Method for Permanent Bonding of Wafers

Specification

This invention relates to a method for bonding of a first solid substrate which contains a first material, especially semiconductor wafers, to a second solid substrate, especially semiconductor wafers ~~as claimed in Claim 1~~.

The objective in permanent or irreversible bonding of solid substrates is to produce a connection as strong and especially as permanent as possible, therefore a high bond force, between the two contact surfaces of the solid substrates. For this purpose, in the prior art there are various approaches and production methods, especially the welding of the surfaces at higher temperatures.

All types of materials, predominantly however metals and ceramics, are permanently bonded. One of the most important systems of permanent bonding is metal-metal systems. Cu-Cu systems have appeared increasingly in recent years. The development of 3D structures specifically requires mostly the joining of different functional layers. This joining is more and more often done by way of so-called TSVs (Through Silicon Vias). The contact-making of these TSVs with one another very often takes place by copper contact sites. At the instant of bonding very often there are full-value, serviceable structures, for example microchips, on one or more surfaces of the solid substrates. Since different materials with different coefficients of thermal expansion are used in microchips, increasing the temperature during bonding is not desirable. This can lead to thermal expansions and thus thermal stresses which can destroy parts of the microchip or its vicinity.

The known production methods and the approaches which have been followed to date often

used. By a combination of grinding and polishing, roughnesses in the nanometer, often even in the subnanometer range, are produced. In most cases so-called CMP methods are used. It is a chemical-mechanical polishing process. Regardless of how long or how precisely grinding is done, a residual roughness which cannot be eliminated always results. This residual roughness upon contact of two surfaces always leads to formation of pores in the nanometer and subnanometer range.

Embodiments~~The object~~ of this invention ~~is therefore to~~ devise a method for careful production of a permanent bond between two solid substrates with a bond force as high as possible at a temperature which is simultaneously as low as possible.

According to an aspect, there is provided a method for bonding of a first solid substrate to a second solid substrate which contains a first material with the following steps, especially the following sequence: formation or application of a function layer which contains a second material to the second solid substrate, making contact of the first solid substrate with the second solid substrate on the function layer, pressing together the solid substrates for forming a permanent bond between the first and second solid substrate, at least partially reinforced by solid diffusion and/or phase transformation of the first material with the second material, an increase of volume on the function layer being caused, wherein the function layer is formed or applied on a surface of the second solid substrate in an average thickness between 0.1 nm and 25 nm, and wherein gaps present due to unevenness of the surface are closed by expansion of the volume of a contact surface formed by the function layer.

~~This object is achieved with the features of Claim 1. Advantageous developments of the invention are given in the dependent claims.~~ All combinations of at least two of the features given in the specification, the claims and/or the figures also fall within the framework of the invention. At the given value ranges values which lie within the indicated boundaries will also be considered disclosed as boundary values and will be claimed in any combination.

The basic idea of embodiments of this invention is to apply or create at least on one of the solid substrates a function layer with a first material which reacts with a second material of the other solid substrate especially after contact-making or production of a prebond between the solid substrates, and thus forms an irreversible or permanent bond between the solid substrates. The two solid substrates need not necessarily form a prebond with one another. Simple contact-making without formation of a prebond is also possible. As per embodiments of~~claimed in~~ the invention the "reaction" is solid diffusion and/or a phase transformation. Before and/or after formation/application of the function layer on the first and/or second substrate, cleaning of the solid substrates or of the solid substrates generally takes place, especially by a rinsing step. This cleaning should generally ensure that there are no particles on the

surfaces which would result in unbonded sites.

The function layer and the material contained in the function layer create the technical possibility of inducing a reaction (first material with the second material) which increases the bond rate and which strengthens the permanent bond directly on the contact surfaces between the solid substrates after producing the temporary or reversible bond in a controlled manner, especially by deformation of at least one of the contact surfaces (preferably the contact surface formed by the function layer) by the reaction, gaps present due to unevenness of the surfaces/contact surfaces being closed, especially in conjunction with pressing together by applying pressure to the solid substrates against one another. Deformation is an expansion of the volume in general, a phase transformation or plasticization which leads to a change in the shape of the crystallites and/or amorphous regions of the surface.

