Thermal Characterization of a Three-Dimensional (3D) Chip Stack

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Abstract

In order to determine appropriate cooling solutions for 3D chip stacks in various cases, it is important to have a better understanding of the total thermal resistance of a 3D chip stack. For this purpose, precise thermal resistance measurements and modeling of each component of a 3D chip stack are important. The thermal resistance of interconnection is considered to be one of the thermal resistance bottlenecks of a 3D chip stack. In this study, a steady-state thermal resistance measurement method is employed for the thermal resistance measurement of interconnection. The thermal resistance of the 200 μm pitch C4's (Pb97Sn3) jointed samples are measured and the thermal conductivity of C4's is derived to be 18 – 24 W/mK. With regard to the thermal resistance of a silicon substrate, the thermal resistance of a silicon substrate with various interconnection pitches and diameters has already been modeled by considering the concentrated heat flow to interconnection, as presented in ICEP 2008.[15] Based on the modeled data, the thermal resistance reduction by underfill with various interconnection pitches and diameters is also studied.

Keywords: Three-Dimensional (3D) Chip Stack, Thermal Resistance, Interconnection, C4 (Controlled Collapse Chip Connection), Underfill, Back-End-of-the-Line (BEOL)

1. Introduction

Three-dimensional integrated circuits (ICs) are receiving increased attention for system performance enhancements without relying on further device scaling. However, because of the limited contact area and the higher circuit densities, the cooling of 3D ICs is challenging. We need better understanding of the total thermal resistance of 3D ICs, so that we can decide on appropriate cooling solutions for 3D ICs in various applications. For this purpose, we need precise thermal resistance measurements and modeling for each component of a 3D IC.

Extensive modeling studies have been carried out to investigate the thermal characteristics of 3D chip stacks. For example, Chiang et al.[1] calculated the power consumption of 3D ICs by incorporating active layers and interconnect joule heating. Other than the study by Chiang et al, Im et al.[2] studied the temperature rise of 3D ICs in two bonding cases, and Puttaswamy et al.[3, 4] further proposed a thermal management solution based on architectural level optimization, and Das et al.[5] investigated the temperature of a stacked FFT (Fast Fourier Transform) datapath with various numbers of stacks. Hua et al.[6] also performed thermal modeling of 3D ICs in greater detail. Chiang et al.[7–9] and Gplen et al.[10] and

Yu et al.[11] studied the effect of thermal-vias.

In contrast to wide-range modeling studies, experimental studies are quite lacking. In particular, there are very few experimental studies on the thermal resistance of the interconnections, even though the interconnections are regarded as one of the thermal resistance bottlenecks of a 3D chip stack. As Gurrum et al.[14] pointed out, the interconnections between chips and printed circuit boards (PCB) are key to the thermal resistance of a conventional 2D chip-to-board configuration, so in a 3D chip stack, the interconnections between stacked chips should also be considered in a similar way as an important factor in the thermal resistance of a 3D chip stack. Yamaji et al.[12] measured the contact thermal resistance between underfill and a chip with laser flash method. Based on their measurement results, they performed a numerical analysis of the total thermal resistance of a 3D chip stack. However, they found it difficult to measure the thermal resistance of the interconnections with the laser-flash method and they pointed out that a careful attention was necessary to achieve a uniform temperature distribution in the sample when using the laser-flash method on heterogeneous specimen, such as stacked chips with interconnections. Sweet et al.[13] measured the

thermal resistance of 3D multi-chip modules by embedding polysilicon heaters and diode thermometers. They also did modeling with the finite element method and compared the measured results with the modeled values. However, the differences between the measured results and the modeled ones were simply attributed to the thermal resistance of the interconnections and the causes were left unclear.

