

Experiment-Based Modeling of Wafer-to-Wafer Bonding for 3D Integration

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Abstract— Wafer-to-wafer (W2W) bonding is a key technology for advanced packaging and three-dimensional device architectures, where precise control of bonding dynamics and resulting wafer distortion is required. Such control must be based on clear understandings of both surface conditions and mechanical deformation. Conventional bonding simulations have been discussed separately from experimental analyses. Thus, it remains difficult to accurately reproduce experimental bonding behavior across different materials and interface conditions using a single simulation framework. In this study, we develop a novel simulation framework that uses experimentally measured values as input parameters. The framework incorporates adhesion energy measured by the double-cantilever beam (DCB) method into a modified Lennard-Jones adhesion model. The simulated bonding dynamics and bonding-induced in-plane displacement are compared with experimental observations. The proposed framework provides a practical route toward connecting experimental bonding characteristics with wafer-scale bonding simulation.

Keywords—Wafer bonding, In-plane distortion, Bond wave, 3D Integration

I. INTRODUCTION

Wafer-to-wafer (W2W) bonding has attracted considerable interest for a wide range of semiconductor technologies, including advanced logic architectures such as backside power delivery network (BSPDN) and complementary FET (CFET), as well as 3D flash memory and CMOS image sensor [1-4]. Depending on the target application, various bonding configurations, wafer deformation profiles, bonding materials, and interface designs must be considered. These include wafers with different initial shapes, such as flat, bowl-shaped, umbrella-shaped, and saddle-shaped wafers, as well as diverse film stacks and bonding interfaces.

Recently, many studies have investigated bonding dynamics and subsequent wafer distortion using numerical simulations

and experimental approaches [5,6]. However, both studies have often been conducted independently and are not yet sufficiently integrated. In particular, only limited efforts have been made to quantitatively connect wafer bonding simulations with experimental bonding-surface properties, such as surface activation, interfacial adhesion, and material-dependent bonding behavior. This lack of connection makes it difficult to predict bonding dynamics for specific combinations of bonding materials, interface properties, and wafer deformation profiles.

In this work, we address this issue by developing an experimentally informed wafer bonding model. Adhesion energy measured by the double-cantilever beam (DCB) method is incorporated into a modified Lennard-Jones adhesion model as an effective parameter representing the bonding-surface condition. The objective of this study is not to directly resolve individual surface-chemical contributions, such as hydroxyl density, adsorbed water, or capillary condensation, but to reflect their combined effect through experimentally measured adhesion energy. The simulation results are then compared with experimental bond wave speed and bonding-induced in-plane displacement to evaluate the validity of the proposed framework.

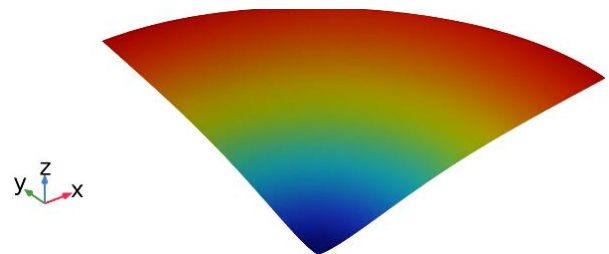


Fig.1 Simulation geometry of deformed wafers for the wafer-to-wafer bonding model.

II. SIMULATION METHODOLOGY

A. Overview of Simulation Model

In this study, the top wafer was modeled as an elastic body with anisotropic Young's modulus [7], while the bottom wafer was treated as a rigid body. A quarter model of a 300-mm wafer was used to reduce computational cost, and symmetry boundary conditions were applied to the two symmetry planes. The wafer thickness was set to 775 μm , and the wafers were assumed to be initially flat. The initial interfacial gap was set to a sufficiently small value. Preliminary analyses indicated that variations in the initial wafer gap and wafer chucking conditions affected wafer distortion only marginally and did not significantly influence bond front propagation under the conditions investigated in this study. The outer edge of the wafer was treated as open to atmospheric pressure, and bonding was initiated from the wafer center.

The simulation model strongly couples wafer deformation with pressure generation in the interfacial fluid gap. As the upper wafer approaches the lower wafer, the interfacial pressure and adhesion force are calculated and fed back to the wafer deformation. Bonding was judged to occur when the local separation between the two wafer surfaces became smaller than a geometrical bonding threshold of 15 nm. This threshold was used only as a numerical criterion for bonding completion and was distinguished from the characteristic adhesion length used in the Lennard-Jones adhesion model. The definitions of the adhesion force model and the interfacial fluid model are described in the following subsections.

B. Definition of Adhesion Energy

In practical wafer bonding, the effective adhesion force originates from several interfacial interactions, including van der Waals forces, hydrogen bonding, and capillary-related interactions. These interactions depend strongly on the bonding-surface condition and the separation distance between the two wafer surfaces. As the interfacial gap decreases, the attractive interaction between the surfaces increases and governs the final stage of bond-front propagation [8,9].

