EFFECT OF ISLAND NUMBER DENSITY ON THE SURFACE EVOLUTION DURING MOLECULAR BEAM EPITAXY

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A combined simulation-analytical model is developed to describe the surface morphology evolution during molecular beam epitaxy. The effect of island number density on transition from one level growth to multilevel growth has been studied. It is shown that decrease in the island number density (increase in the area per island) can involve such a transition even at fixed substrate temperature and growth rate.

INTRODUCTION

Combination of molecular beam epitaxy (MBE) and modern in situ diagnostic techniques such as scanning tunneling microscopy and reflection high energy electron diffraction (RHEED) offers an attractive approach to the fabrication of novel semiconductor devices based on the unique properties of low-dimensional systems with quantum dots, quantum wires, and δ-doping layers. However, a detailed understanding of MBE growth mechanisms has not been achieved yet. For instance, the island number density is believed to be controlled by substrate temperature $T$ and growth rate $R$. However, it has been recently been shown that the value of the island number density can be influenced by other factors. For example, the presence of the surface defects facilitates island nucleation on the Si/Si(111) $7 \times 7$ surface, where the nucleation occurs preferentially at domain boundaries of the $7 \times 7$ reconstruction [1]. The low density of these defects on the well-annealed substrate results in a low island number density on the original surface [1]. The surface reconstruction could be different for the original substrate and the grown layer [2] and, therefore, the island number density could also be different on these surfaces. In addition, the island number density depends strongly on the presence of surfactants [3,4]. So, for fixed values of $T$ and $R$, different values of the island number density may be achieved.

In the present paper, the effect of island number density on the surface evolution and the shape of the RHEED intensity oscillations was studied based on the model developed earlier [5]. This model combines a computer simulation of the random process of 2D-nucleation and an analytical description of island growth. In the present work, the model [5] is modified to describe these processes congruently. The low-temperature case, where desorption is negligible, was considered. The characteristic (for the silicon growth on Si(111)) values of the surface potential barriers and the growth rate were used.

MODEL

General statements

Assuming the 2D-nucleation growth mode, we consider an ideal flat surface without vicinal steps. Neglecting non-uniformity in the distribution of islands, one can divide the surface into equal cells with area $S_0$, so that only one island can start to grow inside each of them. While the island is spreading, the next layer island can eventually appear on its surface, etc. As a result, a pyramid consisting of 2D islands is formed in each cell. The cell area $S_0$ can be estimated as $S_0 = 1/N_o$, where $N_o$ is the island number density. We assume islands having the form of circular discs with a monolayer (ML) height. To simplify description of the coalescence stage of growth the square cells were replaced by round ones with radius $\rho_0 = \sqrt{S_0}/\pi$. The cells are considered not to overlap. The flux via the cell boundary is taken to be zero in accordance with the mean field approximation [6].
The continuity equation

In the case of complete condensation the continuity equations for the concentration of adsorbed atoms \( n(r) \) normalized to the surface site density has the form [6]

\[
\frac{D_s}{r} \frac{d}{dr} \left( r \frac{dn}{dr} \right) + F = 0,
\]

(1)

where \( D_s = a^2 \nu \exp\left(- \frac{E_{\text{diff}}}{k_B T} \right) \) is the surface diffusion coefficient (\( a \) is the atomic spacing; \( \nu \) is the frequency factor; \( E_{\text{diff}} \) is the activation energy for the surface diffusion; \( k_B \) is Boltzmann’s constant); \( F \) is the incoming flux normalized to the surface site density (at complete condensation it is numerically equal to the crystal growth rate \( R \) expressed in ML/s). Assuming the island growth to be limited by the surface diffusion, the boundary conditions for Eq. (1) can be written as [6]

\[
\frac{dn}{dr} \bigg|_{r=0} = \frac{dn}{dr} \bigg|_{r=p_0} = 0,
\]

\[
n(p_i) = \bar{n}, \quad i = 1 \ldots m,
\]

(2)

where \( p_i \) is the radius of the \( i \)th level island in the pyramid; \( m \) is the height of the pyramid (in monolayers); \( \bar{n} \) is the equilibrium adatom concentration.

The diffusion problem (1) – (2) has been solved in [6] for the case of the two-level pyramid \( (m = 2) \). The case of arbitrary number of layers in the pyramid is considered below.

Island spreading

Let us define the lateral growth rate of an island \( V_i = dp_i / dt \) as the sum of the fluxes entering the island step from the lower and the upper terraces: \( V_i = J_{i+1} + J_i \), where \( J_{i+1} = -D_s (dn/dr) \big|_{r=p_{i+1}} \) and \( J_i = D_s (dn/dr) \big|_{r=p_i} \). Solution of Eqs. (1) – (2) gives

\[
V_1 = \frac{F}{4p_1} \left[ 2p_0^2 - \frac{p_1^2 - p_2^2}{\ln(p_1 / p_2)} \right];
\]

\[
V_i = \frac{F}{4p_i} \left[ \frac{p_{i-1}^2 - p_i^2}{\ln(p_{i-1} / p_i)} - \frac{p_i^2 - p_{i+1}^2}{\ln(p_i / p_{i+1})} \right], \quad 1 < i < m;
\]

\[
V_m = \frac{F}{4p_m} \left[ \frac{p_{m-1}^2 - p_m^2}{\ln(p_{m-1} / p_m)} \right].
\]

(3)

It follows from Eq. (3) that the lateral growth rate of the given island depends on the radii of the neighboring islands of the pyramid. As the moments of new island formation are unknown in advance (nucleation is a random process), the integration of Eqs. (3) is impossible in the general case.

Island nucleation

Formation of islands in a new crystal layer can be regarded as the result of a random redistribution of adsorbed atoms. Its rate is determined by the characteristic time for the surface diffusion jumps \( \tau_{ij} = \frac{1}{\nu} \exp\left(\frac{E_{\text{diff}}}{k_B T} \right) \). During this time, only a single jump is on average, possible for an adatom. The redistribution can be considered as a sequence of independent random trials carried out at equal time interval \( \tau_{ij} \). The probability of a successful outcome (i.e., formation of a new island on the top of the pyramid) is [5]

\[
p = J \tau_{ij},
\]

(4)