

Method for depositing a silicon germanium layer on a substrate

5 The invention relates to a method for depositing a silicon germanium (SiGe) layer on a substrate.

Background

Semiconductor devices using SiGe channels represent an interesting alternative to respective devices based on silicon, only. In order to provide a SiGe layer for the
10 integration of SiGe channels, a SiGe layer has usually to be heteroepitaxially deposited atop a substrate, e.g. a silicon single crystal wafer. It is well known that misfit dislocations (MD), threading dislocations (TD) and dislocation pile-ups (DP) of threading dislocations are formed in the course of the deposition process due to a lattice-mismatch of the substrate and the heteroepitaxial SiGe layer.

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Many attempts have been made to reduce problems connected with the presence of MD, TD and DP as well as with a cross-hatch roughening the surface of the heteroepitaxial SiGe layer.

20 US 2010 0 291 761 A1 proposes the provision of a stress compensating SiGe layer deposited on the back side of the substrate.

US 2010 0 317 177 A1 discloses a method which comprises depositing a first SiGe layer on the substrate and a second SiGe layer atop the first SiGe layer.

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According to US 2004 0 075 105 A1 the formation of DP can be reduced through a method comprising forming a substantially relaxed cap layer on a first semiconductor layer, which has a plurality of TD distributed substantially uniform across its surface.

30 Recently, a thesis (Fabrizio Rovaris, Continuum modeling of heteroepitaxy at the mesoscale: tackling elastic and plastic relaxation, University of Milano-Bicocca DEPARTMENT OF MATERIALS SCIENCE, Academic year 2019/2020) was published reporting that the presence of a high-defective region at the edge of the

substrate provides a reservoir of threading arms ready to relax as soon as the growing film reach the critical thickness and that, as effect, a significant reduction of the density of TD is observed by eliminating the random nucleation of loops for the first stages of the relaxation. The author of the thesis, having co-worked with the inventors
5 of the present invention, did not publish that the high-defective region at the edge of the substrate had been obtained by the deposition of a stress compensating SiGe layer on the back side of the substrate.

Summary of the invention

10 It is an object of the present invention to further reduce the TD density of a SiGe layer heteroepitaxially deposited on a substrate.

The object is met by a method for heteroepitaxially depositing a silicon germanium layer on a substrate, comprising:

- 15 providing a mask layer atop the substrate;
removing an outer section of the mask layer to provide access to an annular-shaped free surface of the substrate in an edge region of the substrate surrounding a remainder of the mask layer;
depositing a cylindrical silicon germanium layer atop the annular-shaped free surface
20 of the substrate;
removing the remainder of the mask layer; and
depositing the silicon germanium layer atop the substrate and atop the cylindrical silicon germanium layer, the silicon germanium layer contacting an inner lateral surface of the cylindrical silicon germanium layer.

25 SiGe buffer layers on silicon single crystal substrates relax by heterogeneous nucleation at preferential nucleation sites, as no pre-existing dislocations exist in the substrate. It is well known that the edge of Si wafers exhibits mechanical defects, that serve as preferential nucleation sites. Strain energy is building up in the epitaxial layer
30 during growth and once the activation energy for this process is reached, dislocations rapidly nucleate at these sites, forming thick dislocation bundles. These bundles of misfit dislocations lead to the formation of threading dislocation pileups, as they are effective in blocking the glide of other dislocations. As dislocations are blocked, more

dislocations need to be nucleated to relax the layer completely, which leads to a higher threading dislocation density (TDD). For a more controlled relaxation process and prevention of misfit dislocation bundles, an evenly distributed source of dislocations is needed, that has a low activation energy.

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The present invention proposes a way to implement such source in an edge region of the SiGe layer. This edge reservoir consists of a relaxed or partially relaxed SiGe layer (hereinafter referred to as cylindrical SiGe layer) that is deposited before the SiGe layer. The SiGe layer has a vertical contact to or both, a vertical and a horizontal
10 contact to the cylindrical SiGe layer. Preexisting dislocations contained in this edge reservoir are used to relax the SiGe layer in the initial phase of relaxation by gliding freely towards the center of the wafer upon reaching the critical thickness, leaving behind extremely long misfit dislocation segments without being blocked. This process prevents the formation of thick dislocation bundles by heterogeneous nucleation at the
15 wafer edge, thus preventing the formation of DP and lowering the overall TDD.

Although the following description is dealing with the deposition of a SiGe layer on a silicon single crystal substrate, other substrates like silicon-on-insulator (SOI) wafers may be used, as well. According to a preferred embodiment of the invention, the
20 substrate is a silicon single crystal wafer having a diameter of 200 mm or 300 mm.

