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GE/SI QUANTUM DOTS FORMATION BY THE METHOD OF MOLECULAR BEAM EPITAXY[1]

This scientific work is devoted to the phenomenological description of Ge/Si(100) quantum dots formation processes in the method of molecular beam epitaxy.

Keywords: *quantum dots, silicon, germanium, nanoheterostructures.*

Deposition of SiGe on Si substrate can be described in the first approximation as a classic process of Stranski–Krastanov growth, where QDs formation is governed by competing kinetic and thermodynamic processes. Self-organization of QDs develops through classical stages of islands nucleation and growth. However, growth of SiGe films includes in fact a number of far more complicated mechanisms, which are not taken into consideration by the simplified Stranski–Krastanov growth scheme and which demand more detailed studying, as they influence indirectly on the structure of emerging QDs.

On the initial stages layer-by-layer growth of Ge on Si is realized. After the Ge wetting layer exceeds some critical thickness due to mass transfer with the help of surface diffusion, small 3D islands emerging begins. They appear either as a result of nucleation from 3D nucleus when sufficient strain is accumulated, or by a nucleationless mechanism from morphological instability, forming so called quasi-periodic arrays of islands. With the increasing of de-posited material thickness quite a number of metastable morphological structures such as pyramids with square or rectangle base (hut-clusters) arise. The second stage of coherent islands formation is their independent development, usually proceeding without changes in their geometrical form. In the Ge/Si system with the islands size increasing transition from hut-clusters to so called dome-clusters with typical lateral size of 50–100 nm is observed. After continuous exposition of the structure the next stage of islands ensemble evolution, on which interaction between clusters becomes important, may take place. As a result, dislocated islands with sizes about 1 μm emerge. In this growth scheme processes on initial stages are still ambiguous. The question about driving forces of these processes demands solution. Mechanisms of hut- to dome-clusters transition also remain a subject of scientific discussions.

Another extremely important factor, which is not included in the simple Stranski–Krastanov model, is surface anisotropy. Experiments on growing QDs on substrates with various orientations demonstrate realization of completely different growth modes and surface morphology for structures on Si(100) and Si(111) surfaces. In particular, for certain orientations of substrate metastable strained morphologies may be absent.

Besides that, epitaxy of different materials and doping may become one of the ways of strain relaxation. Impurity introduction increases concentration of inhomogeneities in islands that in turn changes the growth mode and affects quantum dots properties.

Thus, there is a necessity to determine balance between basic driving forces of nucleation and growth of QDs to predict or manage processes of their self-organization for the purpose of improvement of their physical properties.

For creation of different semiconductor devices it is necessary, first of all, to define the QDs arrays typical characteristics essential for achievement of the goals set for devices. For example, to make the QDs suitable for creation of devices operating at room temperature it is necessary to satisfy the following claims:

1) QDs have small enough size for appearance of sufficiently deep localized states;
2) QDs in the ensemble of islands show high homogeneity by their size and shape;
3) QDs have the maximum possible surface density;
4) the system remains coherently strained, that is contains no defects or dislocations.

Therefore investigators pay the maximum attention to reaching growth conditions required for obtaining of such structures. Managing the self-organized islands properties is one of the rapidly developing

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directions. Fulfillment of above demands may be possible thanks to combining achievements of applied physics.

Thus, the task for researchers today is to develop dense and homogeneous arrays of ultra small QDs creation technologies on the large scale substrates [1].

For effective applying in various devices it is necessary to create heterostructures with narrow size distribution of QDs, because such distribution provides optimal conditions for occurrence of quantum effects. Homogeneity of islands critically depends on growth parameters such as temperature, Ge thickness and deposition rate, and some other factors. Desirable size distribution of QDs can be reached only by thorough fitting and permanent control of growth conditions.

In [2] it was reported, that at a growth temperature 600 °C, Ge growth rate of 0,02 nm/s and the Ge coverage of 1,5 nm high uniformity in dot size was achieved. The dots were all dome-shaped with the mean lateral size of 70 nm and the height of about 15 nm. The areal density and the height deviation of the islands was about $3 \cdot 10^9$ cm^{-2} and 3 %, respectively.

Another way to achieve homogeneity is deposition on the Si substrate layers of Ge_xSi_{1-x} with various percentage of Ge. For example, in work [1] results of $Si_{0,75}Ge_{0,25}$ layers deposition on Si(100) surface are represented. Obtained sample consisted of coherently strained QDs with the form of truncated pyramids with side edges in the direction {111} and top surface (100). The mean base size was 135 nm and the dots height was about 80 nm. These results demonstrate the possibility of high uniformity achievement in quantum dots arrays of Ge on Si(100).

