SEMINCONDUCTOR WAFER BONDING: SCIENCE AND TECHNOLOGY

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Abstract: After shortly covering the history of wafer bonding and conventional wafer bonding performed with hydrophilic or hydrophobic surfaces in air and discussing some applications, we will concentrate on silicon wafer bonding under ultra-high vacuum conditions at room temperature which leads to strong covalent bonding. Finally, molecular dynamics simulations of ultra-high vacuum room temperature bonding processes of silicon surfaces will be presented.

1. INTRODUCTION AND HISTORY

It has been known since almost a century that mirror polished and flat pieces of solids adhere to each other at room temperature provided dust particles between the surfaces can be avoided. Lord Rayleigh, in 1936, was the first to investigate this phenomenon systematically for fused quartz [1]. He determined the energy to separate the two pieces again (in the following termed surface energy) to be about 0.1 J/m^2 per surface. This energy is more than an order of magnitude lower than the corresponding value for the covalent bonding within quartz (SiO_2) and was later-on attributed to Van-der-Waals bonding or hydrogen bridge bonds between the surfaces.

In the last decade this adhesion phenomenon has been developed mainly for semiconductor and especially silicon wafers in terms of the bonding of whole wafers [2, 3]. Generally for actual applications in the area of silicon-on-insulators (SOI), power devices and silicon-based micromechanics for sensors and actuators the bonded wafers have to be heat-treated at elevated temperatures to increase the bonding strength of the bonded pair. For an overview on the basics of wafer bonding and on applications the reader is refered to conference proceedings [4-6] and recent review articles [7-12]. The present paper will first deal with conventional wafer bonding which is performed in air at room temperature (section 2) before switching in section 3 to the fairly new possibility of performing wafer bonding under ultra-high-vacuum (UHV) conditions at room temperature (RT) which allows to reach covalent bonding strength already at room temperature without any subsequent heat treatment. In section 4 results of molecular dynamics simulations of UHV bonding will be shown. Let us mention here that semiconductor wafer bonding is one of the very few areas in which a scientific understanding of certain molecular processes allows almost immediate applications. Therefore, we will mainly discuss the science of wafer bonding and mention technological applications only in passing. Frequently, the applications of the combination of materials by wafer bonding is not so much restricted by technical limitations but rather by our imagination in which way combinations of materials may be used profitably.

2. CONVENTIONAL WAFER BONDING

Conventional wafer bonding for technological applications has mainly been developed for hydrophilic silicon wafers which are covered with either a thermally grown oxide or a thin native oxide layer and one or two additional monolayers of water. Alternatively, hydrophobic wafer bonding involves silicon surfaces covered with hydrogen after the native oxide layer has been removed by a dip in diluted HF. In both cases, the contacting procedure is performed at room temperature under normal ambient conditions. The wafer surfaces have to be flat and smooth enough and particles between the surfaces have to be avoided. Wafer bonding in a particle free environment may be accomplished either in a conventional cleanroom of class 10 or better or in a specifically designed "microcleanroom" which may be used in a normal laboratory.

After the two wafer touch each other the bonding may be initiated by locally slightly pressing the two wafer together which starts a self-propagating expansion of the bonded area over the whole wafer within a few seconds (Fig. 1, [13]). The strength of the adhesion after RT bonding character-ized by the surface energy measured by the crack opening method [7] is in the order of 0.1 J/m^2 (or 100 erg/cm^2) for hydrophilic silicon wafers (as mentioned in the introduction) and about ten times lower for hydrophobic wafers [14, 15]. Heat-treating the bonded wafers leads to an increase of the surface energy as shown in Fig. 2 for heat treatments leading to saturated energy values which below 300°C partly involve many days of heating. Shorter heating treatments generally lead to lower values of the surface energy.

Most present technological applications rely on heat treatments around 1100°C. For many applications involving the presence of temperature sensitive layers in or on the silicon wafers (etch-stop layers, metallization layers, devices) reaching high surface energies at lower temperatures or even at room temperature (termed low-temperature wafer bonding) would be highly desirable. Although there are a number of approaches for low-temperature wafer bonding based on modifi-cations of the chemistry of the bonding surfaces [16-18] in the present paper we will only discuss the approach of performing bonding under UHV conditions at room temperature.

