Semiconductor layer structure and method for fabricating a semiconductor layer structure

The invention relates to a semiconductor layer structure and to a method for fabricating a semiconductor layer structure.

For realizing modern components for high-power electronics and also optoelectronics, the prior art usually uses substrates which can only be fabricated in a very complicated and hence cost-intensive manner. Furthermore, said substrates often have a high defect density.

An alternative for producing cost-effective and high-quality substrates consists in depositing a thin layer (a few tens of nm) of the desired substrate material on a high-quality and cost-effective substrate, such as, for example, on a silicon wafer. This yields lattice-matched substrates which enable a low-defect epitaxial deposition of further layers.

However, significant physical properties are determined by the substrate in this case, in particular the coefficient of thermal expansion. This is problematic because, by way of example, the growth of III-V compound semiconductors such as GaN by means of metal organic chemical vapor deposition (MOCVD) is often effected at comparatively high temperatures of above 1000°C in order to ensure a sufficient quality for component fabrication. If a layer deposited at such high temperatures is cooled on a substrate having a significantly lower coefficient of thermal expansion, then firstly a tensile stream of the deposited layer occurs and in the further course of events the layer often cracks, which renders it unusable.

Journal of Crystal Growth 280, 346-351 (2005), N.H. Zhang et al., proposes the use of interlayers of differing composition and/or structure during the deposition, which are intended to compensate for the strains that arise.

One obvious disadvantage is the complicated process implementation, since in general different process steps and parameters are necessary for the production of the interlayers than for the deposition of the desired layer.

In principle, so-called "compliant substrates" or matched substrates constitute another possibility. These are understood to be substrates in which a thin layer of the desired substrate material is applied to another substrate in such a way that there is only a weak mechanical coupling between said substrate and the applied layer.

A method of this type is described for example in Journal of Electronic Materials 29(7), 897-900 (2000), Hobart et al. In this case, firstly an $Si_{1-x}Ge_x$ layer is deposited on an SOI ("silicon-on-insulator") wafer, the buried silicon dioxide layer additionally being doped with boron and phosphorus. This borophosphosilicate layer has the property of being able to flow viscously starting from temperatures of approximately 800°C, which enables a stress relaxation of any layers deposited thereon.

The problem is manifested in this case, however, in that deposited layers bulge out on these substrates. The reason for this is due to the high viscosity of the borophosphosilicate layer and the necessity of thermal contraction of the deposited layer when cooling to room temperature. Since the fabrication of modern semiconductor components places high demands on the planarity of the layers, this is a serious

disadvantage. Such bulging out has hitherto been possible to be achieved in such material systems only - as described in the above publication - by a patterning of the substrates, which is undesirable in many cases.

Further disadvantages arise from the complexity of the fabrication of such substrates. Use is usually made of SOI ("silicon-on-insulator") wafers based on technologically complex processes such as the "smart-cut" process or high-dose oxygen ion implantation ("SIMOX" method).

Other methods for fabricating such virtual substrates, as described for example in EP 1437764 A1 and WO2004/082001 A1), deliberately fabricate a defect region in the substrate in order to enable relaxed layers on non-lattice-matched substrates, in particular for the purpose of producing strained silicon layers on relaxed $Si_{1-x}Ge_x$ layers which were grown on silicon.

An ion implantation step is employed here which serves to produce a defect region below the layer already deposited beforehand or a deposited layer system. During a subsequent thermal aftertreatment, said defect region leads to the formation of dislocations and stacking faults in the original substrate, which have a relaxing effect on the deposited layer or the layer system. A prerequisite for these methods is thin low-defect layers on the silicon substrate which can relax by means of a thermal aftertreatment after the ion implantation step.

There is the problem in this case, however, that the defect regions produced remain stable only over short times and anneal with a longer process duration.

This is associated with the fact that Ostwald ripening takes place that is to say that the cavities coarsen their size distribution by vacancy diffusion and

combine to form a small number of larger cavities. As a result, the density of the cavities produced becomes so low that, for energetic reasons, dislocations or stacking faults no longer form between the cavities. This problem occurs in the case of long process times at high temperatures such as, for example, during the deposition of a layer by means of MOCVD on said layer structure. Since relaxation of the layer structure during cooling is no longer possible on account of the excessively low density of cavities, cracking of the deposited layer occurs.

Possibly increasing the cavity density solves this problem only to a limited extent since, starting from a critical density of said cavities, it is possible for the deposited layer to split off - particularly during subsequent high-temperature processes at temperatures greater than or equal to 1000°C.

Therefore, the example embodiments of the present invention may provide substrates for stress- and crack-free deposition of semiconductor materials and also a method for fabricating substrates of this type.

In a first aspect of the invention, there is provided a method for fabrication a semiconductor layer structure, comprising the following steps: a) provision of a substrate made of a semiconductor material; b) application of a layer made of a second semiconductor material to said substrate for the purpose of producing a semiconductor layer structure; c) implantation of gas ions of one or more atom types, selected from a group of hydrogen and noble gases, into the semiconductor layer structure for the purpose of producing a layer comprising cavities in the semiconductor layer structure; d) application of at least one epitaxial layer to the semiconductor layer structure, characterized in that substrate contains silicon and layer contains silicon carbide, that in step b) layer is provided by uncovering

a buried silicon carbide layer produced by implantation of carbon ions into substrate, and that impurity atoms of one or more atom types, selected from a group of oxygen, nitrogen and carbon, with a dose of utmost $5x10^{17}$ cm^{-2} are implanted into the semiconductor layer structure fur the purpose of thermally stabilizing the cavities produced by implantation of gas ions in layer.

