

DISLOCATION AND STRESS MANAGEMENT BY MASK-LESS PROCESSES USING SUBSTRATE PATTERNING AND METHODS FOR DEVICE FABRICATION

Cross Reference to Related Applications

5 This application claims the benefit of U.S. Provisional Application No. 61328203, filed 27 April 2010, the content of which is incorporated herein by reference and relied upon.

Field of the Invention

10 The invention relates to structures and methods for eliminating threading dislocations, layer cracking and wafer bowing in the epitaxial growth of lattice mismatched and thermally mismatched layers by using patterned substrates. Since materials choice and layer thicknesses are virtually unlimited, the invention can be applied also to the fabrication of devices requiring thick epilayers for their proper functioning, such as multiple junction solar cells, light emitting diodes, semiconductor lasers, radiation imaging detectors and thermo-electric devices. The invention is viable also for the fabrication of microelectronic, opto-electronic and photonic circuits requiring smaller thicknesses of mismatched epilayers.

Background of the invention

20 Attempts to extend Moore's Law by introducing new optical and electrical functionalities to the CMOS platform, realization of high-efficiency solid state lighting, manufacturing of concentrator photovoltaic cells, the fabrication of imaging detectors, especially for high-energy electromagnetic and particle radiation, and the fabrication of thermo-electric devices all require - in one form or another - the integration of crystalline materials with dissimilar lattice parameters on top of each other. This can occur basically in two different ways, either by wafer bonding or by "heteroepitaxial growth". This application belongs to the second method of combining materials, especially to materials the lattice parameters of which differ by more than a few tenths of a percent, and which may widely differ in their thermal expansion coefficients.

Problems related to lattice mismatch

30 When two mismatched materials are grown epitaxially on top of each other, their difference in lattice parameter (misfit) results in mechanical stress, which, when exceeding a certain limit, is relieved either by elastic or plastic relaxation. Under normal circumstances, when a deposit with sufficiently large misfit is made on a single crystalline substrate, stress relaxation can occur elastically, by means of surface corrugation, for example in the form of islands. Elastic relaxation cannot, however, proceed on a flat film. By contrast, for lower misfit, an epitaxial film may remain flat, while stress is relieved plastically by so-called misfit dislocations, once a certain critical film thickness has been exceeded. Eventually, no matter how large the misfit, plastic relaxation by interfacial misfit

dislocations always occurs. Whenever an interface with a significant density of misfit dislocations is incorporated in the active region of a device, e.g., a transistor, its performance may be degraded to a large extent. Interfaces containing misfit dislocations therefore usually need to be spatially separated from the active region of a device. Unfortunately, however, keeping interfaces with misfit dislocations at a distance from the active region of a device often does not guarantee its proper performance. In fact, it rarely happens that dislocations are localized exclusively at the interface between the two materials in the form of misfit dislocations. Misfit dislocations are usually rather accompanied by threading arms extending to the surface of the growing film. Also these threading dislocations can be very detrimental to the functioning of a device if they traverse the active region of a heteroepitaxially grown layer stack. The density of threading dislocations should therefore in general be kept as low as possible.

Problems related to thermal expansion mismatch

The dislocation problem, arising from the lattice misfit, is not the only obstacle to be overcome when epitaxially growing dissimilar materials on top of each other. In many instances the mismatch of the thermal expansion coefficients is equally serious, especially when layers with relatively large thicknesses are needed, for example in devices like high-brightness light emitting diodes for general lighting purposes, multiple junction solar cells, radiation detectors, thermoelectric generators, and many more.

The mismatch of thermal expansion coefficients may lead to wafer bowing upon cooling to room temperature after the epitaxial growth, seriously hampering subsequent processing steps, such as photolithography and patterning, or also further epitaxial growth. The different thermal expansion of epitaxial layers and substrate may even cause the former to crack, either right after epitaxial growth or during any subsequent temperature cycling, which necessarily occurs for example during the operation of concentrator photovoltaic cells (see for example V.K. Yang et al., Journal of Applied Physics **93**, 3859 (2003), the entire disclosure of which is hereby incorporated by reference).

The problem of wafer bowing has been addressed in various ways in the past. One approach consisted in introducing interlayers with reduced crystallinity functioning as stress relaxation layers (see for example US patent application number US2008/0308909 to Masahiro Sakai et al., the entire disclosure of which is hereby incorporated by reference). Another approach involved backside coating of the substrate by some material exerting the opposite stress upon wafer cooling (see for example US patent application number US2003/0033974 to Tetsuzo Ueda, the entire disclosure of which is hereby incorporated by reference). Unfortunately, however, reducing wafer bowing may even increase the tendency of the overlayer to crack, because wafer bowing is associated with partial elastic stress relief.

An alternative way for reducing wafer bowing has been described for example in US patent application number US2008/0233716 to Kazuhide Abe, the entire disclosure of which is hereby

incorporated by reference. Therein, deep grooves are formed in a silicon carbide film perpendicular to the direction along which bending on a semiconductor wafer occurs, thereby reducing said bending.

In a related approach, a mechanical stress absorbing system has been designed in which about 10 μm deep and 1 μm wide grooves are formed in a support substrate, onto which a nucleation layer is transferred from a transfer substrate by wafer bonding techniques (see for example US patent application number US2006/0216849 to Letertre et al., the entire disclosure of which is hereby incorporated by reference). In order to effectively relieve stress during temperature incursions in thick epitaxial layers grown onto the nucleation layer, a stress absorbing buffer layer is additionally needed underneath the nucleation layer, similar to the interlayer described in US patent application number US2008/0308909 to Masahiro Sakai et al., the entire disclosure of which is hereby incorporated by reference. Stresses are supposed to be absorbed by defect generation, local material displacement or creep, depending on the nature of the buffer layer. These stress relief mechanisms need to be very effective, when layer cracking and wafer bending are to be eliminated, in case of thick epitaxial layers with large lateral dimensions, i.e., extending essentially across the whole wafer. Material displacement or creep would therefore have to occur over macroscopic distances, which is very unlikely to happen in practice.

The same applies to a related approach in which the relaxation of misfit stress in epitaxial SiGe/Si(001) layers is assumed to occur by a slipping process, the SiGe epilayer thereby remaining cubic. Here, a thin SOI substrate is used instead of a bulk silicon substrate (see for example US patent number US5,759,898 to Ek et al., the entire disclosure of which is hereby incorporated by reference). Despite of a comparatively low viscosity at sufficiently elevated temperatures, it seems highly unlikely that this slipping process would ever happen on a macroscopic scale.

While wafer bowing and layer cracking are severe practical problems arising typically at layer thicknesses beyond 1 μm , threading dislocations, intimately related to plastic strain relaxation, are normally present already at smaller layer thickness for significant lattice misfits of the order of a fraction of a percent or more.

There have been many attempts to lower threading dislocation densities (TDD) in blanket films, such as compositional grading of buffer layers (see for example US patent number US5,221,413 to Brasen et al., the entire disclosure of which is hereby incorporated by reference). Alternatively, buffer layers containing high defect densities may facilitate dislocation nucleation and annihilation (see for example H. Chen et al., Journal of Applied Physics **79**, 1167 (1996), the entire disclosure of which is hereby incorporated by reference).

Still other methods involve epitaxial growth of parts of a layer at different substrate temperatures, one example being a Ge base layer deposited at low substrate temperature, followed by a second Ge layer at higher temperature (see for example US patent number US6,537,370 to Hernandez et al., the entire disclosure of which is hereby incorporated by reference). The idea behind

this was to suppress or at least reduce island formation by the Stranski-Krastanow mechanism at the early stage of growth, since merging islands and rough surfaces result in larger TDDs.

In addition, post-growth thermal annealing was shown to enhance dislocation glide and annihilation. Cyclic thermal annealing appears to be particularly efficient. Here, the temperature is cycled between a first value above the brittle/ductile transition (i.e., close to the melting point of the epitaxial layer) and a second value below the first. A significant reduction of the TDD was observed for example in Ge films epitaxially grown on Si(001) substrates by using this procedure (see for example US patent number US6,635,110 to Luan et al., the entire disclosure of which is hereby incorporated by reference). The method does not, however, solve the problem of wafer bowing and crack formation, when Ge in the form of blanket films is grown to substantial thicknesses of several micrometers, and the TDD still remains very high, of the order of typically $2 \cdot 10^7 \text{ cm}^{-2}$ for 1 μm thick films.

Problem solving by limited area epitaxy using dielectric masks

Whenever epitaxial layers are grown in the form of continuous films onto a substrate characterized by a significant lattice and thermal expansion mismatch, one is faced with the problems of excessive TDD as soon as the misfit strain starts relaxing plastically, as well as wafer bowing and crack formation at larger thicknesses.

It was realized long ago that a significant further reduction of TDDs can only be achieved by reducing the epitaxial growth area, i.e., by making the epitaxial structures small. This can be achieved by providing the substrate with a dielectric mask, exposing the substrate surface only within openings previously defined by lithography and etching. The idea behind is, that with sufficient layer thickness, threading arms arising from the interface will exit the sides of the epitaxial structure, rather than reaching the upper surface.

The concept was applied to various semiconductor combinations, such as Si, Ge, III-V materials, II-VI materials (see for example UK patent application number GB2 215 514 to Goodfellow et al.). Similarly, the concept was applied to GaAs mesas grown into oxide openings on Si(001) by molecular beam epitaxy (MBE) or chemical vapour deposition (CVD), any material deposited on the oxide mask being removed in a chemical etching step (see for example US patent number US5,158,907 to Fitzgerald, the entire disclosure of which is hereby incorporated by reference). The technique, also termed "epitaxial necking", was shown to be effective not only in reducing TDDs in GaAs mesas grown on Si by MBE, but also in eliminating cracks (see for example Fitzgerald et al., Journal of Electronic Materials **20**, 839 (1991), the entire disclosure of which is hereby incorporated by reference).

The idea of causing defects to terminate at non-crystalline sidewalls, has, in addition to "epitaxial necking", become known also under the name of "Aspect ratio trapping (ART)" (see for example International patent application number WO2008030574 to Bai et al., the entire disclosure of

which is hereby incorporated by reference). Limiting the epitaxial growth area, in combination with the cyclic thermal annealing mentioned before, was also shown to lead to a drastic reduction of TDDs in Ge mesas grown epitaxially on Si(001) (see for example US patent number US6,635,110 to Luan et al., the entire disclosure of which is hereby incorporated by reference).

