Ge/Si ELONGATED QUANTUM DOTS FORMATION MODELLING WITH RESPECT TO THE ENERGY OF EDGES

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Abstract — In this work refining of mathematical model for calculation of parameters of self-organised quantum dots (QDs) of Ge on Si grown by the method of molecular beam epitaxy (MBE) is done. It was shown that elongated islands emerge later than pyramidal clusters. Calculations of QDs surface density and size distribution function for wedge-like clusters with different length to width ratio were performed. The absence of special geometry of islands for which surface density and average size of islands reach points of extremum that was predicted earlier by the model not taking into account energy of edges was revealed when considering the additional contribution of edge formation energy.

МОДЕЛИРОВАНИЕ ФОРМИРОВАНИЯ УДЛИНЕННЫХ КВАНТОВЫХ ТОЧЕК Ge/Si С УЧЕТОМ ЭНЕРГИИ РЕБЕР

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Аннотация — В работе проводится уточнение математической модели расчета зависимостей параметров самоорганизующихся квантовых точек (КТ) германия на кремнии от условий роста в методе молекулярно-лучевой эпитаксии (МЛЭ) с учетом новых данных о величине удельной энергии ребер квантовой точки. Показано, что клиновидные островки образуются позднее, чем пирамидальные. Проведены вычислительные эксперименты по определению поверхностной плотности и функции распределения по размерам клиновидных КТ с различным отношением длины основания к его ширине. Обнаружено, что при учете вклада дополнительной энергии образования ребер отсутствует выделенная геометрия КТ, для которой поверхностная плотность и средний размер островков достигают экстремальных значений, предсказывавшаяся ранее моделью, не учитывающей энергии ребер.

I. Introduction

Semiconductor materials containing nanosized Ge clusters are popular for application in optoelectronics since the 1990s. They are used in development of photodetectors, solar cells and light emitting devices.

The one of the most promising Si/Ge heterostructures production methods is molecular-beam epitaxy. 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.

It is known that ensemble of nanoislands of Ge on Si(100) surface consists of pyramidal (hut-) and elongated (wedge-) clusters, which are pyramids with square and rectangle base, respectively. But the differences in the kinetics of formation of these two types of clusters in quantum dots arrays are still studied poorly [1, 2].

In [3, 4] an attempt was made to study kinetics of wedge-like QDs formation with the help of the model, based on the classical nucleation theory and proposed in [5]. This model relies on the expression for change of free energy of atoms during transition from the wetting layer to the island taking into account change in free energy due to formation of additional facet surface, elastic strain relaxation, and lessening of atoms attraction to substrate [5]. Meanwhile, the contribution in change of the free energy due to formation of additional edges in the island is not taking into account as it is thought to be negligibly small. But at the same time results obtained in [6, 7] show that taking into account the contribution of edge energy is essential for explanation of some recently discovered effects during growth of QDs of germanium on silicon. In [8] an attempt is made to develop kinetic model accounting for the contribution into free energy of island formation due to edge energy. The aim of this work is to compare growth kinetics of pyramidal and wedge-like clusters with various length to width ratios with respect to the contribution of additional edge energy into change in free energy during formation of islands.

II. Main Part

For calculations we used the kinetic model of Ge QDs on Si growth developed in [8]. This model allows us to define temperature dependencies of QDs surface density N and size distribution function for different growth rates V. Calculations of parameters of pyramidal and wedge-like clusters with different length to width ratio r were carried out. From comparison of the nucleation rates for islands with square and rectangle base it is shown that elongated islands with higher r emerge later but their nucleation doesn't progress more intensively as it was predicted earlier [3, 4] (see figure 1).

Modelling of QDs growth dynamics allows us to estimate surface density and size distribution function for the different shaped islands. Results of numerical experiments show that for the same growth conditions average size of elongated islands with small length to width ratio r is larger than for pyramidal clusters when taking into account additional energy of edges. Their size variation and surface density are smaller (see figures 2, 3, 4).

It must be noticed, however, that surface density and average size of the elongated islands change monotonically with the ratio increasing as opposed to the results of previous modelling [4]. There is no singular geometry of QDs with $r = 2$ for which 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 1 to 10 surface density decreases gradually and the average size increases, both reaching their extrema at $r = 1$ that correspond to pyramidal clusters with square base.

