Elongated quantum dots of Ge on Si formation modelling

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Abstract. Quantum dots (QDs) of Ge on Si grown using the method of molecular beam epitaxy (MBE) are examined in this paper. A comparative analysis of growth kinetics of elongated QDs with different length to width ratio was carried out. Calculations of pyramidal and wedge-like clusters formation energy were made. The increase in islands’ surface energy, elastic strain relaxation, and the decrease in the atoms’ attraction to substrate were taken into account. By using a well-known model based on the generalization of classical nucleation theory it was shown that elongated islands emerge after pyramidal clusters but begin to dominate in the QDs array on the later stages of growth. Calculations of QDs surface density and size distribution function for wedge-like clusters with different length to width ratio were performed. The existence of a special geometry of islands was discovered. Surface density and the average size of islands reach points of extremum for this geometry. Theoretical conclusions correlate with the experimental results.

1. Introduction

Heterostructures with QDs of Ge on Si have great importance for the development of semiconductor technology. Growth of Ge on Si attracts much attention from researchers in connection with the many possible uses of Si/Ge-based semiconductor materials in optoelectronics. Materials containing nanodimensional inclusions of Ge embedded in Si matrices make it possible to create light-emitting devices and photodetectors that may successfully compete with traditional optoelectronic devices based on III-V compounds.

Molecular-beam epitaxy is one of the most promising Si/Ge heterostructures production methods. There are two basic types of Ge QDs on Si(001) surface. They are so called hut- and dome-clusters. The morphology of Ge islands during the growth process can be controlled by changing the temperature of substrate, Ge deposition rate, and the total thickness of Ge layer.

Investigations of Ge QDs arrays on Si(001) have shown that the ensemble of hut-clusters is not homogenous [1, 2]. There are numerous morphologically different types of hut-clusters. Two basic kinds of hut-clusters are pyramidal (hut-) and elongated (wedge-) clusters, which are pyramids with a square or rectangular base, respectively. Both types of clusters have the same width to height ratio that is approximately equal to 10. The width of wedge-like cluster is usually less than the lateral size of the hut-cluster. Since these two types of clusters have a different morphology, structural transitions between them are restricted. It was also revealed that wedge-like clusters dominate in QDs arrays grown at low temperatures, and their fraction increases with the growth of deposited Ge thickness [1, 2]. But the role of different types of clusters in quantum dots arrays formation kinetics is still poorly researched.
The aim of this work is to develop the kinetic model of differently shaped self-organized Ge/Si(001) QDs parameters calculation and to compare growth kinetics of pyramidal and wedge-like clusters with various length to width ratios.

2. Theoretical model, results and discussion

For calculations we used the kinetic model of Ge QDs on Si growth developed in [3, 4]. This model, based on a generalization of classical nucleation theory, allows us to define temperature dependencies of QDs surface density \( N \) and size distribution function for different growth rates \( V \). For the estimation of QDs growth kinetics, first of all, thermodynamic parameters of Ge/Si system, such as free energy and equilibrium thickness of wetting layer, were defined.

The free energy of pyramidal islands with a rectangular base and constant contact angle \( \varphi \) is a function of the number of atoms \( i \) in the island and is represented by

\[
\Delta F(i) = Ai^{2/3} - B\zeta i, \tag{1}
\]

where \( \zeta = h / h_{eq} - 1 \) is the wetting layer superstress, \( h \) is the Ge wetting layer thickness, \( h_{eq} \) is its equilibrium thickness. In this equation, free energy is expressed in \( k_B T \) units, where \( T \) is the substrate temperature and \( k_B \) is the Boltzmann constant.

With respect to different geometrical shapes of QDs parameters \( A \) and \( B \) will be defined as

\[
A = \frac{r[\gamma(\varphi)/\cos \varphi - \gamma(0)]\alpha l_0^2}{k_B T}, \tag{2}
\]

\[
B = \frac{[1 - Z(\varphi)]\lambda e_0^2 d_0^2}{k_B T} \ln \left\{ \frac{\Psi_0}{d_0 [1 - Z(\varphi)]\lambda e_0^2} \right\}, \tag{3}
\]

where \( r \) is the island’s length to width ratio, \( \gamma(0) \) and \( \gamma(\varphi) \) are the specific surface energies of the base and the lateral faces of pyramid, \( \varphi \) is the angle between the lateral face and the base of the island, \( l_0 \) is the mean distance between atoms on the surface, \( Z(\varphi) \) is the coefficient of elastic relaxation, \( \lambda \) is the material’s modulus of elasticity, \( e_0 \) is the lattices’ mismatch, \( d_0 \) is the height of one monolayer (ML), \( \Psi_0 \) is the wetting energy density on the substrate surface, and \( \alpha \) is the geometrical factor depending on the island’s shape:

\[
\alpha = \left( \frac{12d_0 e_0^2 \tan \varphi}{(3r - 1)l_0} \right)^{1/3}. \tag{4}
\]