Limited area epitaxy, even when combined with thermal annealing, is not, however, sufficient by itself for complete removal of threading dislocations, even when feature sizes are kept very small. To understand this, it is necessary to consider the nature of the dislocations. In cubic semiconductors the most common dislocations are so-called 60-degree dislocations, where Burgers vectors and dislocation lines enclose an angle of 60 degrees with one another, and are both located in {111} glide planes (see for example Blakeslee, Mat. Res. Soc. Symp. Proc. **148**, 217 (1989), the entire disclosure of which is hereby incorporated by reference). Such dislocations can reach the edge of epitaxial regions by gliding under the influence of stress, or simply reach the interface to the dielectric once the epitaxial structure is sufficiently high, such that their glide plane no longer cuts through the growth front. There are, however, also so-called sessile dislocations with dislocation lines perpendicular to the interface. They are not affected by stress, and can only be induced to deflect from their vertical orientation by interacting with inclined surface facets. It has indeed been shown that the mechanism of dislocation deflection is present in faceted GaN islands, and can lead to a significant reduction of the TDD (see for example Knoke et al., J. Cryst. Growth **310**, 3351 (2008), the entire disclosure of which is hereby incorporated by reference). Surface faceting is expected to have the same effect for group IV and for compound semiconductors (see for example International patent application number WO2008030574 to Bai et al., the entire disclosure of which is hereby incorporated by reference).

Instead of forming limited epitaxial regions in the form of mesas it has been argued that large area heteroepitaxy of mismatched materials with low TDDs should be possible by introducing dislocation sinks in the form of substrate pits. This provides the additional advantage of substantially planar surfaces (see for example European patent application number EP0 505 093 to Bean et al., the entire disclosure of which is hereby incorporated by reference).

A further extension of the technology of TDD reduction involved combining the described patterning by means of dielectric masks with selective epitaxy, followed by epitaxial lateral overgrowth (ELO). For the example of Ge on Si(001) it was argued that by continuing the process until coalescence one may hope to obtain essentially defect-free blanket films (see for example Langdo et al., Applied Physics Letters **76**, 3700 (2000), the entire disclosure of which is hereby incorporated by reference). Obviously, however, the problems of wafer bowing and layer cracking would come into play upon increasing the layer thickness further.

In addition, for epitaxial necking to be efficient, the aspect ratio between the height and width of the mask openings should at least be approximately equal to one. For films with thicknesses below about 1 μm it is therefore necessary to use submicron-lithography for defining the size of the mask

openings. Even smaller dimensions of the openings are required when elastic relaxation is to contribute significantly to the relaxation of the misfit strain (see for example US patent application number US2008001169 to Lochtefeld et al., the entire disclosure of which is hereby incorporated by reference).

5 All methods relying on the epitaxial growth into dielectric windows are furthermore limited by the heights of window sidewalls, since the masks cannot be made arbitrarily thick. This also limits the heights of the regions where dislocation trapping may occur.

Still an alternative approach involved the use of selective epitaxial growth on *protrusions* of crystalline substrate material surrounded by a dielectric mask rather than growth into pits formed in
10 such a mask. In this approach, a buffer layer of Si nanowires is formed on a Si substrate, the nanowires standing perpendicular to the substrate surface and being surrounded by dielectric material through which they protrude. A compound semiconductor is selectively deposited onto the nanowire tips, followed by ELO until a continuous compound semiconductor layer is formed (see for example US patent application number US2008149941 to Li et al., the entire disclosure of which is hereby
15 incorporated by reference). While this approach may as well be effective in reducing the TDD in the compound semiconductor layer, it cannot eliminate the problems associated with the thermal mismatch, when the compound semiconductor layer extends across the whole wafer. As described before, the compound semiconductor layer would have to slip across the substrate over macroscopic distances during cooling from the growth temperature. This is not likely to happen in practice, since
20 neither is a dielectric layer arbitrarily soft, nor could the Si nanowires withstand the shear forces occurring during cooling.

The technology described above, i.e., substrate patterning allowing for “epitaxial necking” or ART, has been applied to the fabrication of electronic and optoelectronic devices made from lattice mismatched materials (see for example US patent application number US2009039361 to Li et al., the
25 entire disclosure of which is hereby incorporated by reference).

The possibility to replace Ge-wafers by Si-wafers as substrates for multi-junction solar cells has been identified as another important application of ART. This application implies the epitaxial growth of relatively thick layer stacks, unless cells are grown on both sides of the substrate. In this latter approach, taking the example of a triple-junction cell, the sub-cell with an intermediate bandgap
30 of about 1.1 eV is made from the Si substrate, while the sub-cell with the largest bandgap is typically made from InGaP, by an ART process applied for example to the top surface, as well as the sub-cell with the smallest bandgap by another ART process on the bottom surface of the substrate (see for example US patent application number US2009065047 to Fiorenza et al., the entire disclosure of which is hereby incorporated by reference). The approach of fabricating sub-cells on both sides of a
35 Si-wafer minimizes the problem of thermal layer cracking because of relatively thin epilayers. The narrow trenches of 300 – 500 nm typically used in ART may in addition allow for some elastic

relaxation, as well as the somewhat compliant nature of the SiO₂ mask. In view of frequent thermal cycling during solar cell operation, it may, however, still be disadvantageous to have a structure composed of laterally varying thermal properties. Moreover, the concept requires the use of wetting layers, which, in addition to the dislocation trapping regions, absorb some of the solar radiation, thus lowering the cell efficiency.

The problems with thermal mismatch appear to become even more significant when multi-junction solar cells are grown on the same side of a Si substrate by using ART and ELO processes. It has been suggested to replace the conventional triple-junction cell, featuring a bottom sub-cell made from Ge, by a triple-junction in which all sub-cells are made entirely from III-V materials (see for example International patent application number WO2010033813 to Fiorenza et al., the entire disclosure of which is hereby incorporated by reference). Although the Ge no longer acts as an active material in this type of cell, it was nevertheless suggested to form first a coalesced Ge layer by an ART + ELO process, before growing the active III-V layer stack. Coalescence is, however, accompanied by the generation of large TDDs in the regions where the growth fronts from neighbouring windows meet. This serious problem encountered in continuous layer formation by ART + ELO has not been solved to date (see for example Fiorenza et al., ECS Transactions 33, 963 (2010), the entire disclosure of which is hereby incorporated by reference). Furthermore, the coalesced Ge layer and the active III-V layers together, are necessarily at least 5 µm thick, such that wafer bowing and layer cracking must be expected to become serious obstacles during further device processing and solar cell operation.

Growth on mask-less patterned surfaces

Approaches leading to continuous layers

In an alternative class of patterning procedures the dielectric mask material is removed from the substrate wafer before epitaxial growth begins, or, alternatively, the patterning is performed without any mask at all. For Si substrates this is possible by using an electrochemical process called anodization, by means of which porous Si is formed. Such porous Si substrates have been used in the fabrication of group III nitride layers, with a Ge layer deposited on the porous Si substrate before the compound semiconductor layers (see for example US patent application number US2005199883 to Borghs et al., the entire disclosure of which is hereby incorporated by reference). The Ge interlayer was believed to reduce the thermal stress arising from the difference in thermal expansion parameters of the Si substrate and group III-nitride material. The porous Si layer on the other hand should accommodate the large lattice mismatch of the Si substrate and the nitride layer. As a result, fewer dislocations should be present in the nitride film, and layer cracking and substrate bowing should be avoided. While these arguments are valid on a small scale, they have to fail to a large extent on a

wafer scale, since a continuous group III-nitride layer would have to slip across the substrate by macroscopic distances during cooling from the growth temperature.

Alternatively, an epitaxial layer may be grown on a flat substrate first. Hereafter, stripes are etched into the layer in a manner in which part of the substrate is removed in between the remaining stripes. In a following selective growth process the material grows laterally from the remaining stripes, forming a suspended film over the etched substrate regions. The process, termed "pendeo-epitaxy", was first applied to epitaxial GaN layers on SiC substrates (see for example T. Zheleva et al., Journal of Electronic Materials **28**, L5 (1999), the entire disclosure of which is hereby incorporated by reference). While TDDs can be drastically reduced by the pendeo-epitaxy process, the problems associated with the thermal expansion mismatch remain for the same reasons as in all other approaches in which continuous layers are eventually formed on a thermally mismatched substrate.

In a further approach, the substrate was patterned in a way such as to form an array of weak posts of submicron size and with an aspect ratio above 0.5. A continuous GaN layer was then grown on top of the posts by pendeo-epitaxial methods (see for example US patent number US6,380,108 to Linthicum et al., the entire disclosure of which is hereby incorporated by reference). The weak posts are configured to crack due to the thermal expansion coefficient mismatch between the substrate and the GaN layer. Upon cooling from the growth temperature at least some of the weak posts should hence crack, thereby relieving stress in the GaN layer. The problem here is again that in order to be effective on a wafer scale, the majority of the posts would have to crack, leading to layer separation from the substrate. While this may indeed be desirable in some applications, it is inconceivable to avoid layer separation and yet release the stress on a wafer scale, again for the same reasons as explained above.

Approaches involving nanorods

As explained above, irrespective of the details of the fabrication procedure it has hardly been possible by prior art techniques to substantially reduce the TDD, and eliminate layer cracking and wafer bowing in the case of continuous layers, unless the total layer thickness is kept comparatively low. Upon relaxing the limited film thickness constraint, the only option to tackle all of these problems appears therefore to be one in which layer coalescence is avoided altogether. Besides providing a solution to the practical problems of layer cracking, wafer bowing and dislocation reduction, the use of discontinuous films may have other advantages. One such advantage is the possibility to employ larger In contents in the active layer of group III-nitride LEDs, without deteriorating the internal quantum efficiency, and, simultaneously achieving higher light extraction efficiency, as shown for InGaN quantum well active regions incorporated into GaN nanorods (see for example US patent application number US2007077670 to Kim et al., the entire disclosure of which is hereby incorporated by reference).

In the latter example a GaN buffer layer was first grown on planar sapphire wafers by an MOCVD process known to those working in the field. The nanorods were subsequently formed by using low substrate temperatures favouring vertical over lateral growth.

