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# Faceting and nanostructure effects in Si and SiGe epitaxy☆

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A R T I C L E I N F O

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A B S T R A C T

Epitaxy in Si technologies has to be integrated in the flow of fabrication; in most cases, it has to be selective and deposition takes place in extremely small patterns.
In a first part, Si or SiGe epitaxy faceting is presented and discussed. Today, the global view is that, at first order, faceting is a kinetic phenomenon, controlled by deposition kinetic anisotropies. On the contrary, in a second part we show that highly faceted structures tend to decrease their surface energy by thermal rounding and that this phenomenon is very important when considering very small (20–40 nm) patterns.
The main part reports on the combination of faceting with small size effects. Experiments consist in depositing $Si_{0.72}Ge_{0.28}$ selectively in very narrow (35–80 nm) lines oriented either along <110> or <100> crystal axis on (100) Si wafers. Preliminary observations clearly demonstrate an important {100} faceting that is often not observed or reported in literature. Our results also evaluate the lateral overgrowth of selective epitaxies. <110>-oriented lines lead to a certain lateral epitaxial overgrowth that is limited by {111} facets whereas epitaxies in <100> lines present a much larger (>2 times) overgrowth bordered by {100} facets.
Finally, we demonstrate that the edge effects have to be taken into account. Firstly, the amount of epitaxial material deposited in narrow lines depends on the line orientation, and then we propose the concept of "anisotropic loading effect". Secondly, we found that deposition rates in small patterns are not constant with time. This corresponds to "time-nonlinear loading effects" that were never conceptualized in literature.


## 1. Introduction

Si, SiGe, SiC and Ge heteroepitaxial growths (epi) are of great interest in Si-based technologies as they allow dramatic performance improvements or even new device fabrication at a minimal additional cost. These materials have to be integrated in more and more complex technologies/devices, i.e. with lower thermal budgets; and the present trends in epi are mainly: higher Ge and C contents, higher stresses, various crystal orientations and smaller lateral sizes. In majority of cases, deposition has to be selective and, in any case, its morphology that plays a very important role has to be controlled. Stress, growth anisotropy and small size effects have then to be examined. This contribution will firstly review main anisotropic effects in epi, and will then report observations when deposition takes place in very small active zones. That way, we will propose 2 concepts of "non standard" loading effects.

## 2. Faceting background

From a general point of view, SiGe/Si epi morphology, strained hetero-epi, is considered to be mainly controlled by islanding and faceting. However, islanding or Stranski–Krastanov growth, well documented in literature and not specific to nanostructures, will not be considered in the present contribution. On the other hand, as seen later, another mechanism, named here as thermal rounding has to be taken into account.

Faceting is a long concern in Si and SiGe selective epi growth (SEG) [1]. As illustrated in Fig. 1, it consists in the fact that the deposition morphology tends to be limited by certain dense planes, {111} and {311} being the most current ones. More recently, a certain effort has been made in order to provide more extensive and more accurate experimental results. Thus, faceting results have been reported for different configurations, different materials and different processes, i.e. SEG, non-SEG and even HCl chemical etching [2–3]. In each case, facets were found to behave very similarly. Fig. 2 reports the transmission electron micrograph cross-section (XTEM) of a Si/SiGe epi deposited on a wafer that already presents different dense planes on its top surface. It appears that flatness of each zone is respected during deposition and that deposited thickness is specific to the plane. Thus, facets are stable enough and are propagating during epi. This kind of experiments and characterizations also allowed to determine the kinetics of the main planes. As an example, the kinetics found in Si SEG carried out with the usual $H_2/SiH_2Cl_2$ (DCS) chemistry are reported in Fig. 3 in the form of Arrhenius plots. We observe that the (100) plane has the highest kinetics and the highest activation energy, especially as compared to {311}. As a consequence, the ratio $r_{311}$, defined as the growth rate ratio between {311} planes and

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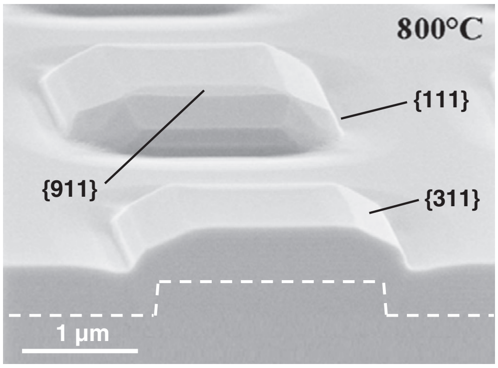


**Fig. 1.** XSEM observation of faceting in Si epi. Full sheet epi was run with $H_2/SiH_4$ chemistry on (001) Si wafers with a structured surface. Patterns consist in Si relief with <110>-aligned vertical Si sidewalls prepared via anisotropic dry etch. The initial wafer morphology is underlined (dashed-line) on the cross-section.

(001) ones, significantly varies with temperature, it decreases from 0.82 to 0.44 when the temperature is increased from 700 °C to 850 °C.

