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AlN-AlN Wafer Bonding and Its Thermal Characteristics

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Homogeneous bonding was successfully demonstrated on 150 mm Si wafers by face-to-face fusion bonding of two clean and smooth aluminum nitride (AlN) layers. Characterization result from XPS confirms the layer composition and reveals that approximately 5 nm of the layer surface was partially oxidized during processing. The as-bonded wafer pair is nearly void and particle free with a high bonding strength of 1263.0 mJ/m², enabling it to withstand the subsequent process steps. In addition, the AlN-AlN bonded wafers appear to have the best heat dissipation capability when compared with other bonded wafers, which used SiO₂ or Al₂O₃ as the bonding layer.

Wafer bonding allows heterogeneous integration of two materials that have similar or very different lattice parameters and thermal properties, via an intermediate bonding layer or direct bonding. One of the most prominent applications of wafer bonding is silicon-on-insulator (SOI) (1-5), and it can also be extended to germanium-on-insulator (GOI) (6, 7) or other III-V groups integration (8, 9). First direct bonded SOI was reported by Lasky et al. in 1986 (3). Since then, SOI fabricated from wafer bonding has been gaining ground from the conventional Si substrate in ultra-large scale integrations (ULSI) and micro-electro-mechanical systems (MEMS) as the starting substrate (10), which benefits from its on-insulator structure. The “on-insulator” advantages make it possible to attain mechanical stability close to Si substrate and excellent electrostatic control, such as attenuated short-channel effects (11), reduced parasitic capacitance and absence of latch-up (12). As the most common buried insulator material, SiO₂ has already shown extensive popularity in a couple of optical devices (13-15). However, the low thermal conductivity of SiO₂ (1.46 Wm⁻¹K⁻¹) limits the heat dissipation efficiency and degrades the advantages of SOI. Also, the degraded heat dissipation path deteriorates its heat transfer efficiency to the underlying bulk Si layer, leading to severe self-heating effect. This effect is magnified further by device scaling for performance improvement, which constrains the applicability of SOI in electronics, especially in the cases where high temperature and power dissipation are expected. In order to address this problem, numerous efforts have been dedicated to exploring for novel buried insulator materials with high thermal conductivity. For example, Puurunen et al. had confirmed the possibility to utilize TiO₂ as the buried insulator in the formation of SOI by wafer bonding, whereas an Al₂O₃ under-layer was required (16). Additionally, SOI formed through Al₂O₃-Al₂O₃ wafer bonding was successfully demonstrated (4). This was

accomplished with the assistance of surface activation carried out at room temperature. Besides TiO_2 and Al_2O_3 , another promising candidate is AlN , which has excellent properties including high thermal stability, good dielectric properties and excellent heat dissipation capability with a thermal conductivity of $134 \text{ Wm}^{-1}\text{K}^{-1}$ (17). Moreover, its thermal expansion coefficient is close to that of silicon (18), thus the thermally induced stress can be potentially relieved. Furthermore, its feasibility as a buried insulator layer for SOI had been proven from bondability (19) and heat transfer efficiency (20) aspects.

In this paper, the AlN - AlN fusion bonding is investigated to examine its bonding quality and to verify its superiority as the buried insulator in terms of heat dissipation capability. It shows the possibility of fabricating bonded wafers with enhanced thermal conductivity through room temperature AlN - AlN fusion bonding. Its strong heat dissipation capability is verified by COMSOL simulation and experimental results obtained from resistance thermal detector (RTD).

Experimental

All Si wafers used for bonding were p-type, 150 mm Si (100) test grade wafers, thickness of $625 \pm 25 \mu\text{m}$, total thickness variation (TTV) $< 10 \mu\text{m}$ and with the resistivity in the range of 10 - 20 $\Omega\cdot\text{cm}$. Firstly, the wafers were pre-cleaned by the standard RCA cleaning method for the purpose of organic and metallic contaminants removal. Then, a 20 nm AlN thin film was sputtered onto the pre-cleaned Si surface with a deposition rate of 7.14 nm/s. While for comparative study, a 20 nm of SiO_2 and Al_2O_3 was deposited via PECVD and ALD system, respectively. After deposition, a pre-annealing step was provided to densify the AlN thin film, allowing outgassing of incorporated gases. This process helped to eliminate voids formation at the bonding interface in the subsequent processes and was significantly important in improving the bonding quality. Pre-anneal was carried out at 450 $^\circ\text{C}$ for 1 hr. During pre-

