boundaries (Perreault et al 1992).

iv) In the plan-view images some of the samples showed linear structures running at an angle of about 30° to a <110> direction. Their spacing is about 50 nm. Diffraction contrast experiments proved that these structures are not related to 60° dislocations. Cross-sectional samples prepared from different {110}- and {100} planes showed a zigzag-like structure in one {100} plane with the same periodicity (50 nm). Samples of all the other planes only show the dislocation network ({110} samples) or dot-like contrasts referring to oxide islands (the other {100} plane). As shown in Fig. 3, a terrace-like structure is reconstructed from all these images. Their nature is not yet known. Terraces may be caused by stress relaxation of the rotational misorientation.

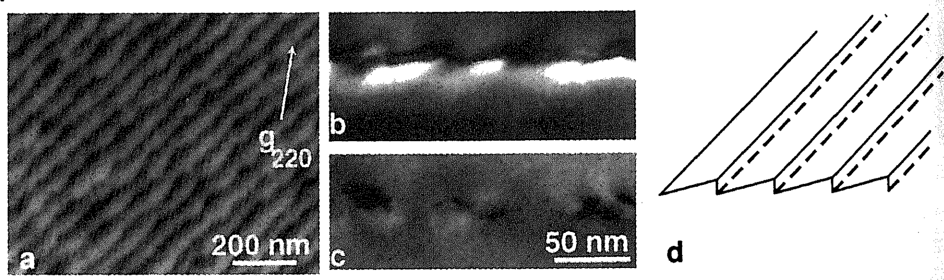

Fig. 3: Terrace-like structure in the interface. TEM-plan-view (a) and cross-sectional images of 2 different {100} planes (b,c). Schema of the terrace structure (d).

CONCLUSIONS

It is shown that the interfaces of bonded hydrophobic wafer pairs and such pairs bonded under UHV conditions correspond to grain boundaries having a twist and a tilt component. MD-simulations for clean and reconstructed surfaces (as obtained under UHV conditions) explain the generation of dislocation networks during bonding by the relaxation of interfacial atoms and the formation of covalent bonds. Furthermore, the defect structure in interfaces of wafers bonded under atmospheric conditions is more complex. Besides the screw dislocation network, interactions of screw dislocations with 60° dislocations, resulting from the miscut of the samples used, are observed more frequently. These interactions may be caused by the high annealing temperatures applied. In some cases, instead of the screw dislocation network, a terrace-like structure forms which may constitute a form of adapting the rotational misorientation, at least partially.

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Dislocation structure in interfaces of bonded hydrophobic silicon wafers: experiment and molecular dynamics

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ABSTRACT: The defect structure in interfaces of directly bonded hydrophobic silicon wafers is studied by HVEM and HREM. It is shown that the twist component of the boundary causes a screw dislocation network, while the tilt component or a miscut are compensated by arrays of 60° dislocations. Interactions occur between both especially during annealing at higher temperatures. For annealing at temperatures below 1000°C the structure of the interface is more or less analogous to that of wafer pairs bonded under UHV conditions at room temperature without any subsequent heat treatment. Molecular dynamics simulations of the latter revealed that the screw dislocation network is caused by the relaxation of atoms into a mosaic-like structure with the formation of covalent bonds via the interface.

1. INTRODUCTION

Silicon wafer direct bonding has become of increasing interest for silicon-on-insulator (SOI) and power devices as well as for micromechanics and sensors. Here, wafers used for wafer bonding are covered with either a thin native oxide or a purposely grown thermal oxide which has been rendered hydrophilic by cleaning procedures. At room temperature, the initial bonds are hydrogen bonds caused by the presence of OH-groups at the interface, while at higher temperatures they are transformed into stable Si-O-Si bonds. The interfaces are atomically flat without any defects. Alternatively, silicon surfaces may be treated with diluted HF, which removes the native oxide layers and directly covers the silicon surface with hydrogen, thus rendering the surfaces hydrophobic. Here, van der Waals forces are generally assumed to be the origin of the attractive force at room temperature. At higher temperatures, they are transformed into Si-Si bonds. Depending on the misorientation between both wafers, dislocation networks are generated in the interface: the twist component causes a network of pure screw dislocations, while the tilt component is compensated by a periodic array of 60° dislocations. Both dislocation fractions were extensively investigated after annealing at T ≥ 1100°C (e.g. Gafiteanu et al 1993, Benamara et al 1994, 1995).

The present paper analyzes the interfacial defects of bonded hydrophobic wafer pairs occurring at lower temperatures (> 800°C). Furthermore, these interfacial defects are compared to the interfaces of wafer pairs bonded under ultra-high vacuum (UHV) conditions at room temperature without any subsequent heat treatment.

2. EXPERIMENTAL

Czochralski-grown silicon wafers (diameter 4 in., (100) orientation, p-type) were used for the experiments. The tilt component (cut-off) of all wafers is below ± 1°. After cleaning in standard