To represent this distance-dependent attraction in a wafer-scale simulation, the adhesion force was modeled using a modified Lennard-Jones-type potential (L-J potential). The adhesive stress was expressed as

$$\sigma_{adh}(\delta) = -\frac{8 G_{adh}}{3 \delta_{adh}} \left[\left(\frac{\delta_{adh}}{\delta + \delta_{adh}} \right)^3 - \left(\frac{\delta_{adh}}{\delta + \delta_{adh}} \right)^9 \right] \quad (1)$$

where G_{adh} is adhesion energy, δ is the local wafer gap, and δ_{adh} is the characteristic adhesion length of the Lennard-Jones-type potential [5]. In this study, G_{adh} was determined from DCB measurements and used as an effective parameter reflecting the bonding-surface condition. The parameter δ_{adh} was set to 50 nm to define the interaction range of the adhesion model. The relationship between the adhesion stress and wafer gap used in the present model is illustrated in Fig. 2.

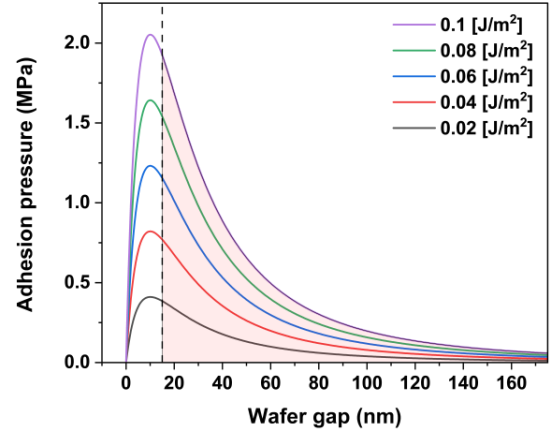


Fig. 2. Schematic adhesion-force curve modeled using the L-J potential. The shaded area indicates the effective adhesion energy evaluated within the bonding threshold.

Increasing G_{adh} enhances the attractive stress and interfacial attraction. A value of $\delta_{adh} = 50$ nm was selected to ensure stable wafer-scale calculations. The painted region in Fig.2 is effective total adhesion energy imposed on upper wafer, because attractive interaction stops systematically at the threshold of 15 nm away from bottom wafer.

C. Definition of Interfacial Fluid Model

The interfacial fluid behavior was described using a Reynolds-type thin-film model, which enables efficient calculation of the pressure distribution within the wafer gap and its coupling with wafer deformation during bond-front propagation.

The present model should be interpreted as an effective wafer-scale thin-film model rather than a molecular-scale description of the final nanometer-scale gap. The Reynolds-type formulation is expected to be valid over most of the interfacial fluid region. However, nanoscale effects may become important during the final stage of bonding. These effects include slip, rarefaction, surface roughness, adsorbed water layers, and surface forces, which are not explicitly included in the present model. To ensure numerical stability, an effective overlap region below the nominal lower-wafer surface was introduced as a regularization domain for evaluating interfacial pressure and adhesion during the final approach. This overlap region does not represent physical wafer penetration but serves as a numerical treatment that enables wafer-scale bonding dynamics to be simulated without directly resolving molecular-scale nanogap physics.

III. BONDING EXPERIMENT

Bonding experiments were performed to measure adhesion energy and bond wave speed for validation of the simulation framework. Thermally grown SiO_2 wafers were used for the bonding experiments. Different bonding-surface conditions were prepared to obtain a range of adhesion energies and bond

wave speed for comparison with the simulation. The experimentally measured adhesion energy and bond wave speed were used for validation of the simulation framework.

We observed bond wave propagation using an infrared camera. The bond wave speed was calculated from the temporal change in the bond-front position. To obtain adhesion energy, a thin blade with a thickness of 0.1 mm was pre-positioned at the wafer edge to form a non-bonded region, and the non-bonded length L was measured after bonding. A schematic view of bond wave propagation and adhesion energy measurement is shown in Fig. 3.

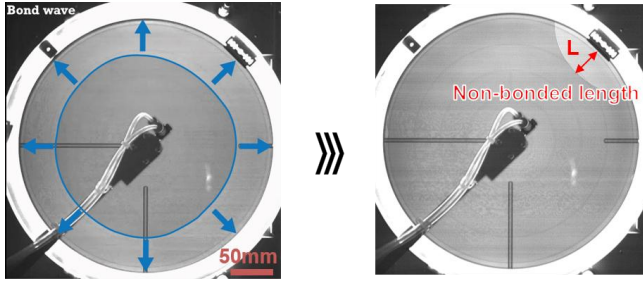


Fig.3 Bond front propagation and adhesion energy measurement

The adhesion energy was calculated using the DCB method as expressed in Eq.2

$$G_{adh} = \frac{3}{16} \frac{E t_w^3 t_b^2}{L^4} \quad (2)$$

where E is young's modulus, L is non-bonded length, t_b is blade thickness, and t_w is wafer thickness.

For hydrophilic bonding surfaces, adhesion energy can evolve with time after bonding because of interfacial reactions, water redistribution, and strengthening of interfacial bonds [10]. Therefore, to compare adhesion energy with bond wave propagation, the earliest measurable adhesion energy after bonding completion was used in this study.

