Method for Coating and Bonding of Substrates

Specification

This invention relates to a method for coating of a first substrate with a first diffusion bond layer and to a method for bonding.

The objective in permanent or irreversible bonding of 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 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, semimetals, semiconductors, polymers and/or ceramics, are permanently bonded. One of the most important systems of permanent bonding is metal-metal systems. Mainly 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 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 to thermal stresses and/or stress induced voiding (SIV) which can destroy parts of the microchip or its vicinity.

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

- low contamination.
- no application of force, or application of force as low as possible.
- temperature as low as possible, especially for materials with different coefficients of thermal expansion.

The reduction of the bond force leads to more careful treatment of the structure wafer and thus to a reduction of the failure probability by direct mechanical loading, especially when the insulating layers between the metallic conductors are made from so-called "low-k" materials.

Current bonding methods are designed primarily for high pressures and temperatures. Mainly avoiding a high temperature is of essential importance for the welding of future semiconductor applications, since different materials with different coefficients of thermal expansion generate thermal stresses which cannot be ignored during heating and cooling processes. Furthermore, the diffusion of doping elements as the temperature rises is increasingly becoming a problem. The doped elements should not leave the intended three-dimensional region after the doping process. Otherwise the physical properties of the circuits would fundamentally change. In the best case this leads to deterioration, in the worst and most probable case to unserviceability of the component. Mainly memories are very susceptible due to degradation of the dielectric and the associated shortened storage time during thermal processes. On the other hand, there are memories in which 3D technology is being increasingly used to raise the capacity and performance.

Embodiments of this invention provide a method for careful production of a permanent bond between two substrates with a bond force as high as possible at a temperature which is simultaneously as low as possible and/or at an average process time.

According to a first aspect of the present invention, there is provided a method of coating a first substrate with a first diffusion bond layer, the method comprising: forming a first intermediate layer on a first surface of the first substrate, the first intermediate layer having an average grain diameter H′ parallel to the first surface and an average grain diameter V′ transverse to the first surface; and depositing the first diffusion bond layer on the first intermediate layer, the first diffusion bond layer being formed of a first material and having an average grain diameter H parallel to the first surface and an average grain diameter V transverse to the first surface, the average grain diameter H being less than 1 μm, wherein the average grain diameter H′ is greater than the average grain diameter H, and wherein the average grain diameter V′ is greater than the average grain diameter V

According to a second aspect of the present invention, there is provided a method of bonding a first substrate to a second substrate coated with a second diffusion bond layer, comprising the steps of: coating the first substrate with a first diffusion bond layer, the coating comprising: forming a first intermediate layer on a first surface of the first substrate, the first intermediate layer having an average grain diameter H′ parallel to the first surface and an average grain diameter V′ transverse to the first surface; and depositing the first diffusion bond layer on the first intermediate layer, the first diffusion bond layer being formed of a first material and having an average grain diameter H parallel to the first surface and an average grain diameter V transverse to the first surface, the average grain diameter H being less than 1 μm; contacting the first diffusion bond layer of the first substrate with the second diffusion bond layer of the second substrate; and pressing the substrates together to form a permanent metal diffusion bond between the first and second substrate, wherein the average grain diameter H′ is greater than the average grain diameter H, and wherein the average grain diameter V′ is greater than the average grain diameter V.

According to a third aspect of the present invention, there is provided a method of coating a first substrate with a first diffusion bond layer, the method comprising: forming a first intermediate layer on a first surface of the first substrate, the first intermediate layer having an average grain diameter H′ parallel to the first surface and an average grain diameter V′ transverse to the first surface; forming a second intermediate layer on the first intermediate layer, the second intermediate layer having an average grain diameter H″ parallel to the first surface and an

average grain diameter V″ transverse to the first surface; and depositing the first diffusion bond layer on the second intermediate layer, the first diffusion bond layer being formed of a first material and having an average grain diameter H parallel to the first surface and an average grain diameter V transverse to the first surface, the average grain diameter H being less than 1 μm, wherein the average grain diameter H′ is greater than the average grain diameter H, wherein the average grain diameter V′ is greater than the average grain diameter V, and wherein H″ is less than H′ and greater than H, and V″ is less than V′ and greater than V.

