Formation of rippled surface morphology during Si/Si (100) epitaxy by ultrahigh vacuum chemical vapour deposition*

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The Si epitaxial films are grown on Si (100) substrates using pure Si_2H_6 as a gas source using ultrahigh vacuum chemical vapour deposition technology. The values of growth temperature T_g are 650 °C, 700 °C, 730 °C, 750 °C, and 800 °C. Growth mode changes from island mode to step-flow mode with T_g increasing from 650 °C to 700 °C. Rippled surface morphologies are observed at T_g = 700 °C, 730 °C, and 800 °C, but disappear when T_g = 750 °C. A model is presented to explain the formation and the disappearance of the ripples by considering the stability of the step-flow growth.

Keywords: step-bunching, Ehrlich–Chwoebel barrier, elastic repulsion, fluctuation

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1. Introduction

Because of its good electrical, mechanical and thermal properties, Si is a dominant material in modern microelectronic and optoelectronic industry and has received much attention. In Si device fabrication, the Si epitaxial layer is widely used in order to grow a 'new substrate' which is atomically clean and smooth for the Si-based heteroepitaxy, or to obtain a layer with different doping levels or doping types.[1,2] Among a variety of growth methods, the ultra high vacuum chemical vapour deposition (UHVCVD) technology has a high background vacuum and therefore the epitaxy can be operated at relatively low temperature.[3,4] As a result, high quality films and abrupt doping can be realized.

An interesting surface morphology of the Si layer are the ripples that appear when quick thick ($\sim 1\mu$m) homoepitaxial film is grown. The rippled surface is like a series of hills and valleys several nanometers in height and a few micrometers in period, which is unfavorable for Si material growth and device fabrication. In general, the ripple surface morphology is believed to be caused by step-bunching on the vicinal surface during growth. The steps originate from the unintentional miscut of the Si substrate.

Pidduck *et al.*[5] performed detailed studies on the rippled surfaces of Si epitaxial films grown by molecular beam epitaxy (MBE) and vapour phase epitaxy (VPE). Their results showed that the ripple formation was independent of impurities or defects. The direction of the ripples is found to depend on the surface misorientation but not in a simple manner, i.e., the ripples are not always parallel to the step edge under atmospheric condition. Besides, the angle between the ripple and step edge under atmospheric condition for the Si epitaxial layer grown by MBE is different from that for VPE. They assume that the stable step edge is parallel to the ripples during growth, and consider that the ripples are formed by step-bunching. Myslivecek *et al.*[6] investigated the ripple morphologies of Si grown by MBE at different temperatures (350 °C–550 °C). They also believed that the step-bunching leads to the rippled surface. Wingerden *et al.*[7] has another idea, they linked the ripples to kink bunching,

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and considered the ripple formation as a specific case of step edge instability.

In this paper, we investigate the rippled surface morphology of the Si epitaxial layer grown by UHVCVD technology. The growth temperature dependence of the surface morphology is investigated in a range of 650 °C–800 °C. The ripples are observable when the growth temperatures are 700 °C, 730 °C, and 800 °C, but unobservable at 750 °C. This phenomenon has not been reported and studied, to our best knowledge. We present a simple model to explain the formation and the disappearance of the ripples by examining the stability of the growth.

2. Experimental details

A cold wall UHVCVD started on an Si (100) substrate with a resistivity of 2 Ω·cm–4Ω·cm. The substrate was cleaned using an improved RCA wet-chemical cleaning recipe, i.e., using H_2O_2:H_2SO_4=1:4, H_2O_2:NH_4OH:H_2O=2:1:5, HF:H_2O=1:10, H_2O_2:HCl:H_2O=7:1:2 solutions sequentially to clean the substrate. Before growing, the substrate was degassed at 300 °C for several hours in the pre-treatment chamber and then deoxided in the growth chamber by being heated to 930 °C for 5 minutes. And then, the homoepitaxy of Si on Si (100) was processed at growth temperature T_g with a pure Si_2H_6 flow of 6 sccm. The values of growth temperature T_g were 650 °C, 700 °C, 730 °C, 750 °C, and 800 °C separately.[8] The Si epitaxial layers were all 1-μm thick.