3.UHV ROOM TEMPERATURE SILICON BONDING

3.1.Small area bonding

The basic idea of UHV RT bonding is the following: After proper cleaning silicon surfaces should not be covered with any adsorbates under UHV conditions and therefore if brought into close contact strong covalent Si-Si bonds between the two surfaces should develop already at room temperature. Our first approach consisted of an attempt to bond small area (<1cm^2) (100) silicon pieces in a UHV chamber under application of a fairly high pressure [19] after sputter cleaning the surface with a 1 keV argon beam. The equipment located at the MPI of Metal Research in Stuttgart has been described in ref. [20]. Only a small percentage of the original area was successfully bonded with a bonding strength in the order of covalent bonding. Cross-sectional TEM of the bonding inter-face (Fig. 3a) showed the presence of an amorphous silicon layer probably due to the sputter clean-ing process. The fact that the amorphous layer decreased its layer thickness by recrystallization only slightly even after a prolonged heat treatment at 650°C, contrary to what is expected for amorphous silicon, suggests that the sputtering process induced the incorporation of carbon atoms

Fig. 1 Infrared picture of initiation and propagation of a bonding or contact wave during bonding of 4" silicon wafers. a) local starting of the contact wave, b) extension after about 2 seconds, and c) complete bonding after about 5 seconds. The radial dark line comes from the tong used to initiate the bonding process. From ref. [13].
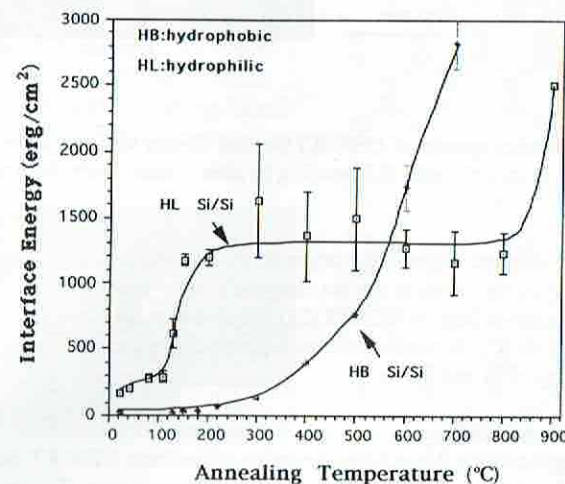

Fig. 2 Surface energy of bonded hydrophilic or hydrophobic silicon wafers as a function of annealing temperature [15].
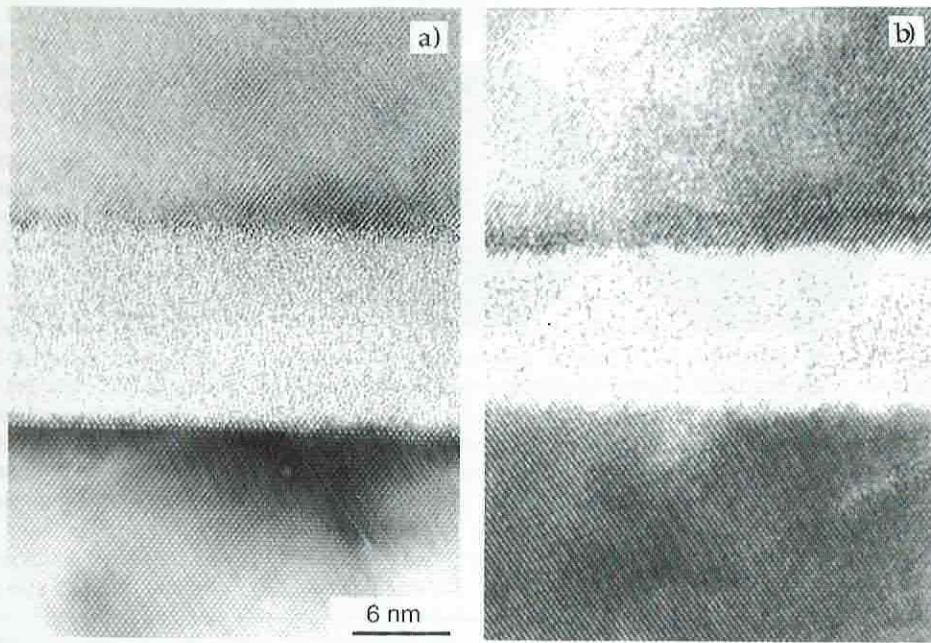
Fig. 3 Cross-sectional TEM micrographs of UHV RT bonded silicon wafers sputter-cleaned with an 1 keV Ar beam [19]. a) directly after RT bonding b) after 1 hour 650°C heat treatment

coming from hydrocarbon contamination of the original silicon surfaces) into the amorphous silicon zone. The incorporated carbon will slow down the recrystallization process.

In the meantime, the group of Suga at RCAST [21] has also managed to bond small areas of silicon under pressure in UHV at RT. In these conference proceedings the same group reports also on successful UHV RT bonding of Si and GaAs.