In a second aspect of the invention, there is provided a semiconductor layer structure, comprising a substrate made of silicon, on which a layer containing silicon carbide is situated, furthermore a region having impurity atoms of one or more atom types selected from oxygen, nitrogen and carbon, which region is situated either in layer or below the interface between layer and substrate and which contains silicon carbide precipitates, additionally a layer within the region having impurity atoms, which layer comprises cavities of hydrogen or noble gas bubbles produced by ion implantation, furthermore at least one epitaxial layer applied to layer and also a defect region comprising dislocations and stacking faults within the layer comprising cavities, the at least one epitaxial layer being crack-free, and a residual strain of the at least one epitaxial layer being less than or equal to 1 GPa.

Also disclosed is a method for fabricating a semiconductor layer structure, comprising the following steps: a) provision of a substrate made of a semiconductor material; b) application of a layer made of a second semiconductor material to said substrate for the purpose of producing a semiconductor layer structure; c) implantation of light gas ions into the semiconductor layer structure for the purpose of producing a layer comprising cavities in the semiconductor layer structure; d) stabilization of said cavities by impurity atoms of a specific species; e) application of at least one epitaxial layer to the semiconductor layer structure.

The substrate provided in a) is preferably a wafer made of monocrystalline silicon.

Furthermore, the use of semiconductor wafers fabricated by means of bonding methods is also preferred.

The use of an SOI ("silicon-on-insulator") wafer as a substrate is likewise preferred.

However, the substrate may also comprise polycrystalline semiconductor material.

The substrate may furthermore also be layer structures comprising a silicon layer, a silicon-germanium (SiGe) layer or a germanium layer.

Generally, all substrates on which monocrystalline or polycrystalline layers can be deposited are suitable.

The layer made of a second semiconductor material that is to be applied in step b) is preferably a monocrystalline silicon carbide layer.

However, a silicon-germanium layer or a layer structure comprising a silicon-germanium layer is also preferred as layer to be applied in step b).

The application of the layer made of a second semiconductor material for the purpose of producing a semiconductor layer structure in step b) of the method according to the invention is preferably effected by means of chemical vapor deposition (CVD), molecular beam epitaxy (MBE) or by ion beam synthesis (IBS).

Depending on the method used for applying the layer in step b), preferred layer thicknesses are 0.5 nm to 100 μm in the case of CVD, 0.5 nm to 5 μm in the case of MBE and 0.5 nm to 1 μm in the case of IBS.

The layer thickness of the layer applied in b) is particularly preferably 1-500 nm, independently of the method used.

In step c) of the method, light gas ions are implanted into the semiconductor layer structure.

The implantation of the gas ions may be effected in a depth range below an interface between applied layer and substrate or else within the layer applied in b).

Here an implantation energy is chosen in the first case such that the cavities arise just below an interface between the substrate and applied layer, that is to say preferably within the range of 0-500 nm below that interface.

By means of the implantation of light gas ions, cavities or bubbles are produced in the semiconductor layer structure.

The implanted gas ions are preferably hydrogen ions.

Implantation of noble gas ions of one or more atom types selected from a group of helium ion, neon ions and argon ions is also preferred.

The implantation of noble gas ions may also be an implantation of mixtures of said atom types or else a combination of separate implantations of said atom types.

By way of example, it is possible, therefore, to combine a helium ion implantation with a neon ion implantation.

However, a combination of an implantation of hydrogen ions and an implantation of noble gas ions of one or

more atom types selected from a group of helium ions, neon ions and argon ions is also preferred.

By way of example it is possible, therefore, to combine an implantation of hydrogen ions with an implantation of helium ions.

For a, for example, 70 nm thick SiC layer on a silicon substrate, an implantation energy of 22 keV for helium ions and a dose of approximately 2×10^{16} cm^{-2} are chosen, by way of example. This then leads to a defect region of approximately 0-70 nm below the interface between applied layer and substrate.

Lower implantation energies can be chosen in order to produce the defect region within the applied layer.

The implantation energies, depending on the thickness and type of the deposited layer, preferably lie within the range of 1 keV-2 MeV.

The implantation energies particular preferably lie within the range of 10-200 keV.

In this case, however, implantation energies of 20-50 keV are especially to be preferred.

The point in time at which the cavities arise can be controlled by way of the choice of the implantation temperature:

If low implantation temperatures and high doses are chosen, cavities having a certain size are already produced directly after the implantation.

It has proved to be advantageous, however to choose higher implantation temperatures of approximately 400°C in order firstly to produce only seeds for cavities, which, after suitable stabilization thereof by impurity

atoms, even during subsequent long high-temperature processes at temperatures of 900-1250°C and with treatment durations of 2 hours or longer result in a narrow cavity distribution with average cavity diameters of approximately 10 nm.

In particular, it is possible to prevent the layer from splitting off later in a high-temperature process up to a temperature of 1250°C.

The choice of the doses of the hydrogen or noble gas ions to be implanted is dependent on the type and thickness of the applied layer and also on the implantation energy.

The doses of the hydrogen and/or noble gas ions to be implanted preferably lie within the range of 1×10^{13} - 1×10^{17} cm^{-2}.

Doses within the range of 1×10^{15} cm^{-2} - 5×10^{16} cm^{-2} are particularly preferred.

It is known to the person skilled in the art that the resulting concentrations of impurity atoms are dependent on the implanted dose and on the thermal outdiffusion. The required doses are therefore preferably determined experimentally.

A tilting of the semiconductor layer structure relative to the ion beam during the implantation is likewise preferred.

The semiconductor layer structure is preferably tilted by an angle of 0-60° with respect to the ion beam.

Angles of 0-30° are particularly to be preferred, angles of 0-15° being especially to be preferred.

In step d) of the method, the cavities in the semiconductor layer structure are stabilized by impurity atoms of one or more atom types selected from a group of oxygen, nitrogen and carbon.

This is effected, in the case where in the substrate and/or in the applied layer, impurity atoms of those atom types are already present at least in the region of the layer comprising cavities, preferably by means of a thermal treatment of the semiconductor layer structure produced at at least 600°C.