Instead of letting nanorods nucleate spontaneously, precise position control of nano-LEDs was obtained by patterning a substrate prior to nitride semiconductor growth. This has been demonstrated for example on Si(111) substrates, patterned in the form of an array of pillars of submicron size, and a height of about 5 μm . In this prior art the height of the epitaxial structures formed on mask-less substrates was comparatively small (less than 2 microns) and MOCVD deposition occurred equally in between the Si pillars (see for example Fündling et al., Physica Status Solidi A 206, 1194 (2009), the entire disclosure of which is hereby incorporated by reference). For the AlGaIn/InGaIn material system nitrogen-rich growth conditions and plasma-assisted MBE are necessary to favour vertical with respect to lateral growth rates to the extent necessary for nanowires to grow (see for example Stoica et al., small 4, 751 (2008), the entire disclosure of which is hereby incorporated by reference). For many devices it is, however, desirable to achieve structure heights of more than a micron. Some devices even require considerably larger height (or layer thickness), such as multiple-junction solar cells, especially for example triple junction solar cells of the conventional kind with Ge forming the bottom sub-cell. Yet taller structures of dozens of microns are necessary for example for X-ray detection.

An attractive way to achieve columnar growth in the AlGaIn/InGaIn material system has been found to be possible by means of low-energy plasma-enhanced vapour phase epitaxy (LEPEVPE) (see for example WO2006097804 to von Känel, the entire disclosure of which is hereby incorporated by reference).

It is an object of the present invention to provide means by which lattice matched and lattice mismatched semiconductor layers can be grown epitaxially in a mask-less process on pre-patterned substrates.

It is another object of the present invention to provide means by which semiconductor layers can be grown epitaxially in a mask-less process on pre-patterned substrates with different thermal expansion coefficients.

It is another object of the present invention to provide means by which lattice mismatched semiconductor layers with a low threading dislocation density can be grown epitaxially in a mask-less process on pre-patterned substrates.

It is another object of the present invention to provide means by which thermally mismatched, crack-free semiconductor layers can be epitaxially grown in a mask-less process on pre-patterned substrates.

It is another object of the present invention to provide means by which thermally mismatched semiconductor layers can be grown in a mask-less process on pre-patterned substrates without causing substrate bowing.

It is another object of the present invention to provide means by which growth of lattice and thermally mismatched semiconductor layers is restricted to the elevated regions of pre-patterned substrates.

It is another object of the present invention to provide means for fabricating semiconductor light emitting diode structures, monolithically integrated on thermally and lattice mismatched, pre-patterned substrates in a mask-less process.

It is another object of the present invention to provide means for fabricating microelectronic circuits monolithically integrated on thermally and lattice mismatched, pre-patterned substrates in a mask-less process.

It is another object of the present invention to provide means for fabricating semiconductor laser structures, monolithically integrated on thermally and lattice mismatched, pre-patterned substrates in a mask-less process.

It is another object of the present invention to provide means for fabricating imaging detectors, such as infra-red and X-ray pixel detectors, monolithically integrated on thermally and lattice mismatched, pre-patterned substrates in a mask-less process.

It is another object of the present invention to provide means for fabricating thermo-electric devices monolithically integrated on thermally and lattice mismatched, pre-patterned substrates in a mask-less process.

It is another object of the present invention to provide means for fabricating multi-junction solar cells, monolithically integrated on thermally and lattice mismatched, pre-patterned substrates in a mask-less process.

It is another object of the present invention to provide means for monolithically integrating devices requiring lattice and/or thermally mismatched semiconductor layers onto pre-patterned, CMOS-processed substrates in a mask-less process.

It is another object of the present invention to provide means for monolithically integrating devices requiring lattice and/or thermally mismatched semiconductor layers in a back-end CMOS-process.

Summary of the invention

The present invention provides means for fabricating active layer stacks of lattice matched, lattice mismatched and thermally mismatched materials on patterned substrates in mask-less processes. Substrates are patterned in the form of elevated regions, separated by narrow channels, the depths of which may exceed the smallest dimensions of elevated regions. A combination of elastic stress relaxation, and elimination of threading dislocations by annihilation, glide towards the edges of said elevated regions, line extension on slip planes during growth, or dislocation line deflection by surface faceting, minimizes threading dislocation densities. Layer cracking is prohibited, and wafer

bowing minimized, by avoiding material grown onto elevated substrate regions to merge. The invention can be applied to the fabrication of monolithically integrated photonic, opto-electronic, microelectronic and thermo-electric devices on lattice mismatched substrates.

Brief description of the drawings

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Figs. 1(a) to Fig. 1(b) are schematic views of a patterned wafer in top view and in cross-section.

Fig. 2 is a schematic process flow.

Figs. 3(a) to Fig. 3(c) are schematic cross-sections of a patterned wafer after epitaxial growth without and with surface faceting, and after renewed surface flattening.

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Fig. 4 is a schematic cross-section of a patterned wafer with groups of patterns.

Fig. 5 is a schematic cross-section of a layer grown on a patterned wafer after merging of epitaxial regions.

Fig. 6 is a schematic cross-section of a patterned wafer with oxidized bottoms and side walls.

Figs. 7(a) to Fig. 7(e) are schematic top views and cross-sections of patterned wafers with variations of patterns.

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Figs. 8(a) to Fig. 8(c) are SEM images of a patterned Si wafers in perspective view (a) and in plan view (b), (c).

Figs. 9(a) to Fig. 9(b) are perspective views of SEM images of different epitaxial structures grown by LEPECVD on patterned Si substrates.

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Fig. 9(c) is a top view of epitaxial structures grown by MBE on patterned Si substrates.

Fig. 9(d) is a perspective view of SEM images of epitaxial structures grown by selective CVD on patterned Si substrates.

Fig. 9(e) is a cross sectional view of epitaxial structures grown on patterned Si substrates with corresponding simulation.

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Figs. 10(a) to Fig. 10(b) are dark field STEM images of cross-sections through an 8 μm thick Ge epilayer on a patterned Si substrate.

Fig. 10(c) is a plan view of the boundary between patterned and unpatterned regions of a Ge epilayer after defect etching.

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Fig. 11(a) is a bright field cross-section TEM image of a 8 μm thick Ge epilayer on patterned Si substrate, the epilayer consisting of individual pillars

Fig. 11(b) is a bright field cross-section TEM image of a 8 μm thick Ge epilayer on patterned Si substrate, the epilayer consisting of regions with fused pillars.

Fig. 12(a) is a perspective view SEM image of a Ge layer grown on a patterned Si substrate showing regions of merged Ge-pillars.

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Fig. 12(b) is a plan view SEM image of a Ge layer grown on a patterned Si substrate showing regions of merged Ge-pillars.

Fig. 13(a) is a SEM image in perspective view of tall pillars.

Fig. 13(b) is a SEM image in perspective view of tall ridges.

Fig. 13(c) is a SEM image in plan view of the tall pillars shown in **Fig. 13(a)**.

Fig. 14(a) is a SEM cross-section image of a 30 μm thick Ge epilayer on a patterned and unpatterned Si substrate

Fig. 14(b) is a corresponding X-ray reciprocal space map of the Ge epilayers of **Fig. 14(a)** around the Si(004) and Ge(004) reflections.

Fig. 14(c) are intensity curves for the symmetrical (004) reflection of the Ge epilayers of **Fig. 14(a)** and of a Ge wafer.

Fig. 14(d) are enlarged views of X-ray reciprocal space maps around the Ge(004) reflections of the Ge epilayers of **Fig. 14(a)**.

Figs. 15(a) to Fig. 15(b) are Nomarski interference contrast images of a compositionally graded SiGe layer grown on a patterned Si substrate.

Fig. 16 is a schematic process sequence for device fabrication.

Fig. 17 is a schematic process for device fabrication by wafer flipping and bonding.

Fig. 18 is a schematic process for device fabrication by wafer bonding.

Detailed description of the preferred embodiment(s)

As described above, the present invention relates to the monolithic integration especially of lattice mismatched and/or thermally mismatched semiconductor layers in an epitaxial growth process, and to devices made from monolithically integrated semiconductor structures. In particular, the invention relates to layer/substrate combinations with different lattice parameters and thermal expansion coefficients. Although the invention relates foremost to the monolithic integration of electronic, opto-electronic and photonic functionalities on a silicon (Si) substrate or silicon-on-insulator (SOI) substrate, it applies also to the integration of functional layers and devices fabricated on other substrate materials, such as germanium (Ge), germanium-on-insulator (GeOI), gallium arsenide (GaAs), indium phosphide (InP), indium antimonide (InSb), cadmium telluride (CdTe), silicon carbide (SiC), sapphire (Al_2O_3), aluminium nitride (AlN), gallium nitride (GaN), or any other single crystal substrate.

The semiconductor materials monolithically integrated onto anyone of these substrates can for example be a group IV material, like C, Si, Ge, Sn, and combinations thereof, or any compound semiconductor materials. Compound semiconductor materials may be III-V materials, for example nitrides like GaN, AlN, InN and their alloys; or arsenides, like AlAs, GaAs, InAs and their alloys; or phosphides, like AlP, GaP, InP and their alloys; or antimonides, like GaSb, InSb, and their alloys. The compound semiconductor materials may also be alloys of group III phosphides and arsenides.

Alternatively, compound semiconductor materials may be II-VI materials, for example sulphides, like ZnS, CdS and their alloys; or selenides, like ZnSe, CdSe, and their alloys; or tellurides, like ZnTe, CdTe, HgTe, and their alloys. The compound semiconductor materials may also be alloys of group IV sulphides, selenides and tellurides, such as PbS, PbSe, and PbTe, or any combination thereof.

5 A first embodiment of the invention is shown schematically in Figs. 1(a) and 1(b). A substrate **100** is patterned in the form of two sets of perpendicular grooves or trenches **120**, leaving in between elevated regions **110** as shown in Fig. 1(a). Elevated regions **110** may for example be of square shape, with w indicating the dimension of the squares. The grooves **120** of width d are etched to a depth h . The width d of the grooves may be smaller or larger than the sides w of the squares. The etch depth h is preferably about equal to or larger than the width d of the grooves. In one preferred aspect of the embodiment, the depth h is much larger than the width d of the grooves, for example up to ten times as large.