At the same time, a theoretical frame was built in order to give a better insight of the underlying mechanisms of faceting [4–5]. The present view of faceting is illustrated in Fig. 4 for a given configuration, i.e. between two $SiO_2$ vertical walls. Fig. 4a and b gives the evolution of Si SEG with deposition temperature. Thin SiGe markers were introduced in order to visualize the formation and propagation of facets. At 850 °C, {311} facets appear and enlarge in such a way that the (001) plane is completely occluded after the fourth Si film. On the contrary, at 750 °C, no facets, neither {111} nor {311} ones, appear. Fig. 4c and d reports the theoretical morphologies considering that deposition morphology is fully determined by plane kinetics. On one hand, dashed lines represent the most advanced positions of the (001), {311} and {111} planes allowed by their relative kinetics $r_{ijk}$ (see Fig. 3). On the other hand, bold lines draw the morphology that would correspond to the most limiting of these planes. Thus, we concluded that faceting in SEG results primary from kinetics anisotropy and not from surface energy anisotropy [4].

## 3. Thermal rounding

Despite its important role, thermal rounding has not been studied to a so large extent as faceting. As a general rule, epi has the tendency to reduce its internal energy that includes the surface or interface energy given by:

$$E_s = \int_S g_s dS,$$

$\gamma_s$ being the anisotropic surface or interfacial energy and S the corresponding surface. Besides surface energy anisotropy that is moderate,

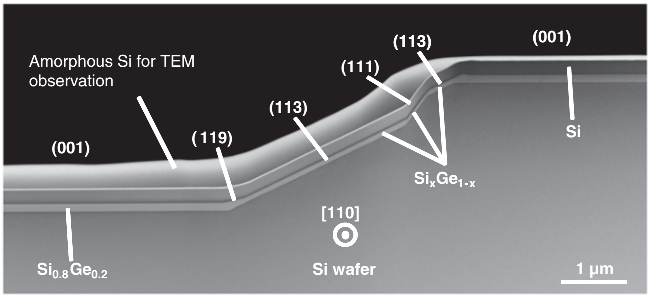


**Fig. 2.** Dark field XTEM observations of a $Si/Si_{0.8}Ge_{0.2}$ stack deposited with $H_2/SiH_4/GeH_4$ chemistry on <110>-(001) Si wafer after surface relief creation.

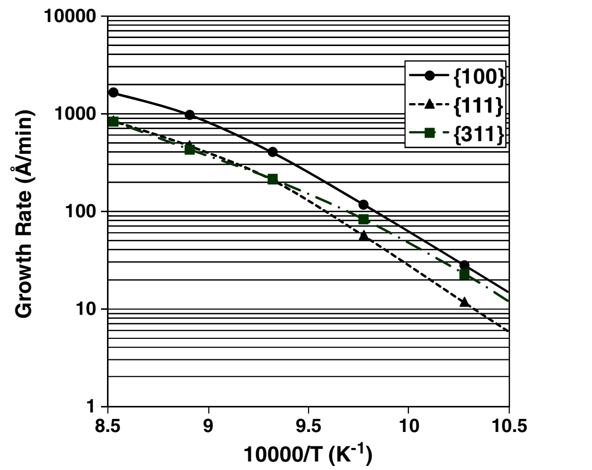


**Fig. 3.** Arrhenius plots of growth kinetics of the (001), {311} and {111} planes in Si selective epi using $H_2$/DCS chemistry: $P_{total} = 2000$ Pa, $P_{DCS} = 4.7$ Pa and T varied from 700 °C to 900 °C modulo 50 °C.

chemical potential is related to the local curvature and then atoms have tendency to migrate from zones with high positive curvature towards lower curvature leading then to a reduction of the mean curvature. This mechanism takes place as soon as surface atoms get a significant mobility: during deposition if temperature is high enough or even more effectively after deposition.

Fig. 5 reports the morphology of SiGe SEG when submitted to different post-deposition $H_2$anneals. SEG was deposited in [100]-aligned patterns on (001) substrates. In this configuration, there are no limiting dense planes such as {111} or {311} ones and consequently no large facets, and horizontal and vertical planes that limit epi are supposed to be {100} ones. In Fig. 5a, where no significant post-deposition anneal was applied, morphology corresponds more or less to a conformal deposition. On the contrary, with increasing post-deposition thermal budgets, morphology dramatically evolves and tends towards quasi cylindrical or spherical shapes, Fig. 5b and c. In this case, and even for moderate thermal budgets, because of the small size of epitaxial area and of a high atom mobility during $H_2$ anneal, the final morphology of SEG is dominated by thermal rounding.

## 4. Small size effects in SEG

### *4.1. Experimental details*

As advanced applications often require epi deposited in very small (10–40 nm) areas with different crystal orientations, this part reports behavior of SiGe SEG in narrow lines and compares results as a function of the line orientation. Two types of (100) Si wafers, with different in plane orientations, were patterned via a $SiO_2$ shallow trench isolation (STI) in order to obtain trenches oriented along <110> or <100> axis. Epi were carried out using the DCS/$GeH_4/H_2$ chemistry in a 300 mm industrial RTCVD (Rapid thermal chemical vapor deposition) reactor. The deposition temperature was 620 °C and gas flows chosen in order to maintain good deposition selectivity and to obtain Ge content around 28%. For most of the results reported below, the wafer unloading procedure was adjusted in order to minimize the thermal budget after the deposition step, i.e. lamp heating system was switched off. This way, the morphology is thought to really correspond to the as-deposited morphology, i.e. very close to the morphology during deposition. For comparison purpose, some other samples were prepared with similar SiGe selective epitaxial growth (SEG) but with a significant post-deposition thermal budget. Finally, deposition morphologies were extensively characterized via scanning electron microscopy (SEM) and different variants of TEM using Hitachi S9380