In this case, the impurity atoms may be present in dissolved form, in the form of compounds with the substrate material, or as precipitates.

A separate thermal treatment is not necessary, however, nor is it preferred if the application of the at least one epitaxial layer in accordance with step e) is effected at a temperature of at least 600°C.

Sufficient densities of areal defects such as are required for a relaxation of the deposited layer are not achieved below said temperature.

A thermal treatment of the semiconductor layer structure at very high temperatures of 1300°C or higher is possible, in principle. However, the dynamic behavior of Ostwald ripening must be taken into consideration here, which may lead to undesirable effects at such temperatures, even in the case of impurity-atom-stabilized cavities. It is primarily necessary to prevent the applied layer from chipping off, and also an excessively great decrease in the density of the cavities on account of coarsening. Therefore, the thermal treatment of the semiconductor layer structure and the deposition of epitaxial layers on the semiconductor layer structure are preferably effected at temperatures of 600-1250°C.

If impurity atoms of one or more atom types which are preferably selected from a group of nitrogen, oxygen and carbon are not present in sufficient concentration in the substrate or at least in the region of the cavities produced, an implantation of ions of said atom types into the semiconductor layer structure is preferably effected in step d).

In this case, the implantation is preferably chosen such that the concentration maximum of the impurity atoms and the concentration maximum of the implanted gas ions coincide or at least lie in a similar depth range.

Therefore, implantation energies of 10-200 keV are preferably chosen.

Finally, in accordance with step e) at least one epitaxial layer is applied to the semiconductor layer structure.

That at least one epitaxial layer is preferably a layer made of monocrystalline silicon.

The at least one epitaxial layer preferably comprises a nitride compound semiconductor.

Said at least one epitaxial layer preferably comprises semiconductor material having a significantly different, namely higher, coefficient of thermal expansion in comparison with the semiconductor material of the substrate.

By way of example, all the compound semiconductors have a greatly different, namely a greater, coefficient of thermal expansion in comparison with silicon, cf. Table 1.

The deposited layers are typically II-IV and III-V compound semiconductors. In particular, they are layers composed of: $Al_xGa_{1-x}N$, $Al_xGa_yIn_{1-x-y}N$, $Al_xGa_yIn_{1-x-y}P$, $Al_xGa_{1-x}Sb$, $Al_xGa_yIn_{1-x-y}N_aSb_{1-a}$, $Al_xGa_yIn_{1-x-y}N_aP_bSb_{1-a-b}$, GaAs, ZnO, CdTe, CdS, CdSe and CdS_xSe_{1-x}.

In particular, layer stacks as a combination of the above compound semiconductors are also conceivable and preferred.

Material	Coeff.of lin. thermal expansion (cub.) [10^{-6}/K]	Coeff.of lin. thermal expansion (hex., α_a) [10^{-6}/K]	Coeff.of lin. thermal expansion (hex., α_a) [10^{-6}/K]
Si	2.6		
GaN		5.59	3.17
3C-SiC	3.8		
6H-SiC		4.3	4.7
ZnO		6.51	3.02
AlN		4.15	5.27

Table 1: Coefficients of thermal expansion for selected semiconductor materials

In this case, these layers may, of course, be doped with impurity atoms of any desired type according to their intended application.

Depending on the desired orientation or crystal structure (100)-, (110)-, (111)- or else misoriented semiconductor wafers may be used in the case where silicon is used as substrate.

If the semiconductor layer structure is a silicon carbide layer on a silicon wafer, the deposition of nitride compound semiconductors and thus the fabrication of starting materials for applications in optoelectronics are preferred.

In this case, the silicon carbide layer is preferably between 1 nm and 500 nm thick.

The layer thickness particularly preferably lies within the range of 30 nm to 150 nm, layer thicknesses of between 50 nm and 100 nm being especially to be preferred.

The thickness of the deposited nitride layer preferably lies - according to the later application - within the range of 100 nm to 100 µm, layer thicknesses within the range of 200 nm to 20 µm being particularly preferred and layers having thickness of between 500 nm and 5 µm being especially to be preferred.

If a layer structure made of GaN/AlN on a silicon carbide layer on silicon is involved, then it is possible to achieve threading dislocation densities of less than or equal to 10^{10} cm^{-2}, preferably within the range of 10^{6} - 10^{10} cm^{-2}.

Also disclosed is a semiconductor layer structure, comprising a substrate made of semiconductor material, on which a layer made of a second semiconductor material is situated, furthermore a region enriched with impurity atoms, which region is situated either in the layer made of a second semiconductor material or at a specific depth below the interface between the layer made of a second semiconductor material and the substrate, additionally a layer within the region enriched with impurity atoms, which layer comprises cavities produced by ion implantation, furthermore at least one epitaxial layer applied to the layer made of a second semiconductor material and also a defect region comprising dislocations and stacking faults within the layer comprising cavities, the at least one epitaxial layer being largely crack-free, and a

residual strain of the at least one epitaxial layer being less than or equal to 1 GPa.

In this case, in the context of example embodiments, cracks are to be understood as a stress-induced cracking of the at least one epitaxial layer, it being possible for said cracking to proceed right into the substrate.

Cracks of this type can be ascertained by means of optical microscopy, scanning electron microscopy, atomic force microscopy or X-ray topography.

The residual strain of the at least one epitaxial layer is preferably less than or equal to 370 MPa.

The roughness of the at least one epitaxial layer is preferably less than or equal to 7.0 nm RMS, particularly preferably 0.5-2.0 nm RMS.

The substrate made of semiconductor material is preferably a wafer made of monocrystalline silicon.

The provision of an SOI wafer as substrate is also preferred.

Moreover, a semiconductor wafer fabricated by means of a bonding method is also preferred as substrate.