Parameter \( \alpha \) defines the relationship between the lateral width of the island \( L \) and the number of atoms in it:

\[
i = \left( \frac{L}{\alpha l_0} \right)^3. \tag{5}
\]

The value of elastic relaxation coefficient \( Z \) may be calculated within the Ratsh–Zangwill model. This model assumes that the effective parameter of lattice mismatch decreases from underlying to top layers because top layers contain additional relaxed atoms near the island edge [5, 6].

Then the islands’ nucleation rate \( I \), QDs surface density \( N \), rate of atoms’ arrival to the island, and QDs size distribution function were calculated.

Using the Zeldovich formula [7], for the nucleation rate elongated islands we will obtain the following dependence on the wetting layer superstress

\[
I(\zeta) = \frac{a}{\zeta l_0^2} \zeta(\zeta + 1)e^{-\Delta F(i)}, \tag{6}
\]
where $i_c$ is the critical size at which the free energy is at its maximum:

$$i_c = \left(\frac{2A}{3Bc}\right)^\frac{1}{3},$$

(7)

$\tau$ is the characteristic time of atoms incorporation processes:

$$\tau = \frac{3\ell_0^4 \nu}{4(r+1)\alpha BD},$$

(8)

$D$ is the coefficient of diffusion of atoms from the wetting layer to the islands, $\nu$ is the cut-off parameter of the elastic strain field [5].

Parameter $a$ is defined as

$$a = \frac{3B}{4\sqrt{\pi}A}.$$  

(9)

Calculations of parameters of pyramidal and wedge-like clusters with different length to width ratios $r$ were carried out. For calculations the following material values were selected [3, 5]:

$\lambda = 1.27 \cdot 10^{12}$ dyn/cm$^2$, $\epsilon_0 = 0.042$, $d_0 = 0.145$ nm, $l_0 = 0.395$ nm, $\Psi_0 = 450$ erg/cm$^2$, $\gamma(0) \approx \gamma(\varphi) = 800$ erg/cm$^2$, $\varphi = 20^\circ$, $h_{eq} = 3$ ML, $\nu = 10$, $D = 6 \cdot 10^{-13}$ cm$^2$/s.

From a comparison of the nucleation rates for islands with square and rectangular bases it is shown that elongated islands with higher $r$ emerge later and their nucleation progresses more intensively (see figure 1). It may explain, in our opinion, the increase of wedge-like clusters fraction in QDs arrays during the later stages of growth [1, 2, 8].

![Figure 1](image1.png)  
**Figure 1.** Time dependence of nucleation rate for elongated islands with $r = 1..5$ in Ge/Si(001) system at substrate temperature $T = 470$ °C and deposition rate $V = 0.07$ ML/s.

![Figure 2](image2.png)  
**Figure 2.** Size distribution function for wedge-clusters of Ge on Si(001) with $r = 1..2$ at substrate temperature $T = 470$ °C and deposition rate $V = 0.07$ ML/s.

Modelling of QDs growth dynamics allows us to estimate surface density and size distribution function for the differently shaped islands. Results of numerical experiments show that for the same growth conditions the average size of elongated islands with a small length to width ratio $r$ is smaller than for pyramidal clusters (see figures 2 and 3). Their size variation is also smaller and surface density is higher, which makes them more attractive for possible device applications.

It must be noted, however, that surface density and average size of the elongated islands change non-monotonically with the ratio increasing (see figure 4).
There is a singular geometry of QDs with $r \approx 2$ for which the average size of the dot reaches its minimum and surface density inversely has its maximum value (for the given growth conditions). With the increase of the length to width ratio from 2 to approximately 7, the surface density decreases gradually and the average size increases, both reaching at $r \approx 6–8$ values that correspond to those of pyramidal clusters with square base. With the further increasing of $r$ the tendency of average size growth and surface density reducing remains constant.

3. Conclusions

Thus, an attempt to develop a kinetic model of the initial stages of growth of different shaped QDs of Ge on Si(001) was made. This model allows us to define the quantum dots size distribution function and their surface density for a given growth temperature, Ge deposition rate and other growth conditions. These are the characteristics which indirectly influence the parameters of nanoheterostructures-based semiconductor optoelectronic devices. Based on theoretical estimations it has been shown that there is an optimal type of QDs with the length to width ratio of 2:1. For this cluster geometry in the equal growth conditions maximum surface density is obtained and the average dot size has its minimum value.

References

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