The reflection high energy electron diffraction (RHEED) measurements show the 2×1 surface reconstruction patterns for all samples, which indicates good crystal quality of the epitaxial films. During the epitaxy, the growth mode (island mode or step-flow mode) could not be monitored because the RHEED measurement could not be performed at the pressure during growth. The surface mophologies of the epitaxial layers were examined by the atomic force microscope (AFM) under atmospheric condition, because no *in situ* scanning tunneling microscope was available in our UHVCVD system. The misorientation of the substrate is evaluated by the double-crystal X-ray diffraction measurements, the results indicates a $\theta \approx 0.25°$ miscut angle in the [011] direction

3. Results and discussion

3.1. Vicinal Si (100) surface

The 0.25° misorientation leads to monatomic-height steps on the vicinal Si (100) surface below 800 °C.[9] On the Si surface, two neighbouring atoms dimerize to form a 2×1 structure along the [011] direction which reduces the number of dangling bonds at the expense of inducing a large surface stress in order to minimize the surface energy.[10] The stress is anisotropic on the vicinal surface, that is, there are tensile strains perpendicular to the dimmer rows and compressed strains along the dimer rows.[11] Because of the stress anisotropy, the dimer rows on adjacent terraces rotate 90° across steps of monatomic height along the [011] direction.[12] Therefore, if the steps are along the [011] direction (i.e., the step edge is along the $[01\bar{1}]$ direction), there are two types of monatomic steps on the vicinal Si (100) surface: one is S_B step if the step edge is perpendicular to the upper-terrace dimer rows, the other is S_A step if the step edge is parallel to the upper-terrace dimer rows. As shown in Fig. 1(a), the vicinal surface consists of evenly distributed T_A and T_B terraces if the step is along the [011] direction. The terraces are labeled according to the step type at their down step edge as T_A or T_B terraces. For the steps along other directions, the step is no longer pure S_B or S_A step, the terrace is no longer pure T_B or T_A terrace either. Instead, each step is the mixture of S_A and S_B steps, each terrace is the mixture of T_A and T_B terraces. The composition of S_A

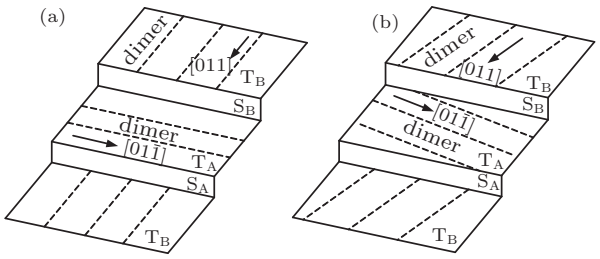


Fig. 1. Steps and terraces on the vicinal Si (100) surface. The dimer row aligns along the dash line. (a) If the steps are along the [011] direction (i.e., the step edge is along the $[01\bar{1}]$ direction), the vicinal surface consists of evenly distributed T_A and T_B terraces. The S_A step edge is parallel to the upper-terrace dimer rows, while the S_B step edge is perpendicular to the upper-terrace dimer rows. The terraces are labeled according to the step type at their down step edge as T_A or T_B terraces. (b) If the steps are not along the [011] direction, each step is a mixture of S_A and S_B steps, each terrace is a mixture of T_A and T_B terraces. The step with high (low) S_B composition is labeled as the S_B (S_A) step, and the terrace with high (low) T_B terrace the T_B (T_A) terrace.

step or T_A terrace is determined by the direction of the step edge. For convenience, we call the step with high (low) S_B composition the S_B (S_A) step, the terrace with high (low) T_B terrace the T_B (T_A) terrace as shown in Fig. 1(b).

3.2. Surface morphology of Si epitaxial layer

The surface morphologies of samples grown at different temperatures (T_g = 650 °C, 700 °C, 730 °C, 750 °C, 800°C) are shown in Fig. 2. The surface morphology is very sensitive to the growth temperature. For the sample grown at 650 °C, the surface is rough and filled with two-dimensional (2D) islands, with a root mean square (RMS) roughness of 4.70 nm.

