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Self-organization of Ge layers on Si surfaces at high temperatures

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Abstract

Conditions for self-organization during heteroepitaxial growth are found, which provide the most exhaustive strain relaxation due to fast high-temperature generated surface and bulk diffusion. In particular, they lead to the ordered SiGe island formation on Si(100) and lateral nanowires on Si(111). The found approach can be used to prepare new self-organized heterostructures of other materials.

1. Introduction

Self-organization during heteroepitaxial growth provides the possibility for the fabrication of semiconductor heterostructures with quantum dot arrays that exhibit unique optoelectronic properties. In order to obtain their best performance, they should be prepared on the base of the ordered three-dimension (3D) islands of identical sizes. Since the self-organization occurs to reduce the lattice strain, the formation of ordered island arrays provides the most exhaustive strain relaxation. It was found that the island ordering can be realized when the nucleation of islands does not occur randomly along the surface, but their locations are governed by the elastic strain distribution generated by underlying patterned structures [1]. The surface morphology formation usually takes place via surface processes which can limit the realization of strain relaxation. The facilitated strain relaxation is suggested to occur in the conditions close to thermodynamic equilibrium, which can be realized, for example, in liquid phase epitaxy [2]. We demonstrate here that the conditions for island ordering can be implemented during molecular beam epitaxy (MBE) of Ge on Si(100) at high temperatures, when the islands are formed by means of the nucleationless process via gradual changes in the surface morphology in the conditions close to the dynamic equilibrium between the growth of islands and their decay through the Ge diffusion into the substrate. The Ge deposition on Si(111) in such conditions leads to lateral nanowire or disc-like island formation depending on the temperature**.**

2. Critical conditions for SiGe island formation on Si(100) at high temperatures

The island formation at high temperatures occurs in the conditions when a significant amount of deposited Ge diffuses into the substrate [3]. There is the Ge deposition rate (R_{dep}) at which the dynamic equilibrium between the growth of islands on the surface and their decay due to the Ge diffusion into the substrate is realized. This rate can be referred to as the critical rate (R_c) for the island formation, similar to the critical oxygen pressure at which the quasi-equilibrium conditions between the silicon oxide growth and decomposition on Si surfaces take place [4]. The value of R_c can be determined by obtaining the island height dependence on R_{dep} [Fig. 1(a)].

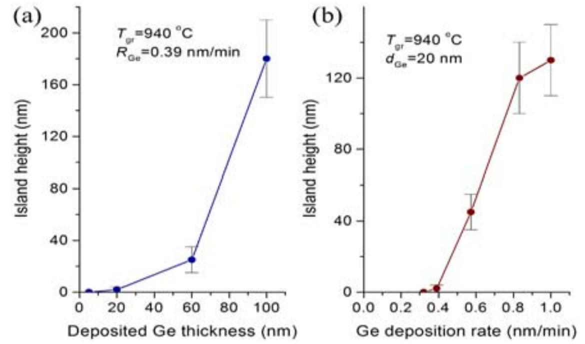

Fig. 1. Dependences of the island height (a) on the deposited Ge amount for the Ge deposition rate of 0.39 nm/min and (b) on the Ge deposition rate for the deposited Ge amount of 20 nm at 940 °C.

If ΔR=R_{dep}-R_c <0, all deposited Ge atoms diffuse into the substrate. However, if after the deposition of a certain Ge amount at a given temperature and R_{dep} the formation of islands is not observed, they can appear when the deposited Ge amount increases [Fig. 1(b)].

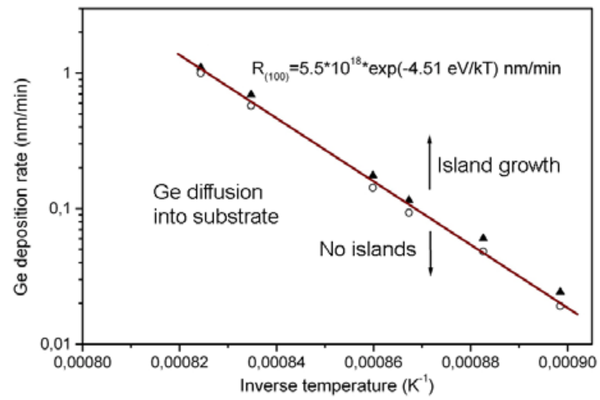

Fig. 2. Critical conditions for the island formation during 5 (data A) and 100 nm (data B) Ge depositions on Si(100) at high temperatures. The solid and open symbols represent the conditions at which the islands appear or not on the surface, respectively.

Since R_c depends on the of Ge deposition amount, its temperature dependence is reasonable to be obtained for several given amounts of Ge depositions. Such temperature dependences show, in particular, that R_c is about 2.5 times bigger for the deposition of 5 nm than that for 100 nm. It can be noted that, in order to prepare ordered island arrays, rather large Ge depositions of about 20 nm or larger must be carried out in the conditions close to the dynamic equilibrium. It is required for the gradual surface morphology development.