Solid substrates as per embodiments of~~claimed in~~ the invention are those solid substrates whose material is able to react or mix as material with another supplied material to form a mixed material with a higher molar volume, as a result of which growth on the function layer is caused, especially on valleys of the surfaces of the solid substrates which form on gaps. The following combinations of materials are especially advantageous, either due to the possibility of forming mixed crystals, of plastically deforming well, of passing through phase transformations which lead to an increase of volume, or due to any other direct or indirect methods named in the specification for closing the gaps in the bond interface:

- Cu-Fe, Cu-Ge, Cu-In, Cu-Li, Cu-Mg, Cu-Mn, Cu-Nb, Cu-Nd, Cu-Ni, Cu-Si, Cu-Sn, Cu-Zn, Cu-Zr, Cu-Ti, Cu-W, Cu-Ti, Cu-Ta, Cu-Au, Cu-Al, Cu-Cu,
- W-Fe, W-Ge, W-In, W-Li, W-Mg, W-Mn, W-Nb, W-Nd, W-Ni, W-Si, W-Sn, W-Zn, W-

Zr, W-Ti, W-Ti, W-Ta, W-Au, W-Al,

- Ti-Fe, Ti-Ge, Ti-In, Ti-Li, Ti-Mg, Ti-Mn, Ti-Nb, Ti-Nd, Ti-Ni, Ti-Si, Ti-Sn, Ti-Zn, Ti-Zr, Ti-Ta, Ti-Au, Ti-Al,
- Ta-Fe, Ta-Ge, Ta-In, Ta-Li, Ta-Mg, Ta-Mn, Ta-Nb, Ta-Nd, Ta-Ni, Ta-Si, Ta-Sn, Ta-Zn, Ta-Zr, Ta-Ti, Ta-W, Ta-Ti, Ta-Ta, Ta-Au, Ta-Al,
- Au-Fe, Au-Ge, Au-In, Au-Li, Au-Mg, Au-Mn, Au-Nb, Au-Nd, Au-Ni, Au-Si, Au-Sn, Au-Zn, Au-Zr, Au-Ti, Au-W, Au-Ti, Au-Ta, Au-Au, Au-Au, Au-Al,
- Al-Fe, Al-Ge, Al-In, Al-Li, Al-Mg, Al-Mn, Al-Nb, Al-Nd, Al-Ni, Al-Si, Al-Sn, Al-Zn, Al-Zr, Al-Ti, Al-W, Al-Ti, Al-Al, Al-Al, Al-Al,

The following mixed forms of semiconductors are also conceivable as solid substrates:

- III-V: GaP, GaAs, InP, InSb, InAs, GaSb, GaN, AlN, InN, $Al_xGa_{1-x}As$, $In_xGa_{1-x}N$
- IV-IV: SiC, SiGe,
- III-VI: InAlP.
- nonlinear optics: $LiNbO_3$, $LiTaO_3$, KDP (KH_2PO_4)
- solar cells: CdS, CdSe, CdTe, $CuInSe_2$, $CuInGaSe_2$, $CuInS_2$, $CuInGaS_2$
- conductive oxides: $In_{2-x}SnxO_{3-y}$

Although the aforementioned binary, tertiary and quaternary phase systems generally have extremely low edge solubilities, due to their covalent bonding affinity they behave in a rather brittle manner, occur mostly as single crystals and only very rarely as polycrystals, the properties claimed for metals as per embodiments of~~claimed in~~ the invention can also occur in semiconductor systems. It should be noted that the surface roughnesses of current semiconductor wafers can be reduced to such a degree that the gaps which are to be closed as per embodiments of~~claimed in~~ the invention can only have a volume in the angstrom

range. It is a fact that even for poor edge solubility of a multicomponent system components can dissolve in the main component even if only in the ppm range. Therefore the ideas as per embodiments of~~claimed in~~ the invention will and should be considered as disclosed even for nonmetallic systems.

It is especially advantageous as per embodiments of~~claimed in~~ the invention if contact-making of the solid substrates after application of the function layer takes place as near as possible in time, especially within 2 hours, preferably within 30 minutes, even more preferably within 10 minutes, ideally within 5 minutes. This measure minimizes possible unwanted reactions such as oxidation of the function layer or of the surfaces of the solid substrates.

As per embodiments of~~claimed in~~ the invention there can be means for inhibiting these reactions of the function layer and/or of the surfaces of the solid substrates before the contact surfaces make contact, especially by passivation of the reaction layer of the solid substrates, preferably by exposure to N_2, forming gas or an inert atmosphere or under a vacuum or by amorphization. In this connection treatment with plasma which contains forming gas, especially consists largely of forming gas, has proven especially suitable. Here forming gas is defined as gases which contain at least 2%, better 4%, ideally 10% or 15% hydrogen. The remaining portion of the mixture consists of an inert gas such as for example nitrogen or argon. Systems with an inert atmosphere or vacuum atmosphere can preferably be implemented as systems in which the transfer of the solid substrates from one process chamber to the next process chamber takes place by means of a solid substrate handling system which can carry out the transfer of the solid substrates completely in a controlled, adjustable atmosphere, especially a vacuum atmosphere. These systems are known to one skilled in the art.

