

FIG. 1

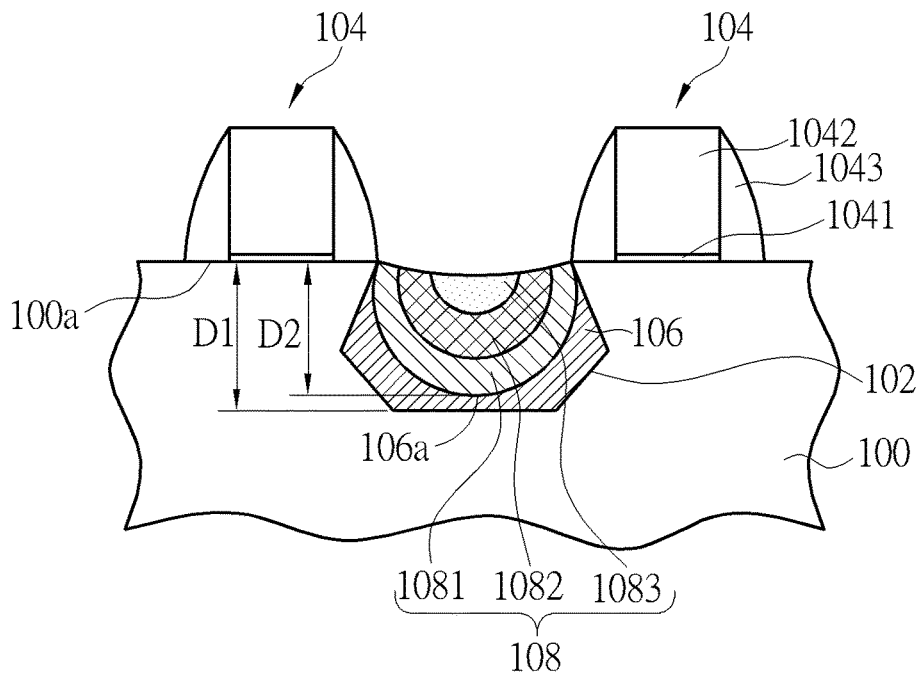


FIG. 2

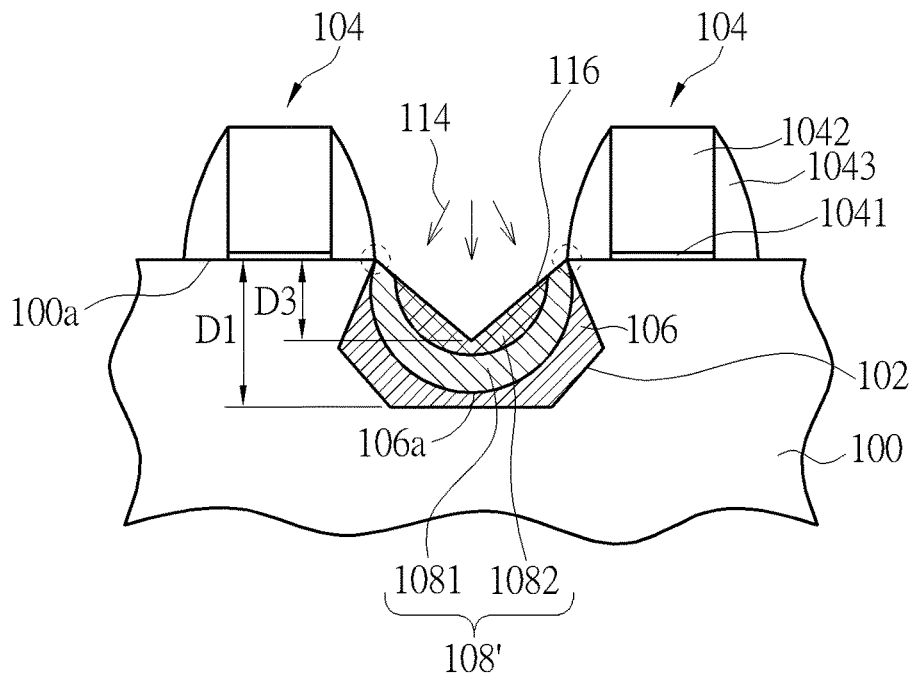


FIG. 3

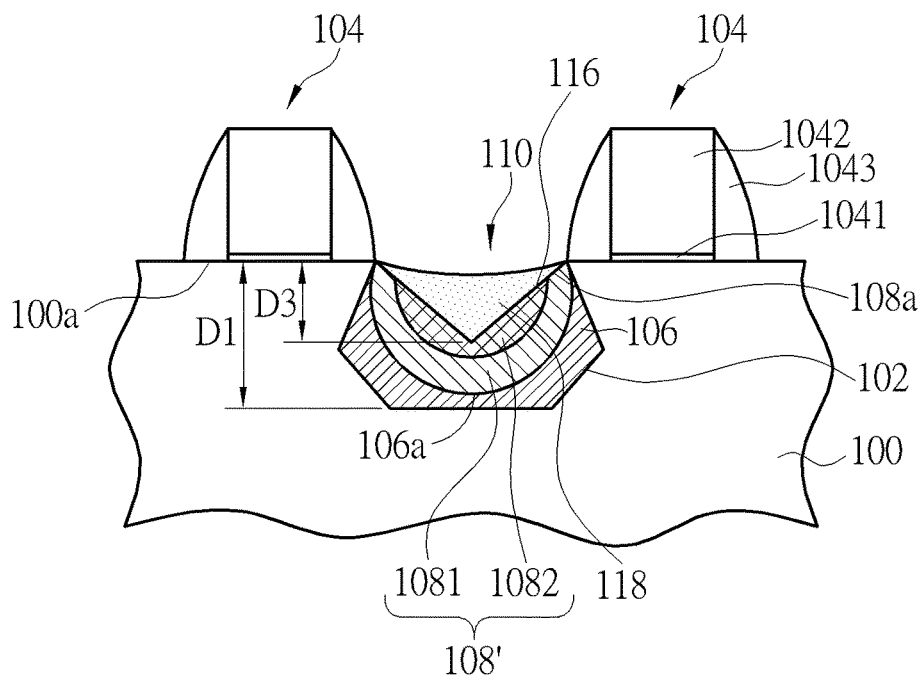


FIG. 4

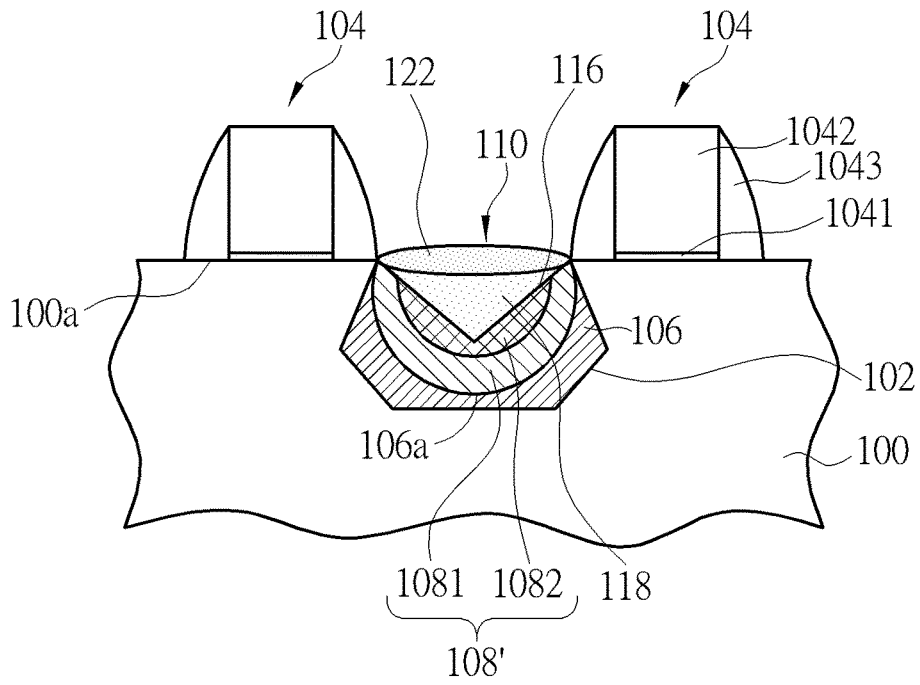


FIG. 5

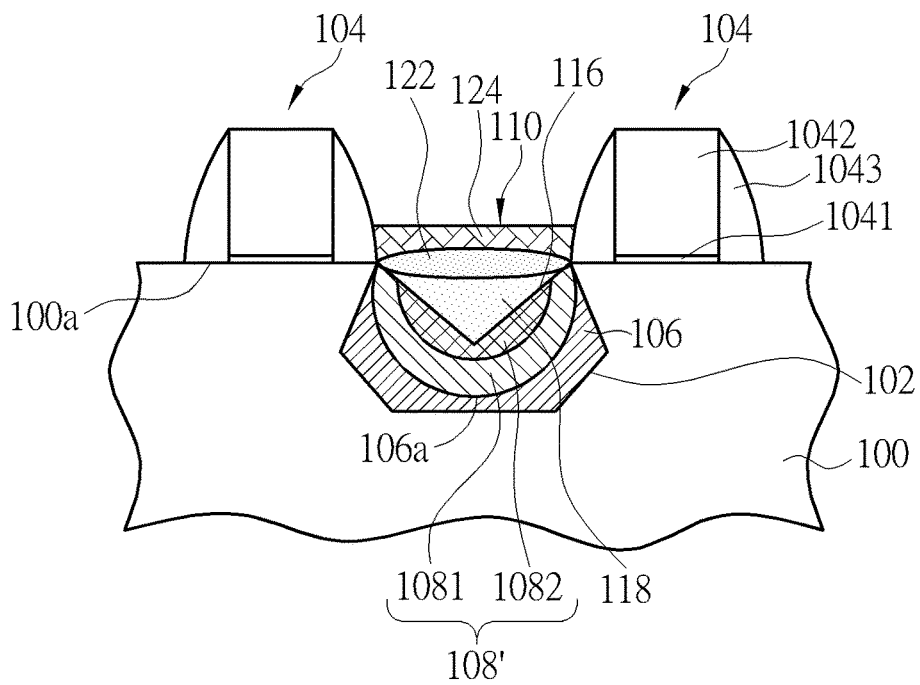


FIG. 6

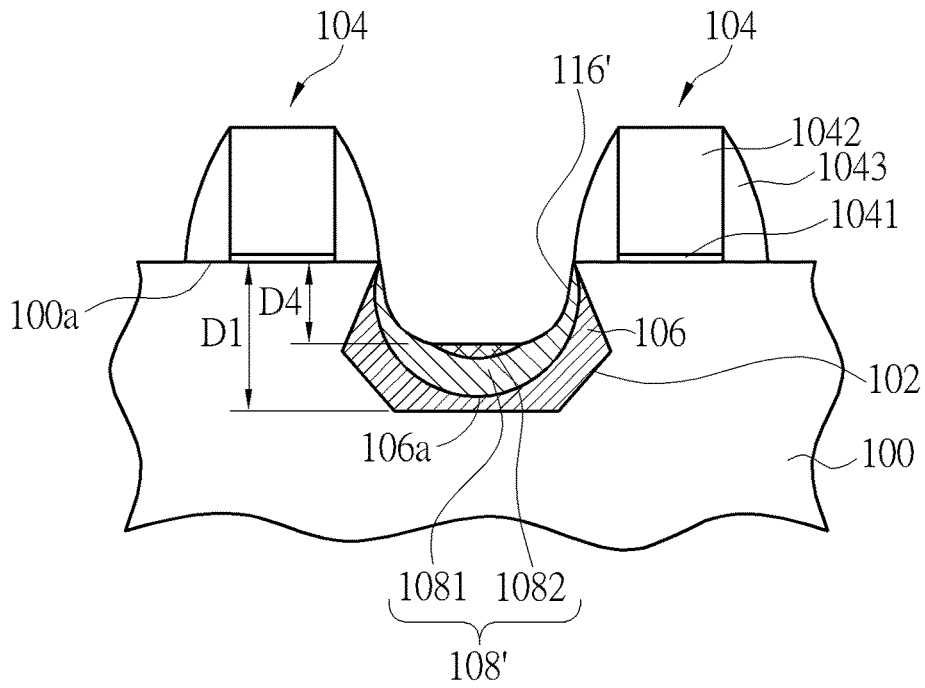


FIG. 7

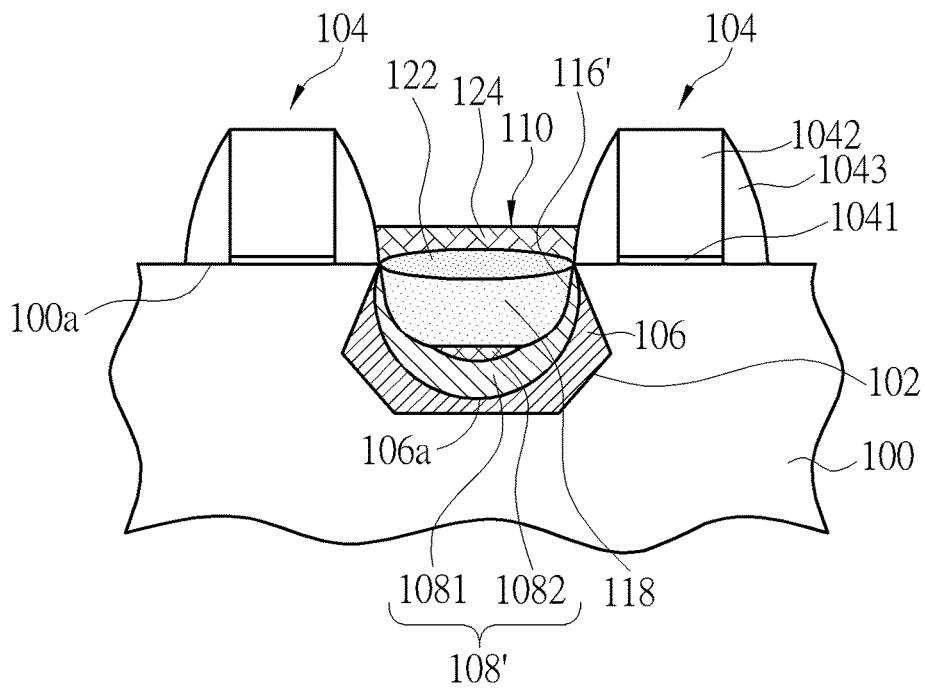


FIG. 8

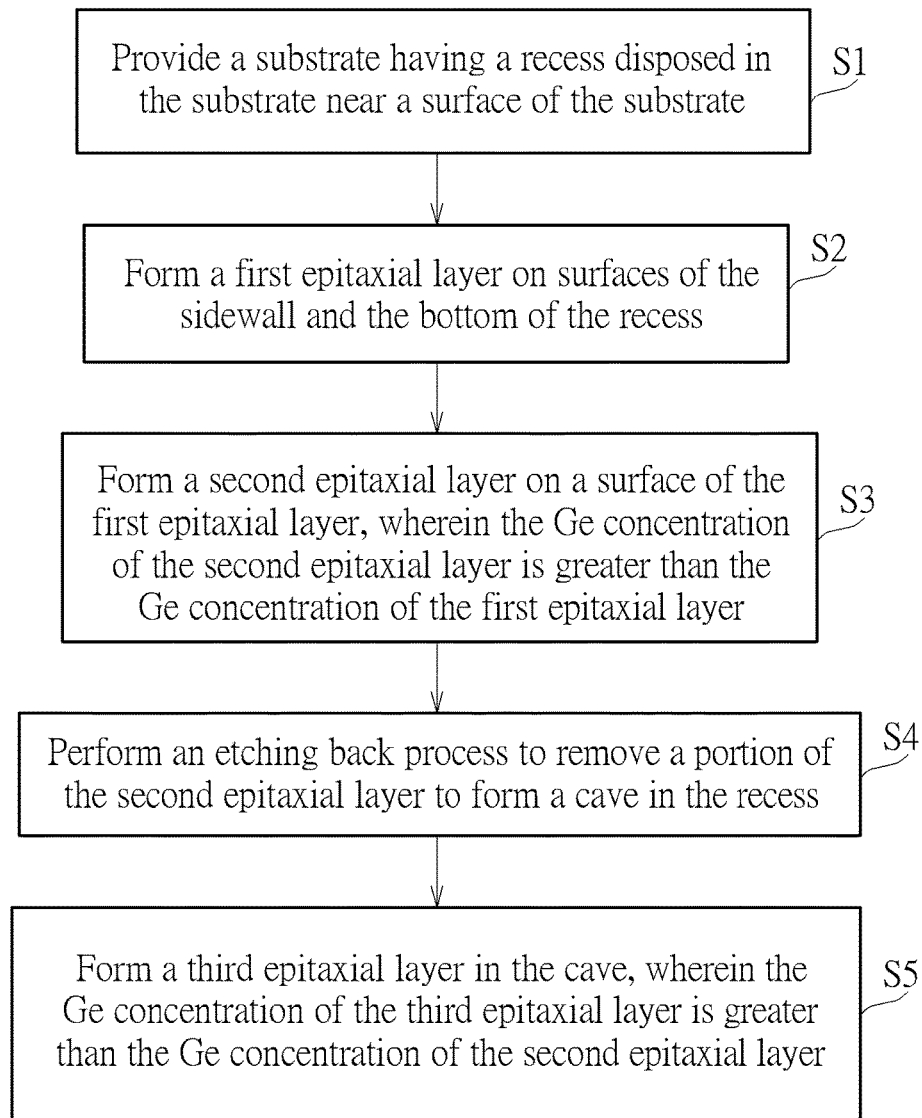


FIG. 9

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EPITAXIAL STRUCTURE OF SEMICONDUCTOR DEVICE AND MANUFACTURING METHOD THEREOF

BACKGROUND OF THE INVENTION

1. Field of the Invention

The present invention relates to an epitaxial structure of semiconductor device and a manufacturing method thereof, more particularly, to an epitaxial structure of semiconductor device with improved strain effect and a manufacturing method thereof.

2. Description of the Prior Art

