Applied Surface Science 465 (2019) 10–14

Contents lists available at ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

Full Length Article

Electromigration effect on the surface morphology during the Ge deposition on Si(1 1 1) at high temperatures

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ARTICLE INFO

Keywords:
Electromigration
Si/Ge heterostructures
Ge growth on Si(1 1 1)
Nanostructures

ABSTRACT

The directional atom drift under direct electric current (DC) flowing through a sample is a unique tool for the surface morphology manipulation, which was previously studied in detail for Si surfaces. We show that electromigration can significantly influence the heterostructures growth process. Without electromigration, the surface morphology is formed under the action of two driving forces determined by a surface and strain energy minimization. DC shifts the balance between them in favor of one of them, depending on the DC direction, producing unusual surface nanostructures during the Ge deposition on Si(1 1 1) at 850–900 °C. When electromigration inhibits the surface energy minimization, the high atomic steps are formed. Their edges became wavy and unstable when the step edges reached the height larger than 15 nm. The instability induced disintegration of the step edges with the flat-shaped islands formation.

1. Introduction

The heterostructures formation during their growth at sufficiently high temperatures occurs through the self-organization governed by free energy minimization. However, this is often limited by the kinetic factors, i.e. rates of surface processes. The use of high temperatures makes the growth to be nearly a thermodynamically equilibrium process. One of the interesting phenomena affecting the surface morphology formation at high temperatures is electromigration, which occurs when the direct electric current (DC) flows through a sample. When Si samples are heated to high temperatures, the dominant processes are the generation of adatoms and their surface diffusion and evaporation. If Si samples are heated using DC, the atom drift becomes spatially directed due to electromigration. This leads to the rearrangement of atomic steps, in particular, to the step bunching, depending on the sample temperature and the DC direction with respect to atomic steps [1–7]. The step bunching under electromigration conditions was observed in the high-temperature epitaxy of the materials, such as SiC [8] and graphene nanoribbons on 6H-SiC (0001) substrates [9]. Recently, a strong surface electromigration effect was observed for metals, namely, in the vicinal W(1 1 0) surface morphology formation [10]. The surface electromigration phenomenon was extensively investigated in the theoretical studies, and it was associated with the interaction between the applied electric field and an effective charge for surface atoms [11–14]. Here, we report on the first observation of the electromigration effect in the epitaxial growth of semiconductor heterostructures, i.e. for the Ge growth on Si(1 1 1).

In the middle temperature range (~500 °C) the Ge growth on Si (1 1 1) was studied in detail, and it occurs through the Stranski-Krastanov growth mode [15–18]. At temperatures higher than 750 °C, the new growth phenomena were observed recently [19,20], and they were associated with the solid-state dewetting of SiGe layers on Si (1 1 1) [20]. The dewetting, probably, occurs also at lower temperatures, such as 600 °C, but at an essentially lower rate. It consists in the three-dimensional (3D) island growth under the post-growth annealing without the Ge deposition [21], which is accompanied by the deep trenches formation along the island perimeter [17,22]. The use of higher temperatures of about 850 °C and relatively low Ge deposition rates leads to the formation of flat triangular shaped islands and lateral nanowires [23]. The appearance of large flat terraces and high atomic steps at their edges was observed at 850–900 °C [24]. The study of high-temperature growth is important because of the processes which occur on Ge and Si surfaces only at high temperatures. This is related to their reactions with carbon, in particular, to the formation of SiC and graphene layers [25–27]. A specific aspect is that this electromigration can strongly influence the surface morphology formation at such high temperatures.

We study the surface morphology evolution during the deposition of

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https://doi.org/10.1016/j.apsusc.2018.09.119
Received 13 May 2018; Received in revised form 31 August 2018; Accepted 14 September 2018
Available online 18 September 2018
0169-4332/

various Ge amounts on Si(1 1 1) when the sample was heated to the temperatures of 850 and 900 °C by using either the alternating current (AC) or DC. We found that the Ge deposition led to the formation, in particular, of wide (1 1 1) terraces with edges in the shape of high steps. The atomic step height exhibited a strong dependence on the DC direction. The obtained experimental results suggest that the surface morphology formation occurs under conditions of competition between the minimizations of surface and strain energies, which act against each other. At the same time, the difference in their changes as a function of the atomic step height in the wide range is small. This allows a relatively small contribution from electromigration to have a significant effect on the balance between them. Under these conditions, the surface morphology, which is formed during the high-temperature growth of the SiGe heterostructures, becomes very sensitive to electromigration.

2. Experimental details

The Ge deposition on Si(1 1 1) was performed using the solid-source molecular-beam epitaxy technique in an ultrahigh-vacuum chamber with a base pressure of about 1×10^{-10} Torr. The chamber was equipped with a scanning tunneling microscope (STM) manufactured by Omicron. The $10 \times 2 \times 0.3\,mm^3$ samples were cut from an *n*-type Si (1 1 1) wafer with a miscut angle of less than 10′ and a resistivity of 5–20 Ω cm. Clean Si surfaces were prepared by flash AC or DC heating at 1250–1300 °C. The sample temperature was measured using an IMPAC IGA 12 pyrometer. A Knudsen cell with a BN crucible was used for the Ge deposition, which rate was calibrated using submonolayer Ge growth on Si(1 1 1) at relatively low temperatures [28].

The apparent atomic step height being measured by STM can depend on the bias voltage and the chemical composition of samples [29]. The calibration of our STM for height measurements was carried out using the atomic steps on Si(1 1 1), for which the step height is almost independent of the bias voltage. It has been shown that the presence of Ge atoms on the step edges on Si(1 1 1) causes a relatively small changes in step height, which is proportional to the changes in the lattice constant [30,31]. The surface layers of our samples consisted of SiGe with the Ge content ranging from 0 to 10%. It is reasonable to expect that in this case the dependence of the apparent step height on the Ge content is insignificant.