.2. Self-propagating, large area bonding

For many practical applications it would be desirable to perform UHV RT bonding for whole wafers and without the necessity of applying pressure over the whole area. The question is whether self-propagating wafer bonding can be initiated under UHV conditions by locally pressing the two wafer together just as in the case of conventional wafer bonding in air. Our recent experiments [13, 2] involving 4" (100) Si wafers demonstrate that this is actually possible.

We first bonded two Si wafers hydrophobically in air, brought the bonded wafers into a UHV chamber and separated the two wafers under UHV conditions. The separated wafers were heated
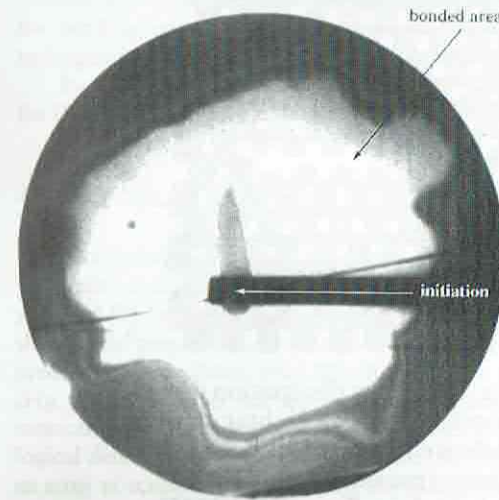

Fig.4: Infrared transmission image (in situ) of room-temperature UHV bonded silicon wafer (bright areas correspond to self-propagating bond wave; 4 inch wafer, (100)-orientation)

Fig.5: Cross-sectional transmission electron micrograph of the interface of two (100) silicon wafer bonded at room temperature in UHV
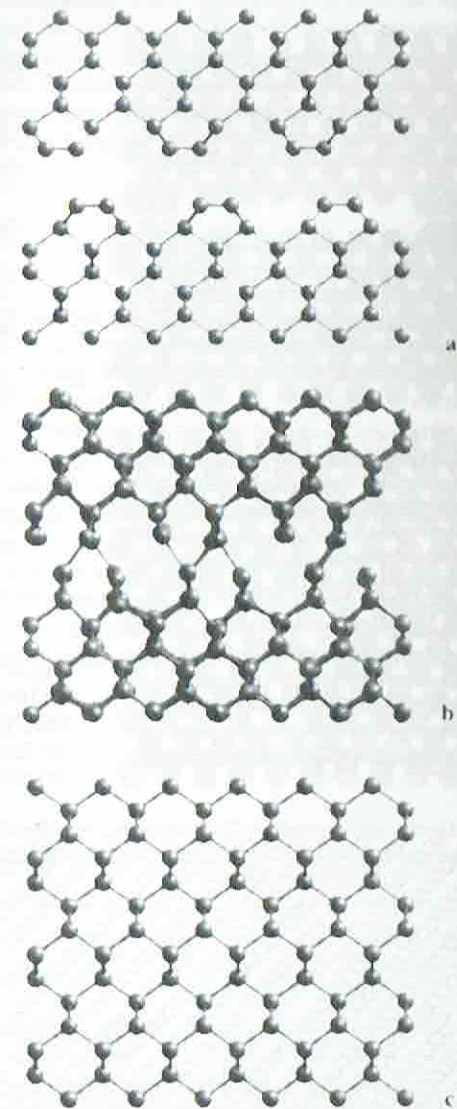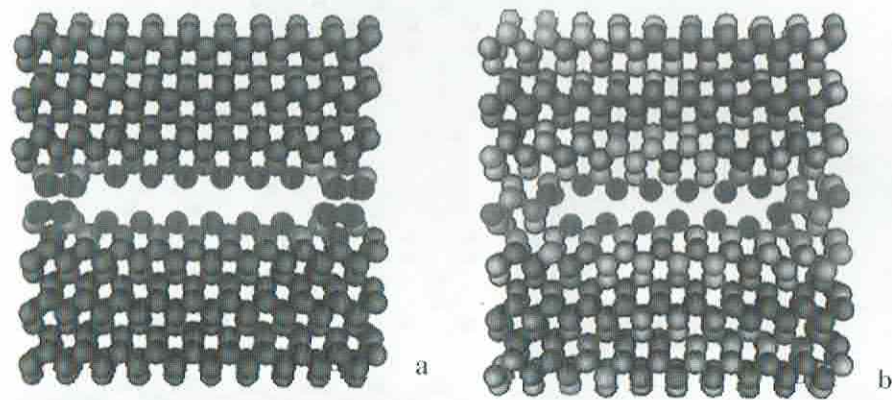