The semiconductor integrated circuit (IC) industry has experienced rapid growth. In the course of IC evolution, strained source/drain features have been implemented using epitaxial (EPI) semiconductor materials to enhance carrier mobility and improve device performance. For example, when forming a metal-oxide-semiconductor field effect transistor (MOSFET), silicon germanium (SiGe) may be epitaxially grown to form source and drain features. Various techniques directed at shapes, configurations, and materials of these source and drain features have been implemented to further improve transistor device performance. Although many approaches have been developed for their intended purposes, they have not been entirely satisfactory in all respects. For example, in a conventionally formed SiGe bulk structure, the Ge concentration in Ge region is not as high as expectation, and the Ge region with higher concentration has a certain distance to channel region.

SUMMARY OF THE INVENTION

It is one of the objectives of the present invention to provide an epitaxial structure and manufacturing method thereof, wherein the formed epitaxial structure has improved distribution and arrangement of Ge region with high concentration.

According to an embodiment of the present invention, an epitaxial structure of semiconductor device is provided. The epitaxial structure of semiconductor device includes a substrate, a recess, a first epitaxial layer, a second epitaxial layer, and a third epitaxial layer. The recess is formed in the substrate and disposed near a surface of the substrate, wherein the recess has a recess depth. The first epitaxial layer is disposed on surfaces of a sidewall and a bottom of the recess. The second epitaxial layer is disposed on the surface of the first epitaxial layer, wherein the germanium (Ge) concentration of the second epitaxial layer is greater than the Ge concentration of the first epitaxial layer. The third epitaxial layer is disposed on the surface of the second epitaxial layer, wherein the Ge concentration of the third epitaxial layer is greater than the Ge concentration of the second epitaxial layer, and the depth of the third epitaxial layer is about $\frac{1}{2}$ to about $\frac{3}{4}$ of the recess depth.

According to an embodiment of the present invention, a manufacturing method of an epitaxial structure is further provided. The manufacturing method includes providing a substrate, wherein a recess is disposed in the substrate near a surface of the substrate; forming a first epitaxial layer on surfaces of a sidewall and a bottom of the recess; forming a second epitaxial layer on a surface of the first epitaxial, wherein a germanium (Ge) concentration of the second epitaxial layer is greater than a Ge concentration of the first epitaxial layer; performing an etching back process to remove a portion of the second epitaxial layer to form a cave in the recess; and forming a third epitaxial layer in the cave,

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wherein a Ge concentration of the third epitaxial layer is greater than the Ge concentration of the second epitaxial layer.

