of a few \( 10^{10} \) cm\(^{-2} \) within an InAs coverage \( \theta \) increment of \( \sim 0.2 \) ML. This rapidly increasing period in island density within the 0.2-ML increment in InAs deposition is generally regarded as the 2D-3D transition process for MBE InAs/GaAs(001). The 2D-3D transition is not the conventional SK mechanism, during which a large amount of InAs material is transferred between the 2D InAs wetting layer and the ensemble of 3D InAs islands [3–6]. Leonard et al. [1] pointed out that during the 2D-3D transition the number density \( N \) of 3D InAs islands increases with InAs coverage \( \theta \) according to a power law \( N \propto (\theta - \theta_c)^\alpha \). In discussing their observation on variation of the average size of 3D InAs islands with \( \theta \), Kobayashi et al. [7] implicitly divided the 2D-3D transition process into two successive stages. In their initial stage of the 2D-3D transition, \( N \) is low and the 3D islands were isolated from each other, and these islands grow at the same rate. In the latter phase, the size-limiting effect [7, 8] sets in, and InAs material was transported between the islands.

In this work, the 2D-3D transition process in MBE InAs/GaAs(001) was investigated step-by-step using atomic force microscope (AFM). It was observed that the evolution of the 3D InAs islands in both the total volume \( V \) and number density \( N \) with InAs coverage \( \theta \) can be divided into two distinctive phases during the 2D-3D transition. In the first phase, both \( V \) and \( N \) increase rapidly according to a power law; while in the second phase, the increase in \( V \) as well as in \( N \) with \( \theta \) is much more gradual.

2 Experimental

The sample for an AFM observation was fabricated by depositing 2.0 ML of InAs on GaAs(001) substrate at substrate
temperature $T=500$ °C under the conventional MBE conditions for the self-assembly of InAs QD: As-rich and 0.1 ML/s growth rate. The substrate temperature was calibrated by the de-oxidation of the surface of GaAs (001) substrate at 580 °C, and was monitored by the infra-red pyrometer. The GaAs (001) substrate was not rotating during the InAs deposition to obtain an InAs film with the thickness varying from 1.5 to 3.0 ML across the 5.5-cm diameter in the [110] direction to obtain an InAs film with the thickness varying from 0.0068 ML in each step. The exact shape of the InAs islands is unknown, especially in their initial growth process, but their base shape is nearly rotationally symmetrical in the AFM images. The total volume $V$ of the ensemble of the 3D InAs islands is assumed to be proportional to $N \times w^2 \times h$, where $N$, $w$ and $h$ are the number density, average width and height, respectively, of the 3D InAs islands obtained by statistically averaging on the AFM images of $1 \times 1$ µm$^2$ in size.

The AFM observation was focused on the regions of the sample surface where $\theta$ is in the range of $1.65–1.81$ ML, which corresponds to the 2D-3D transition of the SK mode. The AFM measurement was made every 0.25 mm along the [110] diameter of the substrate with InAs increasing by 0.0068 ML in each step. The exact shape of the InAs islands is unknown, especially in their initial growth process, but their base shape is nearly rotationally symmetrical in the AFM images. The total volume $V$ of the ensemble of the 3D InAs islands is assumed to be proportional to $N \times w^2 \times h$, where $N$, $w$ and $h$ are the number density, average width and height, respectively, of the 3D InAs islands obtained by statistically averaging on the AFM images of $1 \times 1$ µm$^2$ in size.

### 3 Results

Successive AFM images reveal that the 3D InAs islands with a height above 1 nm begin to appear at $\theta \sim 1.65$ ML, and their number density $N$ increases steadily from below $10^6$/cm$^2$ to $7 \times 10^9$/cm$^2$ at $\theta \sim 1.81$ ML, beyond which $N$ increases more gradually to $(8–9) \times 10^9$/cm$^2$ until $\theta \sim 2.2$ ML, then island coalescence occurs and large dislocated islands begin to appear. Such behavior is similar to what are usually reported in literature. Figure 1 (a) is the log-log plot of island number density $N$ against extra InAs deposition $(\theta - \theta_c)$ with $\theta_c = 1.65$ ML. It can be seen from the figure that, approximately, the evolution of $N$ with InAs coverage $\theta$ in the 2D-3D transition can be divided into two successive phases with a transition region around $(\theta - \theta_c) \sim 0.05$ ML and $N \sim (1–2) \times 10^{10}$/cm$^2$. The very initial phase proceeds drastically with the increase of InAs deposition, and the second phase is more gradual. The experimental data can be fitted with two straight lines of different slope, implying that the two phases in the 2D-3D transition are consistent with the different power law $N \propto (\theta - \theta_c)^{\alpha}$ with $\alpha = 1.94$, while the second phase proceeds much more gradually and the total volume increases with a very small rate. It should be noted that in the estimation of $V(= N \times w^2 \times h)$, some constant factor is inevitably missing, and the estimated value is not precise. However, the general trend of the variation in $V$ with $\theta$ should be true. The large portion ~70% of the total increment in $V$ in the 2D-3D transition occurs in the first phase with the InAs deposition extending from 1.65 ML to 1.72 ML. In this period, the nominal InAs coverage $\theta$ increases by only ~0.07 ML, while the total island volume $V$ increment is ~0.3 ML. In the second phase, from $\theta \sim 1.72$ ML up to $\theta \sim 1.81$ ML, $V$ increases by only ~0.15 ML, roughly consistent with the amount of material from the InAs impinging flux. It is generally assumed that the transferring of InAs material between the 2D InAs wetting layer and the ensemble of 3D InAs islands extends over the whole 2D-3D transition [6]. However, the observation in this work shows that the material transferring occurs mainly in the very initial period of the 2D-3D transition, while the later stage is basically a conventional growth process. In plotting the total island volume as a function of InAs coverage for the same system, Placidi et al. [6] obtained a linear relation. Obviously, our result is inconsistent with their’s, and the discrepancy needs further investigation.

![Fig. 1 Variations in both the island density (a), and total island volume (b) against extra InAs deposition $(\theta - \theta_c)$ with $\theta_c = 1.65$ ML in the 2D-3D transition of MBE InAs/GaAs (001).](image)