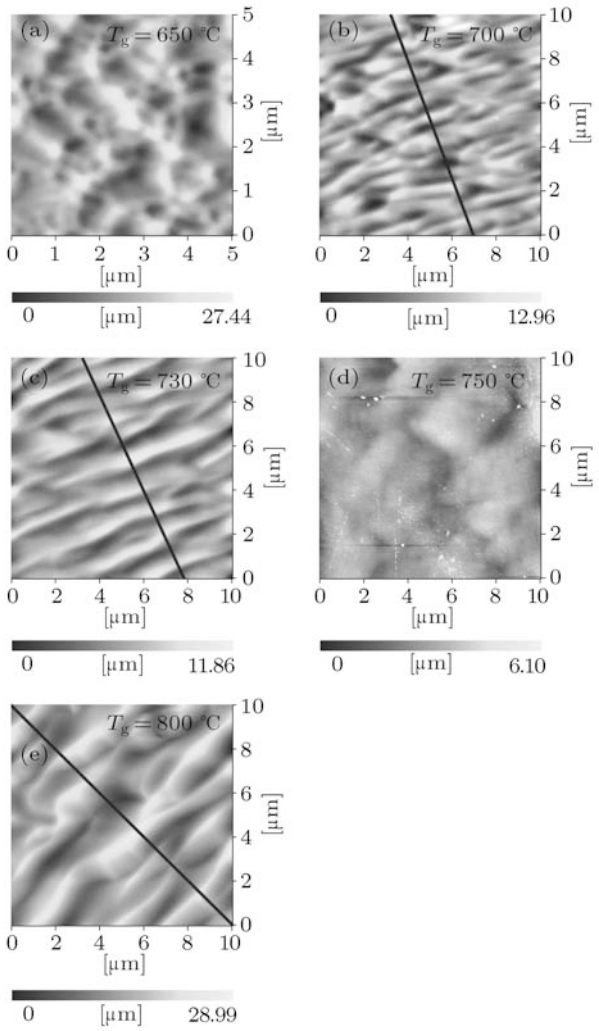


Fig. 2. Surface morphologies under different values of growth temperature T_g = 650 °C (a), 700 °C (b), 730 °C (c), 750 °C (d), and 800 °C (e). The RMS roughnesses are 4.70, 2.54, 1.70, 0.73, 3.40 nm, respectively. The height profiles along the lines in the AFM image of sample at T_g = 700 °C (b), 730 °C, (c), and 800 °C (e) are shown in Fig. 5.

In this case, the diffusion coefficient is low, as a result, the adatom tends to stay still on the T_A or T_B terrace and meets another adatom to form a cluster at a high probability. The clusters have much lower mobility than a single adatom, they finally stop on the terrace, becoming a nucleation centre and leads to the 2D island surface morphology.

When T_g = 700 °C and 730 °C, the surfaces became smoother and free of islands with roughnesses of 2.54 nm and 1.70 nm, respectively. However, ripples can be seen on the surface. Considering the ±10° azimuth accuracy of the AFM measurement, the directions of the ripples are approximately along the [010] direction. Obviously, the growth mode changes from island mode to step-flow mode, and during growth the steps propagate along the direction perpendicular to the step edge. Under these temperatures, the diffusion coefficient is high enough so that the adatoms are able to migrate into the kink of the step edge. The growth mode transition from island mode to step-flow mode during Si growth using the molecular beam epitaxy technology has been reported.[13] When T_g = 750 °C, the epitaxial film was very smooth with an RMS roughness of 0.73 nm and the ripples disappeared. When T_g reached 800 °C, the ripples appear again approximately along the [010] direction and the surface becomes rougher with an RMS roughness of 3.40 nm.

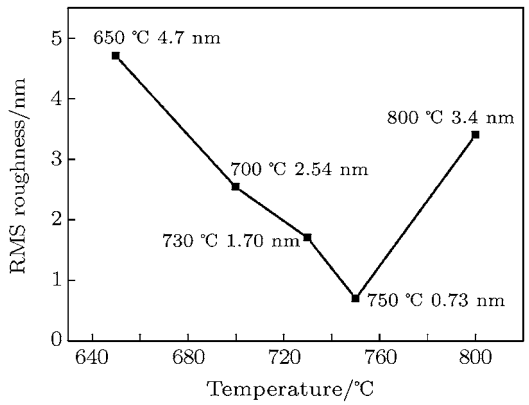


Fig. 3. Temperature dependence of the surface RMS roughness.