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 substrates a diffusion bond layer of a material which has a microstructure with a grain as fine as possible, and thus a grain boundary surface as large as possible. As per embodiments of the invention mainly grain boundaries are preferred which run normally to the substrate surfaces which are to be bonded. This is achieved as per embodiments of the invention by controlled setting of the layer thickness of the diffusion bond layer which constitutes a limiting criterion for the grain size. The two substrates can, but need not necessarily, prebond with one another. Simple contact-making without formation of a prebond is also possible. As per embodiments of the invention the term "reaction" should be understood as solid diffusion. Before and/or after formation/application of the diffusion bond layer(s) on the first and/or second substrate, cleaning of the substrate or of the 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. Ideally all steps of deposition and/or bonding as per embodiments of the invention take place in a closed system which is preferably flooded with inert gas, more preferably evacuated so that a cleaning step after coating can be omitted.

Embodiments of this invention form the diffusion bond layer at least on the contact surface between the first and second substrate with an average grain diameter H parallel to the contact surface or substrate surface smaller than 1 μm.

The diffusion bond layer which is formed in this way and which has a small average grain

diameter creates the technical possibility of causing faster diffusion directly on the contact surfaces between the substrates and thus enabling the permanent bond primarily at low temperatures and furthermore strengthening it, and increasing the bond speed.

Hereinafter deformation is defined as a change of the surface and/or of the bulk as a result of diffusion.

All elements of the periodic table, mainly the metals, semimetals, lanthanoids and actinoids are possible as materials as per embodiments of the invention for the diffusion bond layer.

Preferably, embodiments of the invention are used for Cu-Cu bonds.

The following mixed forms of semiconductors are conceivable as 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: $In_{2-x}SnxO_{3-y}$

It is especially advantageous as per embodiments of the invention if contact-making of the substrates after application of the diffusion bond 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 metal diffusion bond layer or of the surfaces of the substrates.

Oxide removal before the actual bonding process is also possible. The oxide can be removed for example by wet-chemical means or with corresponding reducing gases. Any known

chemical and/or physical methods for oxide reduction can be used.

As per embodiments of the invention there can be means for inhibiting these reactions of the metal diffusion bond layer and/or of the surfaces of the substrates before the contact surfaces make contact, especially by passivation of the surfaces of the 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 substrates from one process chamber to the next process chamber takes place by means of a substrate handling system which can carry out the transfer of the substrates completely in a controlled, adjustable atmosphere, especially a vacuum atmosphere. These systems are known to one skilled in the art.

The diffusion bond layer is applied by one or more of the following methods:

- CVD especially PECVD, LPCVD, MOCVD or ALD
- PVD especially sputtering or vapor deposition
- epitaxy especially MBE, ALE
- electrochemical deposition processes
- currentless deposition processes

Embodiments of the invention thus solve the problem of better welding of the surfaces of two coated substrates which have been brought into contact with one another by using the microstructure properties of the uppermost layer, the diffusion bond layer. Embodiments of the invention thus relate to a method

and a process for adjusting the microstructure of the uppermost deposited layer by the controlled deposition of thin layers by means of chemical and/or physical processes such that its grain interface is as large as possible. Preferably the grain boundaries run normally to the substrate surface.

The grain size which is small as per embodiments of the invention yields an extremely increased grain boundary surface and thus accordingly larger diffusion paths; this promotes the welding of the two material layers during bonding. The idea as per embodiments of the invention therefore consists in increasing the flow of those atoms which diffuse along the grain boundaries by increasing the grain boundary surface.

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 400°C, especially between room temperature and 300°C, preferably between room temperature and 200°C, even more preferably between room temperature and 100°C, especially during a maximum 12 days, preferably a maximum 1 day, even more preferably a maximum 1 hour, 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 determined for example with the so-called Maszara test.

The bond strength can be increased especially advantageously in that the two substrates have a diffusion bond layer with a grain size which is very small as per embodiments of the invention, and thus a very large grain boundary surface. This enables increased diffusion flow in both directions which accordingly supports the bond process.