However, the substrate may also comprise polycrystalline semiconductor material.

However, a substrate comprising a silicon layer, a silicon-germanium layer or a germanium layer may also be involved.

The region enriched with impurity atoms is preferably enriched with impurity atoms of one or more atom types selected from a group of oxygen, nitrogen or carbon.

The layer comprising cavities within the region enriched with impurity atoms is preferably produced by implantation of light gas ions.

The implanted gas ions are preferably hydrogen ions.

The implanted gas ions are preferably noble gas ions of one or more atom types selected from a group of helium ions, neon ions and argon ions.

Furthermore, it is also preferred for the cavities to have been produced by combinations of implantations of noble gas ions of one or more atom types, selected from a group of helium ions, neon ions and argon ions.

By way of example, the cavities may have been produced by an implantation of helium ions and an additional implantation of neon or argon ions. Corresponding gas mixtures are also conceivable for producing the cavities.

However, the production of said cavities by a combination of an implantation of hydrogen ions and an implantation of noble gas ions of one or more atom types selected from a group of helium ions, neon ions and argon ions is also preferred.

A combination of hydrogen- and helium-implanted cavities shall be mentioned as an example here.

The layer made of a second semiconductor material that is situated on the substrate is preferably a monocrystalline silicon carbide layer, particularly preferably ion-beam-synthetized silicon carbide on a substrate made of monocrystalline silicon.

The relative expansion of the lattice constant of silicon carbide is less than 0.2% in said silicon

carbide layer, which corresponds to a residual strain of the silicon carbide layer of less than 1 GPa.

The residual strain of the at least one epitaxial layer deposited on the silicon carbide layer is then less than or equal to 370 MPa.

Also disclosed is a semiconductor layer structure, comprising a layer made of ion-beam-synthetized silicon carbide on a substrate made of monocrystalline silicon, a relative expansion of the lattice constant of silicon carbide in said layer as measured by means of high-resolution X-ray diffraction being less than or equal to 0.2%.

In this case, the lattice constant and the relative expansion thereof are measured for example by means of high-resolution X-ray diffraction (HR-XRD). The measured shift relative to the unstrained value for the lattice constant produces the specified value for the residual strain of the material by conversion by means of the elastic properties, that is to say by means of the elastic constant of the semiconductor material.

The layer made of a second semiconductor material that is situated on the substrate may also be a layer structure comprising a monocrystalline silicon carbide layer on polycrystalline silicon carbide.

The at least one epitaxial layer on the semiconductor layer structure preferably comprises semiconductor material having a significantly different, namely higher, coefficient of thermal expansion in comparison with the semiconductor material of the substrate.

A first epitaxial layer preferably comprises a nitride compound semiconductor. A second epitaxial layer comprising a nitride compound semiconductor is preferably applied to the semiconductor layer

structure. The first epitaxial layer preferably comprises aluminum nitride, and the second epitaxial layer preferably comprises gallium nitride.

Optoelectronic semiconductor components which, after activation emit light having an energy of 0.1-7.0 eV can be fabricated on semiconductor layer structures of this type.

The layer made of a second semiconductor material situated on the substrate is also preferably an SiGe layer or a layer structure whose topmost layer is an SiGe layer. In this case, the epitaxial layer is preferably an epitaxial silicon layer which is applied on that SiGe layer or that layer structure comprising SiGe.

The method and the semiconductor layer structure will be explained below using particularly preferred embodiments and for the case of a semiconductor layer structure comprising 3C-SiC on silicon.

It has been shown that the method is particularly well suited to depositing a comparatively thick crack-free layer having a thickness of between 100 nm and 100 µm, that is to say a thickness of 2.5 µm, for example, which comprises $Al_xGa_{1-x}N$ having a high coefficient of thermal expansion, for example, on an ion-beam-synthetized semiconductor layer structure, such as 3C silicon carbide on silicon, for example, which has a low coefficient of thermal expansion, at high temperatures of approximately 1100°C which are typical of metal organic chemical vapor deposition (MOCVD).

This is because in the context of example embodiments it has been ascertained that the introduction of a defect

structure into an ion-beam-synthetized semiconductor layer structure is advantageous for the later crack- and stress-free deposition of nitride compound semiconductors.

For this purpose, preferably, in a 3C-SiC-Si semiconductor layer structure, by implantation of light gas ions, such as hydrogen, helium, neon or argon (or else combinations thereof), a defect-rich region is produced just below, that is to say preferably within a depth interval of 0-500 nm below, the interface between 3C-SiC and silicon, which region comprises gas-filled bubbles or cavities and, if appropriate, additionally a dislocation network and stacking faults between said bubbles or cavities. The abovementioned implantation can likewise only be effected into the 3C-SiC layer which results in a cavity structure accompanied by defects above the interface.

During the later growth of a material having a higher coefficient of thermal expansion at high temperature, that is to say at least 600°C up to at most just below the melting point of silicon - this defect structure has the effect that during the cooling operation, the upper part of the silicon substrate can plastically relax thermal stresses by virtue of dislocations and stacking faults being formed between the bubbles or cavities and/or silicon being incorporated into said cavities.

Primarily the formation of dislocations and stacking faults and also the incorporation of silicon into cavities would have the effect that a tensile strain of the layer or layers applied to the layer structure, during the cooling operation, would be reduced dynamically and be absorbed by the region of the layer structure near the surface.

A problem that is already known in the prior art is posed by the typical growth rates (typically 1 µm/h) and hence long process times at high temperatures which are present in the MOCVD deposition of III-V semiconductor layers, since cavities fabricated by ion implantation are subject to the phenomenon of Ostwald ripening and the small cavities are coarsened by vacancy diffusion. This leads to a decrease in the density of said cavities with respect to time. The formation of dislocations thus becomes less favorable energetically since the energy of a dislocation rises with its linear expansion, which may have the effect that dislocations are no longer formed and a relaxing effect is no longer present.