The substrate patterning may take place by means of lithography and etching steps well known to experts in the field. First, a lithography step is used to define the pattern. Depending on the size of the features to be etched into the substrate, either optical photolithography, or holographic exposure, or X-ray lithography, or electron beam lithography, or nano-imprinting, may be used. The exposed pattern may then be transferred to the substrate by wet chemical or dry etching steps. Especially the patterning of Si wafers is very well known to anyone working in the field. Grooves **120** may be etched to depths h of many microns, for example by deep reactive ion etching (DRIE) (see for example the "Bosch process" described in US patent number US5,501,893 to Laermer et al., the entire disclosure of which is hereby incorporated by reference). Depending on the lithography and etching process used, the size w of elevated regions **110** may vary from a sub-micron scale, for example 100 nm, to a scale of many micrometers, for example 10 μm . For some applications size w of elevated regions **110** may be chosen to be even larger, for example up to 100 μm or even 500 μm . The width d of grooves **120** may likewise vary from a few tens of nanometers to a few micrometers, for example 2-5 μm . The etch depth h may vary from a fraction of a micrometer to a few micrometers, or even many micrometers, for example 20 μm . It is advisable to keep the aspect ratio h/w about equal to one or even larger than one, in a preferred aspect of the embodiment even much larger than one, such as for example ten.

30 Another aspect of the embodiment is shown in Fig. 1(b). Here, elevated substrate regions **130** may be faceted instead of being flat. Vertical grooves **120** may have height h_1 , and the facets may extend to height h_2 . Surface facets **130** may be formed by etching and/or deposition techniques well known to experts working in the field. Elevated substrate regions **130** may be advantageous for the deflection of dislocations towards the edges of epitaxial patches during the growth (please see also Fig. 3).

Referring now to Fig. 2, a process sequence **200** may include steps of patterning a substrate, **210**, ex-situ cleaning the patterned substrate by methods well known to anyone working in the field, including for example an optional step of surface passivation, **220**, loading the substrate into the epitaxial reactor, **230**, and performing an optional in-situ cleaning step **240**. This cleaning step **240** may consist of any number of sub-steps well known to anyone working in the field, such as thermal annealing steps, designed to remove physisorbed hydrocarbon molecules and moisture, or annealing in the presence of a flow of hydrogen gas, or thermal desorption of a thin surface oxide in UHV. The temperature of the clean substrate is then adjusted in accordance with the needs of the first epitaxy step **250**, which may consist of the epitaxial growth of a lattice-matched material, such as the substrate material itself, or of a lattice mismatched, or of a thermally mismatched material, followed by an optional annealing step **260**. The substrate temperature may then be readjusted according to the needs of a second epitaxy step **250** of a lattice mismatched and/or thermally mismatched material. Depending on the epitaxial growth technique and the process parameters used, the vertical growth rate may be chosen to be higher than the lateral growth rate during epitaxy step **250**. In a preferred aspect of the embodiment, the vertical growth rate may be chosen to be even much higher than the lateral growth rate, for example ten times as high or even more. In accordance with Fig. 3(a), most of the semiconductor material may be deposited in the form of isolated patches **330** with surfaces **326** on top of elevated substrate regions **110**, **310**. Some of the material may also be deposited on the bottom of trenches **120**, **320**, and to a lesser extent on the sidewalls **350** of trenches **120**, **320**, unless said trenches are chosen to be very narrow, or have already been narrowed down in a previous epitaxy step. In other words, according to the invention, process sequence **200** may lead to a very different layer structure than can be anticipated from prior art, even for thick epitaxial layers. Instead of coalescing into a continuous film, the layers grown in step **250** may be composed of isolated patches epitaxially grown on elevations **110**.

Isolated epitaxial patches **330**, evolving into pillars as growth proceeds, may have a profound influence on the dislocation structure, as may be seen from Fig. 3(b). Here, dislocations **370** lying in glide planes inclined to the interfacial plane may reach sidewalls **351** even in the absence of any glide motion, because such glide planes all cut through the sidewalls sooner or later during growth. If surfaces **326** of isolated epitaxial patches **330** have inclined facets **360**, **361**, **362** during growth, then vertical, sessile dislocation lines **380** may be additionally deflected into dislocation lines **381**, extending towards sidewalls **351** by interacting with inclined facets **361**, **362**, **360**. Faceting may be achieved by choosing process conditions during epitaxial growth step **250** such that horizontal top facets **331**, **332** shrink during growth, while inclined facets **361**, **362** expand. This may require for example a lower deposition rate and higher substrate temperature during epitaxial growth step **250**, in order to increase the surface diffusion length, for example favouring the growth of more stable facets. Once a sufficient height of epitaxial pillars has been attained, depending on the width w of substrate

patterns **110**, all sessile vertical dislocation lines **380** have been successfully deflected into tilted lines **381** extending to sidewalls **351**.

As shown in Fig. 3(c), processing conditions of epitaxial growth step **250** may be changed again at this point, such as to favour horizontal top facets **326** to expand again at the expense of inclined facets **360**. All threading dislocations **370**, **381** may thus have reached sidewalls **351** by the time inclined facets **360** have been satisfactorily reduced in size in order to facilitate further processing with essentially horizontal top surfaces **360**. By swapping process conditions **250** and **260** back and forth between faceted and planar pillar growth, the morphology of the final structure may thus be tuned in a wide range, while forcing all dislocation lines to end at sidewalls **351**, where they cannot do any harm.

The growth step **250** may also be followed by an optional annealing step **260**, whereupon the dislocation structure of the grown layer may change, for example by means of glissile threading dislocations moving to the edges of regions **110**, **351**. Steps **250** and **260** may be repeated a number of times, for example in order to increase the thickness of a given semiconductor material, or to form a stack of different materials on top of one another, while choosing conditions such that layer patches **330** remain isolated.

In another aspect of the embodiment, elevated substrate regions **110** may be too large for complete inclined facets **360** to form. Dislocations **380** may still be removed from horizontal flat areas **326** by a suitable choice of epitaxial growth step **250** of process sequence **200**. Such a choice may include the well known concept of compositional grading (see for example US patent number US5,221,413 to Brasen et al., the entire disclosure of which is hereby incorporated by reference). For shallow grading rates a growing graded layer on top of a mismatched substrate corresponds to a system of low effective lattice mismatch, and vertical dislocations **360** are not expected to form. On the other hand, dislocation glide to the sidewalls of epitaxial patches **330** is expected to happen very efficiently, as long as the dimensions of elevated substrate regions **110**, **310** are chosen to be no larger than about $10\text{ }\mu\text{m}$ (see for example Hammond et al., Applied Physics Letters **71**, 2517 (1997), the entire disclosure of which is hereby incorporated by reference). While the grading rate has to be kept low for continuous graded layers, for example $10\%/ \mu\text{m}$, in order to facilitate dislocation glide, this is no longer necessary for structures of micron size or even smaller. According to the invention, the grading rate can thus be increased to as much as $100\%/ \mu\text{m}$, or even $200\%/ \mu\text{m}$, depending on the size of elevated substrate regions **110**, **310**. Isolated epitaxial patches **330** can therefore be chosen to be thin, with heights **312** for example as low as $0.5\text{ }\mu\text{m}$, even when said patches incorporate a graded layer.

The optional use of compositional grading may be used for any material system forming miscible alloys in a non-negligible concentration range. Such examples may be SiGe, InGaAs,

HgCdTe, PbTeSe, InGaN, and any others suitable for electrical, electro-optical and further applications.

After completion of the final layer stack, the substrate may be cooled, and removed from the epitaxy reactor in step 270. Depending on the application, device fabrication steps 280 may follow, in general consisting again of many sub-steps known to those working in the field. It is understood that many variations of process sequence 200 may be applied, including repetitions of the whole sequence after completion of step 280, with or without an additional patterning step 210.

For epitaxial growth step 250 any of the methods may be used, which are known to experts working in the field, such as molecular beam epitaxy (MBE), chemical vapour deposition (CVD), metal-organic chemical vapour deposition (MOCVD), or magnetron sputter epitaxy (see for example International patent application number WO9604677 to von Känel et al., the entire disclosure of which is hereby incorporated by reference), or low-energy plasma-enhanced chemical vapour deposition (LEPECVD) (see for example US patent number US7,115,895 to von Känel, the entire disclosure of which is hereby incorporated by reference), or low-energy plasma-enhanced vapour phase epitaxy (LEPEVPE) (see for example WO2006097804 to von Känel, the entire disclosure of which is hereby incorporated by reference).

Referring now to Fig. 4, an aspect of a second embodiment is shown, in which trenches 420, 430, etched into substrate 400 may have unequal widths d_1 and d_2 , where for example d_2 is larger than d_1 . This may be achieved by choosing corresponding feature sizes of the lithographic structures defined during substrate patterning step 210. As is well known to those working in the field, unequal widths of trenches 420, 430 may lead to unequal depths h_1 and h_2 during a reactive ion etching or chemical etching step. As may be seen in Fig. 5, elevated substrate features 410, 510, may therefore give rise to epitaxial regions consisting of merged structures 570 with sidewalls 576 above narrow trenches 420, 520, while wider trenches 430, 530 remain open. On the bottom 540 of narrow trenches 420, 520 less or negligible material may be deposited during epitaxial growth step 250 and optional annealing step 260 than on the bottom 580 of wider trenches 430, 530. Likewise, the side walls 550 of narrow trenches may receive less or negligible material during epitaxial growth step 250 and optional annealing step 260 than the side walls 560 of wider trenches 430, 530.

Merged structures 570 may be formed above narrow trenches 420, 520 by choosing conditions during epitaxial growth steps 250 and optional annealing steps 260, well known to experts working in the field, such as reducing deposition rates and increasing substrate temperatures, causing an increase of surface diffusion lengths, in order to reduce the ratio between vertical and lateral growth velocities. The size 514 of epitaxial structures 570 may be chosen arbitrarily by choosing the spacing between wider trenches 430, 530. It is, however, advisable to choose this size in accordance with the mismatch of thermal expansion coefficients and thickness 512 of the deposits, in order to avoid layer cracking and wafer bowing during cooling to room temperature or during any thermal cycle.

In one aspect of the embodiment processing steps **250, 260**, of processing sequence **200** may be chosen in such a way as to favour voids **590** to form, in merged structures **570**, above narrow trenches **420, 520**. The presence of voids **590** may be a way of relieving thermal stress in merged structures **570** or a means to lower dislocation densities during island merging.

It is understood that in other aspects of the embodiment, more than two different trench widths and more than one spacing between wider or narrow trenches may be chosen, as well as many different shapes and sizes of elevated substrate regions.