The critical conditions presented in Fig. 2 allow them to be well approximated by the exponential function $R_c(T)=R_0\times\exp(-E_a/kT)$, where R_0 is the pre-exponential factor and E_a is the effective activation energy. The obtained E_a was found to be about 4.5 and 5.0 eV for the Ge depositions of 5 and 100 nm, respectively. As expected, these values are in agreement with the activation energy of Ge diffusion in Si.

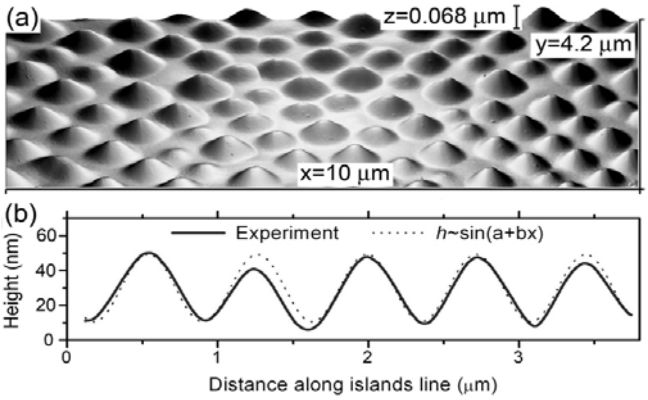

Fig. 3. (a) and (b) STM images of the surfaces obtained by 20 nm Ge deposition on Si(100) at 925 °C with the deposition rate of 0.39 and 0.57 nm/min, respectively. (c) The solid line represents the height profile along islands array on the surface shown in (a). The dotted line is the approximation of the experimental height profile by the sinusoidal function.

The size, shape and spatial distribution of islands on the surface strongly depends on ΔR. The islands grown in the conditions close to the dynamic equilibrium have an oval shape and a tendency to lateral ordering [3]. Moreover, they form a smooth surface shape at their base (Fig. 3).

3. Ge deposition on Si(111) at high temperatures

Other 3D SiGe structures were observed after Ge depositions on Si(111) at temperatures around 850 °C in the conditions closed to the dynamic equilibrium. Their formation proceeds through the nucleation of islands which then develop into long straight and winding nanowires (NWs) (Fig. 4). The NWs are formed in spite of their larger surface area size, in comparison with disk-like islands of the same base size, and longer perimeters at which the lattice strain is known to be the strongest. The general reason for the NW formation is the minimization of the strain energy by means of elongation instead of flat 3D structures isotropic-like growth, as has been theoretically demonstrated [5]. Additional factors that govern the NW shape formation are different for the straight and winding NWs. The crystallographic orientations of NWs on the Si(111) surface and their probable SiGe composition suggest that the energy barrier for the dislocation net work formation at the NW/substrate interface is responsible for the straight shape of the NWs and for their certain width [6].

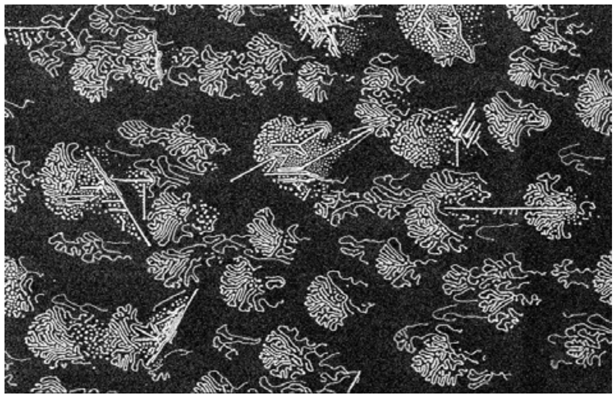

Fig. 4. SEM images of NWs grown by 5 nm Ge deposition on Si(111) at 840 °C.

4. Conclusions

We obtained the critical rate for Ge deposition on Si(100) at temperatures in the range of 840 – 960 °C, at which the dynamic equilibrium between the growth of islands and their decay by means of the Si-Ge intermixing with the Ge diffusion into the substrate is realized. The SiGe islands grown in the conditions close to the dynamic equilibrium are formed via a nucleationless process, exhibiting a tendency to ordering. The islands arrays are characterized by homogeneous distributions of the lattice strain and the SiGe composition in the direction along the surface. It is expected that SiGe/Si heterostructures, fabricated on the basis of such islands arrays, may possess a narrow spectrum of electronic states, which is required for the realization of electronic and optical resonances. In contrast to the growth on Si(100), Ge deposition on Si(111) leads to the formation several different surface morphologies composed of 3D disk-like islands, lateral nanowires or 3D large thin islands depending on the temperature and the deposited Ge amount. The large thin islands exhibit a tendency to form a complete 2D SiGe layer as the deposited Ge amount increases.

Acknowledgements

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