For the provision of the cylindrical SiGe layer at the edge of the substrate, a masking approach is pursued. In principle, any masking mechanism for temporarily excluding a surface area of the substrate from deposition with an SiGe layer may be used.
25 According to a preferred embodiment of the invention, an oxidic material like SiO₂ is used as masking material, e.g. a low temperature oxide (LTO). An LTO may be deposited atop of the substrate by chemical vapor deposition (CVD) at temperatures between 300 °C and 500 °C in an atmosphere containing silane (SiH₄) and oxygen (O₂). Alternatively, other known methods for depositing an oxidic layer may be used or
30 the oxidic layer may be grown through dry oxidation in a rapid thermal anneal (RTP) furnace at temperatures between 850 °C and 1200 °C.

Next, the mask layer is removed in an edge region of the substrate for providing an annular-shaped free surface of the substrate that extends from the edge of the substrate towards the center of the substrate. The mask layer in the edge region may be removed e.g. by wet etching with hydrofluoric acid or with ammonium fluoride and hydrofluoric acid or by plasma etching with e.g. CF_4 or the like. According to an embodiment of the invention, the mask layer in the edge region of the substrate may be removed by putting the substrate face down on a support and by introducing HF fumes in a process chamber, the HF fumes diffusing between the support and the mask etch away a mask portion having a width of up to 1.5 mm.

According to an embodiment of the invention, the annular-shaped free surface of the substrate radially extends from the edge towards the center of the substrate over a distance which is preferably not less than 200 μm and not more than 1.5 mm. The width of the annular-shaped free surface of the substrate may even be as small as the length of an edge portion of the substrate, where the thickness of the substrate decreases, or may be even smaller.

Next, the cylindrical SiGe layer is epitaxially deposited on the annular-shaped free surface of the substrate. According to an embodiment of the invention, CVD under atmospheric pressure is performed for the deposition of the cylindrical SiGe layer. Details of the deposition process are well known and e.g. discussed in US 2010 0 317 177 A1. Alternatively, the deposition may be performed under reduced pressure and at lower temperatures. According to an embodiment of the invention, the composition of the cylindrical SiGe layer is $\text{Si}_{1-x}\text{Ge}_x$, wherein $0.01 \leq x \leq 1$. According to a further preferred embodiment of the invention, the cylindrical SiGe layer has a thickness of not less than 10 nm and not more than 10 μm , and the cylindrical SiGe layer is partially or fully relaxed. The mentioned properties of the cylindrical SiGe layer allow to properly control the TDD of the cylindrical SiGe layer, which is crucial for meeting the object of the invention. The TDD of the cylindrical SiGe layer is preferably at least $1.0 \times 10^3 \text{ cm}^{-2}$.

After the provision of the cylindrical SiGe layer in the edge region of the substrate, the remaining mask layer, which is surrounded by the cylindrical SiGe layer is removed

and the surface of the substrate that was covered with the mask layer becomes accessible for the deposition of an SiGe layer contacting the surface of the substrate and an inner and upper surface of the cylindrical SiGe layer. According to a preferred embodiment of the invention, the SiGe layer is epitaxially deposited via CVD under atmospheric pressure. According to a further preferred embodiment of the invention, the composition of the SiGe layer is $\text{Si}_{1-x}\text{Ge}_x$, wherein $0.01 \leq x \leq 1$. According to an embodiment of the invention, the SiGe layer is a graded buffer layer or a constant composition layer. The SiGe layer is partially or fully relaxed and contacts the substrate and an inner surface of the cylindrical SiGe layer or the substrate and both, an inner and an upper surface of the cylindrical SiGe layer. The content of germanium of the cylindrical SiGe layer may be lower, equal to or higher than the germanium content of the SiGe layer. The SiGe layer has a thickness, which is preferably not less than $0.01 \mu\text{m}$ and not more than $10 \mu\text{m}$.

The threading dislocations contained in the cylindrical SiGe layer cause the SiGe layer to relax by gliding towards the center upon reaching the critical thickness. The result is a reduction of the pile-up density and the threading dislocation density, as well as an improvement of surface roughness and the overall uniformity compared to prior art approaches.

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The invention is disclosed with reference to drawings hereinafter.

Brief description of the figures

Fig. 1 represents a sectional view of an embodiment of the wafer in its final state of production.

Fig. 2 represents a sectional view displaying an edge region of the wafer shown in Fig. 1.

Fig. 3 differs from Fig. 2, only, that the edge region of the wafer is shown in an intermediate state of production of the wafer.

Fig. 4 is top-view representation of the wafer according to Fig. 3.

Fig. 5 displays in top-view representation of states of the wafer in the course of the claimed process starting with the substrate and ending with the intermediate state of production of the wafer according to Figs. 3 and 4.

Fig. 6 shows the evolution of TD starting with the intermediate state of production of the wafer according to Fig. 3 and ending with the final state of production according to Fig. 2.