Referring now to Fig. 6, a third embodiment with substrate pattern **600** is shown, in which sidewalls **350, 550, 560, 650** and bottoms **340, 540, 580, 640** of trenches **120, 320, 420, 430, 520, 530, 620** are coated with dielectric layer **630**. On elevated regions **110, 410, 610** the clean substrate is exposed as before. This may be achieved by processes well known to experts working in the field. The patterned substrate may for example be coated with dielectric layer **630**. Subsequently, this dielectric layer may be removed from elevated regions **110, 410, 610** for example by protecting bottoms **340, 540, 580, 640** and side walls **350, 550, 560, 650** of trenches **120, 320, 420, 430, 520, 530, 620** with a protective layer while it is being etched. Dielectric layer **630** may for example be a thermal oxide formed on a patterned Si substrate. Layer **630** may be advantageously used by choosing a selective epitaxy process in epitaxial growth step **250**. Side walls **350, 550, 560, 650** may thus be prevented from being covered independent of the widths of trenches **120, 320, 420, 430, 520, 530, 620** by using a selective epitaxy process in growth step **250**.

It is understood that simple substrate pattern **600** is but an example of arbitrarily different substrate patterns that may be used. Moreover, substrate pattern **600** with coated side walls and bottoms of trenches **120, 320, 420, 430, 520, 530, 620** may be combined with patterned substrate regions wherein dielectric coatings **630** have not been applied.

Referring now to Figs. 7a to 7d, various embodiments are shown, exhibiting examples of variations of substrate patterns. It should be understood by any expert working in the field that there may be many more possible patterns, giving rise to dislocation-free and crack-free epitaxial regions after execution of steps **250, 260** of processing sequence **200**. In Fig. 7a, elevated substrate regions **710** are rectangular in shape. Long sides **714** of the rectangles may be oriented along a symmetry direction of the substrate, for example along $\langle 110 \rangle$ or $\langle 100 \rangle$ for a cubic substrate with surface normal $\langle 001 \rangle$. The $\langle 100 \rangle$ orientation may favour dislocation glide, or simply dislocation line extension during growth, to the edges of isolated patches **330** during execution of steps **250, 260** of processing sequence **200**.

It is advisable to keep the aspect ratio h/w_1 between the depth h of trenches **720** and the short side **718** of rectangular elevated regions **710** larger than one, in preferred aspects of the embodiments much larger than one, such as for example ten. This may enhance the elastic contribution of misfit

stress relaxation along the direction of short sides **718**, during execution of steps **250**, **260** of processing sequence **200**.

Referring now to Fig. 7b, a substrate pattern is shown, where elevated regions **710**, **730**, **740** have different sizes and shapes. The width of trenches **720**, **722**, **724**, **726** may be chosen such that after execution of steps **250**, **260** of processing sequence **200**, epitaxial layers formed on elevated substrate regions **710**, **730**, **740** do not form a continuous film.

Referring now to Fig. 7c, it may be seen that elevated substrate regions **750** do not need to have square shapes. By way of example, regions **750** are shown to be circular in shape. Many more shapes are possible, as long as trenches **720** are designed such that after execution of steps **250**, **260** of processing sequence **200** epitaxial layers formed on elevated substrate regions **750** do not form a continuous film.

Referring now to Fig. 7d, an embodiment is shown in which elevated substrate regions **710**, **730**, **740**, **750**, **760**, are spaced too far apart to prevent layers deposited in between from cracking. Regions outside of trenches **780** surrounding substrate regions **710**, **730**, **740**, **750**, **760**, may therefore be coated with a dielectric layer **790**. Likewise, bottoms and side walls of trenches **780** may be coated with a dielectric layer. The dielectric coatings **790** may for example be a thermal oxide formed on a patterned Si substrate. Semiconductor material may be prevented from growing on dielectric regions **790** if a selective epitaxy process is used in step **250** of processing sequence **200**.

Referring now to Fig. 7e, it may be seen that the substrate patterning need not lead to straight side walls of trenches **120**, **320**, **420**, **430**, **520**, **530**, **620**, **720**, **722**, **724**, **726**, **780**. In fact, the formation of under-etched trenches may be very advantageous for several reasons. First of all, under-etching reduces the width of substrate posts beneath elevated regions **710**, compared to equally sized regions **710**, defined by vertical side walls. Elastic relaxation of the substrate may therefore be enhanced, and thus the density of misfit dislocations lowered to some extent. Second, side wall coverage may be greatly diminished or even eliminated altogether for sufficient under-etching, even when trenches are not chosen to be very narrow, and even in the absence of dielectric layer **630** and in the absence of selective area epitaxy during epitaxial growth step **250**. This may be advantageous for all applications in which the electrical properties of elevated substrate features **110**, **310**, **410**, **510**, **610**, **710**, **730**, **740**, **750**, **760**, are altered by the deposition of material on the side walls during execution of steps **250**, **260** of processing sequence **200**.

It is understood that Figs. 7a to 7e are only examples of substrate patterns according to the invention. Substrate patterns may be combinations of these patterns, or any patterns of different shape and symmetry, for example face-centered square or hexagonal symmetry, as long as they contain elevated regions **110**, **310**, **410**, **510**, **610**, **710**, **730**, **740**, **750**, **760** separated by trenches suitable for the epitaxial growth of isolated patches on top.

*Examples*Substrate patterning

Referring now to Figs. 8(a)-8(c), scanning electron microscopy (SEM) images **800** of patterned substrates may be seen in perspective (a) and plan (b)-(c) view. Here, the substrate is a Si(001) wafer which was patterned by standard photolithography and the Bosch process, leading to the ripples on the side walls of Si pillars **810**. In Fig. 8(a) pillars **810** are about 1.8 μm wide, while the width of trenches **812** is about 2.2 μm . The plan view SEM image of Fig. 8(b) shows two different kinds of trenches with widths of about 1.7 μm for narrow trenches **830** and 2.9 μm for wider trenches **840**, while pillars **820** are about 1.3 μm wide. Wider trenches **840** are about 8 μm deep, and narrow trenches **830** slightly less.

Fig. 8(c) shows other examples of patterns, A1, B1, C1 and D2, composed of elevated substrate regions **850**, **860**, **870** and **880** of different size and distance. Many more substrate patterns have been examined with elevated features ranging from submicron to tens of microns in size, and with trench width variations in a similar range.

Epitaxy on patterned substrates

(1) Isolated features: Examples of islands and ridges

Referring now to Figs. 9(a) to 9(e), SEM images patterned Si(001) substrates **900** are shown, on which various epitaxial layers were grown by using steps **250** and **260** of processing sequence **200**. Fig. 9(a) are perspective views of pure Si, $\text{Si}_{0.6}\text{Ge}_{0.4}$ alloy, and pure Ge pillars **915** grown to a height of about 8 μm . As is well known to researchers working in the field of Ge/Si heteroepitaxy, the lattice mismatch between pure Si and Ge is about 4.2% at room temperature. The mismatch of thermal expansion coefficients is even larger, amounting to about 125% at room temperature. Apart from being characterized by a high density of TDDs, continuous Ge layers beyond a thickness of a few micrometers are therefore bound to crack, and to induce significant layer bowing.

The image of Fig. 9(a) shows, however, that neighbouring Si, SiGe and Ge regions **915** grown onto Si pillars do not touch, when processing conditions **250** and widths of trenches **812**, **830**, **840**, are chosen such as to favour vertical with respect to lateral growth. By contrast, processing conditions **250** have been chosen by taking into account the different surface diffusion lengths for Si, SiGe, and Ge, at given substrate temperature and deposition rate. In this way, spacings **910** between adjacent pillars **915** are nearly the same for all three materials. According to the figure, there is little under-etching of the Si pillars in this example. A small amount of side-wall deposition **920** can therefore be seen in addition to some deposition at the bottom **912** of the Si trenches, occurring mostly at the beginning of the growth.

Fig. 9(b) is a perspective SEM view of a cleaved cross-section through Ge ridges **960** oriented along the $\langle 1-10 \rangle$ direction of the substrate. Conditions of process step **250** have again been chosen in such a way that neighbouring ridges **960** remained separated by narrow trenches **968**. A small amount of sidewall deposition **962** can again be seen, in addition to some deposition at the bottom **966** of the Si trenches, occurring mostly at the beginning of the growth. Note that the horizontal top facet **970** of the Ge ridges is a (001) facet, while inclined facets **980** are {113} facets.

According to high-resolution X-ray diffraction measurements (see also Fig. 14), the pillars and ridges shown in Fig. 9(a) and (b) are fully relaxed. For example the pure Ge structures can therefore be used as templates for the growth of GaAs. Fig. 9(c) shows an example in which GaAs has been grown onto Ge ridges similar to the ones in Fig. 9(b). Similar to the Ge itself, the GaAs ridges are faceted, with (001) facets **990** on top and inclined facets **991**. Note that the surface diffusion lengths have not been optimized in the example shown, such that trenches **992** have nearly closed.

Fig. 9(d) shows an example of a patterned Si(001) substrate, where sidewalls **650**, **810**, **830**, **840** have been oxidized before selective Ge growth. As a result, Ge deposition **994** has occurred only on top of Si pillars, while no material has nucleated on sidewalls **996** and bottoms **998** of trenches.

Fig. 9(e) finally shows a simulation and corresponding SEM image of a cross-section through Ge ridges **960**. In this case Si ridges **964** and trenches **965** are about 2 μm wide and 8 μm high. According to the simulations, the self-aligned vertical growth visible in Figs. 9(a), (b) and (e) is quite general and results from a combination of two main factors. The first factor is a kinetic one, concerning the short diffusion length along the surface of epitaxial structures **915**, **960** (some 100-200 nanometers, in any case smaller than typical facet sizes), preventing transfer of the deposited material from one facet to another, at least within the prototypical times for crystalline incorporation. In this framework, the facets grow nearly independently, at a rate determined by the incoming flux and the velocity for crystalline incorporation. The second factor is one related to the peculiar kind of patterning, i.e. the mutual geometric shielding of the incoming flux by the elevated substrate regions, whereby reactant supply to sidewalls of pillars **915** and ridges **960** and to bottoms **912**, **966** of trenches is greatly reduced (from 50% to about 0.1%) with respect to the reactant supply available to top facets **914**, **970**, **980**, **990**. The sidewalls of pillars **915** and ridges **960**, receiving a progressively smaller flux when coming close to one another, eventually stop growing laterally, expanding almost exclusively vertically instead, as is well known to the experts working in the field. According to the simulation, the predominance of vertical over lateral growth visible in Figs. 9 requires a careful balance of deposition rates and substrate temperatures in steps **250**, **260** of process sequence **200**, thereby ensuring that the surface diffusion length becomes sufficiently small. This may be achieved for example by using high deposition rates in a plasma-enhanced CVD process such as LEPECVD. The experimental results of Figs. 9(a), (b) and (e) have been obtained by such a process, at growth rates of about 4 nm/s. Alternatively, in a thermal CVD process, preferably precursors decomposing at low

substrate temperatures should be used, in order to guarantee low diffusion lengths at comparatively low deposition rates. The selective Ge deposition shown in Fig. 9(d) has been achieved in such a way, with germane decomposition occurring already at substrate temperatures below 500° C. The growth was performed in a two-step process, wherein a thin template is first formed at 330° C at a very small rate of about 4 nm/min, followed by the main deposition at 500° C, at a rate of 25 nm/min. For the growth of compound semiconductors, an additional degree of freedom comes into play, since surface diffusion constants depend also on the ratio between anion and cation supply. The example of GaAs shown in Fig. 9(c) has been obtained by solid source MBE at a substrate temperature of 520° C, with arsenic supplied from a cracker cell, and gallium in the usual elemental form. In this case the deposition rate was chosen to be very small, of the order of 0.1 nm/s, and the surface diffusion length was kept small by choosing a low III/V ratio of about 1:20.