Figure 1. Formation process for AlN - AlN bonding and RTD on the bonded wafers.

annealing, the furnace was purged with N₂ gas to minimize the contact with air or moisture. Then, the pre-annealed wafers underwent 15 s Ar plasma activation for surface hydrophilicity enhancement, and were cleaned by de-ionized (DI) water rinse and dried with spin dryer. Prior to the fusion bonding, the properties of AlN thin film, such as roughness and film composition, were measured by atomic force microscope (AFM) and x-ray photoelectron spectroscopy (XPS). AlN-AlN bonding was initiated at room temperature. Then, the bond was strengthened by annealing at 300 °C in N₂ ambient for a duration of 3 hr. The formation process of AlN-AlN bonding is illustrated in Figure 1. The bonding quality was verified by both infrared (IR) imaging and cross-sectional scanning electron microscope (SEM), while the post-annealing bonding strength was calculated based on Maszara's crack opening method (21).

RTD was then patterned and formed on the bonded wafers, followed by *I-V* measurement to verify the thermal characteristics of the bonding layer. After the bond strengthening annealing, Si on one side of the bonded structure was removed by grinding and wet etching. Next, RTD patterns, also known as Au line Kelvin structures, were formed by lithography, metal deposition, and lift-off processes. The dimension of zig-zag line in the RTD patterns was 1445 μm in length, 15 μm in width (as shown in Figure 2), and the thickness of Au line was 150 nm. Here, a 30 nm thick chrome layer was used to promote the adhesivity.

Figure 2. Top-view of the RTD pattern for thermal characteristics measurement.

Results and Discussion

AlN Thin Film Characterizations

XPS measurement was performed to verify the composition and oxidative stability of the AlN thin film. Owing to the sputter deposition method, a large amount of gases was incorporated in the thin film. These gases would out-diffuse and cause the formation of voids when the annealing temperature is increased to above 100 °C. With increasing the annealing time and temperature, the voids are enlarged and finally lead to large debonded areas around the wafer center region. In order to eliminate voids formation, a pre-anneal process was provided at 450 °C. However, it is reported that the AlN thin film is prone to oxidation when exposed to air (22). Also, annealing at a high temperature accelerates the oxidation. With these concerns, XPS was carried out on a 30 nm-thick AlN thin film sample using monochromatic Al K-α source for composition examination. Al 2*p* peak and N 1*s* peak were observed at binding energy of 73.8 eV and 396.9 eV (as shown in Figure 3). These results coincide with previously reported values (19), confirming that the sputtered thin film is AlN. Only the first 5 nm is oxidized with surface oxygen concentration of 20.8 at%, while the rest thin film has nearly 1:1 atomic ratio between Al

Figure 3. XPS analyses: (a) Al 2p and (b) N 1s spectra for pre-annealed AlN sample.

Figure 4. Atomic concentration profiles of pre-annealed AlN sample by XPS.

and N. According to the atomic concentration diagram (in Figure 4), there is a slight mismatch in the stoichiometric ratio of AlN at the surface region. This indicates that the AlN thin film was partially oxidized by H₂O or O₂ in the air and/or air leakage into the N₂ furnace. When the film is sputter-etched, the atomic concentration of oxygen drops to 5.2 - 5.7%. The possible sources introducing oxygen into the thin film are the impurities from source materials and gas incorporation during sputtering caused by the relatively high chamber pressure.

Direct wafer bonding only occurs when the stringent requirements in surface morphology and roughness are fulfilled. Thus, well control of surface roughness is essential in obtaining successfully bonded wafers, where root mean square (RMS) roughness need be less than 0.5 nm for polar group passivated surface (23). Smooth and adhesive thin film was sputtered with RMS of 0.133 nm in a 5 $\mu\text{m} \times 5 \mu\text{m}$ AFM scan area as shown in Figure 5a. The roughness value is further reduced to 0.120 nm after the pre-anneal process, which is shown in Figure 5b. The smoothening in surface roughness is originated from both the surface oxidation process (24) and the removal of incorporated gases. Though Ar plasma activation roughens the surface (as shown in Figure 5c), the RMS value of activated surface, which is 0.328 nm, is still within the bonding requirement. Thus, it allows direct wafer bonding when bringing two such wafers into intimate contact.