This study primarily aims to experimentally obtain the thermal resistance of the interconnections. The thermal resistance measurement results of copper-tin (CuSn) interconnection has been shown in the previous ICEP,[15] and in this paper, we discuss the thermal resistance of C4, which is one of major interconnections for high-end applications. The term “C4” is an abbreviation for “Controlled Collapse Chip Connection” and refers to Pb97Sn3 (a mixture of 97% (by weight) lead (Pb) and 3% tin (Sn)). Secondly, based on the modeled thermal resistance of a silicon with various interconnection pitches and diameters,[15] the thermal resistance reduction by underfill in various interconnection pitches and diameters is studied.

In this paper, the term “interconnections” refers to joinings (for example, interconnections between two silicon substrates).

2. Measurement Method

2.1 Measurement tool

Our previous steady-state thermal resistance measurement method appears in the reference,[15] however there are some new modifications are performed since then, so it is explained here.

Our steady-state thermal resistance measurement method uses liquid metal as the thermal interface material (TIM, which is applied between a sample and the measurement tool) as shown in Figure 1. This involves two Cu blocks, a heater, a cooler, four K-type thermocouples (T_1 , T_2 , T_3 , T_4), and a sample which is sandwiched between the two Cu blocks. Each of the four K-type thermocouples is paired with another K-type thermocouple that is kept at 0°C. (A total of eight K-type thermocouples are used in the measurements.) The four pairs of thermocouples are regulated by a Pt-resistive-thermal-sensor (Testo 735). The diameter of the eight thermocouples is 1 mm in this study, and future studies with thinner thermocouples should improve the accuracy. In order to realize the one-dimensional heat flow, the horizontal dimension of the Cu blocks should be large enough compared to the vertical dimension of the Cu blocks. On the other hand, the sample fabrication tends to be difficult as the horizontal dimension

Fig. 1 Steady-state thermal resistance measurement method (cross-section view).

increases. Considering these two factors, the horizontal dimension of the Cu blocks and the sample is set to be 21.5 mm × 16.5 mm, and the vertical dimension of the Cu block is set to be 20 mm. The measurements are performed at controlled temperatures to reduce the heat loss from the measurement tool to the surroundings. The surrounding temperature is controlled at $(T_4 - (T_3 - T_4) / 6)$, which is the temperature of the bottom of the Cu block. Liquid metal (a mixture of 75.5% (by weight) indium (In) and 24.5% gallium (Ga)) is applied between a sample and the two Cu blocks to minimize the contact thermal resistance. The thermal conductivity of In is 82 W/mK and that of Ga is 41 W/mK and this mixture is liquid at room temperature, so it can be compressed into a very thin film. For intimate contact between liquid metal (InGa) and a sample, the top and bottom surfaces of a sample are coated with 20 nm thick titanium (Ti). The thermal resistance of 20 nm Ti (thermal conductivity : 21.9 W /mK) is calculated to be lower by several orders of magnitude than the thermal resistances of samples in this study. The characteristics of InGa liquid metal TIM lead to the small contact thermal resistance and the resulting fluctuation of the contact thermal resistance is also small.

2.2 Derivation of the thermal resistance of liquid metal TIM

The thermal resistance of a sample is derived with Equation 1. The thermal resistance of the liquid metal TIM is derived from the measurements of two different thick silicon substrates as depicted in Figure 2. The composition of the interfaces (liquid metal between a silicon and Cu) in this derivation is the same as in the measurements of the actual jointed samples (the C4 jointed samples.) The

Thermal resistance of a sample (K/W)

$$= \frac{T_t - T_b \text{ (K)}}{\text{Heat flow (W)}} - 2A$$

Thermal resistance
of liquid metal TIM

Where

$$T_t = T_2 - (T_1 - T_2)/6$$

$$T_b = T_3 + (T_3 - T_4)/6$$

$$\text{Heat flow (W)} = \frac{((T_1 - T_2) + (T_3 - T_4)) \times 1/2}{1/398 \times 150 \times 1/B}$$

Thermal conductivity
of Cu (W/mK) Length of
Cu block Horizontal area
of Cu block

Equation 1 Derivation of the thermal resistance of a sample.