Base on the disclosure of the present invention, it is an advantage that a cave is formed before forming the third epitaxial layer with high Ge concentration such that the sequentially formed third epitaxial layer can fill the cave to have a large top area and is arranged adjacent to the channel region, which efficiently improve the strain effect.

These and other objectives of the present invention will no doubt become obvious to those of ordinary skill in the art after reading the following detailed description of the preferred embodiment that is illustrated in the various figures and drawings.

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1 to FIG. 6 are schematic diagrams illustrating the manufacturing method of an epitaxial structure according to a first embodiment of the present invention, wherein:

FIG. 1 is a schematic drawing of a cross-sectional view of the epitaxial structure after performing the first and second steps mentioned in the first embodiment;

FIG. 2 is a schematic drawing in a step subsequent to FIG. 1;

FIG. 3 is a schematic drawing in a step subsequent to FIG. 2;

FIG. 4 is a schematic drawing in a step subsequent to FIG. 3;

FIG. 5 is a schematic drawing in a step subsequent to FIG. 4; and

FIG. 6 is a schematic drawing in a step subsequent to FIG. 5.

FIG. 7 and FIG. 8 are schematic diagrams illustrating the manufacturing method of an epitaxial structure according to a second embodiment of the present invention, wherein:

FIG. 7 is a schematic drawing of a cross-sectional view of the epitaxial structure following the process illustrated in FIG. 2; and

FIG. 8 is a schematic drawing in a step subsequent to FIG. 7.

FIG. 9 is a schematic diagram illustrating the process flow of the manufacturing method of an epitaxial structure according to the present invention.

DETAILED DESCRIPTION

To provide a better understanding of the present invention to the skilled users in the technology of the present invention, preferred embodiments will be detailed as follows. The preferred embodiments of the present invention are illustrated in the accompanying drawings with numbered elements to elaborate on the contents and effects to be achieved.

Please refer to FIG. 1 to FIG. 6 and FIG. 9. FIG. 1 to FIG. 6 are schematic diagrams illustrating the manufacturing method of an epitaxial structure according to a first embodiment of the present invention, which also illustrate the cross-sectional views of the epitaxial structure. FIG. 9 is a schematic diagram illustrating the process flow of the manufacturing method of an epitaxial structure according to the present invention. First, as shown in FIG. 1 and FIG. 9, the step S1 is performed to provide a substrate 100, wherein a recess 102 is disposed in the substrate 100 near the surface 100a of the substrate 100. The substrate 100 may be a semiconductor substrate (such as a silicon substrate), a silicon containing substrate (such as a silicon carbide substrate), an III-V group-on-silicon (such as GaN-on-silicon)

substrate, a graphene-on-silicon substrate, a silicon-on-insulator (SOI) substrate or an epitaxial layer containing substrate, but not limited thereto. The formation of the recess **102** may comprise one or more etching process, including but not limited to a dry process such as a plasma etching process, a wet etching process, or a combination of both. For example, an etchant such as carbon tetrafluoride (CF₄), HF, tetramethylammonium hydroxide (TMAH), or combinations of thereof, or the like may be used to perform the wet etch process, so as to form the recess **102**. The formed recess **102** has a recess depth **D1** which is, but not limited to, about 500-1000 angstroms in this embodiment.

In addition, two gate structures **104** are selectively formed on the surface **100a** of the substrate **100**, wherein each of the gate structures **104** includes a gate insulating layer **1041** disposed on the surface **100a** of the substrate **100**, a gate portion **1042** disposed above the dielectric layer **1041**, and a spacer **1043** surrounding the gate portion **1042**. In this embodiment, the recess **102** is formed in the source/drain region near the gate structures **104**. More specifically, the formed recess **102** is disposed between the two adjacent gate structures **104**. The gate insulating layer **1041** may be composed of dielectric material such as oxides or nitrides, but not limited thereto. The gate insulating layer **1041** could also be composed of pad oxide or a high-k dielectric layer composed of HfSiO, HfSiON, HfO, LaO, LaAlO, ZrO, ZrSiO, or HfZrO. The gate portion **1042** may be a silicon layer including an amorphous silicon layer, a polysilicon layer, a single silicon layer with doped silicon layer, or a composite silicon layer with combination of aforementioned silicon layers. The gate portion **1042** may also include metal materials or be composed of metal layer and other functional or optional layers (not shown), such as work function layer(s) and barrier layer(s). In addition, a cap layer (not shown) may be selectively disposed on the gate portion **1042**. The spacer **1043** can be a single layer or a composite layer, which may be composed of high temperature oxide (HTO), silicon nitride, silicon oxide or silicon nitride (HCD-SiN) formed by hexachlorodisilane (Si₂Cl₆), but not limited thereto.