Figure 5. AFM images of (a) as-sputtered, (b) pre-annealed, and (c) activated AlN layer.

AlN-AlN Bonding Quality

The IR imaging results in Figure 6a show that AlN thin film exhibits very good bondability when two of them are bonded face-to-face. The good bondability can be attributed to the sufficiently clean and flat surface with low surface roughness. Only very few unbonded areas were observed due to the presence of particles, which were trapped during wafer handling and can be eliminated with careful control of contamination

Figure 6. IR images of bonded Si/AlN-AlN/Si wafer (a) before, (b) after bond strengthening annealing in N_2 ambient, and (c) with crack opening.

Figure 7. (a) Cross-sectional SEM image bonded Si/AlN-AlN/Si wafer and (b) SEM EDX elemental mapping for Al

sources. This led to a respectable AlN-AlN bonded interface. After annealing, no obvious void enlargement or new void formation was found, which indicates that out-gassing is not significant. The low out-gassing level is due to the pre-anneal process introduced prior to wafer bonding. Cross-sectional SEM image, which can be seen from Figure 7a, reveals that the bonded layer is uniform without defect at the microscale. The thickness of the bonded layer is 35.4 nm, the small deviation corresponds to the knocked-off layer during Ar plasma activation. An Al-rich layer was detected by Energy Dispersive X-Ray (EDX) Analysis compositional mapping as shown in Figure 7b, qualitatively proving that the bonding layer is AlN.

The bonding strength is estimated using the crack opening model. A crack is introduced by inserting a razor blade, thickness of $2y$, into the edges of the bonded wafer pair. Then, the crack propagates along the interface, giving rise to a crack length L . Substituting the value of L into the following equation:

$$\gamma = \frac{3Et^3y^2}{8L^4} \quad [1]$$

the bonding strength γ can be calculated. Where E is the elastic modulus of Si (100), and t is the thickness of a single wafer. Based on this method, the crack length of the bonded sample is 21.9 mm and the bonding strength is estimated to be 1263.0 mJ/m^2 , which is sufficiently high to withstand the subsequent process steps. The mechanism behind this strong bond formation is still under investigation.

Bonded Wafers Thermal Characteristics

According to the COMSOL simulation results, AlN has shown a great advantage as the insulator layer in terms of heat dissipation capability as compared with conventional insulator materials SiO_2 and the recently widely studied Al_2O_3 . Their heat dissipation capability was investigated and compared by studying the temperature profile across the bonded structure when the material stack was subjected to a heat flux of $1 \times 10^8 \text{ W/m}^2$. From Figure 8, the simulated surface temperature of 40 nm SiO_2 , Al_2O_3 , AlN, Si on Si structures are 35.25, 32.50, 32.42, and 32.42 °C, respectively. 40 nm AlN on Si

Figure 8. COMSOL simulation results (a) schematic view and (b) Cross sectional temperature profile of 40 nm $\text{SiO}_2/\text{Al}_2\text{O}_3/\text{AlN}/\text{Si}$ on Si.

appeared to have the similar temperature profile as direct Si-Si bonded wafers, because they have close thermal conductivity values (AlN: $134 \text{ Wm}^{-1}\text{K}^{-1}$ and Si: $131 \text{ Wm}^{-1}\text{K}^{-1}$). Thus, it can be noted that the presence of AlN thin film does not degrade the thermal property or hinder heat from spreading to the underlying Si substrate.

To further confirm the findings from COMSOL simulation results, *I-V* measurement was carried out on RTDs that had been formed on the bonded wafers with two different bonding intermediate layers: SiO_2 and AlN. This experiment is still in the measurement stage and results will be reported in the future.

Conclusion

In conclusion, a successful void-free AlN-AlN wafer bonding was demonstrated on 150 mm Si wafer. Characterization results verified that the sputtered film was AlN, which was clean, smooth and with only approximately 5 nm partially oxidized top surface. When bonding two such surfaces together, a respectable AlN-AlN bonded interface was achieved with very few unbonded areas. The bond strength reached 1263.0 mJ/m^2 with the addition of 3 hr bond strengthening anneal at 300°C . After the annealing, no obvious void enlargement or new void formation was observed, which was in virtue of sufficient outgassing during the pre-anneal step. In addition, the bonded AlN-AlN layer showed superior heat dissipation capability based on COMSOL simulation results, which was similar to that of Si-Si direct bonding. Its superiority will be further confirmed with experimentally measured results.

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