The structures were grown at 850 and 900 °C. After the growth, each sample was transferred to the STM stage in the ultrahigh-vacuum conditions for STM imaging, which was carried out in the constant-current mode at the bias voltage of −2.0 V and the tunneling current of 10 pA. The sharp STM tips were used. The opening angle of their apexes was usually less than 30°. After electrochemical etching, the sharpening of the W STM tips were carried out by material removing from their apexes from several sides using the 30 kV Ga ion beam of a separate Zeiss 1540 XB cross beam scanning electron microscope. After removing of the samples from the growth chamber, their scanning electron microscope (SEM) images were obtained using a Pioneer microscope manufactured by Raith.

3. Experimental results

The surface morphology obtained by the Ge deposition on Si(1 1 1) at temperatures in the 850–900 °C range has a strong dependence on the Ge deposition rate (R_{Ge}). When $R_{Ge} > 0.4$ nm/min, micron-sized islands are formed surrounded by arrays of flat islands with lateral dimensions of 0.2–0.5 μm and a height of about 20 nm [23]. The micron-sized islands are not formed at 900 °C if R_{Ge} is less than 0.3 nm/min [Fig. 1(a)–(c)], depending on the deposited Ge amount. When a sample surface has an inclination from a Si(1 1 1) plane at an angle of about 0.1°, it is normally covered by atomic steps [32] having the height of one interplanar distance, $d_{(1\,1\,1)} = 0.314$ nm, i.e. one bilayer (BL) thick, and by (1 1 1) terraces with a width $L_o \sim 0.2$ μm. It appeared that the Ge deposition at 900 °C leads to the increase in the (1 1 1) terrace width, as shown in Fig. 1(a)–(c) and 2. This was accompanied by the steps formation at the terrace edges which were much higher than $d_{(1\,1\,1)}$. At the same time, we found that the terrace width (L) and, consequently, the step height strongly depend on the electric current direction with respect to the step edges direction (Fig. 2).

When AC was used, the average height (h_{st}) of atomic steps at the (1 1 1) terrace edges increased to $\sim 10 d_{(1\,1\,1)}$, as the deposited Ge amount (d_{Ge}) was increased to 20 nm. With the further d_{Ge} increase, h_{st} changed insignificantly and could reach $\sim 13 d_{(1\,1\,1)}$ at the 40–60 nm Ge depositions (Fig. 2). The edge shape of the high atomic steps was composed of the set of single steps. They were so narrow and had a high density of kinks on a short length scale along their edges, similar to Ge single steps on Si(1 1 1) observed in [31], that it was difficult to recognize their (1 1 1) terraces in the STM images (Fig. 3).

The use of DC, when DC was in the step-up direction, also leads to the increase in h_{st}, but the increase was approximately 2 times smaller than that at AC [Figs. 1(a, b) and 2]. At the same time, the increase in h_{st} was significantly bigger when DC was in the step-down direction [Figs. 1(c), (d) and 3(a)]. The h_{st} value, in this case, was 3–10 times higher (depending on d_{Ge}) than when AC was used, and it reached $\sim 80 d_{(1\,1\,1)}$ during the 60 nm Ge deposition (Figs. 2 and 3). It is reasonable to assume that the observed electric current effect on the surface morphology originates from the surface electromigration which usually occurs on Si surfaces at high temperatures [1–7].

The obtained results show that electromigration causes the formation of substantially different surface morphologies during the Ge deposition on Si(1 1 1) in comparison with that on bare Si(1 1 1) surfaces. In contrast to the single step bunches formation on bare Si(1 1 1) surfaces [1], in our case, the electromigration produces the high steps formation. As h_{st} reaches a certain value, the steps become unstable when DC in the step-down direction was used (Fig. 3). Firstly, their step edges become wavy at $h_{st} \sim 10$ nm [Fig. 3(a)]. Then the step edges disintegrate producing the formation of flat 3D structures, such as individual islands and short nanowires [Fig. 1(c, e) and 3(b, c)]. This occurs when h_{st} becomes larger than 15 nm, up to ~25 nm. The flat 3D structures height was the same as the height of adjacent steps, i.e. in the range of 15 to 25 nm, depending on d_{Ge} and temperature [Fig. 3(b, c)]. Simultaneously with the high steps, the wide (1 1 1) terraces were formed. It was shown earlier that, when Ge was deposited at 850 °C, the lateral nanowires were formed on wide flat (1 1 1) terraces, and their length reached ~10 μm [23].

4. Discussion

In the case of AC, i.e. without the electromigration effect, the high step formation during the Ge deposition can be explained by the action of strain minimization, as schematically illustrated in Fig. 4(a, b). When a cluster of several Ge atoms is located on a Si surface, the strain acts to compress the cluster. If the Ge cluster is located on the step edge, the compression force is reduced, because a smaller number of Si substrate atoms are involved in the interaction with Ge atoms, as shown in Fig. 4(a). On the contrary, the compression force increases when the cluster is located in front of step edges [Fig. 4(b)]. Such action strain leads to the high steps formation. At the same time, their formation leads to an increase in the number of surface atoms per unit surface area, and, hence, to an increase in surface energy. Consequently, the step height under the dynamic equilibrium conditions is determined by the balance between the forces acting from the surface energy increase and the strain energy decrease. It can be mentioned that the dynamics of surfaces with homogeneous composition and containing high atomic steps can be described on the basis of the discontinuous surface tension [33].

The error bars in Fig. 2 are large, and these are determined by measuring the atomic step heights using the STM data obtained for different surface areas of the samples. The formation of high atomic steps occurs by the movement of single ($d_{(1\,1\,1)}$-thick) atomic steps