Next, the step **S2** is performed to form a first epitaxial layer **106** on surfaces of the sidewall and the bottom of the recess **102**. The first epitaxial layer **106** has a low Ge concentration, which is less than and equal to 30%, or less than and equal to 25%. The Ge concentration of the whole first epitaxial layer **106** may be substantially fixed to a certain value or to a certain range uniformly, such as ranging from 25% to 30%, but not limited thereto. However, the first epitaxial layer **106** may have a gradient Ge concentration upwardly increased. For example, the Ge concentration of the first epitaxial layer **106** may be upwardly increased from about 0% to about 30%. A selective epitaxial growth (SEG) process may be carried out to form the first epitaxial layer **106**. The SEG process may include, but not limited to, a low pressure chemical vapor deposition (LPCVD) process. For example, the SEG process can use dichlorosilane (SiH₂Cl₂, DCS) as a silicon source, germane (GeH₄) as a germanium source, HCl or Cl₂ as an etchant to provide selectivity during the deposition and hydrogen (H₂) as a carrier gas, so as to control selective growth. However, in other embodiments, deposition and etching processes may be separately and independently performed in separate processing steps.

Sequentially, as shown in FIG. 9 and FIG. 2, the step **S3** is executed to form a second epitaxial layer **108** on the surface of the first epitaxial layer **106**. The second epitaxial layer **108** is a bulk epitaxial layer and is directly in contact with the first epitaxial layer **106**, and the bottom boundary

106a of the first epitaxial layer **106** and the second epitaxial layer **108** is positioned around $\frac{2}{3}$ of the recess depth **D1** as an example. The second epitaxial layer **108** formed in the step **S3** of forming the second epitaxial layer **108** substantially fills the recess **102**. The Ge concentration of the second epitaxial layer **108** is greater than the Ge concentration of the first epitaxial layer **106**. It should be noted that second epitaxial layer **106** has a gradient Ge concentration upwardly increased. Preferably, the Ge concentration of the second epitaxial layer **108** is greater than about 30% and less than about 45% or about 40%. For example, the second epitaxial layer **108** may include at least three portions according to different ranges of Ge concentration: the first portion **1081**, the second portion **1082**, and the third portion **1083**, but not limited thereto. The first portion **1081** has a Ge concentration ranges from about 30% to about 35% and is positioned on the surface of the first epitaxial layer **106**. The second portion **1082** has a Ge concentration ranges from about 35% to about 40% and is positioned on the surface of the first portion **1081**. The third portion **1083** has a Ge concentration ranges from about 40% to about 45% and is positioned on the surface of the second portion **1082**. Specifically, the first portion **1081**, the second portion **1082**, and the third portion **1083** are arranged as a part of three concentric circles, which means the first portion **1081** surrounds the lower side of the second portion **1082**, and the second portion **1082** surrounds the lower side of the third portion **1083**. The formation of the second epitaxial layer **108** can include a SEG process, which may adopt the same precursor, material source, and etchant and other process parameters as the formation of the first epitaxial layer **106**. It should be noted that since the Ge concentration of the second epitaxial layer **108** is increased gradient, the flow ratio of the source of Ge to the source of Si may be advanced by steps, for instance. In various embodiments, the second epitaxial layer **108** has a linear distribution of Ge concentration, wherein the boundaries between the first, second, and third portions **1081**, **1082**, and **1083** cannot be clearly defined.

Then, referring to FIG. 3 and FIG. 9, the step **S4** is executed to perform an etching back process **114** to remove a portion of the second epitaxial layer **108** in order to form a cave **116** in the recess **102**. In this embodiment, the sectional cross-sectional profile of the cave **116** preferably is a V-shaped structure, but not limited thereto. The etching back process **114** includes a dry etching process, a wet etching process, or combination thereof. In addition, the etching back process **114** is controlled and tuned to ensure removal of the certain portion of the second epitaxial layer **108** in order to obtain a preferable shape of the cave **116**. For example, etching parameters of the dry and/or wet etching processes can be tuned, such as etchants, etching temperature, etching solution concentration, etching pressure, source power, RF bias voltage, RF bias power, etchant flow rate, and other suitable parameters. In this embodiment, the etching back process **114** is a dry etching process that uses a chlorine-containing gas, such as HCl, Cl₂, other chlorine-containing gases, or a combination thereof. However, other etchant may also be used in the dry etching process, such as a fluorine-containing gas (such as HF, NF₃, SF₆, CF₄, other fluorine-containing gases, or combinations thereof), a silicon-containing gas (such as DCS, SiCH₃, other silicon-containing gas, or a combination thereof), other gas, or a combination thereof. In a preferred embodiment, HCl is used as the etchant because of that HCl may be also used during the SEG processes in the formation of the first epitaxial layer **106** and the formation of the second epitaxial layer **108**, such that the etching back process **114** can be

in-situ performed with the aforementioned SEG processes, in the same chamber of forming the epitaxial layers. Preferably, the etching back process **114** is continuously executed until the opening fringe of the cave **116** (as marked by the dotted circles) is close to the opening fringe of the recess **102**, which means the top opening of the cave **116** reaches the gate structures **104** and close to the channel regions below the gate structures **104**. Alternatively, the etching back process **114** can be continuously carried out until the depth **D3** of the cave **116** reaches about $\frac{1}{2}$ of the recess depth **D1** to about $\frac{3}{4}$ of the recess depth **D1**, wherein the depth **D3** of the cave **116** can be defined by the distance of the lowest point of the V-shaped structure and the top surface **100a** of the substrate **100**. It should be noted that the third portion **1083** of the second epitaxial layer **108** is substantially removed and the upper part of the second portion **1082** and the first portion **1081** of the second epitaxial layer **108** near the gate structures **104** are also removed in the etching back process **114**. The remained second epitaxial layer is numbered as **108'**, composed of the residual first portion **1081** and second portion **1082**.