Measured thermal resistance ($10^{-6} \text{ m}^2\text{K/W}$)	Calculated thermal resistance* of silicon ($10^{-6} \text{ m}^2 \text{ K/W}$)	Thermal resistance of liquid metal TIM ($10^{-6} \text{ m}^2\text{K/W}$)
3-4	2.6	0.4-1.4

Measured thermal resistance ($10^{-6} \text{ m}^2\text{K/W}$)	Calculated thermal resistance* of silicon ($10^{-6} \text{ m}^2 \text{ K/W}$)	Thermal resistance of liquid metal TIM ($10^{-6} \text{ m}^2\text{K/W}$)
4-5	3.4	0.6-1.6

* The value is proportional to the thickness. The thermal conductivity of silicon is assumed to be 148 W/mK.

'Thermal resistance of liquid metal TIM'
= 'Measured thermal resistance' -
'Calculated thermal resistance of silicon'

Fig. 2 Derivation of the thermal resistance of liquid metal TIM.

measured thermal resistances of a 380 μm thick silicon, including liquid metal, the interface between a silicon and liquid metal and the interface between liquid metal and Cu are $3 \times 10^{-6} - 4 \times 10^{-6} \text{ m}^2\text{K/W}$. The calculated thermal resistance of a 380 μm thick silicon is $2.6 \times 10^{-6} \text{ m}^2\text{K/W}$. The calculated thermal resistance is proportional to the silicon thickness and the thermal conductivity of silicon is assumed to be 148 W/mK. Also, the measured thermal resistance of a 510 μm thick silicon, including liquid metal, the interface between a silicon and liquid metal and the interface between liquid metal and Cu are $4 \times 10^{-6} - 5 \times 10^{-6} \text{ m}^2\text{K/W}$. The calculated thermal resistance of the 510 μm thick silicon is $3.4 \times 10^{-6} \text{ m}^2\text{K/W}$. By subtracting the calculated thermal resistance of silicon from the measured thermal resistance, and considering the accuracy of the measurement, the thermal resistance of liquid metal TIM should be between $0 - 2 \times 10^{-6} \text{ m}^2\text{K/W}$.

3. Results and Discussions

3.1 Thermal resistance measurement of 200 μm -pitch-C4 jointed sample

The jointed samples in this study are composed of 200 μm -pitch-C4 sandwiched between two silicon substrates as illustrated in Figure 3. The upper silicon is 725 μm thick, and the lower one is 640 μm thick. The size of the upper silicon is 16.5 mm by 21.5 mm and that of the lower silicon is 20.5 mm by 24 mm. In the following, the size of the lower silicon is taken as 16.5 mm by 21.5 mm (the same as that of the upper silicon), and it is confirmed by modeling that this does not influence the measured thermal resistances in this study.

The thermal resistances of the jointed samples are measured to be $39 \times 10^{-6} - 44 \times 10^{-6} \text{ m}^2\text{K/W}$ (Sample No.1) and $43 \times 10^{-6} - 48 \times 10^{-6} \text{ m}^2\text{K/W}$ (Sample No.2). The thermal conductivity of C4 is derived by comparisons with the modeled values (using the finite-element-method) as follows. The model of the jointed sample is built as depicted in Figure 4 (in which the periodic boundary condition is set at the lateral surfaces of the model). The thermal resistances of the jointed sample are modeled by changing the

Fig. 3 C4 jointed sample (cross-section view).

thermal conductivity of C4 (Figure 5). When the thermal conductivity of C4 is set to be 24 W/mK, the modeled thermal resistance is $39 \times 10^{-6} \text{ m}^2\text{K/W}$. When the thermal conductivity of C4 is set to be 18 W/mK, the modeled thermal resistance is $48 \times 10^{-6} \text{ m}^2\text{K/W}$. Based on these comparisons, the thermal conductivity of C4 is obtained to be 18 – 24 W/mK.