The contact surfaces conventionally show a roughness with a quadratic roughness (R_q) of 0.2 nm. This corresponds to peak-to-peak values of the surfaces in the range of 1 nm. These

empirical values were determined with atomic force microscopy (AFM).

The reaction as per embodiments of~~claimed in~~ the invention is suitable for allowing the function layer to grow by 0.1 to 10 nm, especially 0.1 to 1 nm, preferably by 0.1 to 0.3 nm, for a conventional wafer surface of a circular wafer with a diameter of up to 450 mm, especially locally on gaps between the contact surfaces of the solid substrates.

The (additionally applied) function layer is applied by one or more of the following methods:

- PECVD,
- LPCVD,
- vapor deposition
- epitaxy
- MOCVD
- sputtering

Embodiments of t~~T~~he invention thus solves the problem of better welding of the surfaces of solid substrates which have been brought into contact with one another by on at least one of the surfaces a solid reaction with another material which is located in the function layer being produced which leads to a volume expansion of the corresponding region near the surface and thus closes the gaps or pores which are present due to surface roughness in the interface (boundary surface between the solid substrates which have been brought into contact). It should be mentioned here that the two solid substrates which are to be welded to one another are already for the most part in contact with one another. At the contact sites a volume expansion onto the solid substrates is of course normally not possible since the material in this direction is subject to obstruction of expansion. Still all methods

as per embodiments ofclaimed in the invention which increase the energy state so dramatically that the material spreads into the pores are explicitly mentioned. Either the material expands by the methods as per embodiments ofclaimed in the invention directly into the pores (by way of example but not restrictively here let the volumetric expansion by mixed crystal formation or a phase transformation be mentioned) or the material cannot expand in one direction due to the methods as per embodiments ofclaimed in the invention since it is subject to obstruction of expansion, but fills the nearby pores, since based on the increased energy state it deforms plastically. For the sake of completeness it should be mentioned that plastic deformation can take place by dislocations, twinning or diffusion and in a strict physical sense is not accompanied by a volume expansion. There is no longer any explicit differentiation between plasticization and (residual elastic) volume expansion hereinafter. The term volume expansion will stand for a residual enlargement and/or deformation of a surface part.

The second material can be applied either as a layer to at least one of the two substrates (Figure 2), can penetrate by grain boundary diffusion between the grains of a first especially polycrystalline material into the volume (Figure 3), can alternate in a layer structure with layers of the first material (Figure 4) or can be applied to the second solid substrate by mechanical alloying of microparticles and/or nanoparticles (Figure 5).

This results in higher bond strengths at lower temperatures.

According to one advantageous embodiment of the invention it is provided that formation and/or reinforcement of the permanent bond by diffusion of the second material into the first material takes place especially with formation of a mixed material C.

According to another advantageous embodiment of the invention, it is provided that the formation of the permanent bond takes place at a temperature between room temperature and

200°C, especially between room temperature and 150°C, preferably between room temperature and 100°C, even more preferably between room temperature and 50°C, especially during a maximum 12 days, preferably a maximum 1 day, even more preferably a maximum 1 hour, at best a maximum 15 minutes.

Here it is especially advantageous if the irreversible bond has a bond strength of greater than 1.5 J/m^2, especially greater than 2 J/m^2, preferably greater than 2.5 J/m^2.

The bond strength can be increased especially advantageously in that during solid diffusion and/or phase transformation a mixed material C with a greater molar volume than the molar volume of the second material and of first material is formed. In this way growth on the second solid substrate or on the function layer is effected, as a result of which gaps between the contact surfaces can be closed by the chemical reaction as per embodiments of~~claimed in~~ the invention. As a result, the distance between the contact surfaces, therefore the average distance, is reduced, and dead spaces are minimized.

To the extent prior to application/formation of the function layer plasma activation of the surfaces of the solid substrates takes place especially with an activation frequency between 10 and 600 kHz and/or a power density between 0.075 and 0.2 watt/cm^2 and/or with application of a pressure between 0.1 and 0.6 mbar, additional effects such as smoothing of the contact surface are effected. Here application of pressure is defined as the pressure of the working atmosphere during plasma activation.

In another advantageous embodiment of the invention it is advantageously provided that the solid diffusion and/or phase transformation is limited to one surface layer (3o) of the first solid substrate (1) with a maximum initial density D less than 1 μm, especially less than 100 nm, preferably less than 10 nm, even more preferably less than 1 nm.