However, such big islands do not claim to be device-oriented since quantum properties become apparent only for sufficiently smaller QDs. To date achievement of such homogeneity allied with small sizes of QDs meets certain technological difficulties. It is especially complicated by the tendency of QDs to bimodal size distribution on late stages. Thereby, for potential applications it is necessary to learn how to govern islands size distribution.

A special place takes growth and self-organization of quantum dots in multi-layer structures, containing embedded layers with quantum dots, which greatly effect the islands growth and ordering. That is because for quite a number of applications it is very important to create ordered arrangement of islands. In some cases ordering can occur spontaneously due to repulsive elastic forces between islands. This trend of spontaneous ordering can be intensified by stacking several layers with quantum dots (one above another) separated by thin layers of silicon.

Besides that, due to outstanding significance of multi-layer structures containing layers with quantum dots it is important to create such structures with given properties. Such multi-layer heterostructures with quantum dots have great applied importance because of their new potentialities, such as electron connection of clusters in vertical direction, formation of 3D lattices, consisting of quantum dots, frequently called «artificial atoms» [3].

It should be noted that creation of multi-layer structures with 100 or more layers is technologically difficult and practically unreasonable because the quality of *p*–*n*-junction in this situation is reducing. While making multi-layer structure, in particular assuring occurrence of inter-mediate band, materials with different crystal lattices constants are used. It causes appearance of built-in mechanical strains and, if the total thickness of multi-layer structure is rather high, of structural defects such as misfit dislocations.

For multi-layer structures with self-organized QDs in top layers reduction of critical thickness of Stranski – Krastanov transition was found out. This effect is caused by local deformation of the thin layer above the QDs. Emerging of dots in the top layers occurs with lesser thickness of deposited material exactly above the islands of underlying layer. As a result of such nucleation in multi-layer structures with thin enough intermediate layers vertical ordering of QDs is observed. Successive depositing of layers with Ge QDs leads to improvement of ordering of islands by their size and area. Elastic deformation field distortions from cluster penetrate on various distances into the spacer layer depending on accumulation of QDs and the volume of particular dot. On the spacer surface areas of preferential nucleation of QDs appear. Adjusting spacer thickness it is possible to filter influence of weak QDs [3].

As an explanation of Stranski – Krastanov transition nature benefit in elastic energy of the system is usually named. This occurs due to relaxation of the top of the QD that compensates loss in surface energy of the system originating from the surface area increasing in comparison with plain layer. Energy change due to weakening of at-traction of adatoms to the substrate, breaking into the energy balance also influences the transition critical thickness. An expression for this energy changes essentially for multi-layer structures in comparison with the modeling of single layer. When considering multi-layer systems, the

value of free energy should be calculated with respect to influence of all the deposited strained layers. It considerably complicates modeling of QDs formation kinetics and requires an adequate theoretical model. In the simplified case it is necessary to introduce some phenomenological parameter that has a form of exponential factor to the elastic energy of the system with some characteristic length called attenuation depth. Layers situated deeper than this length do not influence the Stranski – Krastanov transition [4].

Another phenomenon also defining the Stranski – Krastanov transition is segregation, that is depletion of the solid solution and enhancement of the surface layers by Ge atoms. It is especially important to take into account the segregation effect when Ge and Si atoms concentration distribution between layers is calculated. It also plays an important role for the further computing of critical thickness for depositing on the Si surface of Ge_xSi_{1-x} layers with various percentage of Ge [5].

Finally, as soon as islands on the initial stage have a form of pyramids with square or rectangle base [1], it is necessary to create model that takes into account co-existence of these two forms of clusters. We assume it is possible by accounting of change in side walls square and base perimeter and area. We have also recomputed the Ratsch–Zangwill coefficient of elastic relaxation for the elongated islands.

From comparison of the nucleation rates for islands with square and rectangle base it is obvious that elongated islands emerge a bit later and their nucleation progresses more intensively. It may explain, in our opinion, the increase of wedge-like clusters fraction in QDs arrays on the later stages of growth.

Results of estimations show that surface density N of islands of both types decreases gradually with the Ge de-position rate V reduction and with growth temperature T increase. On the contrary, average size of islands increases with temperature T or with deposition rate V decrease. It may be explained by the fact that with temperature or Ge flux increase the diffusion length of adatoms in the substrate decreases. Thereafter, the area of adatoms collecting and islands size decrease, while surface density increases.

Meanwhile we may derive the general rule that at the same growth conditions average size of wedge-like clusters lesser and surface density is higher than for pyramidal islands with square base. It makes rectangular dots more attractive for device application.

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