Silicon layer transfer by hydrogen implantation combined with wafer bonding in ultrahigh vacuum

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A layer transfer method was developed by combining in situ photothermal activation of hydrogen passivated surfaces, ultrahigh vacuum bonding, and hydrogen-implantation induced splitting. Structural and electrical investigations showed that ultrathin, single crystalline silicon layers can be transferred to appropriate substrates without the involvement of an intermediate layer such as an oxide or solder. Significant current flow across such produced silicon-silicon bonded interfaces was observed, making this approach very attractive for material integration. © 2006 American Institute of Physics. [DOI: 10.1063/1.2387410]

State-of-the-art electronic applications often require high quality single crystalline layers on top of various substrates. Hydrophilic bonding of silicon wafers followed by implantation induced splitting is already established for producing silicon-on-insulator (SOI) wafers but lacks in providing the solution for direct transfer (no intermediate layer). Hydrophobic bonding suffers from low initial fracture strength and usually cannot be combined with hydrogen-implantation induced splitting because typically blistering occurs before the bonding energy has reached a sufficiently high value to allow layer splitting. A recent approach based on lithographic patterning and layer splitting requires high temperature annealing following hydrophobic bonding (>1100 °C), a major drawback when transfer between different materials is desired. Moreover, the required removal of SOI handle wafer by backetching is both expensive and time consuming.

By replacing the traditional bonding procedures with ultrahigh vacuum (UHV) bonding combined with laser induced photodesorption of hydrogen, we were able to achieve direct transfer of ultrathin Si(100) layers onto Si(100)-(2×1) substrates on a large scale.

The layer transfer requires three steps: (i) implantation of the device wafer with a relatively high hydrogen dose, (ii) bonding of the device onto the host substrate, and (iii) annealing of the bonded pair in order to achieve the splitting.

The main inherent challenges are the crystallinity of the transferred layers and a sufficiently low electrical resistivity of the device-substrate interface.

Upon implantation hydrogen generates displacement damage in the form of interstitials, vacancies, and complexes. Given a sufficiently high dose, these point defects agglomerate along the [100] and [111] planes, generating areas with a high number of broken bonds called platelets. Already present in high concentrations, H is quickly trapped at these surfaces, passivating the broken bonds. During annealing the trapped H dissociates from complexes and diffuses into the platelets, forming H2 molecules. Due to the pressure increase the platelets expand into microcracks which join together in the same plane, causing material exfoliation.

For the experiments, 100 mm high quality single crystalline silicon wafers 500 µm thick, (100) oriented, with doping concentrations of 1017 cm−3 were implanted with H2 molecules. The implantation was performed under 7° tilt in order to minimize ion channeling, using doses of 5 × 1016 ions/cm2 and energies of 130 keV.

After implantation, the silicon wafers underwent RCA cleaning. The native SiO2 layer was removed by short dipping in aqueous HF solution. The two dangling bonds (DBs) on each surface atom are terminated by hydrogen, leading to a Si(100)-(1×1):H structure. The surface thus created is quite stable and requires in situ heating to about 500 °C in order to desorb the hydrogen passivating the surface DB. Upon hydrogen desorption, Si–Si dimers are formed and the surface undergoes a (2×1) reconstruction, with only one DB per surface atom. When two such surfaces are joined in UHV, covalent bonds are formed at room temperature (RT) by breaking the (2×1) reconstruction, due to the high energy of unpassivated silicon surfaces.

Implantation induced splitting is also a thermally activated process, the onset time having an exponential dependence on the annealing temperature. Typically, it takes about 1 s to develop blisters on a wafer surface heated at 350 °C, making it impossible to apply standard thermal desorption on implanted wafers without rendering them unbondable by the development of surface blisters. Instead, a photothermal desorption approach was used by means of short KrF (5 eV) excimer laser pulses. A direct Si–H photochemical bond breaking is not possible since an electron would require at least 6–6.5 eV to be promoted from the Si–H σ bonding orbital to the unoccupied σ* antibonding orbital, as shown by electron-field emission from a scanning tunneling microscope tip. This result was further confirmed by photochemical versus photothermal desorption experiments performed with F2 (7.9 eV) and XeCl (4.0 eV) lasers. As a consequence, energy densities as high as 600 mJ/cm2 had to be used in order to yield significant hydrogen desorption by energy transfer from the hot carriers in the substrate to vibrationally excited states of the Si–H bonds.