The RMS roughness of the surface as a function of the growth temperature is shown in Fig. 3. The direction of the ripples and the substrate misorientation under atmospheric condition of all samples are indicated in Fig. 4. The angle between the miscut vector [100] and the normal line is $\theta = 0.25°$. Before growth, the step edge direction is $[01\bar{1}]$ which is perpendicular to the miscut vector [100]. But during growth,

the stable step edge is parallel to the direction of ripples as indicated by Pidduck *et al.*[5] The ripple height profiles of samples grown at 700 °C, 730 °C, and 800 °C along the direction perpendicular to the ripple in Figs. 2(b), 2(c), and 2(e) are shown in Fig. 5. As can be seen in Fig. 5, the average heights and periods of the ripple 'hills' are 2.2 nm and 800 nm, 3.1 nm and 1300 nm, 5.2 nm and 1470 nm for sample grown at 700 °C, 730 °C, and 800 °C respectively. The average height and period both become larger at higher growth temperatures.

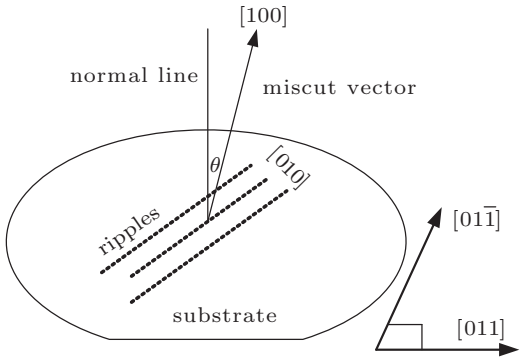


Fig. 4. Schematic diagram of the miscut vector of the Si (100) substrate and the ripples on the surface. The angle between the miscut vector [100] and the normal line is $\theta = 0.25°$. Before growth under atmospheric condition, the step edge direction is along [01$\bar{1}$], but during growth, the stable step edge is parallel to the direction of the ripples.

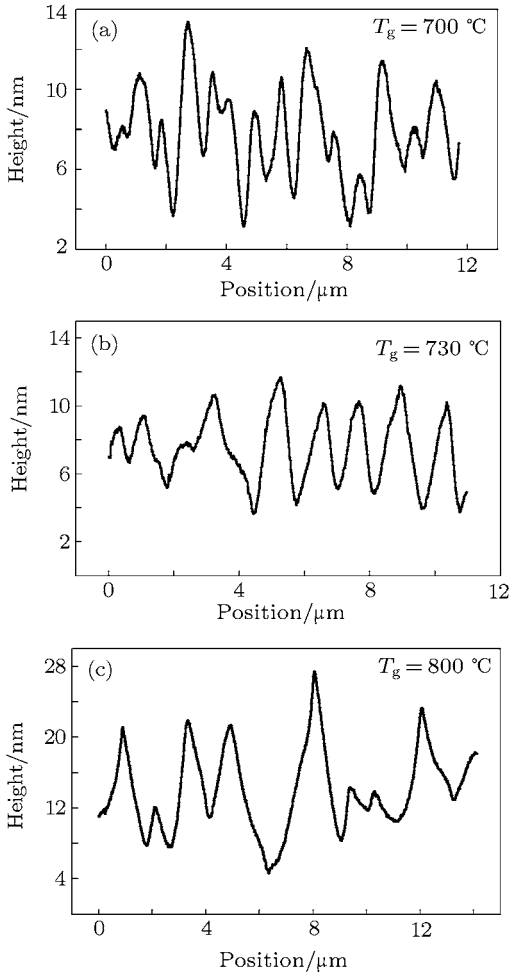


Fig. 5. The ripple height profiles of samples grown at 700 °C (a), 730 °C (b), and 800 °C (c) along the line in the AFM image which is perpendicular to the ripples. The average heights and periods of the ripple 'hills' are 2.2 nm and 800 nm, 3.1 nm and 1300 nm, 5.2 nm and 1370 nm for samples (a) T_g = 700 °C, (b) 730 °C, and (c) 800 °C respectively.

