

Self-propagating room-temperature silicon wafer bonding in ultrahigh vacuum

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Wafer bonding of commercial 4 in. silicon wafers has been performed at room temperature under ultrahigh vacuum conditions. After local initiation of the bonding process the bonding area is self-propagating just as in the case of wafer bonding under atmospheric conditions. The room-temperature bonded wafers, without any additional heat treatment show a bonding strength typical for bulk material. © 1995 American Institute of Physics.

Mirror polished and flat pieces of solids adhere to each other provided dust particles between the surfaces of the two solids are avoided. This adhesion phenomenon was first systematically investigated by Lord Rayleigh in 1936 for pieces of fused quartz.¹ He already determined the energy required to separate the two pieces again to be in the order of 0.1 J/m² per surface (termed surface energy γ). This energy is more than an order of magnitude lower than the corresponding value for the covalent bonding within quartz (SiO₂) and was later on attributed to van-der-Waals forces or hydrogen bridge bonds between water molecules adsorbed on the quartz surfaces. Fifty years after Lord Rayleigh's pioneering paper, the same type of adhesion phenomena was used to bond silicon wafers to each other intended for applications in the area of silicon-on-insulator (SOI) and power devices.^{2,3} For silicon wafers covered with a thermally grown oxide (corresponding to fused quartz) or a native oxide room-temperature bonding works well if the surfaces are hydrophilic and covered by one or two monolayers of adsorbed water molecules. Silicon wafers dipped in hydrofluoric acid (HF), which removes the native oxide, covers the silicon surfaces with hydrogen and makes them hydrophobic, also bond well but show a much lower surface energy γ of about 0.02 J/m². In order to increase the bonding strength of the adhesion the room-temperature bonded wafers have to be subsequently heated to more than 700 °C to reach the bonding strength of the bulk material.⁴⁻⁶ For a number of applications it would be desirable to be able to reach the bulk bonding strength by room-temperature bonding without the requirement of an additional heating step. In this context, the question arises whether it is possible to bring the flat and clean surfaces of two silicon wafers without any adsorbed foreign atoms or molecules together at room temperature so that covalent bonds will form directly at room temperature. The present letter deals with this question.

Parallel to performing wafer bonding experiments at room temperature under ultrahigh vacuum (UHV) conditions, we investigated the possibility of the formation of covalent bonds between two clean (100) silicon surfaces at room temperature by means of molecular dynamics simulations. The program used is based on a simulator developed

by Garofalini^{7,8} because macroscopic relevant systems solely can be simulated applying classic molecular dynamics with semiempirical potentials. Modifications of the potentials and the method itself, however, are necessary to include a more realistic surface reconstruction and interaction. A detailed description of the simulation method and the resulting interface structures will be published elsewhere.⁹ Here, the results are discussed which are relevant for the following experimental investigations. For describing the interaction potential between silicon atoms we modified the parameters in the potential originally suggested by Stillinger and Weber¹⁰ in such a way, that the experimentally observed spontaneous surface reconstruction of the (100) surface in terms of dimer formation is reproduced by the molecular dynamics simulation. The rescaled potential has an increased interaction distance of 3.99 Å and gives a dimer bond length in correspondence with experiments and *ab initio* calculations. The energy dissipation and the dynamic bonding behavior are controlled by transfer rates for the kinetic energy. While the outermost atomic layers of the structure model are cooled during the molecular dynamics calculation a macroscopic heat conduction is simulated. Then two slabs of silicon with reconstructed (100) surfaces are brought in parallel position at a distance of about 3.8 Å. A schematic cross section is shown in Fig. 1(a). After less than 10⁻¹³ s, the dimers broke up and the first bonds between the two surfaces had formed [Fig. 1(b)] before, finally, a perfect crystal formed across the interface [Fig. 1(c)]. Since in actual bonding experiments, we have to take into account rotational misorientations and surface steps these situations were also simulated. These simulations also predicted the formation of covalent bonding at room temperature, although for topological reasons no perfect crystal but grain-boundary-like interface structures developed.