It had already been known from Nuclear Instruments and Methods B 175-177 (2001), 132-139, Donnelly et al., that the phenomenon of Ostwald ripening or the coalescence of smaller bubbles to form larger cavities can be attenuated, for example by implantation of carbon or oxygen into a region in which a defect region composed of bubbles is subsequently produced, for example by means of helium implantation followed by a thermal treatment. This would be sought in particular for the purpose of stabilizing the cavities in order to optimize gettering of metallic impurities.

In the context of example embodiments presented here, it has been ascertained that cavities produced by ion implantation in silicon can be stabilized by implantation of oxygen, nitrogen or carbon ions or combination of implantations of said ion types, even at high temperatures, in particular far beyond the time and temperature range of 900°C and 30 minutes considered by Donnelly.

In this case, the impurity atoms can be introduced by ion implantation also after the production of the helium bubbles into the relevant depth range.

In particular, it is thereby possible to realize higher surface densities of the cavities and thus higher densities of relaxing defect structures, whereby extensive relaxation of the deposited layers can be achieved. Only this enables a deposition of epitaxial layers of semiconductors having a greatly different coefficient of thermal expansion in comparison with silicon.

In particular, by means of a high density of cavities, it is possible to reduce the distances between the latter to an extent such that defect structures comprising dislocations and stacking faults become energetically so favorable that these can be formed between said cavities up to low temperatures at approximately 600°C. Dynamic relaxation of an epitaxial layer on the semiconductor layer structure is consequently possible.

If no cavities were present, or if the density of cavities were low, the distance between two cavities would also be large and, consequently, dislocations and stacking faults would be energetically unfavorable since the energy of said defects is dependent on their expansion. Therefore, production of a high density of stable cavities is to be striven for.

In particular, the cavities must also be thermally stable, that is to say are not permitted to coalesce and form a thermal separating layer in a temperature range of 25-1250°C.

Furthermore the cavities must also be mechanically stable in order to permit further component-relevant process steps. It is known to the person skilled in the art that the thermal stability of the cavities can be increased or decreased further by a higher or lower oxygen implantation dose, respectively.

In particular, it should be pointed out that typical deposition times and temperatures in the case of MOCVD are higher than corresponding parameters for gettering of impurities.

It has been ascertained in experiments that a post-implantation of the impurity atoms for the purpose of stabilizing the cavities is preferable to a pre-implantation. In comparison with a post-implantation, with otherwise identical parameters, pre-implantation leads to blistering, that is to say to the detachment of parts of the layer structure from the substrate. It is therefore possible to achieve higher cavity densities, and hence also higher densities of relaxing defects, by means of a post-implantation of the impurity atoms.

The inventors have furthermore recognized that the stabilizing effect can in this case be attributed, on the one hand, to the formation of strong Si-O or Si-C bonds which first have to be broken for alteration of an expanded cavity. On the other hand, the diffusivity of helium and vacancy complexes is reduced by an impurity atom implantation, which greatly restricts an Ostwald ripening of helium bubbles or cavities.

As a result, the density of cavities remains high even for long periods of time at high temperatures - that is to say for several hours and at temperatures of 1050°C or higher) - and the formation of dislocations for a desired plastic relaxation remains energetically favorable.

Consequently, the combination of the production of an ion-beam-synthetized layer structure with the provision of a high-temperature-stable defect region within the starting substrate produces an ideal substrate for the

deposition of semiconductor layers or structures having greatly different coefficients of thermal expansion.

Ion-beam-synthetized semiconductor layer structure can be fabricated by a procedure in which ions are implanted into a specific depth of a substrate, the latter is then treated thermally, as a result of which in the substrate a buried monocrystalline layer and also, above and below the monocrystalline layer, transition regions form and the upper substrate layer and also the transition region lying above the monocrystalline layer are subsequently removed, as a result of which the monocrystalline layer is uncovered.

An implantation of the desired ion type under corresponding conditions results in the production firstly of small epitaxial crystallites of the intended compound composed of substrate atoms and implanted ions. In a thermal treatment step, said crystallites coalesce and form a contiguous monocrystalline layer.

The fabrication of a buried 3C-SiC layer in silicon by implantation of carbon ions into a silicon substrate shall be mentioned here as an example.

In order that the compound semiconductor layer produced is brought to the surface, in a subsequent step the substrate covering layer and also the transition region lying above the monocrystalline layer are removed. A chemical etching treatment is preferably carried out for this purpose. As an alternative, however, said layer may also be uncovered by means of oxidation and subsequent chemical removal of this oxide formed or by polishing or else by reactive ion etching or plasma etching.

Optionally, the uncovered surface of the monocrystalline layer can then subsequently be smoothed by chemical mechanical means or by a thermal treatment

step at high temperatures, typically to a surface roughness of 5 nm RMS or less.

RMS roughness values of 1 nm RMS or less are preferred, particularly preferably 0.5 nm RMS or less.

A further possibility for smoothing the surface is afforded by the use of ion beams of cluster ion beams.

In order then to produce a thermally stable defect structure comprising dislocations and stacking faults in this ion-beam-synthetized semiconductor layer structure firstly carbon, oxygen or nitrogen ions or combinations thereof are implanted into the semiconductor layer structure produced with a dose of at most 5×10^{17} cm^{-2}.

In this case, the ion energy is preferably chosen such that the maximum of the implantation profile lies just below, that is to say typically a few tens of nm below the interface between substrate and the ion-beam synthetized layer.

However, the implantation energy may also be chosen such that the implantation maximum lies within the ion-beam-synthetized layer.

Furthermore, the temperature during the implantation is to be chosen such that no amorphization of the semiconductor layer structure occurs, that is to say principally only point defects are produced. In the case of pure silicon, therefore, the temperature is typically to be chosen above 130°C, so that an ion-beam-induced amorphization no longer occurs here.