Then, as shown in FIG. 4 and FIG. 9, the step **S5** is performed to form a third epitaxial layer **118** in the cave **116**, wherein the Ge concentration of the third epitaxial layer **118** is greater than the Ge concentration of the second epitaxial layer **108**. Preferably, the third epitaxial layer **118** fully fills the cave **116** and has a fixed high Ge concentration ranges from about 40% to about 45%. The composition concentration of the third epitaxial layer **118** may be uniform in this embodiment. The formation method and parameters of the third epitaxial layer **118** may be referred to the aforementioned paragraphs of the formation of the first epitaxial layer **106** and the second epitaxial layer **108**, thus redundant description will not be repeated herein. After the formation of the third epitaxial layer **118**, the manufacture of the epitaxial structure **110** of semiconductor device according to the present invention is completed. Therefore, the epitaxial structure **110** of semiconductor device according to the present invention includes a substrate **100**, a recess **102**, a first epitaxial layer **106**, a second epitaxial layer **108'**, and a third epitaxial layer **118**. The recess **102** is formed in the substrate **100** and disposed near the surface **100a** of the substrate, wherein the recess **102** has a recess depth **D1**. The first epitaxial layer **106** is disposed on surfaces of the sidewall and the bottom of the recess **102**. The second epitaxial layer **108'** is disposed on the surface of the first epitaxial layer **106**, wherein the Ge concentration of the second epitaxial layer **108'** is greater than the Ge concentration of the first epitaxial layer **106**. In addition, the third epitaxial layer **118** is disposed on the surface of the second epitaxial layer **108'**, wherein the Ge concentration of the third epitaxial layer **118** is greater than the Ge concentration of the second epitaxial layer **108'**, and the depth **D3** of the third epitaxial layer **118** is about $\frac{1}{2}$ to about $\frac{3}{4}$ of the recess depth **D1**.

According to the present invention, since the third epitaxial layer **118** with the highest and fixed Ge concentration fully fills the cave **116**, the boundary **108a** between the top portion of the third epitaxial layer **118** and the second epitaxial layer **108** is close to the opening fringe of the recess **102**. Therefore, the third epitaxial layer **118** with high Ge concentration has a large top area covering a portion of the substrate **100** that is positioned between the gate structures **104** and is in contact with the channel region positioned below the gate structures **104**, such that the strain of channel can be effectively improved. In addition, since most part of the third epitaxial layer **118** is deposited on the second

portion **1082** with a medium range of Ge concentration, not the first portion **1081** of the second epitaxial layer **108**, the third epitaxial layer **118** with high Ge concentration can be formed with good crystalline structure, without dislocation and stacking fault. Moreover, the V-shaped cave **116** also provides an advantage to further avoid dislocation when depositing the third epitaxial layer **118**.

In addition, after the formation of the third epitaxial layer **118** of the present invention, a SiGe cap layer and a doped silicon cap (Si-cap) layer may be further formed on the third epitaxial layer **118**. Referring to FIG. 5, the SiGe cap layer **122** is deposited on the third epitaxial layer **118**, wherein the Ge concentration of the SiGe cap layer **122** may be decreased upwardly in gradient from about 40% or 45% to about 0%, for instance. In this situation, the SiGe cap layer **122** may have a linear distribution of Ge concentration from bottom to top. Then, as shown in FIG. 6, a Si-cap layer **124** is formed to cover the SiGe cap layer **122**, wherein the Si-cap layer **124** may be doped with dopants such as boron. The SiGe cap layer **122** and the Si-cap layer **124** may be deposited through CVD processes, but not limited thereto. After the formation of the Si-cap layer **124**, other fabrication processes of semiconductor device may be further performed.

The epitaxial structure of semiconductor device of the present invention and the manufacturing method thereof are not limited by the aforementioned embodiment, and may have other different preferred embodiments. To simplify the description, the identical components in each of the following embodiment are marked with identical symbols. For making it easier to compare the difference between the embodiments, the following description will detail the dissimilarities among different embodiments and the identical features will not be redundantly described.

Please refer to FIG. 7 and FIG. 8. FIG. 7 and FIG. 8 are schematic diagrams illustrating the manufacturing method of an epitaxial structure according to a second embodiment of the present invention, wherein FIG. 7 shows the profile of the epitaxial structure following the process illustrated in FIG. 2. As shown in FIG. 7, this embodiment is different from the first embodiment in that the cave **116'** formed during the etching back process (not shown in FIG. 7 and FIG. 8) has a profile of U-shaped structure in sectional view. The depth **D4** of the U-shaped cave **116'** is about $\frac{1}{2}$ to about $\frac{3}{4}$ of the recess depth **102**. With reference to FIG. 8, after forming the cave **116'**, the third epitaxial layer **118** is deposited to fully fill the cave **116'**, and the SiGe cap layer **122** and the Si-cap layer may be optionally formed on the third epitaxial layer **118**. Therefore, the third epitaxial layer **118** of the epitaxial structure **110** in the second embodiment of the present invention has a U-shaped boundary. Similarly, the top part of the third epitaxial layer **118** has a large area near the channel region, and the strain effect can also be improved.