The value (18 – 24 W/mK) is considered to include the components, such as the thermal resistance of intermetallic compounds, the contact thermal resistances between a silicon and metals of interconnections, and the contact thermal resistances between metals of interconnections. For the contact thermal resistance between metals of interconnections, Bai et al.[16] measured the contact thermal resistance between eutectic lead-tin (PbSn) solder and Cu to be from 1.1×10^{-6} to $3.3 \times 10^{-6} \text{ m}^2\text{K/W}$. Although the metal compositions in Bai's

study differ from those in this study, it is estimated that the contact thermal resistances between metals of interconnections contribute little to the thermal conductivity of C4 obtained in this study.

Also the difference of the measured thermal resistance between sample No.1 and sample No.2 is estimated to be caused by the variation of interconnections. The thermal conductivities of intermetallic compounds were studied by Terada et al.[17] and Jacobsson et al.,[18] and they reported that the thermal conductivities of intermetallic compounds depend on whether they are in an ordered crystal phase or in a disordered phase. They noted that the thermal conductivities in the ordered crystal phase are higher than those in the disordered phase. The phases of the intermetallic compounds of C4 in this study are not yet investigated, which are subjects of our future study.

3.2 Effect of underfill

In most cases of 3D chip stacks, underfill is supposed to be used for the improvement of mechanical reliability. Underfill is also expected to reduce the thermal resistance of 3D chip stacks, and its effect is examined by modeling.

In the previous ICEP,[15] the thermal resistance of a silicon with various interconnection pitches and diameters was modeled employing a μm -scale model. Based on it, the thermal resistance reduction by underfill with various interconnection pitches and diameters is studied. The μm -scale models in Figure. 6 are used (the C4 interconnection height is $7.5 \mu\text{m}$.) and the thermal conductivity of underfill is assumed to be 0.4 W/mK. The thermal resistance of the model is derived by the difference between the average temperature of the top surface and that of the bottom surface of the model and they are depicted in Table1. It indicates when the area ratio of interconnection is the same in $10 \mu\text{m}$ pitch, $20 \mu\text{m}$ pitch, $50 \mu\text{m}$ pitch, $100 \mu\text{m}$

Fig. 4 The model of the C4 jointed sample (cross-section view).

Fig. 5 Modeled temperature distribution of the C4 jointed sample.

Fig. 6 μm -scale model of two silicon with one interconnection. (A : when air is filled, B : when underfill (0.4 W/mK) is filled.) (cross-section view).

Table 1 Dependence of the thermal resistance reduction by underfill on the interconnection pitch and diameter. The thermal resistance reduction by underfill is calculated as follows. The difference between the modeled thermal resistance when air is filled and that when underfill is filled, is divided by the modeled thermal resistance when air is filled.

Interconnection pitch (diameter)	10 μm (5 μm dia.)	20 μm (10 μm dia.)	50 μm (25 μm dia.)	100 μm (50 μm dia.)	200 μm (100 μm dia.)	500 μm (100 μm dia.)
Modeled total thermal resistance ($10^{-6} \text{ m}^2\text{K/W}$) (air (Fig.6(A)))	2.88	2.95	3.11	3.42	4.09	28.85
Modeled total thermal resistance ($10^{-6} \text{ m}^2\text{K/W}$) (underfill (Fig.6(B)))	2.70	2.75	2.88	3.12	3.61	12.30
Thermal resistance reduction by underfill (%)	6.3	6.9	7.4	8.8	11.7	57.4

pitch and 200 μm pitch, the thermal resistance reduction by underfill gradually rises as the pitch increases. (i.e., the difference between the modeled thermal resistance when air is filled and that when underfill is filled, divided by the modeled thermal resistance when air is filled, increases as the pitch increases.) When the interconnection diameter is the same in 200 μm pitch and 500 μm pitch, as the pitch increases, the thermal resistance reduction by underfill significantly rises.