Moreover, an excessively great outdiffusion of the implanted hydrogen or noble gas is to be restricted by way of the temperature; consequently, the implantation

should take place at a temperature of less than or equal to 800°C.

The implantation temperatures are preferably 130-800°C, implantation temperatures of 250-500°C being particularly to be preferred.

The choice of the implantation temperature can be used to influence whether cavities are formed as early as during the implantation, or not until in a later thermal treatment step. In order to obtain narrow cavity distributions with small average cavity diameters, higher implantation temperatures (~ 400°C) have proved to be useful.

In a subsequent ion implantation step, the cavities are then formed preferably by implantation of light gas ions, for example by implantation of hydrogen, helium, neon or argon ion or combinations of ion implantations of said atom types, which may lead to the later formation of compressive stresses in the silicon and the formation of dislocations.

The implantation energy is preferably chosen such that the density maximum of cavities lies within the maximum of the implantation profile of the oxygen, carbon or nitrogen implantation step.

A subsequent thermal treatment step leads, on the one hand, to the formation of larger cavities and at the same time, by means of compound formation between the implanted oxygen, carbon or nitrogen atoms and the substrate, for example, in the case of silicon, to the formation of Si-O, Si-C or Si-n bonds, which makes it considerably more difficult for the cavities formed to experience a thermally activated diffusive size coarsening.

This suppresses the process of Ostwald ripening and thus counteracts the decrease in the density of the cavities.

The result, therefore, is a semiconductor layer structure having a high density of comparatively small cavities of a few nanometers below the interface between ion-beam synthetized layer and original substrate. Furthermore, there is a high density of other defects at this location, which promotes the formation of interstitial defect agglomerates and dislocations.

If a layer or a layer system comprising a semiconductor material having a greatly different coefficient of thermal expansion in comparison with the semiconductor material of the starting substrate (and hence the entire semiconductor layer structure produced) is then deposited on to said semiconductor layer structure at a temperature of at least 600°C, dislocations and stacking faults formed during the cooling of the layer structure in the defect-rich zone between the cavities still present numerously and densely on account of the stabilization achieved by means of impurity atoms.

The deposited semiconductor layer structure relaxes elastically by means of a plastic deformation in a defined region - namely in the region comprising the cavities, and also defect structures - of the substrate. Consequently, during the cooling operation, the stresses in the layer system that is deposited later are reduced dynamically and a layer deposited on the semiconductor layer structure is prevented from cracking.

This process also reduces the formation of threading dislocations for layer relaxation in the deposited layer or layer structure, since the required number of dislocations for relaxation is greatly reduced.

One possible variation relates to the order of the implantation steps for introducing the cavity-stabilizing impurity atoms and for producing the cavities themselves or for producing the seeds thereof.

Since the cavities are stabilized by compound formation with the impurity atoms only later in a high-temperature treatment step, the order can be chosen arbitrarily here.

In a further alternative embodiment, it is possible to dispense with the separate thermal treatment step after the production of the thermally stable cavity structure if the deposition of a further layer or layer structure is effected at a temperature of at least 600°C. In this case, the production and passivation of the cavities may be effected together with the deposition of the layer or layer structure.

A further variation of the method relates to the provision of the impurity atoms required for the stabilization of the cavities. If the starting substrate itself already comprises impurity atoms of this type, selected from a group of oxygen, carbon, nitrogen or compounds of said elements with the substrate material, then an implantation of said elements is preferably dispensed with if said impurity atoms are present in a high number behind the interface between ion-beam synthetized layer and substrate.

In this case, the impurity atoms may either be dissolved in the substrate and/or be present in precipitates of a compound containing said impurity atoms.

Furthermore, the method described permits the fabrication of substrates for the large-area realization, e.g. of III-V semiconductors since it is

independent of the size of the starting substrates and is therefore dependent only on the availability of said substrates. In particular, conventional silicon wafer diameters of 100 mm, 150 mm, 200 mm, 300 mm shall be mentioned here, 450 mm wafers currently being in the development phase.

In the prior art, by contrast, potential substrates are restricted by the synthesis process to diameters of at most 200 mm for sapphire, 100 mm for 6H- or 4H-SiC.

The short process times required are also particularly advantageous since the implantation doses required for the relaxation lie in the region of at most a few 10^{17} cm^{-2} and the thermal aftertreatment step can either be chosen to be very short (within the seconds range) or - depending on the later processing - can be entirely obviated.

The semiconductor layer structures in example embodiments are suitable in particular for realizing cost-effective light emitting diodes (LEDs) specifically based on III-V semiconductors such as GaN or InGaN, and for the fabrication of Schottky diodes, radiofrequency and high-power components, such as e.g. high electron mobility transistors (HEMTs), which are based primarily on III-V semiconductors such as AlN and GaN, and also SiC.

The subject matter of the invention will be explained in more detail below with reference to examples and with reference to **Figures 1-4.**

Figure 1 shows a semiconductor layer structure, comprising a substrate **1** and a layer **2** having the thickness d1.

Figure 2 shows a semiconductor layer structure, comprising a substrate **1**, a layer **2** having the

thickness d_1 and a region **8** having a specific impurity atom density or a specific impurity-atom-containing precipitate density.

Figure 3 shows a semiconductor layer structure, comprising a substrate **1**, a layer **2** having the thickness d_1 at a depth t_1 an impurity-atom-implanted layer **3** having the thickness d_2, a layer **4** comprising cavities or seeds for cavities, and further layers **6** having the thickness d_3 and **7** having the thickness d_4 having greatly different coefficients of thermal expansion in comparison with the substrate material, which leads to the production of a layer **5** comprising dislocations and stacking faults.