Experiments and simulations hence both show that growth of isolated epitaxial structures on top of elevated substrate regions **110, 310, 410, 510, 610, 710, 730, 740, 750, 760** may be achieved by many different deposition processes by careful choice of steps **250, 260** of process sequence **200**.

Referring now to Figs. 10(a) to 10(c), the results 1000 of a defect analysis of Ge grown onto a patterned Si(001) substrate may be seen. Figs. 10(a) and (b) are dark field scanning transmission electron microscopy (STEM) images obtained on cross-sections through Ge pillars characterized by different facet structures. Top facet **1016** in Fig. 10(a) is a (001) facet parallel to the surface **1011** of Si pillars **1010**. Conditions of step **250** of process sequence **200** have again been chosen such as to ensure finite gaps **1018** between individual Ge pillars. Because of vertical sidewalls of elevated substrate features **1010** and use of non-selective growth, finite coverage has occurred on sidewalls **1012** and bottoms **1014** of the Si trenches. Fig. 10(a) shows that threading dislocations **1020** are confined mostly to deposits on sidewalls **1012** and to the vicinity of the tops **1011** of Si pillars **1010**. In fact, most TDDs move to the edges of the Ge islands within a distance of about one micron from the Ge/Si(001) interface.

One straight dislocation **1024** running up to the top of the Ge pillar can, however, be seen. This dislocation is not deflected because it forms a right angle with respect to surface facet **1016**. No dislocations extending to the top of Ge pillars with inclined facets **1040** shown in Fig. 10(b) have ever been seen.

As is well known by experts working in the field, cross-section TEM analyses are not, however, suitable for a quantitative analysis of dislocation densities. The TEM studies of mismatched layers grown on patterned substrate surfaces were therefore complemented by defect etching and etch pit counting. Fig. 10(c) shows an SEM image the boundary between a patterned and a flat substrate region **1070** onto which a Ge layer has been epitaxially grown in a manner similar to that of Fig. 10(b), i.e., for conditions leading to fully faceted pillar growth. The SEM image was taken after a standard defect etching procedure. The image reveals etch pits **1080** exclusively in the un-patterned

substrate region, but none in inclined facets **1050** on top of pillars and **1060** at the boundary. We may therefore conclude that the mechanism of dislocation deflection by surface facets, as depicted in Fig. 3(b), is very effective for structures with sufficiently large aspect ratios.

5 (2) Merged Ge pillars

Referring now to Figs. 11(a) to 11(b), a comparison of the defect structure of free-standing and merged Ge pillars **1100** on patterned Si(001) may be seen. Fig. 11(a) and (b) are bright field TEM images of cross-sections taken through free-standing Ge pillars (a) and merged pillars (b). In Fig. 11(a) dislocations **1110** can be seen, which have been deflected by interacting with inclined facets during pillar growth. Dislocations **1110** are again confined to a region close to the top of the substrate pillars. Interestingly, no additional dislocations seem to have formed upon pillar merging, as revealed by regions **1120** of Fig. 11(b), located in the gap between Si pillars, where the Ge growth fronts must have met each other during the process of pillar fusion.

Referring now to Figs. 12(a) to 12(b), the marginal generation of dislocations during pillar merging is shown via images **1200**, allowing the reason therefor to be deduced. Fig. 12 (a) is an SEM image in perspective view of an epitaxial Ge layer grown on a patterned Si(001) substrate to a thickness of about 8 μm . Substrate patterning in this case has been similar to the example displayed in Fig. 8(b), consisting of 10 x 10 blocks of closely spaced pillars **820**, spaced by wider trenches **840**. According to Fig. 12(a), the blocks of closely spaced pillars separated by narrow trenches **1220** have merged, while wider trenches **1230** have remained open. A plan view SEM image of a similar structure may be seen in Fig. 12(b). By tuning substrate temperatures during steps **250** and **260** of process sequence, whereby the surface diffusion length may be modified, it has in fact been possible to cause openings **1210**, **1250** between the merged pillars. Despite the fusion of selected pillars, separated by trenches of appropriate width, it may therefore be possible to create surface openings at well-defined locations, where dislocations may escape as in the case of isolated pillars.

According to this example, and in accordance with the second embodiment outlined above, the size of contiguous epitaxial regions may be chosen by defining the width of trenches **420**, **430**, **830**, **840**, the spacing of wider trenches **430**, **840**, and by choosing appropriate conditions during execution of steps **250**, **260** of processing sequence **200**, in order to reduce the vertical with respect to the horizontal growth rate. The squares of merged pillars of Fig. 12(b) are approximately 30 μm long, and consist each of 100 fused Ge pillars. Voids **1210** formed above narrow trenches **1220**, may also help in relieving thermal stress, as outlined in the second embodiment above.

35 (3) Very thick structures, absence of cracks

Referring now to Figs., 13(a) to 13(c), SEM images **1300** are shown. From the SEM image of Fig. 13(a), an example may be seen, where Ge islands, grown onto a Si(001) substrate patterned in the form of pillars, are about 25 μm tall. Conditions during steps **250**, **260** of processing sequence **200**

have been chosen such as to leave a tiny gap **1310** between neighbouring Ge islands, thus avoiding their merging. The SEM image of Fig. 13(b) shows an example of Ge ridges **1330**, about 30 μm tall, grown onto ridges **1320** etched into a Si(001) substrate and oriented along a $\langle 110 \rangle$ direction. Gaps **1310**, **1340** can be tuned to very narrow values, for example as narrow as 50 nm, when steps **250**, **260** of processing sequence **200** ensure a sufficiently short surface diffusion length, and a large ratio of vertical to lateral growth velocities.

The Ge islands of Fig. 13(a) are again entirely stress-free, as revealed by HRXRD. By contrast, thermal stress does develop during cool-down from the growth temperature in areas **1350** outside patterned region **1370** visible in the plan view SEM image of Fig. 13(b). As a result, un-patterned regions **1350** tend to form cracks **1360**, whereas no cracks form in patterned regions **1370**. Furthermore, crack propagation is seen to be inhibited by patterned regions **1370**.

According to the invention it may hence be possible to combine lattice and thermally mismatched semiconductor structures of almost arbitrary thickness by growth on suitable substrate patterns **100**, **400**, **600**, **700**, as long as steps **250** and **260** of process sequence **200** are chosen such as to prevent large contiguous regions to form.

(4) Comparison with perfect substrate material

Referring now to Figs. 14(a) to 14(d), a comparison of X-ray data **1400** obtained on Ge pillars **1410** grown on patterned Si(001) substrates, continuous Ge layers **1420** grown on un-patterned Si(001) substrates, and finally Ge(001) wafer **1426** may be seen. Fig. 14(a) shows SEM images of 30 μm high Ge pillars **1410** and continuous, 8 μm thick Ge layer **1420**, respectively.

In Fig. 13(b) are depicted X-ray reciprocal space maps (RSMs) around the symmetrical (004) reflections from the Si substrate **1402**, **1404**, and the corresponding (004) reflections from Ge pillars **1410** and layer **1420**. Enlarged images of the RSMs in the region of the Ge (004) reflections **1410**, **1420** are shown in Fig. 14(d).

Fig. 14(c) shows a comparison of X-ray scans in the region of the Ge(004) reflection along Q_z . Curve **1410** refers to a measurement obtained on Ge pillars **1410** of Fig. 9(a), curve **1420** to a measurement obtained on continuous Ge layer **1420** of Fig. 9(a), and curve **1426** to the corresponding result obtained on a bulk-Ge wafer. Curve **1410** exhibits sharp peak **1426**, whose position and half width are identical to those of perfect Ge wafer **1426**, proving that Ge pillars **1410** are completely relaxed and of excellent crystal quality. Curve **1410** has a second maximum at higher Q_z value **1424**, stemming from tensile-strained Ge present in trenches **1411**. For continuous layer **1420** the maximum occurs at higher Q_z , from which a tensile strain of about 0.15% can be deduced. It is this thermally induced tensile strain which leads to cracks and wafer bending in the case of thick Ge films.

(5) Compositional grading and patterned growth

Referring now to Figs. 15(a) to 15(b), an example may be seen via images 1500 in which epitaxial growth on elevated substrate regions **110, 310, 410, 510, 610, 710, 730, 740, 750, 760** has been combined with the method of compositional grading, wherein a $\text{Si}_{1-x}\text{Ge}_x$ alloy has been graded from pure Si to pure Ge at a rate of about 10%/ μm . Fig. 15(a) shows the boundary between a flat Si(001) substrate region and a patterned region with squares $15 \times 15 \mu\text{m}$ in size. Isolated epitaxial structures grown on elevated substrate regions of this size are characterized by horizontal facets **1510** bounded by inclined facets **1520**. While the surfaces of flat substrate regions exhibit a pronounced cross-hatch, formed by dislocation bunches **1530**, very few bunches **1530** may be seen in the patterned part.

According to Fig. 15(b) patterned regions with smaller feature sizes of $9 \times 9 \mu\text{m}$ do not exhibit any visible cross-hatch on horizontal facets **1540** at all. This indicates effective dislocation glide to the sidewalls of epitaxial patches **330**, even when elevated substrate regions **110, 310, 410, 510, 610, 710, 730, 740, 750, 760** are many microns in size. Sessile dislocations **380** are not expected to form in a graded structure, because the effective misfit is always small. When compositional grading is being used, epitaxial patches **330** of sufficient height may therefore remain dislocation-free, even when dislocation deflection cannot occur in the absence of inclined facets **360**.