To summarize, the present invention provides an epitaxial structure of semiconductor and a manufacturing method thereof that can improve the strain effect for the channel region by the way of forming a cave after the deposition of SiGe bulk with a gradient Ge concentration and filling the cave with the third epitaxial layer having fixed high Ge concentration. As a result, the third epitaxial layer has a large top area and is very close to the channel region located below the gate structures, so as to gain the expected strain effect. In addition, since the etchant of the etching back process that forms the cave can adopt HCl and/or Cl₂ which may be already used in the deposition process of epitaxial process, the etching back process may be in-situ performed

with the deposition process of epitaxial layers. Accordingly, the total fabrication process is very simple without extra process cost and procedures in comparison with prior-art process.

Those skilled in the art will readily observe that numerous modifications and alterations of the device and method may be made while retaining the teachings of the invention. Accordingly, the above disclosure should be construed as limited only by the metes and bounds of the appended claims.

What is claimed is:

1. An epitaxial structure of semiconductor device, comprising:

a substrate;

a recess in the substrate disposed near a surface of the substrate, wherein the recess has a recess depth;

a first epitaxial layer disposed on surfaces of a sidewall and a bottom of the recess;

a second epitaxial layer disposed on a surface of the first epitaxial layer, wherein a germanium (Ge) concentration of the second epitaxial layer is greater than a Ge concentration of the first epitaxial layer; and

a third epitaxial layer disposed on a surface of the second epitaxial layer, wherein a Ge concentration of the third epitaxial layer is greater than the Ge concentration of the second epitaxial layer and a depth of the third epitaxial layer is about $\frac{1}{2}$ to about $\frac{3}{4}$ of the recess depth.

2. The epitaxial structure of semiconductor device according to claim 1, wherein a cross-sectional profile of the third epitaxial layer is a V-shaped structure or a U-shaped structure.

3. The epitaxial structure of semiconductor device according to claim 1, wherein a boundary between a top portion of the third epitaxial layer and the second epitaxial layer reaches an opening fringe of the recess.

4. The epitaxial structure of semiconductor device according to claim 1, wherein a composition concentration of the third epitaxial layer is uniform.

5. The epitaxial structure of semiconductor device according to claim 4, wherein the Ge concentration of the third epitaxial layer ranges from about 40% to about 45%.

6. The epitaxial structure of semiconductor device according to claim 1, wherein the second epitaxial layer has gradient Ge concentration upwardly increased.

7. The epitaxial structure of semiconductor device according to claim 6, wherein the Ge concentration of the second epitaxial layer is greater than about 30% and less than about 40%.

8. The epitaxial structure of semiconductor device according to claim 1, wherein a composition concentration of the first epitaxial layer is uniform.

9. The epitaxial structure of semiconductor device according to claim 8, wherein the Ge concentration of the first epitaxial layer ranges from about 25% to about 30%.

10. The epitaxial structure of semiconductor device according to claim 1, wherein the first epitaxial layer has gradient Ge concentration upwardly increased.

11. The epitaxial structure of semiconductor device according to claim 10, wherein the Ge concentration of the first epitaxial layer is upwardly increased from about 0% to about 30%.

12. The epitaxial structure of semiconductor device according to claim 1, wherein a bottom portion of a boundary between the first epitaxial layer and the second epitaxial layer is positioned around $\frac{2}{3}$ of the recess depth.

13. A manufacturing method of an epitaxial structure, comprising:

providing a substrate, wherein a recess is disposed in the substrate near a surface of the substrate;

forming a first epitaxial layer on surfaces of a sidewall and a bottom of the recess;

forming a second epitaxial layer on a surface of the first epitaxial layer, wherein a germanium (Ge) concentration of the second epitaxial layer is greater than a Ge concentration of the first epitaxial layer;

performing an etching back process to remove a portion of the second epitaxial layer to form a cave in the recess; and

forming a third epitaxial layer in the cave, wherein a Ge concentration of the third epitaxial layer is greater than the Ge concentration of the second epitaxial layer.

14. The manufacturing method of an epitaxial structure according to claim 13, wherein the recess has a recess depth, and the cave has a depth ranges from about $\frac{1}{2}$ of the recess depth to about $\frac{3}{4}$ of the recess depth.

15. The manufacturing method of an epitaxial structure to claim 13, wherein a sectional cross-sectional profile of the cave has a V shape or a U shape.

16. The manufacturing method of an epitaxial structure according to claim 13, wherein an opening fringe of the cave reaches an opening fringe of the recess.

17. The manufacturing method of an epitaxial structure according to claim 13, wherein the second epitaxial layer formed in the step of forming the second epitaxial layer substantially fills the recess.

18. The manufacturing method of an epitaxial structure according to claim 13, wherein a composition concentration of the third epitaxial layer is uniform.

19. The manufacturing method of an epitaxial structure according to claim 18, wherein the Ge concentration of the third epitaxial layer ranges from about 40% to about 45%.

20. The manufacturing method of an epitaxial structure according to claim 13, wherein a bottom portion of a boundary between the first epitaxial layer and the second epitaxial layer is positioned around $\frac{2}{3}$ of a recess depth of the recess.

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