Figure 4 shows a semiconductor layer structure, comprising a substrate **1**, a layer **2** having the thickness d_1, a region **8** having a specific impurity atom density or a specific impurity-atom-containing precipitate density, at a depth t_1, a layer **3** having the thickness d_2 comprising those impurity atoms, a layer **4** comprising cavities or seeds for cavities, and further layers **6** having a thickness d_3 and **7** having a thickness d_4 having greatly different coefficients of thermal expansion in comparison with the substrate material, and a layer **5** comprising dislocations.

By way of example the substrate **1** in **figure 1** is monocrystalline (111)-oriented silicon.

A buried layer **2** having a thickness of approximately 150 nm is produced by means of high-dose carbon ion implantation (energy E = 180 keV, dose $D = 6.75 \times 10^{17}$ cm^{-2}, temperature T = 550°C), which layer was uncovered by a further amorphizing implantation of helium ions (50 keV, $D = 8.0 \times 10^{16}$/cm^2 at 0°C) and by means of chemical etching in a solution comprising 1:5 HF:HNO_3. This gives rise to an approximately 70 nm

thick ion-beam-synthetized 3C-SiC layer **2** lying at the surface of the substrate **1**.

Afterward, at a temperature of 400°C, He^+ ions are implanted with an energy of 22 keV and a dose of $2 \times 10^{16}/cm^2$ into the region **3**, which until now does not contain impurity atoms.

Directly afterward this is followed by, likewise at a temperature of 400°C, an implantation of $5 \times 10^{14}/cm^2$ O^+ ions at an energy of 85 keV into the region **3**, which is situated a few nm to a few tens of nm below the interface between ion-beam-synthetized layer **2** and substrate **1**.

This results in the formation, in a defined depth range, of a layer **4** with cavities or seeds for the later growth of cavities, the density maximum of cavities approximately coinciding with the maximum of the oxygen concentration.

Firstly, a 150 nm thick layer **6** made of aluminum nitride (AlN) is then deposited on to this semiconductor layer structure by means of MOCVD at a temperature of 1100°C.

After reduction of the temperature to 1080°C, a 3 µm thick layer **7** made of gallium nitride (GaN) is grown from the precursors tetraethylgallium and ammonia. The growth rate is approximately 1 µm/h so that the entire process lasts approximately 3 h.

After the layer has cooled, the deposited layer is largely stress-free and, in particular, exhibits no cracks. This results from the formation of a defect structure comprising cavities **4** and dislocations **5** which dynamically reduces the stresses in the layer structure since that defect structure permits a plastic relaxation between substrate **1** and the nitride-

containing layers **6** and **7**. This occurs without the substrate being torn through laterally in the region of the cavities produced. The resulting semiconductor layer structure is shown in **figure 3**.

One variation of this method is the use of a semiconductor layer structure with an impurity-atom-containing layer **8**, as illustrated in **figure 2**. The oxygen implantation can be obviated in this case. Only cavities are produced by helium implantation, which are then preferably formed at the precipitates. This energetically favorable configuration is likewise largely thermostable.

Afterward, once again a 150 nm thick layer **6** made of AlN and subsequently a 3 μm thick layer **7** made of GaN is grown by means of MOCVD. Upon cooling, a defect structure comprising cavities and dislocations is then formed again and dynamically absorbs the layer stresses caused by the different coefficients of thermal expansion. The resulting layer structure is illustrated in **Figure 4**.

As an alternative to this, in the above example, the immobilization of the cavities can be optimized by the surfaces of the cavities being ideally coated with impurity atom bonds - in this case Si-O bonds - in a thermal treatment step prior to the MOCVD deposition. The need for such a process step is dependent on the process duration and temperature of the MOCVD deposition, since these parameters determine the kinetics of the Ostwald ripening of the cavities or gas-filled bubbles. In particular, such a process step is preferable, particularly in the case of long depositions (> 2h) at high temperatures (> 1000°C). It is primarily possible here to choose the heat treatment conditions such that a sufficient number of stabilizing bonds are formed, but an Ostwald ripening of the cavities largely fails to occur.

A further variation relates e.g. to the use of 3C-SiC layer systems outlined above. In this case, numerous 3C-SiC precipitates are present in the substrate **1** below the ion-beam-synthetized layer **2** in a depth range of typically 0 nm to 200 nm below the interface. This region therefore comprises a silicon matrix with a high density of largely misoriented 3C-SiC precipitates.

During the formation of cavities by means of helium implantation and subsequent high-temperature treatment, it is evident that the cavities are predominantly attached to said precipitates and are also thermally immobilized thereby. What is responsible for this is, on the one hand, the possibility of lowering the total interface energy with respect to the silicon substrate by means of a common interface and, on the other hand the formation of Si-C bonds at the cavity surface. It has been shown, however, that the immobilization effect can be further reinforced by a further implantation of oxygen, so that an even greater relaxation can be achieved. The necessity of such an implantation step thus emerges in each case from the degree of relaxation of the deposited layer that is desired for the respective application.

Patent claims

1. A method for fabrication a semiconductor layer structure, comprising the following steps: a) provision of a substrate made of a semiconductor material; b) application of a layer made of a second semiconductor material to said substrate for the purpose of producing a semiconductor layer structure; c) implantation of gas ions of one or more atom types, selected from a group of hydrogen and noble gases, into the semiconductor layer structure for the purpose of producing a layer comprising cavities in the semiconductor layer structure; d) application of at least one epitaxial layer to the semiconductor layer structure, characterized in that substrate contains silicon und layer contains silicon carbide, that in step b) layer is provided by uncovering a buried silicon carbide layer produced by implantation of carbon ions into substrate, and that impurity atoms of one or more atom types, selected from a group of oxygen, nitrogen and carbon, with a dose of utmost $5x10^{17}$ cm^{-2} are implanted into the semiconductor layer structure fur the purpose of thermally stabilizing the cavities produced by implantation of gas ions in layer.