Applications

As mentioned above, a straightforward application of the invention consists of epitaxially growing a semiconductor layer of some material on a patterned substrate of another material, wherein in general the material of the grown layer adds value to the substrate. This may for example happen by choosing a substrate made of cheap metallurgical grade silicon, onto which high purity, highly perfect Si is grown, for example in the pillar form shown in Fig. 9(a). By combining any of the substrate/layer materials considered before, a virtual substrate of an expensive material may be formed. In many cases an obvious choice would be a silicon substrate of preferably large dimensions coated with some expensive semiconductor, such as GaAs or InP. The product of all such applications may hence be a virtual substrate as a starting point for the subsequent fabrication of devices of any kind.

Referring now to Fig. 16, schematic process sequence **1600** for the fabrication of generic device **1680** may be seen. In step **1602** substrate **1605** is patterned according to process step **210** of processing sequence **200**, defining at least one elevated substrate region **1610**, separated by trenches **1620** from each other and from surrounding areas **1611**. Substrate **1605** may for example be a Si wafer or SOI wafer, or a SiC wafer, which may have undergone a number of optional CMOS processing steps, including implantation steps **1615** underneath elevated substrate regions **1610**. It may be advisable to protect CMOS circuits **1612** by dielectric layers **1614**. Alternatively, substrate **1605** may for example be a Si, SOI, GeOI, SiC, GaAs, InP or sapphire wafer which has optionally been pre-processed in any other way before patterning step **1602**.

In process step **1604**, steps **220** to **270** of process sequence **200** may be applied, whereby epitaxial layer stacks **1630** are formed on exposed elevated regions **1610** of substrate **1605**. In the case that substrate **1605** is a processed CMOS wafer, process step **1604** and all following steps may be chosen to fulfil the requirements for CMOS back end processes. Process step **280** of process sequence **200** may consist of several sub-steps. Sub-step **1606** may consist of filling trenches **1620** with filling material **1650**, which may for example be a polymer or an inorganic dielectric. An optional chemical-mechanical polishing step may subsequently be carried in order to create a planar surface before process step **1608**. Process step **1608** may include a metallization step in which contacts **1660** are formed on epitaxial layer stacks **1630**. Generic device **1680** fabrication may include additional sub-steps, such as for example contacting optional implanted regions **1615**.

Depending on the kind of patterned substrates **100**, **400**, **600**, **700**, and the kind of epitaxial layer stacks formed in steps **250**, **260** of process sequence **200** generic device **1680** may now be applied to encompass photonic circuits consisting of waveguides, modulators, detectors and emitters fabricated from lattice mismatched layer stacks, for example monolithically integrated on a CMOS chip. Generic device **1680** may also encompass electronic circuits fabricated from lattice mismatched layer stacks, for example monolithically integrated on a CMOS chip. Generic device **1680** may also encompass imaging detector arrays, for example monolithically integrated on a CMOS chip, such as infrared imaging detectors and X-ray pixel detectors, where for example every single pixel **1610** may be read out by CMOS circuit **1612**. Generic device **1680** may also be an array of multiple-junction solar cells. Generic device **1680** may be any other combination of opto-electronic, microelectronic and photonic devices fabricated from lattice-mismatched layer stacks monolithically integrated on a single-crystal substrate wafer.

Referring now to Fig. 17, a scheme of alternative fabrication procedure **1700** for generic device **1704** may be seen. Here, patterned wafer **1705** is subjected to process steps **220** to **270** of process sequence **200**, whereby mismatched epitaxial material stacks **1730** may be grown on elevated substrate regions **1710**. Wafer **1705** may then be flipped over and the bonded in a low-temperature wafer bonding process to CMOS-processed wafer **1740**. Wafer **1740** may contain contact pads **1740** contacting layer stacks **1730**. CMOS wafer **1740** may contain CMOS circuits fabricated on surface **1744**, or on surface **1746**, or on both surfaces **1744** and **1746**.

In a variation of this scheme, patterning may be applied not only to wafer **1705** but also on wafer **1740**. During process steps **220** to **270** of process sequence **200** mismatched epitaxial material stack **1730** grown on elevated substrate **1710** regions of wafer **1704** may then for example be p-doped. Conversely, a corresponding mismatched epitaxial material stack grown on wafer **1740** may be n-doped or vice versa. Both wafers **1705** and **1740** may be subjected to additional device processing steps **280** of process sequence **200**, such as well known reactive ion etching and metallization steps,

before the flipping and bonding process is being carried out in order to put specific n-doped and p-doped regions into electrical contact.

The processing sequence just described may for example be applied to the fabrication of thermoelectric generators integrated on a CMOS chip. Here, p-doped layer stacks **1730** on wafer **1705** and corresponding n-doped layer stacks on wafer **1740** may form p-n junction diodes wherein the p-side may be connected to a heat source, and the n-side to a heat sink, or vice versa. Epitaxial layer stacks **1730** may for example consist of SiGe alloys or any other material suitable for thermoelectric applications. In such an application patterned substrates **800** may contain also larger structures for example of dimensions on the order of 100 μm or even more, as long as wafer bowing and layer cracks remain on a negligible scale, since thermoelectric devices suffer less from a high TDD than for example detectors or emitters, or other active devices.

Referring now to Fig. 18, a scheme of alternative device fabrication procedure **1800** for generic device **1804** may be seen. Here, thin patterned wafer **1805** is subjected to process steps **220** to **270** of process sequence **200**. Wafer **1805** may then be bonded to CMOS wafer **1840** in a low-temperature wafer bonding process. CMOS wafer **1840** may have optional contact regions **1835** aligned with active layer stacks **1830**. CMOS wafer **1840** may contain CMOS circuits fabricated on surface **1844**, or on surface **1846**, or on both surfaces **1844** and **1846**.

The patents and articles mentioned above are hereby incorporated by reference herein, unless otherwise noted, to the extent that the same are not inconsistent with this disclosure.

Other characteristics and modes of execution of the invention are described in the appended claims.

Further, the invention should be considered as comprising all possible combinations of every feature described in the instant specification, appended claims, and/or drawing figures which may be considered new, inventive and industrially applicable.

Multiple variations and modifications are possible in the embodiments of the invention described here. Although certain illustrative embodiments of the invention have been shown and described here, a wide range of modifications, changes, and substitutions is contemplated in the foregoing disclosure. While the above description contains many specifics, these should not be construed as limitations on the scope of the invention, but rather as exemplifications of one or another preferred embodiment thereof. In some instances, some features of the present invention may be employed without a corresponding use of the other features. Accordingly, it is appropriate that the foregoing description be construed broadly and understood as being given by way of illustration and example only, the spirit and scope of the invention being limited only by the claims which ultimately issue in this application.

Addendum

The following US patent documents, Foreign patent documents, and Additional Publications are incorporated herein by reference thereto and relied upon:

- 5 **US patent documents**
- 2008/0308909 A1 12/2008 Masahiro Sakai et al.
- 2003/0033974 A1 2/2003 Tetsuzo Ueda
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- 2006/0216849 A1 9/2006 Letertre et al.
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- 15 5,158,907 10/1992 Fitzgerald
- 2008/0001169 A1 1/2008 Lochtefeld et al.
- 2008/0149941 A1 6/2008 Li et al.
- 2009/0039361 A1 2/2009 Li et al.
- 2009/0065047 A1 3/2009 Fiorenza et al.
- 20 2005/0199883 A1 9/2005 Borghs et al.
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- 2007/0077670 A1 4/2007 Kim et al.
- 7,115,895 B2 10/2006 von Känel
- 5,501,893 3/1996 Laermer et al.
- 25 **Other patent documents**
- GB2 215 514 A 9/1989 Goodfellow et al.
- WO2008/030574 A1 3/2008 Bai et al.
- EP0505093 A2 9/1992 Bean et al.
- 2010/033813 A2 3/2010 Fiorenza et al.
- 30 WO9604677 A1 2/1996 von Känel et al.
- WO2006097804 A3 9/2006 von Känel

Additional publications

- V.K. Yang et al., "Crack formation in GaAs heteroepitaxial films on Si and SiGe virtual substrates", *Journal of Applied Physics*, vol. 93, no. 7 (April 1 2003) pp. 3859-3865.
- H. Chen et al., "Low-temperature buffer layer for growth of low-dislocation-density SiGe layer on Si by molecular-beam epitaxy", *Journal of Applied Physics*, vol. 2 (Jan 15 1996) pp. 1167-1169.
- 5 E.A. Fitzgerald et al., "Epitaxial necking in GaAs grown on pre-patterned Si substrates", *Journal of Electronic Materials*, vol. 20, no. 10 (1991) pp. 839-853.
- T.A. Langdo et al., "High quality Ge on Si by epitaxial necking", *Applied Physics Letters*, vol. 76, no. 25 (June 19 2000) pp. 3700-3702.
- 10 A.E. Blakeslee, "The use of superlattices to block the propagation of dislocations in semiconductors", *Materials Research Society Symposium Proceedings*, vol. 148 (1989) pp. 217-227.
- I.Y. Knoke, et al., "Reduction of dislocation density in GaN during low-pressure solution growth", *Journal of Crystal Growth*, vol. 310 (2008) pp. 3351-3357.
- T. S. Zheleva et al., "Pendeo-epitaxy: A new approach for lateral growth of gallium nitride films", *Journal of Electronic Materials*, vol. 28, no. 4 (1999) pp. L5-L8.
- 15 S. Fündling et al., "Three-dimensionally structured silicon as a substrate for the MOVPE growth of GaN nanoLEDs", *Physica Status Solidi A*, vol. 206, no. 6 (March 25 2009) pp. 1194-1198.
- J.G. Fiorenza et al., "Aspect ratio trapping: a unique technology for integrating Ge and III-Vs with silicon CMOS", *ECS Transactions*, vol 33, no. 6 (2010) pp.963-976.
- 20 T. Stoica et al., "Interface and wetting layer effect on the catalyst-free nucleation and growth of GaN nanowires", *small*, vol. 4, no. 6 (2008), pp. 751-754.
- R. Hammond et al., "The elimination of surface cross-hatch from relaxed, limited-area $\text{Si}_{1-x}\text{Ge}_x$ buffer layers", *Applied Physics Letters*, vol. 71, no. 17 (1997) pp. 2517-2519.