3.3. Ripple formation and disappearance

The diffusion of adatoms is highly anisotropic on the terrace. The diffusion parallel to the dimer rows is a factor of 1000 times faster than that perpendicular to them.[14,15] As a result, during epitaxy in step-flow mode, the S_B steps advance faster than the S_A steps. They finally come together to form biatomic steps. For a biatomic step, the speed of the upper S_B step is limited by that of the lower S_A step. However, when the misorientation is smaller than 6° the biatomic step is unstable and tends to relax back to monatomic step at high temperatures during growth.[9,16] Therefore, the S_B steps tend to keep a distance d_{avg} from the S_A steps. According to Poon *et al.*'s work[17] the $d_{avg} \approx 20a_l$ at 500 °C, where a_l is the lattice constant. We will call the S_A and S_B steps the S_B/S_A pair instead of biatomic step in the discussion below. The vicinal surface morphology after this early stage of step-flow growth is shown in Fig. 6(a). It seems that a series of units of S_B/S_A pairs are formed everywhere.

After the early stage of step-flow growth discussed above, the following epitaxy may be unstable or stable, depending on whether several S_B/S_A pairs may catch up with each other or not. If the step-flow growth is unstable, several S_B/S_A pairs may come together to form a 'higher hill' on the vicinal surface. If the step-flow growth is stable, the vicinal surface morphology still consists of a series of S_B/S_A pairs as shown in Fig. 6(a). The stability of the step-flow growth is determined mainly by the competition between two mechanisms: the Ehrlich–Schwoebel (ES) barrier[18] and the elastic repulsion between S_A and S_B steps.[19]

Adatoms which migrate across the terrace of each S_B/S_A pair will encounter the Ehrlich–Schwoebel (ES) barrier which prevents diffusion across the terrace. The ES barrier on clean Si (100) surface is observable[20] and apparently low.[21] The ES barrier has a significant influence on the stability of the S_B/S_A

pairs, depending on whether the ES barrier hinders the diffusion of atoms from lower to upper terraces or hinders the diffusion from upper to lower terraces. According to the work of Mo *et al.*,[14] there is no energy barrier for an adatom to diffuse from the upper T_B terrace to the lower T_A terrace, and the S_B step is a good sink for the adatom. Besides, in their work the denuded zone which was caused by the anisotropic diffusion was not seen on the T_A terrace near the S_A step in low flux, thus there is a barrier which prevents the diffusion from lower T_B terrace to upper T_A terrace. Therefore the ES barrier of the S_B/S_A pair should hinder the diffusion from lower to upper terrace.

If we assume that the step edges of each S_B/S_A pair are straight and the adatom diffusion length is much larger than the terrace width, the motion of the S_B/S_A pairs can be understood in terms of a simple model[16,22] of step flow: $v_n(t) = \mathrm{d}X_n/\mathrm{d}t = k_1W_{n-1}(t) + k_2W_n(t)$, where $v_n(t)$ and $X_n(t)$ are, respectively, the position and the speed of the n-th step of S_B/S_A pairs at time t; k_1 and k_2 are the coefficients. The step index n increases in the direction of step motion. $W_n(t) = X_{n+1}(t) - X_n(\mathrm{t})$ is the width of the terrace in front of the n-th step. As mentioned above, the ES barrier of Si hinders the diffusion from lower to upper terraces, the speed of a step of the S_B/S_A pair now has a positive correlation with the width of the upper terrace: $v_n(t) = k_1W_{n-1}$, $k_1 > 0$. During growth, if the fluctuations advance to the n-th step of S_B/S_A pairs, the $(n-1)$-th terrace width will be larger than that of the n-th terrace: $W_{n-1} > W_n$. As can be seen in Fig. 6(b), before the growth is affected by the fluctuations, the widths of the $(n-1)$-th and the n-th terraces are the same (solid line). After the fluctuations, $W_{n-1} > W_n$ (dash line). As a result the speed of the n-th S_B/S_A pair ($v_n = k_1W_{n-1}$) becomes even faster than that of the $(n+1)$-th step ($v_{n+1} = k_1W_n$): $v_n > v_{n+1}$. The n-th step moves faster and faster while the $(n+1)$-th step moves slower and slower under the effect of the fluctuations. Finally, a structure is formed after two S_B/S_A pairs have met each other. This analysis is also valid if the fluctuations slow down the n-th step. In this situation the n-th step will be caught up by the $(n-1)$-th step and also form a structure composed of two S_B/S_A pairs. Obviously, the fluctuation is a positive feedback to the growth when the ES barrier hinders the diffusion from lower terrace to upper terrace. As shown in Fig. 6(c), the moving speed v_2 of the structure formed by two S_B/S_A pairs is slower than that of one S_B/S_A pair, because the upper S_B/S_A pair cannot move before the bottom S_B/S_A pair advances. Consequently, the S_B/S_A pair tends to catch up with the structure formed by two S_B/S_A pairs, forming an even bigger structure. This process occurs continuously, and pyramid-like structures consisting of several S_B/S_A pairs will be formed, until the pyramid is big enough to prevent the diffusion across steps and the fluctuations. The pyramids which have more S_B/S_A pairs move more slowly than those with less S_B/S_A pairs. The average speed of an S_B/S_A pair is v_1, the speed of a pyramid with m S_B/S_A pairs is v_m, as indicated by Kandel *et al.*,[16] v_1 is approximately m times v_m, i.e. $v_m = v_1/m$. As a result, when the pyramids grow bigger, the speeds of different pyramids become the same. Thus a series of pyramids with uniform size are formed on the vicinal surface as shown in Fig. 6(d). We can draw a conclusion that the ES barrier of Si destabilizes the step-flow growth.