2. The method as claimed in claim 1, wherein the substrate provided in a) is a wafer made of monocrystalline silicon.

3. The method as claimed in claim 1, wherein the substrate provided in a) is an SOI wafer.

4. The method as claimed in claim 1, wherein the layer applied in b) is a layer structure comprising a region containing SiC precipitates and a monocrystalline silicon carbide layer.

5. The method as claimed in claim 4, wherein the at least one epitaxial layer applied in e) comprises a nitride compound semiconductor.

6. The method as claimed in claim 1, wherein the noble gas ions are selected from a group of helium, neon and argon.

7. The method as claimed in claim 1, wherein the energy required by implantation of gas ions in step c) is chosen such that the layer comprising cavities which is produced in the semiconductor layer structure in step c) is situated below an interface between applied layer and substrate.

8. The method as claimed in claim 1, wherein the layer comprising cavities which is produced in the semiconductor layer structure in step c) is situated within the applied layer.

9. The method as claimed in claim 1, wherein prior to implantation of impurity atoms of one or more atom types, selected from a group of oxygen, nitrogen and carbon, a thermal treatment of the semiconductor layer structure at a temperature of at least 600°C is effected.

10. The method as claimed in claim 1, wherein the ion beam in step b) is implanted into the substrate, which is a silicon wafer, the latter is then theated thermally, as a result of which in the substrate a buried monocrystalline silicon carbide layer and also, above and below the monocrystalline silicon carbide layer, transition regions form and the upper substrate layer and also the transition region lying above the monocrystalline silicon carbide layer are subsequently removed, as a result of which the monocrystalline silicon carbide layer is uncovered.

11. A semiconductor layer structure, comprising a substrate ~~(1)~~ made of silicon, on which a layer containing silicon carbide is situated, furthermore a region having impurity atoms of one or more atom types selected from oxygen, nitrogen and carbon, which region is situated either in layer or below the interface between layer and substrate and which contains silicon carbide precipitates, additionally a layer within the region having impurity atoms, which layer comprises cavities of hydrogen or noble gas bubbles pro-

duced by ion implantation, furthermore at least one epitaxial layer applied to layer and also a defect region comprising dislocations and stacking faults within the layer comprising cavities, the at least one epitaxial layer being crack-free, and a residual strain of the at least one epitaxial layer being less than or equal to 1 GPa.

12. The semiconductor layer structure as claimed in claim 11, the residual strain of the at least one epitaxial layer being less than or equal to 370 MPa.

13. The semiconductor layer structure as claimed in claim 11, the roughness of the at least one epitaxial layer being 0.5-7.0 nm RMS.

14. The semiconductor layer structure as claimed in claim 13, the roughness of the at least one epitaxial layer being 0.5-2.0 nm.

15. The semiconductor layer structure as claimed in claim 11, wherein the substrate is a wafer made of monocrystalline silicon.

16. The semiconductor layer structure as claimed in claim 11, wherein the substrate is a SOI wafer.

17. The semiconductor layer structure as claimed in claim 11, wherein the layer is a layer structure comprising a region containing SiC precipitates and a monocrystalline silicon carbide layer.

18. The semiconductor layer structure as claimed in claim 11, wherein the at least one epitaxial layer comprises a nitride compound semiconductor.

19. The semiconductor layer structure as claimed in claim 18, wherein a further epitaxial layer comprising a nitride compound semiconductor is applied to the semiconductor layer structure.

20. The semiconductor layer structure as claimed in claim 19, wherein the layer comprises aluminum nitride.

21. The semiconductor layer structure as claimed in claim 20, wherein the layer comprises gallium nitride.

22. The semiconductor layer structure as claimed in claim 11, a relative expansion of the lattice constant of silicon carbide in layer as measured by means of high-resolution X-ray diffraction being less than or equal to 0.2%.

23. The semiconductor layer structure as claimed in claim 22, the substrate having a diameter of greater than or equal to 100 mm.

24. The semiconductor layer structure as claimed in claim 11, having a defect region comprising dislocations in or below the layer.

25. The semiconductor layer structure as claimed in claim 24, that layer comprising cavities being resistant to thermal cleavage at temperatures of 25-1250°C.

26. The semiconductor layer structure as claimed in claim 18, furthermore comprising one or more epitaxial interlayers situated between layer and the at least one epitaxial layer comprising a nitride compound semiconductor.

27. A semiconductor component, produced on a semiconductor layer structure as claimed in claim 18, which after activation emits light having an energy of greater than or equal to 0.1 eV and less than or equal to 7 eV.

Abstract

Semiconductor layer structure and method for fabricating a semiconductor layer structure

Semiconductor layer structure, comprising a substrate (1) made of semiconductor material, on which a layer (2) made of a second semiconductor material is situated, furthermore a region (3) enriched with impurity atoms, which region is situated either in layer (2) or at a specific depth below the interface between layer (2) and substrate (1), additionally a layer (4) within the region (3) enriched with impurity atoms, which layer comprises cavities produced by ion implantation, furthermore at least one epitaxial layer (6) applied to layer (2) and also a defect region (5) comprising dislocations and stacking faults within the layer (4) comprising cavities, the at least one epitaxial layer (6) being largely crack-free, and a residual strain of the at least one epitaxial layer (6) being less than or equal to 1 GPa.

Method for fabricating a semiconductor layer structure, comprising the following steps: a) provision of a substrate (1) made of a semiconductor material; b) application of a layer (2) made of a second semiconductor material to said substrate (1) for the purpose of producing a semiconductor layer structure; c) implantation of light gas ions into the semiconductor layer structure for the purpose of producing a layer (4) comprising cavities in the semiconductor layer structure; d) stabilization of said cavities by impurity atoms of a specific species; e) application of at least one epitaxial layer (6) to the semiconductor layer structure.

Fig. 3