Epitaxial growth of a nanoscale, vertically faceted, one-dimensional, high-aspect ratio grating in III-V materials for integrated photonics

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Homoeptaxial selective growth of a GaAs nanoscale, high-aspect ratio, one-dimensional (1D) grating with vertical facets is reported. For a pattern direction along [110], the kinetics of faceting in selective molecular-beam epitaxy (MBE) induce (110)-type facets vertical to a GaAs(001) substrate near the boundary between an SiO2 mask and an open substrate area. On a 1.25-μm period, 1D stripe, SiO2-patterned GaAs(001) substrate with an opening width of ~ 300 nm, vertical faceting results in a grating structure consisting of 2.8-μm-high, 820-nm-wide features. Kinetics of faceting in selective MBE is explained as a result of the minimization of total surface energy.

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Facets vertical to a (001) orientation substrate have many important applications in optoelectronic semiconductor devices such as laser diodes. Generally, these facets are generated by cleaving of a semiconductor substrate, which is not compatible with integration processes. An alternative choice for vertical faceting is etching. An etched surface is, however, not strictly vertical to the substrate and suffers from etching damage roughness resulting in light-scattering losses. For integration of laser diodes and other resonator structures into large-scale optoelectronic/photonic circuits, a process which can overcome these problems is required.

In this work, we report a directed self-assembly fabrication technique—a so-called “top-down/bottom-up” process—for the epitaxial growth of vertical facets, which is radically different from cleaving or from “top-down” chemical etching and is compatible with integration processes. Selective epitaxial growth and associated faceting developed for patterned molecular-beam epitaxy (MBE) is employed.

Several papers on patterned GaAs growth have been reported, but (110)-type sidewall facets vertical to a (001) substrate have not previously been achieved. Depending on the growth rate, the thickness and profile of the masking material employed for selective epitaxy, and the direction of the patterns, the resulting facets at a substrate-mask boundary can be vertical. We demonstrate the formation of {110} facets exactly vertical to a (001) substrate surface and with very low surface roughness by directed self-assembly, and interpret the kinetics of faceting in patterned growth as resulting from minimization of the total surface energy.

A 1.25-μm period, one-dimensional (1D) stripe pattern was fabricated in a 30-nm-thick SiO2 mask film prepared on a GaAs(001) substrate, by large-area, i-line interferometric lithography and dry etching. The pattern direction was aligned to [110]. The width of the open stripe in each period was ~ 300 nm. On this patterned substrate, GaAs was deposited at a growth temperature of 595 – 600 °C and a nominal growth rate of 0.03 monolayer/sec, which are the selective growth conditions for MBE. The substrates were rotated at 15 rpm during growth.

Figure 1(a) is a scanning electron microscope (SEM) image taken near the substrate-mask boundary of a GaAs epilayer selectively grown on a very wide stripe (100 μm) SiO2-covered (001) substrate. The deposition amount corresponds to a 300-nm-thick layer per unit area on a large-area unpatterned surface. This is denoted by 300 nm/cm2. The straight substrate-mask boundary is directed along [110]. As schematically shown in Fig. 1(b), the GaAs epilayer laterally grows over the SiO2 mask. The sidewall adjacent to the boundary consists of a tilted (111)B and a vertical (110) facet relative to the (001) substrate plane.

![Figure 1](image_url)

**FIG. 1.** (a) A cross-sectional SEM image of a GaAs epilayer selectively grown on a 100-μm-wide stripe opening fabricated into a 30-nm-thick SiO2-covered GaAs(001) substrate. The deposition amount corresponds to ~ 300 nm/cm2. (b) A schematic illustration of the cross section shown in (a) with facet identification. The dashed lines indicate lateral growth over the SiO2 mask.
Applying the same growth conditions to a periodically SiO\textsubscript{2}-patterned substrate, the vertical faceting results in a grating structure. Figure 2(a) shows a 1.25-\textmu m period 1D grating structure selectively grown on an SiO\textsubscript{2}-patterned GaAs(001) substrate. (b) A magnification of (a). The deposition amount of (a) and (b) is about 1 \mu m/cm\textsuperscript{2}. A bird’s-eye view SEM image of a 1D grating grown under the same growth condition as that employed for (a) except for a thicker growth (\sim 2 \mu m/cm\textsuperscript{2}). (c) A cross section of (c).

![Fig. 2](image_url)

Fig. 2. (a) An SEM image of a 1.25-\textmu m period 1D grating structure selectively grown on an SiO\textsubscript{2}-patterned GaAs(001) substrate. (b) A magnification of (a). The deposition amount of (a) and (b) is about 1 \mu m/cm\textsuperscript{2}. (c) A bird’s-eye view SEM image of a 1D grating grown under the same growth condition as that employed for (a) except for a thicker growth (\sim 2 \mu m/cm\textsuperscript{2}). (d) A cross section of (c).

The vertical sidewalls, a flat bottom, and two (111)B-type facets are clearly maintained up to a 2-\mu m-thick deposition. The actual height and width of each feature is increased to \sim 2.8 \mu m and \sim 820 nm, respectively, with an aspect ratio of about 3.4.