Unlike the ES barrier, the elastic repulsion between S_A and S_B steps tends to stabilize the step-flow growth.[19] The elastic repulsion is caused by the strain anisotropy, i.e., the tensile strain perpendicular to the dimer rows is different from the compressed strain along the dimer rows.[11] In the absence of ES barrier, the elastic repulsion stabilizes the step-flow by preventing the steps from accidentally bunching.[23]

In order to explain the formation and the disappearance of the ripples, we assume that the effect of the elastic repulsion is weaker than that of the ES barrier when $T_g = 700$ °C and 730 °C. As a result, the step-flow is unstable under the effect of the ES barrier and a series of pyramid-like structures are formed on the vicinal surface. The pyramid-like structures lead to a rippled surface morphology when $T_g = 700$ °C and 730 °C.

At a higher temperature ($T_g = 750°$), the energy of adatom is high enough to overcome the ES barrier and the effect of the ES barrier is less important: $D_+/D_- \propto \exp(2E_{ES}/k_BT)$, where E_{ES} is the ES barrier, D_+ and D_- are the diffusion coefficients along and reverse to the ES barrier, respectively. As can be seen, D_+ and D_- tend to be the same at high temperature. However, in this case the elastic repulsion keeps on stabilizing the step-flow. The elastic repulsion is strong enough to prevent the fluctuations. Consequently, the bunching between S_B/S_A pairs cannot occur and the step-flow is stable, which leads to a smooth surface free of ripples.

When $T_g = 800$ °C, the temperature is high

enough so that the dimer vibrates frequently and starts bulking collectively.[24,25] Thus, the strain anisotropy is weakened and the effect of elastic repulsion is no longer strong enough to prevent the fluctuations. Therefore, there is no mechanism to stabilize the step-flow. Accidental bunching between S_B/S_A pairs occurs under fluctuations. After the accidental bunching, a series of S_B/S_A pairs comes together to form a pyramid-like structure. As discussed above, pyramids which have more S_B/S_A pairs move more slowly than those with less S_B/S_A pairs. Finally, rippled surface morphology is formed with a series of pyramid-like structures of uniform size.