Fig.6: Snapshot (cross section) of molecular dynamics simulation for perfectly aligned reconstructed (100) silicon surfaces: a) initial configuration, b) after 0.1ps, c) final configuration

Fig.7: Energy dissipation during bonding at steps (lighter grey values indicate higher potential energy above ground state):
a) Initial configuration (300K),
b) after 12.5fs, c) after cooling (0K).
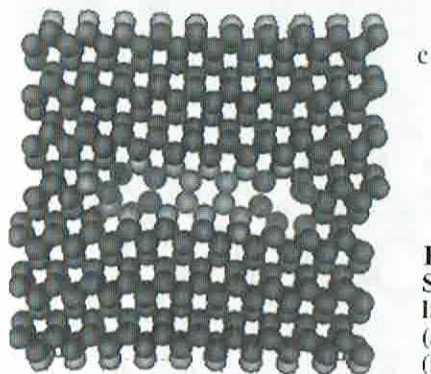
Fig.8: MD-simulation of rotationally misoriented Si(100) wafer bonding, plane view with light (dark) lines for bonds of the upper (lower) surface:
(a) Initial configuration: 4.58° misorientation,
(b) after 1.25ps/300K, 1.25ps/900K and cooling to RT.
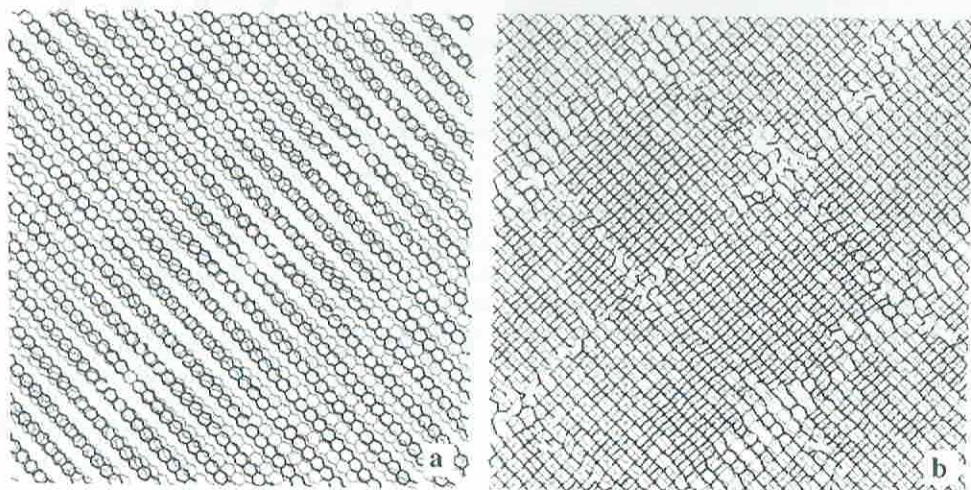
in-situ to above 600°C to desorb the hydrogen from the silicon surfaces. After cooling th[e] room temperature, the wafers were slightly pressed together locally in the UHV cham[ber] initiated a self-propagating bonding process over most of the wafer. The bonded area i[s] gray area in the infrared picture in Fig. 4. Mechanical tests showed that the wafers were [well] bonded. Cross-sectional TEM (Fig. 5) show the almost perfect bonding of the two waf[ers] the bonding interface. Due to the cleaning process consisting of simple thermal des[orption of] hydrogen from the surface no layer of amorphous silicon is present.

In the meantime UHV bonding of 3" silicon wafers has been demonstrated also by [...] the Naval Research Laboratories in Washington [23].

4. MOLECULAR DYNAMICS SIMULATIONS

Molecular dynamics simulations for hydrophilic silicon bonding has been perf[ormed by] Garofalini et al. [24]. Based on a modified simulation package with a modified Stilling[er-Weber] potential [25] we have simulated the UHV RT silicon wafer bonding process. The startin[g ...] showed the proper surface reconstruction as know from experimental results. Molecular [...] predicts the possibility for UHV RT covalent wafer bonding for perfect silicon (100[) ...] (Fig. 6) as well as for real silicon surfaces with mono-atomic or diatomic steps (Fig. 7). B[onding of] rotationally misoriented (100) silicon wafers also leads to covalent bonding but in this [...] logical defects are present (Fig. 8a). After simulating a heat treatment at 1000°C the interf[ace ...] an array of screw dislocations (Fig. 8b) in accordance with experimental results [26]

Presently, we work on the use of molecular dynamics simulations as a tool for [...] whether different materials may be bonded under UHV conditions or in the presence o[f ...] molecular surface layers. In this context, it will also be interesting to find thermally stab[le ...] coverages of silicon, such as Si-F which do not bond and could be used for applications [...] mechanics where bonding should be avoided.

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