Based on the results of the molecular dynamics simulations described above, we expected that room-temperature bonding of clean silicon wafers with high bonding strength should be possible. Bonding for local areas of silicon surfaces had been predicted already by Nelson *et al.*¹¹ in terms of an adhesion avalanche. In order to deal with clean surfaces without adsorbates the bonding experiments had to be performed under UHV conditions. UHV bonding experiments of quartz surfaces polished to optical flatness had already been performed by Smith and Gussenhoven¹² about 20

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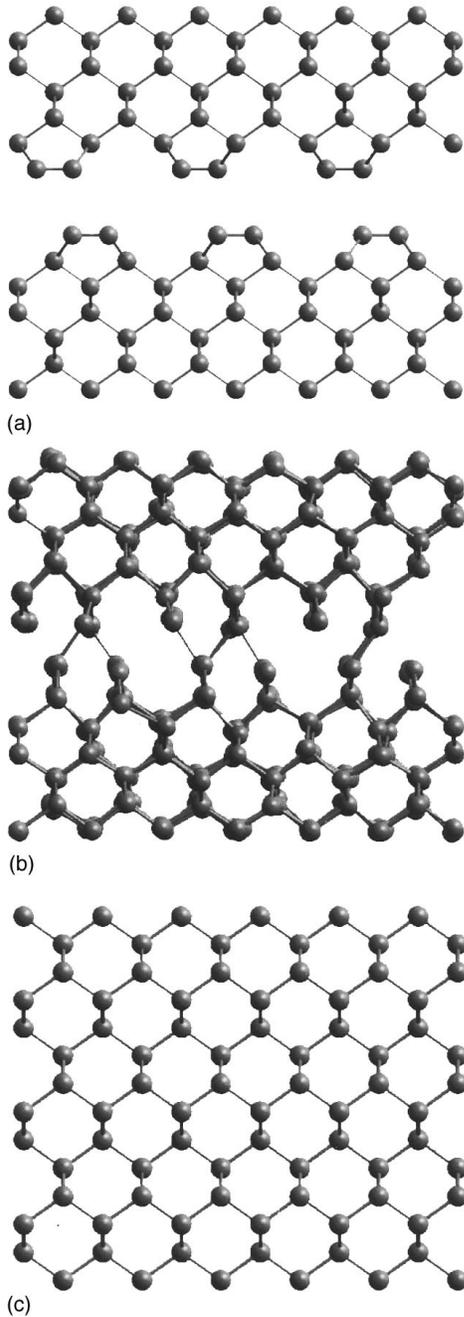


FIG. 1. Snapshot (cross section) of molecular dynamics simulation for perfectly aligned reconstructed (100) silicon surfaces: (a) initial configuration, (b) after 10^{-13} s, and (c) after final configuration.

years ago. Their result was that bonding in UHV is possible but occurs by van-der-Waals interaction and is correspondingly weak. In contrast, the rebonding of the surfaces of partially cleaved germanium crystals in UHV appear to lead to covalent bonds.¹³ Suga and co-workers¹⁴ had bonded silicon and copper (or aluminum) at room temperature under UHV conditions and reached high bonding strengths, but in their case the bonding only occurred under the influence of an external high compressive stress which plastically deformed the metal and the bonded area was limited to the area at which the external stress was applied. The purpose of the

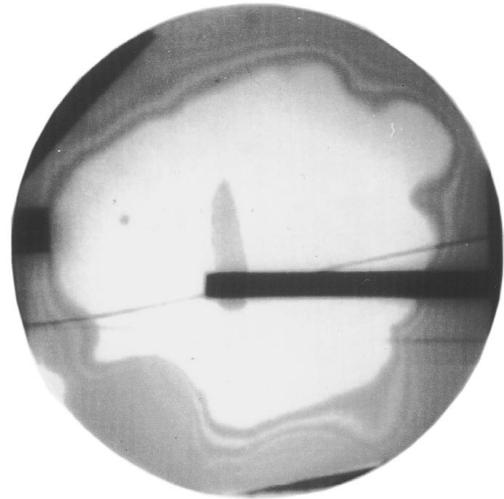


FIG. 2. Infrared transmission picture of room-temperature UHV bonded silicon wafers. The bright wafer areas correspond to bonded areas. The thick black horizontal beam is part of the mechanism to initiate bonding by locally pressing the wafers together. The thin black lines across the wafer come from wires which prevent the two wafers from separating too much before bonding.

experiments described below was to check whether it is possible to get room-temperature covalent bonding over large areas in which the bonding process after initiation by a local external compressive stress is spreading over the wafer in a self-propagating fashion.