It should be noted that in actual 3D chip stacks (3D stacked devices), a wiring layer (in other words “back-end-of-the-line (BEOL)”) exists and the thermal conduction path from a transistor to interconnections is complicated. The effect of underfill is considered to depend on the thermal conduction path, and therefore the thermal conduction path from a transistor to interconnection by incorporating the back-end-of-the-line is modeled as shown in Figure 7 (Two-dimensional model). The structure of BEOL is based on the 45 nm node BEOL[19] and only one continuous BEOL is included in the model. The thermal conductivity of SiCOH is assumed to be 0.59 W/mK (effective thermal conductivity),[20] SiO₂ is 1.3 W/mK, and C4 is 18 W/mK, silicon is 148 W/mK, Cu is 398 W/mK, respectively. Periodic boundary conditions are set at lateral surfaces of the model and the heat density ($1 \times 10^4 \text{ W/m}^2$) is applied at the bottom of the model and the heat transfer coefficient ($0.5 \times 10^4 \text{ W/m}^2\text{K}$) is set at the top of the model. The interconnection area ratio ((i.e. the interconnection area divided by the total chip area)) of Figure7. is 0.2. The modeled temperature distribution is shown in Figure 7(B) and the modeled temperature range is 45 – 45.0213°C. It means the modeled thermal resistance is $2.13 \times 10^{-6} \text{ m}^2\text{K/W}$ (the temperature at the top of the model and that at the bottom of the model are uniform, respectively and therefore the thermal resistance is

Fig. 7 (A) Two-dimensional model of BEOL and an interconnection between two chips. (B) Modeled temperature distribution. (C) Modeled temperature distribution when air is filled (instead of underfill). The thermal conductivity of underfill is assumed to be 0.4 W/mK, SiCOH is 0.59 W/mK, SiO₂ is 1.3 W/mK, C4 is 18 W/mK, silicon is 148 W/mK, Cu is 398 W/mK, respectively.

directly derived from the modeled temperature range). As a reference, the temperature distribution when air is filled (instead of underfill) is also modeled as shown in Figure 7(C) and the modeled thermal resistance is $2.23 \times 10^{-6} \text{ m}^2\text{K/W}$.

The thermal resistance reduction by underfill is calculated to be 4.5%, which is different from Table 1 (6.3%) by 1.8%. This comparison suggests that even when the model varies (Figure 7 is two-dimensional model and BEOL is incorporated, and Figure 6 (Table 1) is three-dimensional model), the derived thermal resistance reduction by underfill does not change significantly. It is estimated that in the $10 \mu\text{m}$ pitch ($5 \mu\text{m}$ diameter) C4 interconnection, underfill with the thermal conductivity of 0.4 W/mK contributes to reduce the thermal resistance around 4.5 to 6.3%.

Further, the thermal resistance reduction by underfill, when the interconnection area ratio is 0.5, is calculated in the same method of Figure 7, and it is below 1%. It indicates that when the interconnection area ratio is high such as 0.5, the thermal resistance reduction by underfill is very small.

4. Conclusions

We experimentally obtained the thermal conductivity of C4 by steady-state thermal resistance measurements. The obtained thermal conductivity of C4 is $18 - 24 \text{ W/mK}$. The thermal resistance reduction by underfill is also investigated by modeling and its dependence on the interconnection pitch and diameter is obtained. Further, the thermal conduction path from a transistor to an interconnection is modeled by incorporating back-end-of-the-line (BEOL) and the thermal resistance reduction by underfill in this thermal conduction path model is also examined. In order to consider appropriate cooling solutions for various 3D chip stack applications, it is necessary to have better understanding of the total thermal resistance of a 3D chip stack. Precise thermal resistance measurements and modeling for each component of a 3D chip stack, described in this paper, are essential for the purpose.

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