Fig. 7 represents a sectional view of another embodiment of the wafer in its final state of production.

Fig. 8 represents a sectional view of still another embodiment of the wafer in its final state of production.

Fig. 9 represents a sectional view of the edge region of the substrate.

List of reference numerals employed

15	1	substrate
	2	cylindrical silicon germanium layer
	3	silicon germanium layer
	4	mask layer
20	5	remainder of the mask layer
	6	annular-shaped free surface of the substrate
	7	edge portion
	l	length of edge portion
	w	width
25	t	thickness
	TD	threading dislocation

In the final state of production, a wafer produced in accordance with the present invention may have the structure displayed in Fig. 1. This structure comprises a substrate 1, a cylindrical silicon germanium layer 2 and a silicon germanium layer 3 contacting an inner and an upper surface of the cylindrical silicon germanium layer 2. In Fig. 2 an edge region of this wafer is shown that extends in the direction of the arrow from the edge of the wafer towards the center of the wafer.

Before the deposition of the silicon germanium layer 3, the wafer is in an intermediate state displayed in Fig. 3. The structure of the intermediate state comprises the substrate 1 and the cylindrical silicon germanium layer 2 which has a radial width w and a thickness t . Fig. 4 represents a top-view of the wafer in the intermediate state.

In order to achieve the intermediate state, a mask layer 4 is provided atop an upper surface of the substrate 1 as shown in Fig. 5. Then, an outer section of the mask layer 4 is removed to provide access to an annular-shaped free surface 6 of the substrate 1 in an edge region of the substrate 1. Next, the cylindrical silicon germanium layer 2 is deposited on the annular-shaped free surface 6 and surrounds a remainder 5 of the mask layer 4. Subsequently, the remainder 6 of the mask layer 4 is removed, as well, to provide the intermediate state for the subsequent deposition of the silicon germanium layer 3 on the substrate 1 and the cylindrical silicon germanium layer 2.

Fig. 6 shows the evolution of TD starting with the intermediate state of production until the final state of production. The threading dislocations contained in the cylindrical silicon germanium layer 2 promote the relaxation of the silicon germanium layer 3 by gliding towards the center once the critical thickness is reached.

In the final state of production, a wafer produced in accordance with the present invention may also have the structure displayed in Fig. 7 or Fig. 8. According to the embodiment displayed in Fig. 7, the silicon germanium layer 3 contacts the surface of the substrate 1 and the inner surface of the cylindrical silicon germanium layer 2 up to a certain height thereof. According to the embodiment displayed in Fig. 8, the silicon germanium layer 3 and the cylindrical silicon germanium layer 2 have the same thickness.

As shown in Fig. 9, the width of the annular-shaped free surface of the substrate may even be as small as the length l of an edge portion 7 of the substrate 1, where the thickness of the substrate decreases, or may be even smaller than the length l .

The description hereinabove of illustrative embodiments is to be understood as being exemplary.

Claims

1. A method for heteroepitaxially depositing a silicon germanium layer (3) on a substrate (1), comprising:
 - 5 providing a mask layer (4) atop the substrate (1);
 - removing an outer section of the mask layer (4) to provide access to an annular-shaped free surface (6) of the substrate in an edge region of the substrate surrounding a remainder (5) of the mask layer (4);
 - depositing a cylindrical silicon germanium layer (2) atop the annular-shaped free
 - 10 surface (6) of the substrate;
 - removing the remainder of the mask layer; and
 - depositing the silicon germanium layer (3) atop the substrate (1) and atop the cylindrical silicon germanium layer (2), the silicon germanium layer (3) contacting an inner lateral surface of the cylindrical silicon germanium layer (2).
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2. The method as claimed in claim 1, comprising providing a low temperature oxide material as mask layer (4).
3. The method as claimed in claim 1 or claim 2, comprising
 - 20 depositing the cylindrical silicon germanium layer (2) atop the annular-shaped free surface (6) of the substrate such that it has a width of not more than 1.5 mm and a thickness of not less than 10 nm and not more than 10 μm .
4. The method as claimed in one of claims 1 to 3, comprising
 - 25 depositing the silicon germanium layer (3) atop the substrate (1) and atop the cylindrical silicon germanium layer (2) such that it has a thickness of not less than 0.01 μm and not more than 10 μm .
5. The method as claimed in one of claims 1 to 4, wherein
 - 30 the silicon germanium layer (3) is a constant composition layer.

6. The method as claimed in one of claims 1 to 4, wherein
the silicon germanium layer (3) is a graded composition layer.
7. The method as claimed in one of claims 1 to 6, wherein
5 the content of germanium of the cylindrical SiGe layer (2) is lower, equal to or
higher than the germanium content of the SiGe layer (3).