ISSN 1063-7826, Semiconductors, 2013, Vol. 47, No. 12, pp. 1595–1597. © Pleiades Publishing, Ltd., 2013.
Original Russian Text © N.O. Krivulin, D.A. Pavlov, P.A. Shilyaev, 2013, published in Fizika i Tekhnika Poluprovodnikov, 2013, Vol. 47, No. 12, pp. 1621–1623.

SYMPOSIUM "NANOPHYSICS AND NANOELECTRONICS", NIZHNI NOVGOROD, MARCH, 2013 (CONTINUATION)

Growth Model of Silicon Nanoislands on Sapphire

N. O. Krivulin^, D. A. Pavlov, and P. A. Shilyaev
Lobachevsky University of Nizhni Novgorod, Nizhni Novgorod, 603950 Russia
^e-mail: krivulin@phys.unn.ru

Submitted April 22, 2013; accepted for publication, April 30, 2013

Abstract—A growth model of silicon nanoislands on silicon by molecular-beam epitaxy is refined. It is shown that silicon islands grow due to the diffusion of material from the wetting layer, with the contribution from direct hits of atoms to this growth being nearly zero.

DOI: 10.1134/S1063782613120117

Nanocrystalline silicon on sapphire is one of a multitude of structural modifications of silicon, in which properties uncharacteristic of this indirect semiconductor appear due to quantum-confinement restrictions. Nanocrystals can be formed in several ways. The most widely used method for obtaining silicon nanocrystals in which confinement effects of the electron spectra are manifested consists in the formation of nanocrystals by the implantation of Si atoms into a dielectric matrix, followed by annealing [1]. This makes it possible to create an effective emission system [2, 3]. In another method, nanosize clusters are formed directly during the course of layer growth. This technique is based on the crystallization process by the Stranski–Krastanov mechanism. The method for obtaining an array of quantum dots (QDs) in a germanium–silicon heterosystem by molecular-beam epitaxy (MBE) has been well studied [4]. The QD sizes in systems of this kind are comparatively large, 10 nm and more, whereas their surface density is at a level of 10^9–10^{11} cm^{-2} [5].

Previously, we have shown that silicon nanocrystals can be formed on the surface of sapphire by MBE [6]. In this case, the maximum density of the islands reaches a value of 10^{11} cm^{-2}, which is comparable with the results obtained for the germanium–silicon heterosystem. In the present work, we discuss the growth mechanism of islands in the silicon–sapphire heterosystem. The data of the cross-sectional transmission electron microscopy of silicon nanoislands on sapphire suggest that growth in the silicon–sapphire heterosystem occurs by the Stranski–Krastanov mechanism [7]. In [8], the growth mechanism of islands for a small degree of coverage is described in detail with consideration for the presence of a wetting layer. This mechanism disregards direct island hits by atoms of the molecular beam. It is considered that the islands grow due to the diffusion of atoms from the surface. Then, two situations are possible: growth of islands from a supersaturated vapor of atoms on the surface of the wetting layer and that via consumption of the material directly from the wetting layer.

During the course of island growth, the layer thickness will remain constant in the first case and will decrease in the second. Data on silicon-on-sapphire structures are thus far insufficient for tracing the thickness-variation dynamics of the wetting layer. The silicon–germanium heterosystem has been well studied, and it was shown that, in this case, island growth during the initial stage of MBE occurs via the consumption of atoms from the wetting layer [8]. The same behavior is observed in the GaAs–InGaAs system. In what follows, we assume that, in the silicon–sapphire system too, growth occurs by the same mechanism and the motion of atoms over the surface of the wetting layer only leads to the growth of the wetting layer itself. A similar model is considered in [8], according to which atoms diffuse from the wetting layer into an island under the action of elastic stresses. In this case, the following formula is used to find the growth rate of islands with a supercritical size, di/dt (i is the number of atoms in an island, and t is time):

$$\frac{di}{dt} = \frac{D}{l_0^2}\frac{\nabla\mu}{k_B T}P, \qquad (1)$$

where D is the diffusion coefficient of atoms of the wetting layer for diffusion caused by the difference in the elastic stresses in the wetting layer and in the island, $\nabla\mu$ is the gradient of the chemical potential at the island boundary, P is the island perimeter, $1/l_0^2$ is the concentration of adsorption sites on the surface, T is temperature, and k_B is the Boltzmann constant.