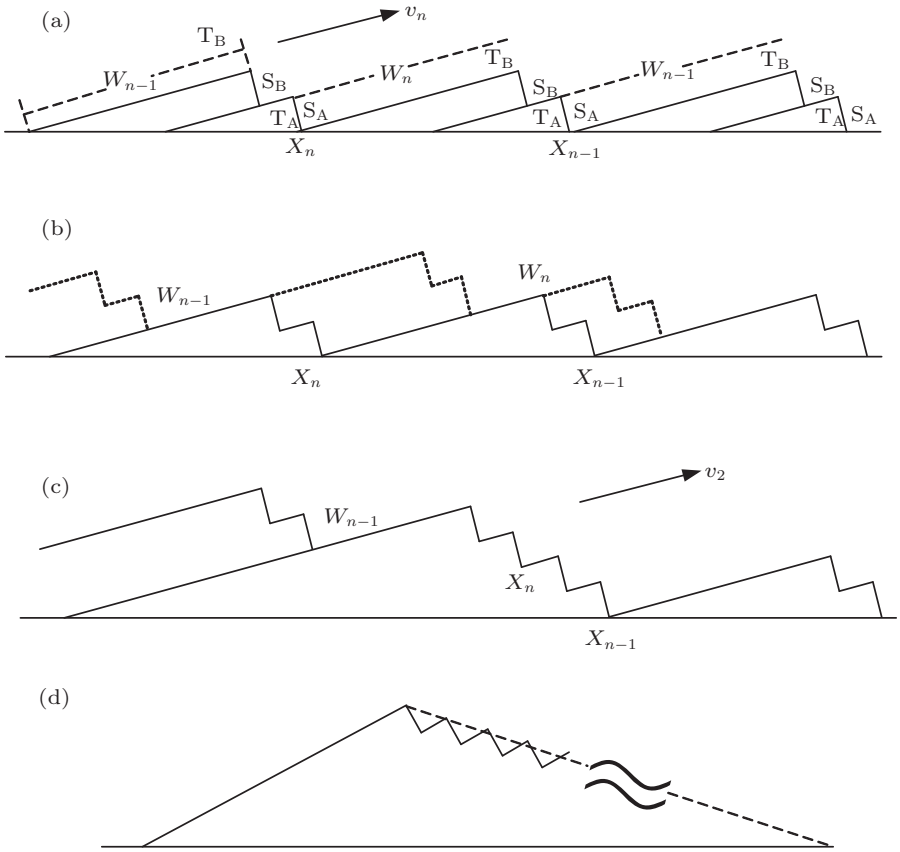


Fig. 6. Schematic diagrams of the evolution of ripples on the epitaxial Si layer surface. (a) After the early stage of the epitaxy, a series of S_B/S_A pairs are formed on the vicinal surface because of the diffusion anisotropy. The step of S_B/S_A pairs advances along the direction of the arrow. X_n and v_n are the position and the speed of the n-th step, W_n is the terrace width in front of the n-th step. (b) If the fluctuations advance to the n-th step, the width of terrace in front of the $(n-1)$-th step will be larger than that in front of the n-th step. In the case when ES barrier hinders the diffusion from lower terrace to upper terrace, the n-th step will catch up with the $(n+1)$-th step. The solid line and the dashed line represent the step structure before and after the fluctuations during growth, respectively. (c) The structure formed by two S_B/S_A pairs moves more slowly than that formed by one S_B/S_A pair, because the upper S_B/S_A pairs cannot move until the bottom S_B/S_A pairs advance to meet them. (d) The bunching keeps on occurring, finally forming a series of pyramid-like structures with several S_B/S_A pairs, until the pyramid is large enough to prevent the diffusion and fluctuations.

4. Conclusion

The Si homoepitaxy is carried out at the values of growth temperature T_g = 650 °C, 700 °C, 730 °C, 750 °C, and 800 °C on Si (100) surface with 0.25° misorientation towards [011] direction. Growth mode changes from 2D island mode to step-flow mode as T_g elevates from 650 °C to 700 °C. When the layer is grown in step-flow mode, a series of S_B/S_A pairs is formed on the vicinal surface at the early stage because of the diffusion anisotropy. The ES barrier of the S_B/S_A pairs, which hinders the diffusion from lower terrace to upper terrace, leading to the formation of ripples when T_g = 700 °C and 730 °C. The elastic

repulsion between S_A and S_B steps tends to stabilize the step-flow. At $T_g = 750$ °C, the effect of the ES barrier vanishes but the elastic repulsion still exists, thus the surface of the epitaxial layer is smooth and free of ripples. When $T_g = 800$ °C, the buckling and the vibration of dimers weaken the elastic repulsion between steps, thus the ripples appear again because of the accidental bunching.

Our model has a limitation in consideration of the competition between ES barrier and elastic repulsion in that there are no detailed data available to support it. Nevertheless, the phenomenon may be important for the Si homoepitaxy using the CVD technology and for Si device fabrication.

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