Figure 3 shows the detailed structure near the substrate-mask boundary for these two gratings. The as-grown samples were treated with dilute HF to remove the SiO\textsubscript{2} mask after the growth for better SEM contrast. The SiO\textsubscript{2} sites indicated in this figure correspond to the positions of the SiO\textsubscript{2} mask during growth. The growth of both grating fingers began from the \sim 300 nm open stripe surface between the SiO\textsubscript{2} stripes. However, lateral growth proceeds in both directions over the mask as indicated by the white arrows in Fig. 3. The apparent lateral growth rate (the lateral width of the SiO\textsubscript{2} mask covered by GaAs/growth time) of the (110)-type facets in Fig. 3(a) is about 4.5 nm/hr, which is similar to that in Fig. 3(b) of \sim 4 nm/hr. The ratio of apparent vertical to lateral growth rates of the grating shown in Fig. 3(b) is \sim 8.

There have been several reports on selective epitaxy on a patterned substrate.\textsuperscript{1-9} Most of these works have been done by metal-organic vapor phase epitaxy (MOVPE). It has been reported that growth on a stripe opening directed to [110] is terminated with forming an isoscales triangular cross section which consists of (111)B sidewalls,\textsuperscript{5} or laterally proceeds over a mask with the evolution into a polygonal cross section without (1\bar{1}0)-type facets as a major sidewall.\textsuperscript{6,7} One of the possible reasons for the absence of vertical faceting in MOVPE is deposition rate, which affects surface migration and diffusion. In MOVPE, we observe the vertical faceting...
similar to that presented in this work when the deposition rate is reduced to \( \sim 0.2 \text{ ML/sec} \). The details of vertical faceting in MOVPE will be reported elsewhere.

Minimization of the total surface energy can explain the vertical faceting. If only a (111)B orientation was available, the cross section of an epilayer selectively deposited on an open substrate surface would tend towards an isosceles triangle, as schematically illustrated in Fig. 4. Since vertical faceting happens at a certain point of the growth, however, the cross section must be changed from a triangle to a pentagon and a shape transition occurs. The total surface energy of the corresponding epilayer varies with this shape transition. In order for such variation to be energetically favorable, the total surface energy per unit length along the stripe direction of a single grating finger having a pentagon cross section \( (E_p) \) must be lower than that having a triangle cross section \( (E_t) \). These energies, \( E_t \) and \( E_p \), can be written as

\[
E_t = 2(a_1 \sigma_{(111)B} - a_1 \sigma_{(001)}) + 2a_2(\sigma_{\text{int-SiO}_2} - \sigma_{\text{SiO}_2}),
\]

\[
E_p = 2(b_1 \sigma_{(111)B} + h \sigma_{(110)} - a_1 \sigma_{(001)}) + 2b_2(\sigma_{\text{int-SiO}_2} - \sigma_{\text{SiO}_2}),
\]

where \( a_i \ (i = 1 \text{ to } 3) \) and \( b_j \ (j = 2 \text{ and } 3) \) are the side lengths indicated in Fig. 4, \( h \) is the height of the [110] vertical sidewalls of the pentagon which can be represented with \( a_i \) and \( b_j \)'s from the conservation of a cross section area in shape transition, and \( \sigma_{\text{int-SiO}_2} \) and \( \sigma_K [K = (111)B, (001), \{110\}, \text{ and SiO}_2] \) are the interfacial energy per unit area between the GaAs epilayer and the SiO\(_2\) mask and a surface energy per unit area of each facet and an SiO\(_2\) film, respectively.\(^{12}\) The interfacial energy between the sidewall of the SiO\(_2\) mask and the epilayer is neglected in Eq. (1) since the thickness of the SiO\(_2\) mask is considerably smaller than that of the epilayer in our gratings. In order for the shape transition, \( E_p < E_t \), which corresponds to \( \sigma_{(110)}/\sigma_{(111)B} < 2b \csc \theta/(a + b) \). At the initiation of the shape transition, it can be assumed that \( a_2 \approx b_2 \) in Fig. 4, which means \( h \rightarrow 0^+ \). By equating them in Eq. (1), the condition of \( E_p < E_t \) is simplified to

\[
\sigma_{(110)}/\sigma_{(111)B} < 1.23.
\]

Generally, it is known that \( \sigma_{(110)} \) is higher than \( \sigma_{(111)B} \) in cubic crystal structure. A theoretical calculation suggests \( \sigma_{(110)}/\sigma_{(111)B} \sim 1.05 \) under As-rich conditions.\(^{13}\) Equation (2) means that the shape transition can occur even for \( \sigma_{(110)} > \sigma_{(111)B} \) implying that the shape transition resulting in vertical facets on a (001) substrate can be explained by the minimization of total surface energy.

The vertical facets shown in Fig. 1(a) and the nanoscale gratings of Fig. 2 can be applied to the cavity mirrors of an integrated semiconductor laser and the semiconductor/air distributed-Bragg reflector of a short-cavity edge-emitting laser diode which requires strict verticality and low scattering. Epitaxial growth of nanoscale high-aspect-ratio 1D gratings has been reported. On a 1.25-\( \mu \text{m} \) period 1D stripe SiO\(_2\)-patterned GaAs(001) substrate with the opening width of 300 nm and the pattern direction parallel to [110], vertical faceting and lateral epitaxy result in a grating consisting of 2.8-\( \mu \text{m}-\text{high}, 820-\text{nm-wide features}. \) Kinetics of vertical faceting in selective MBE has been explained as resulting from the minimization of total surface energy.

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\(^{1}\)See, for example, R. Jambunathan and J. Singh, IEEE J. Quantum Electron. 33, 1180 (1997), and references therein.


\(^{12}\)In Eq. (1), the change of surface energy due to epitaxy is counted but the details of facet boundaries are not considered.