What is claimed is:

1. A structure comprising:
 - 5 a) a patterned crystalline semiconductor substrate with elevated regions (110, 130, 410, 610, 710) bounded by trenches (120, 320, 420, 430, 620, 720); and
 - b) epitaxial semiconductor material deposited on said elevated substrate regions in the form of isolated semiconductor patches (330, 570).
- 10 2. The structure of claim 1 containing mismatched semiconductor materials, wherein:
 - a) the patterned semiconductor substrate is made from a first crystalline semiconductor material; and
 - b) the epitaxial deposit comprises at least one second crystalline semiconductor material, having a lattice mismatch or thermal mismatch to said substrate.
- 15 3. The structure of claim 2, wherein mismatched semiconductor materials are lattice mismatched or thermally mismatched.
- 20 4. The structure of claim 2, wherein said deposit is of sufficient thickness to allow defects associated with the lattice mismatch to exit said patches either through their sidewalls (351, 576) or through any inner openings (590, 1210, 1250).
- 25 5. The structure of claim 1, wherein the depth h of said trenches is at least as large as their width d.
- 30 6. The structure of claim 1, wherein said elevated substrate regions (130) are faceted to allow defects forming in said epitaxial patches to exit through the sidewalls of said patches.
7. The structure of claim 1, wherein sidewalls and bottoms of said trenches are covered with a dielectric layer.
8. The structure of claim 1, wherein said elevated substrate regions have at least one smallest dimension w within the range from 100 nm to about 500 μm .

9. The structure of claim 1, wherein said elevated regions comprise at least one region, the boundary of which is aligned along a high-symmetry direction of said substrate.
10. The structure of claim 1, wherein said trenches comprise at least one trench (720) which is under-etched.
11. The structure of claim 1, wherein said isolated patches have facets (361, 362) during growth, and wherein said facets are inclined to the growth direction to allow deflecting vertical defects (380) into oblique directions (381), such that said defects may exit through sidewalls (351) of said patches.
12. The structure of claim 1, wherein surfaces of epitaxial patches (330, 570) have been modified during epitaxial growth to have horizontal surfaces (326).
13. The structure of any one of claims 1 and 2, wherein isolated patches (330, 570) have widths (314, 514) and heights (312, 512) small enough to inhibit layer cracking and wafer bowing.
14. The structure of claim 2, wherein isolated patches (330, 570) are separated by narrow channels (1310, 1340), comprising widths in the range of about 30 – 300 nm.
15. The structure of claim 1, wherein said semiconductor substrate is one of a group of substrates consisting of Si, SOI, Ge, GeOI, GaAs, InP, InSb, CdTe, SiC, Al₂O₃, AlN and GaN.
16. The structure of claim 2, wherein the at least one second semiconductor material is one of a group of semiconductor materials, consisting of elemental group IV semiconductors and their alloys, and compound semiconductors from group III-V, group II-VI, and group IV-VI, and their alloys.
17. The structure of claim 2, wherein the epitaxial deposit from the at least one second semiconductor material comprises a layer with compositional grading, said graded layer being chosen among a group of alloys consisting of an alloy of group IV, group III-V, group II-VI, and group IV-VI semiconductors, and said graded layer facilitating the gliding of dislocations towards the sidewalls (351, 576) of said epitaxial patches.
18. The structure of claim 2, wherein the epitaxial deposit comprises an active layer stack made from a plurality of semiconductor layers such plurality selected from a group of

semiconductor layers consisting of elemental group IV semiconductors and their alloys, and compound semiconductors from group III-V, group II-VI and group IV-VI, and their alloys.

19. The structure of claim 18, wherein at least one layer of said active layer stack is doped.

20. The structure of any of claims 1-19, wherein the epitaxial layer stack comprises a photovoltaic solar cell.

21. The structure of claim 20, wherein the photovoltaic solar cell is a triple-junction solar cell.

22. The structure of claim 21, wherein the bottom cell of the triple-junction solar cell is a Ge p-n junction solar cell.

23. The structure of claim 17, wherein at least one layer is doped.

24. The structure of any one of claims 1-17 and 23, wherein the epitaxial deposit comprises a photovoltaic solar cell.

25. The structure of claim 24, wherein the photovoltaic cell comprises at least three single-junction solar cells stacked to a multiple-junction solar cell.

26. The structure of claim 2, wherein said semiconductor substrate has undergone CMOS processing.

27. The structure of any one of claims 1-18 and 26, wherein the layer stack comprises at least one high-mobility transistor structure.

28. The structure of any one of claims 1-19, and 26, wherein the layer stack comprises a photonic structure, comprising at least one light-emitting diode structure, or a laser diode structure, or wherein the layer stack comprises a structure for a thermoelectric device.

29. The structure of any one of claims 1-19, and 26, wherein the layer stack comprises an infrared imaging detector structure, comprising pixels communicating with readout circuits of said CMOS processed substrate.

30. The structure of claim 29, wherein the infrared detector is made from Ge.
31. The structure of claim 29, wherein said infrared detector structure is made from an InGaAs alloy.
32. The structure of any of claims 1-19, and 26, wherein the layer stack comprises an X-ray imaging detector structure, comprising pixels communicating with readout circuits of said CMOS processed substrate.
33. The structure of claim 32, wherein said X-ray detector structure is made from Ge.
34. A method of forming the structure of claim 1 having isolated semiconductor patches (330, 570) on elevated regions, the method comprising steps of
- a) forming a patterned crystalline semiconductor substrate, the pattern comprising the elevated regions (110, 130, 410, 610, 710) bounded by trenches (120, 320, 420, 430, 620, 720);
 - b) performing an ex-situ substrate clean;
 - c) loading the substrate into an epitaxy reactor;
 - d) optionally performing an in-situ clean;
 - e) epitaxially depositing at least one semiconductor layer on said elevated regions optionally using an epitaxial growth mode favouring vertical over lateral growth; and
 - f) optionally annealing said at least one semiconductor layer.
35. The method of claim 34, wherein said at least one semiconductor layer comprises a crystalline material having a lattice mismatch or thermal mismatch to said substrate.
36. The method of claim 35, wherein said layer is grown to a thickness sufficient to allow defects associated with said lattice mismatch to exit said patches either through sidewalls (351, 576) or through any inner openings (590, 1210, 1250).
37. The method of claim 34, wherein said trenches are etched to a depth h at least as large as their width w.
38. The method of claim 34, wherein the surface of said elevated substrate regions (110, 130, 410, 610, 710) is faceted by anisotropic etching.

39. The method of claim 34, wherein a dielectric layer is formed on the sidewalls and bottoms of said trenches.

40. The method of claim 34, wherein said elevated substrate regions are patterned with smallest dimensions w within the range from 100 nm to about 500 μm .

41. The method of claim 34, wherein at least one of said elevated regions is aligned with a high-symmetry direction of said substrate.

42. The method of claim 34, wherein at least one of said trenches is under-etched.

43. The method of claim 34, wherein epitaxial growth conditions are tuned during growth, thereby favouring inclined facets (361, 362) to form, and thereby deflecting vertical defects (380) into oblique directions (381), such that said defects may exit through sidewalls (351) of said patches.

44. The method of any one of claims 36 and 43, wherein the growth conditions are modified after all defects have escaped to said sidewalls, thereby changing the surface morphology of said epitaxial patches from inclined to horizontal facets.

45. The method of any one of claims 34 to 44, wherein isolated patches (330, 570) are grown to widths (314, 514) and heights (312, 512) small enough to inhibit layer cracking and wafer bowing.

46. The method of any one of claims 34 and 35, wherein forming isolated patches (330, 570) comprises the formation of narrow channels (1310, 1340) separating said patches, said narrow channels comprising widths in the range of about 30 – 300 nm.

47. The method of claim 34, wherein said semiconductor substrate is anyone chosen from a group of substrates consisting of Si, SOI, Ge, GeOI, GaAs, InP, InSb, CdTe, SiC, Al_2O_3 , AlN and GaN.

48. The method of claim 34, wherein the at least one semiconductor material is one chosen from one of a group of semiconductor materials, consisting of elemental group IV semiconductors and their alloys, and compound semiconductors from group III-V, group II-VI, and group IV-

VI, and their alloys.

5 **49.** The method of claim 34, wherein the epitaxial deposit from the at least one semiconductor material comprises a layer with compositional grading, said graded layer being chosen among an alloy of group IV, group III-V, group II-VI or group IV-VI semiconductors, and said graded layer facilitating the gliding of dislocations towards the sidewalls (351, 576) of said epitaxial patches.

10 **50.** The method of claim 34, wherein the epitaxial deposit comprises an active layer stack made from a plurality of semiconductor layers, comprising elemental group IV semiconductors and their alloys, and compound semiconductors wherein the compound includes at least one constituent selected from a group of constituents consisting of group III-V, group II-VI, and group IV-VI, and their alloys.

15 **51.** The method of claim 50, wherein at least one layer of said active layer stack is doped.

52. The method of claim 51, comprising further the formation of a photovoltaic solar cell structure.

20 **53.** The method of claim 52, wherein said photovoltaic solar cell structure comprises a triple-junction solar cell.

54. The method of claim 53, wherein a Ge p-n junction is formed as the bottom cell of said triple-junction solar cell.

25 **55.** The method of any one of claims 49 to 51, comprising the formation of a photovoltaic solar cell.

30 **56.** The method of claim 55, the formation of said photovoltaic solar cell comprising the formation of at least three stacked single-junction solar cells.

57. The method of claim 34, wherein said substrate has been CMOS processed.

35 **58.** The method of any one of claims 34 to 50 and 57, comprising the formation of a high-mobility electronic structure.

59. The method of any one of claims 34-51, and 57, wherein the formation of the layer stack comprises the formation of a photonic structure, comprising at least one light-emitting diode structure, or a laser diode structure, or wherein the formation of said layer stack comprises the forming a structure for a thermoelectric device.

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60. The method of any one of claims 34-51, and 57, wherein the formation of the layer stack comprises the formation of an infrared imaging detector structure, comprising pixels communicating with readout circuits of said CMOS processed substrate.

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61. The method of claim 60, wherein said infrared imaging detector structure is formed from a Ge layer.

62. The method of claim 60, wherein said infrared imaging detector structure is formed from an InGaAs alloy layer.

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63. The method of any one of claims 34-51, and 57, wherein the formation of the layer stack comprises the formation of an X-ray imaging detector structure, comprising pixels communicating with readout circuits of said CMOS processed substrate.

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64. The method of claim 63, wherein said X-ray imaging detector structure is made from Ge.

65. A semiconductor product made by the method of any one of the claims 34 to 64.

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