A major concern is the temperature profile within the wafer during the laser pulse. The time-dependent heat equation was numerically solved for a depth corresponding to the implantation peak (0.5 µm in our case) and a time range of 0–100 ns. The laser source has been modeled according to Ref. 11, additional contribution of energy losses by radiation being considered. For an energy density of 600 mJ/cm2, the
temperature at 0.5 \, \mu m below the surface reaches a maximum of 700 °C (surface temperature was 980 °C) and decreases to 250 °C in 80 ns. These are appropriate conditions for hydrogen desorption from the surface without onset of blistering of the implanted hydrogen.

One implanted wafer which underwent laser treatment was bonded to a standard, thermally activated silicon wafer at RT in UHV (pressure less than $1 \times 10^{-10}$ mbar) followed by heating to 400 °C in order to achieve splitting. After transfer occurs, only a few bubbles can be observed in an otherwise perfect layer (Fig. 1). Annealing experiments were carried out for 1 h at 1000 °C in H$_2$ atmosphere in order to smoothen the transferred layer.

Structural investigations were performed by means of transmission electron microscopy (TEM) in order to study the distribution of implantation generated defects in the transferred layer (Fig. 2). Towards the end of the implantation region one can see remaining platelets (free inner surfaces) having the appearance of white stripes parallel to the split surface. During the postbonding annealing they grow without causing splitting due to the insufficient gas pressure contained inside them. Other defects surviving the postbonding annealing are point defect agglomerates having a dark contrast. Their distribution is related to the broadening of the implantation peak. The cross-sectional high-resolution TEM micrograph in Fig. 3(a) confirms that direct transfer can be achieved at RT followed by 400 °C annealing. Indeed, two sets of (111) planes cross the bonded interface at an angle of 54.7° without any interruption. The bright spots with a periodicity of 5 nm are given by the strain field of the screw dislocation network which is directly observable in a plane-view image [Fig. 3(b)]. The dislocation distance corresponds to a twist angle $\theta$ of 4.4° between the bonded wafers.

Electrical investigations were done on a $p$-type silicon layer transferred on a $n$-type silicon substrate. Current-voltage ($I$-$V$) characteristics for both as-transferred and annealed $n$+$p$ junctions are depicted in Fig. 4. The as-transferred sample is characterized by a poor rectifying behavior, due to deep levels introduced at the interface by bonding and in the volume of the transferred layer by implantation. Once the sample is annealed, most of the generation-recombination (G-R) centers are removed and the reverse-bias current decreases by two orders of magnitude. For comparison, $I$-$V$ characteristics were simulated using a drift-diffusion model implemented in the software WIAS-TESCA. The bonded interface was modeled using a midgap G-R center having a concentration of $5 \times 10^{11}$ cm$^{-2}$ and surface recombination velocities of 150 and 15 cm/s for electrons and holes, respectively. The measured forward current is lower at higher bias values, in comparison to the simulated characteristic. The effect is related to the nonideal Ohmic contact on the back side of the transferred layer, which acts as a Schottky barrier. The remaining electrical activity is very likely due to a small number of dangling bonds still present at the interface, having an acceptorlike behavior. The surface recombination velocities are small compared to that...
of an unpassivated Si surface \( (2 \times 10^5 \ \text{cm/s}, \text{Ref.} \ 13) \). For the nonimplanted device area, bulk recombination lifetime for electrons and holes of \( 10^{-6} \ \text{s} \) was used for computation. For the transferred layer, values between \( 10^{-9} \) and \( 10^{-6} \ \text{s} \) were used, the best consistency between measured and simulated \( I-V \) characteristics being reached for lifetime of \( 10^{-6} \ \text{s} \). Therefore we concluded that almost complete recovery of the electric properties occurs upon annealing to 1000 °C.

In conclusion, hydrogen-implantation induced layer transfer of silicon layers bonded to another silicon wafer without any intermediate (oxide) layer was accomplished by an UHV-based photothermal activation combined with UHV wafer bonding and subsequent splitting. The resulting transferred thin film/substrate structure was characterized structurally and electrically. The procedure developed will allow the use of the hydrogen-implantation induced layer transfer not only for oxide covered hydrophilic silicon surfaces but also for hydrophobic surfaces, leading to electrically conducting silicon-silicon interfaces without intermediate non-silicon bonding layer.

\[ \text{References} \]