In the case of the silicon–sapphire heterosystem, silicon islands are very close to each other. At an island size of 5–7 nm, the distance between the islands is in the range 5–10 nm. In this case, the contribution from

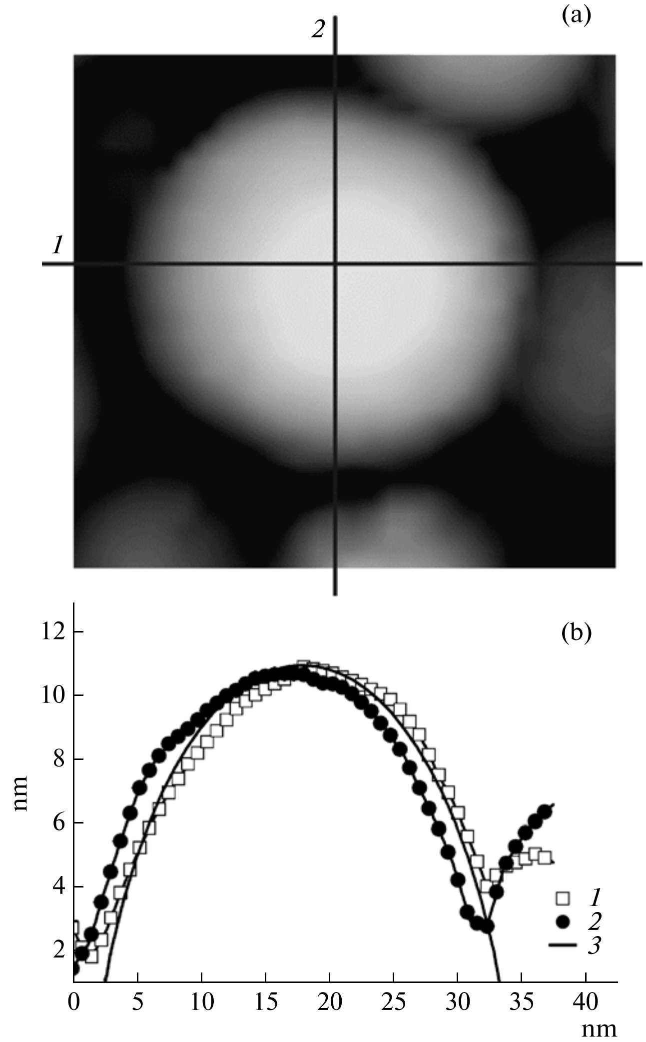

Fig. 1. (a) AFM image of a typical silicon nanoisland on sapphire. (b) (*1*, *2*) Cross-sectional profiles of the given island and (*3*) that of an approximating sphere with a radius $R = 17$ nm.

direct atomic hits to island growth may be important. We made an attempt to take this contribution into account. In this case, the growth rate is expressed as

$$\frac{di}{dt} = SJ, \tag{2}$$

where S is the island-base area, and J is the atomic flux of the substance being deposited. At a growth rate of 2 Å/s, $J \approx 10$ nm^{-2} s^{-1} for Si (100).

It is convenient to calculate the island size, rather than the number of atoms in an island. The island size can be observed experimentally by atomic-force microscopy (AFM) or transmission electron microscopy. Therefore, we replace the number of atoms in an island in formulas (1) and (2) with its lateral size. Figures 1a and 1b show, respectively, the AFM image of a typical silicon island on sapphire and cross-sectional profiles in two perpendicular directions.

The island is well approximated with a spherical segment of radius R (Fig. 1b), protruding above the surface to a height h. Taking that a single silicon atom occupies a volume of $V_s = 0.036$ nm^2, we write the island volume as $V = \pi h^2(3R - h)/3 = iV_s$. The perimeter of the island, $P = \pi l$, and its base area $S = \pi l^2/4$, where l is the lateral size (diameter) of the island. Further, we express R and h in terms of l: $R = h/2 + l^2/8h$. During the course of growth, the l/h ratio varies, but we can consider in the earliest stages of growth that $l = 3h$, then $R = 0.54l$. Finally, we obtain an expression for the island volume $V = 0.47\pi l^3 = iV_s$, whence we express the number of atoms in the island as $i = 0.47\pi l^3/V_s$. Substituting all these results into formulas (1) and (2) and integrating, we obtain the time dependence of the growth rate of the lateral sizes of the islands:

$$l = \sqrt{5.13 V_s \frac{D}{l_0^2}\frac{\nabla\mu}{k_\mathrm{B}T} t + L^2}, \tag{3}$$

for the island growth mechanism due to the supply of material from the wetting layer, and

$$l = 0.64 J V_s t + L \tag{4}$$

in the case of island growth via direct atomic hits. Here, L is the critical nucleus size. L being very small (as a rule, several atoms), it can be neglected in these expressions. Let us now perform a simulation for a growth temperature of 650°C. D and $\nabla\mu$ are unknown for the silicon–sapphire system, but, in the end, all the unknown quantities can be reduced to a single one. In this case, the expression for the lateral size of an island will have the following form: $l = A\sqrt{t}$. We are going to choose coefficient A experimentally. Substituting the necessary values into (4), we obtain expressions for the size of an island upon its growth due to direct hits: $l = 0.128t$.

Figure 2 shows how the lateral sizes X and Y of the islands depend on the growth time. Durign the initial growth stages (at growth durations shorter than 30 s), the experimental data correlate with the simulation results. The best agreement between the experimental and simulation results was observed at $A = 3.8$. It can be seen in this case that growth by direct hits barely gives any contribution.

At deposition times exceeding 30 s, strong disagreement appears between the experimental and simulation results. The real island sizes substantially exceed the calculated values, with the discrepancy becoming more pronounced with increasing deposition time. The reason is that the suggested model disregards the coalescence of islands, whereas this pro-

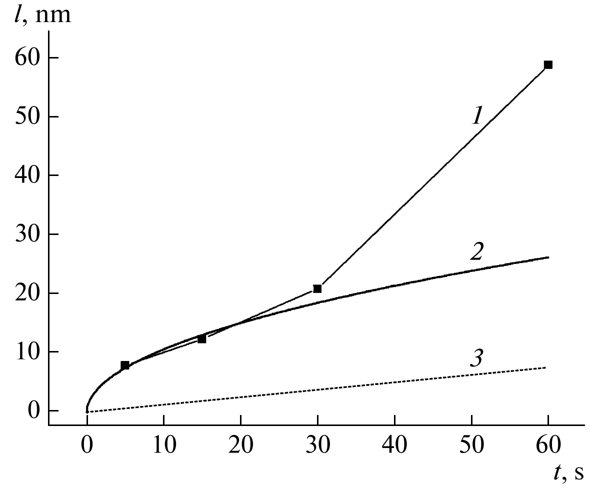

Fig. 2. Lateral sizes of the islands vs. the growth duration at a growth temperature of 650°C and growth rate of 2 Å/s: (*1*) experiment, (*2*) growth at the expense of the wetting layer, and (*3*) growth due to direct atomic hits.

cess is observed in the earliest stages of MBE growth. In the case of coalescence, the islands are combined and their overall size sharply increases.

On the whole, the suggested model adequately describes the growth of silicon nanoislands on sapphire during the course of molecular-beam deposition and confirms the assumption that growth in the silicon–sapphire system is described by the Stranski–Krastanov model.

The study was supported by the Russian Foundation for Basic Research (project no. 12-02-31686).

REFERENCES

1. P. Bettotti et al., J. Phys.: Condens. Matter **14**, 8253 (2002).
2. S. Yanagiya and M. Ishida, J. Electron. Mater. **28**, 496 (1999).
3. Y. Zhu and P. P. Ong, Surf. Rev. Lett. **8**, 559 (2001).
4. O. P. Pchelyakov, Yu. B. Bolkhovityanov, A. V. Dvurechenskii, L. V. Sokolov, A. I. Nikiforov, A. I. Yakimov, and B. Foikhtlender, Semiconductors **34**, 1229 (2000).
5. N. N. Gerasimenko and Yu. N. Parkhomenko, *Silicon: A Material for Nanoelectronics* (Tekhnosfera, Moscow, 2007) [in Russian].
6. D. A. Pavlov, P. A. Shilyaev, E. V. Korotkov, and N. O. Krivulin, Tech. Phys. Lett. **36**, 548 (2010).
7. D. A. Pavlov, P. A. Shilyaev, E. V. Korotkov, N. O. Krivulin, and A. I. Bobrov, Bull. Russ. Acad. Sci.: Phys. **76**, 1002 (2012).
8. V. G. Dubrovskii, *Theoretical Principles of Semiconductor Nanostructure Technology* (St.-Petersburg, 2006) [in Russian].

Translated by M. Tagirdzhanov