For the bonding experiments we used commercially available 4 in. (100) silicon wafer. The wafers were dipped in diluted HF in order to remove the native oxide and render the surfaces hydrophobic and covered with a layer of hydrogen. Two hydrophobic silicon wafers were then bonded in a microcleanroom setup¹⁵ under normal atmospheric conditions at room temperature. The bonded wafer pair was transferred into a UHV chamber which subsequently was pumped down to about 3×10^{-9} Torr. The bonding state of the two wafers, which were held in a vertical position could be observed *in situ* by an infrared camera. Then, by an appropriate manipulator handled from the outside of the UHV chamber, the two wafers were separated by introducing three wedges between the wafers at the rim. That the wafers were actually completely separated could be observed by the infrared camera. In order to a drive off the hydrogen from the silicon surfaces, the two separated wafers were heated in various cycles from 600–800 °C.¹⁶ Due to the desorbing hydrogen gas the pressure in the chamber increased to about 10^{-6} Torr. The two wafers (both standing vertically but separated by a couple of millimeters) were then slowly cooled down to room temperature and UHV conditions of 3×10^{-9} Torr were reached again after sufficiently long pumping. The two separated wafers without hydrogen coverage were then the starting point of our actual room-temperature UHV wafer bonding experiment. By pressing the two wafers locally together by a kind of tong (seen in Fig. 2 as horizontal dark bar) operated from the outside of the UHV chamber, a bonding process was initiated which propagated over most of the wafer area. An infrared picture of the silicon wafers after the

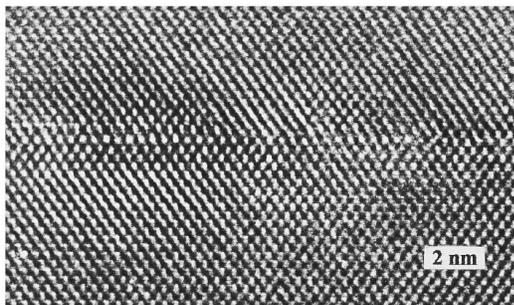


FIG. 3. Cross-sectional transmission electron micrograph of the interface of two (100) silicon wafers bonded at room temperature in UHV without further heat treatment.

bonding process is shown in Fig. 2. The bright areas in Fig. 2 correspond to bonded areas. The lateral propagation speed of the bonded area was so fast that it was beyond what we could resolve with our video equipment, which translates to a value of the lateral bonding speed of much more than 1 m/s. This value is much higher than the typical bonding speed of about 0.01 m/s under atmospheric conditions.¹⁷

The bonded wafers could not be separated anymore by the wedge mechanism (which had been used to separate the wafers bonded in atmosphere) either inside or outside the UHV chamber, but rather induced the breaking off of part of the bonded wafers. Based on experiments of wafers bonded under atmospheric conditions and then subsequently heated for increasing the bonding strength, we conclude that the inability to separate the UHV bonded wafers by the wedges already indicates that the surface energy is higher than about 2 J/m². Pieces of the room-temperature UHV bonded silicon wafers were subjected to tensile test measurements. The samples either fractured at the silicon-glue interface or across the silicon bulk (typically, at a stress of $>3.5 \times 10^7$ N/m²) but in no case at the bonding interface. This result, as well as the fact that it was not possible to separate the bonded wafers by wedges (which were razor blades in our case), again show that strong covalent bonds developed during room-temperature UHV bonding.

The bonding interface of the room-temperature UHV bonded silicon wafers was further investigated by cross-sectional high-resolution transmission electron microscopy. An example is shown in Fig. 3. The interface does not con-

tain any noticeable intermediate layer but does not correspond to a perfect crystal because of the unavoidable misorientations of the two wafers relative to each other.

In conclusion, we have demonstrated that large area, self-propagating, room-temperature covalent wafer bonding of commercially available (100) silicon wafers is possible. We have not yet any results on other crystal orientations, combinations of crystal orientations, other materials such as GaAs and combinations of materials with different thermal expansion coefficients, such as GaAs and Si, for which a room-temperature bonding procedure leading to covalent bonding would be especially desirable. It has also not yet been checked whether the hydrogen drive-off cleaning procedure could be replaced by an inert gas plasma cleaning performed at room temperature. These questions will be addressed experimentally in the near future.

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