IV. RESULTS AND DISCUSSION

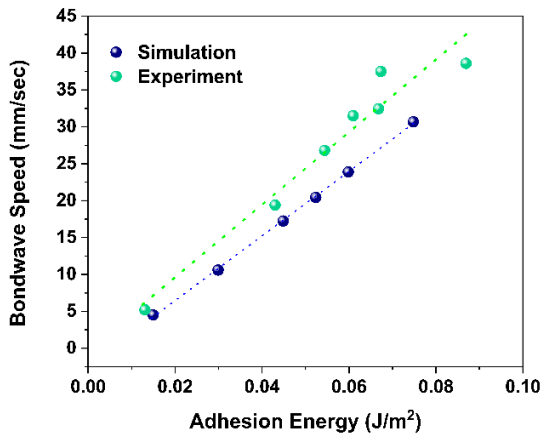


Fig. 4 Correlation between adhesion energy and bond wave speed In the simulation, the bonding threshold was set to 15 nm; therefore, the effective adhesion energy corresponds to approximately three-quarters of the input adhesion energy.

Fig. 4 shows the relationship between adhesion energy and bond wave speed. Both experimental and simulation results indicate that bond wave speed increases with adhesion energy. This trend is consistent with previous reports that bond-front propagation is strongly affected by interfacial adhesion [9]. In the present simulation, the adhesion energy measured by the DCB method was used as an input parameter in the modified Lennard-Jones adhesion model, and the simulated bond wave speeds followed the experimental trend over the investigated adhesion-energy range.

Although the proposed model reproduced the overall trend of bond wave speed, some deviations remained between the simulation and experiment. These deviations may originate from effects that are not explicitly included in the present model, such as interfacial fluid-surface interactions, local surface roughness, adsorbed water transport, capillary condensation, and possible slip or rarefaction in the nanometer-scale gap. Therefore, further model development will be required to quantitatively reproduce bonding behavior under a wider range of bonding-surface conditions.

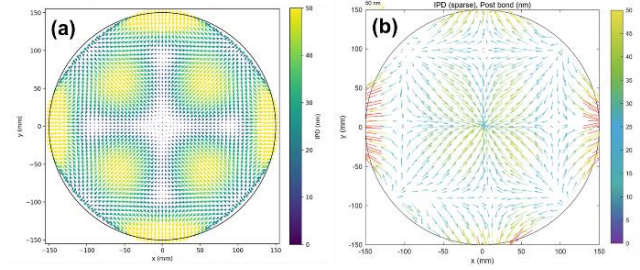


Fig.5 Residual wafer IPD map after linear correction

(a) Simulation (b) Experimental data[11]

Next, the simulation results were compared with experimental observations in terms of in-plane displacement (IPD). Fig. 5 shows the residual wafer IPD map after 6-parameter linear correction. For comparison with the experimental data, the simulation condition yielding the closest bond wave speed was selected. The simulated vector-map pattern showed a similar overall distribution to the experimental result, suggesting that the proposed model captures the main features of bonding-induced wafer distortion.

In particular, the simulation reproduced the anisotropic characteristics of the wafer distortion observed in the experiment. The directional dependence of the IPD distribution, including the preferential distortion pattern associated with the crystallographic orientation of the silicon wafer, was qualitatively consistent with the experimental result. This agreement indicates that the anisotropic elastic properties incorporated in the simulation play an important role in determining the bonding-induced distortion pattern. While some differences remain in the detailed displacement distribution, the simulation results tend to show smaller IPD values than the experimental data. These differences are mainly attributed to the simulation configuration. As shown in Fig. 2, the effective adhesion energy differs from the input adhesion energy because the upper wafer is not allowed to approach closer than 15 nm. This suggests that chemical reactions and surface forces

occurring in the nanoscale gap region may further contribute to IPD enlargement. A previous study also showed that the chemical characteristics of the top surface can have a significant impact on IPD increase [12]. Therefore, the present comparison is intended to demonstrate that the proposed model can qualitatively capture the anisotropic nature and spatial characteristics of bonding-induced wafer distortion observed in experiments.

V. CONCLUSION

In this study, an experiment-informed wafer bonding simulation framework was developed for wafer-to-wafer bonding. Adhesion energy measured by the DCB method was incorporated into a modified Lennard-Jones adhesion model and used as an effective parameter representing the overall bonding-surface condition. The simulated bond wave speed increased with adhesion energy and followed the same trend as the experimental results, indicating that experimentally measured adhesion energy can be used to connect bonding experiments with wafer-scale bonding simulation.

The proposed model was also applied to the analysis of bonding-induced in-plane displacement. The simulated IPD map qualitatively reproduced the anisotropic distortion pattern observed in the experimental data, suggesting that the coupled model of wafer deformation, interfacial fluid pressure, and adhesion force captures the main features of bonding-induced wafer distortion. Although the present framework does not directly resolve individual surface chemistry or molecular-scale nanogap effects, it provides a practical approach for incorporating experimentally obtained bonding characteristics into wafer-scale simulation. Future work will focus on improving quantitative accuracy by including additional interfacial effects, such as fluid-surface interaction, adsorbed water behavior, surface roughness, and nanoscale slip or rarefaction.

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