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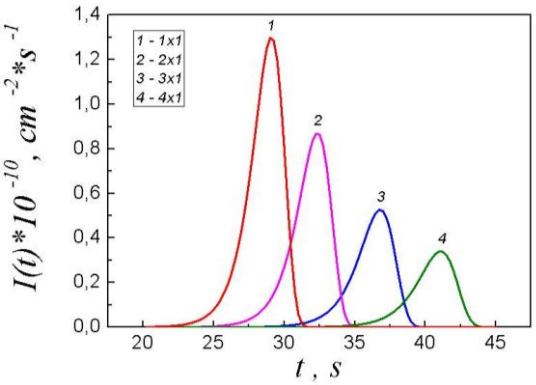

Fig. 1. Time dependence of nucleation rate I(t) for QDs with r = 1..4 in Ge/Si(001) system at substrate temperature T = 470 °C and growth rate V = 0.1 ML/s.

Рис. 1. Временные зависимости скорости нуклеации I(t) для КТ с r = 1..4 в системе Ge/Si(001) при температуре подложки T = 470 °C и скорости роста V = 0.1 МС/с

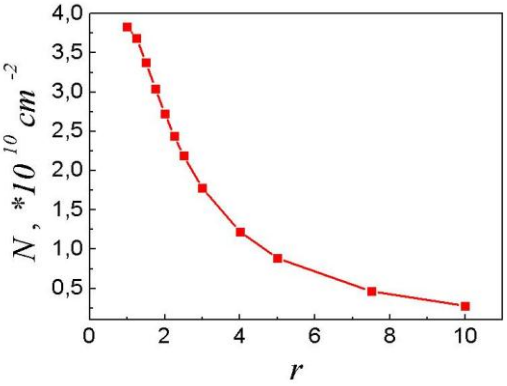

Fig. 2. Surface density of wedge-like clusters of Ge on Si(001) surface as a function of r at substrate temperature T = 470 °C and deposition rate V = 0.1 ML/s.

Рис. 2. Поверхностная плотность клиновидных КТ Ge/Si(001) как функция r при температуре подложки T = 470 °C и скорости роста V = 0.1 МС/с

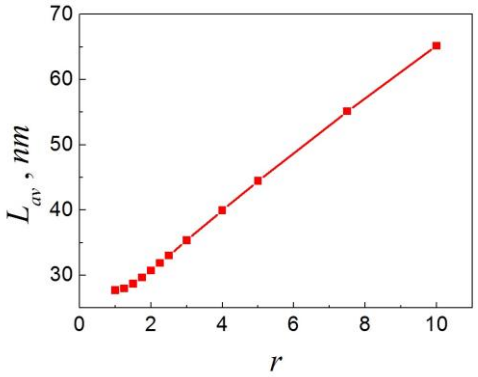

Fig. 3. Average size of wedge-like clusters of Ge on Si as a function of r at substrate temperature T = 470 °C and deposition rate V = 0.1 ML/s.

Рис. 3. Средний размер клиновидных кластеров Ge на Si как функция r при температуре подложки T = 470 °C и скорости осаждения V = 0.1 МС/с

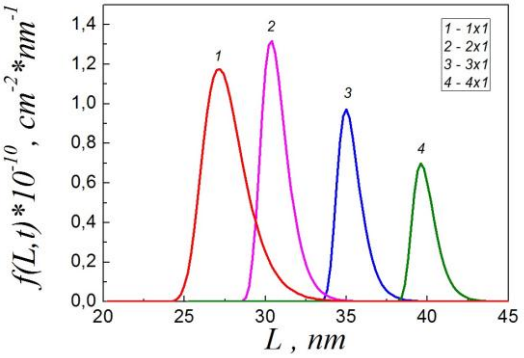

Fig. 4. Size distribution function for wedge-clusters of Ge on Si(001) with r = 1..4 at substrate temperature T = 470 °C and deposition rate V = 0.1 ML/s.

Рис. 4. Функция распределения по размерам клиновидных кластеров Ge на Si(001) с r = 1..4 при температуре подложки T = 470 °C и скорости осаждения V = 0.1 МС/с

III. Conclusion

Thus, in this work an attempt is done to apply different shaped QDs of Ge on Si(100) the kinetic model of initial stages of growth of QDs accounting for additional energy of edges. Estimations with the help of this model show that average size and surface density of clusters monotonically depends on length to width ratio *r* and there is no special geometry of QDs as it was predicted before.

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