The design and optimization of novel elliptic cylindrical through-silicon via and its temperature characterization

Wenbo Guan | Hongliang Lu | Yuming Zhang | Yimen Zhang

Abstract

Through-silicon via (TSV) technology is a key technology to realize multi-layer chips and its structure model and transmission characteristics have attracted much attention. With the continuous reduction of chip size, higher requirements are put forward for the model and transmission characteristics of TSV. A novel elliptic cylindrical TSV structure model is proposed. The influence of axial length ratio, height, dielectric layer thickness, and spacing on the transmission characteristics of TSV is further studied by HFSS software. The results show that the transmission of TSV is facilitated by the decrease of axial length ratio, the decrease of height, the increase of dielectric layer thickness, and the increase of TSV spacing. The TSV structural parameter values are optimized by a single variable method. The optimized TSV structure is compared with the original TSV, traditional cylindrical and conical TSV, and coaxial TSV. It is concluded that the elliptic cylindrical TSV structure has better transmission performance. The temperature characteristics of the elliptic cylindrical TSV are simulated. It is indicated that the transmission characteristics of the elliptic cylindrical TSV are poor at low frequency and better at high frequency when the temperature rises.

KEYWORDS
finite element method, parameter optimization, temperature effect, through-silicon via, transmission characteristics

JEL CLASSIFICATION
Electrical and electronic engineering

1 INTRODUCTION

In the novel integrated circuit technology, three-dimensional (3D) integration technology has many advantages, which can improve performance and functions while reducing costs.1-3 Among them, through-silicon via (TSV) technology occupies an important position in the 3D integration technology, and is the key part of realizing multi-layer chip interconnection.4,5 TSV-based 3D integrated circuits are designed to stack and interconnect chips in the vertical direction.6-8 It provides a promising near-term solution for further miniaturization and performance improvement of...
With the demand for low-cost and high-yield process technology, the successful application of TSV technology requires further optimization of TSV design and model structure. In view of the structural model and electromagnetic characteristics of TSV, domestic and foreign scholars have conducted extensive research and discussion. At present, the common TSV studied are cylindrical TSV, coaxial TSV, conical TSV, and annular TSV. The analytical model of capacitance and inductance for cylindrical TSV is extracted in References 12 and 13, and the accuracy is verified. Based on the theory of electromagnetics, the parasitic capacitance model of conical TSV was established in References 14 and 15. In Reference 16, a coaxial TSV is proposed, which uses SiO$_2$ with low permittivity as the dielectric layer, and the transmission characteristics of the coaxial TSV are simulated. The research in Reference 17 shows that the signal transmission performance of toroidal TSV is almost independent of copper filling rate. In addition, Reference 18 studied the electrical signal transmission and mechanical reliability of TSV with different geometry. The results show that rectangular TSV has good characteristic impedance and better mechanical reliability.

With the size of TSV continues to decrease, the system puts forward higher requirements on the transmission characteristics of TSV in a wider frequency band. In addition, due to the high power density and chip temperature in 3D stacking structure, the temperature influence on the performance of TSV is critical in its modeling, characterization, and design. In order to further improving the transmission characteristics of TSV, a novel TSV structure, that is, elliptical cylindrical TSV, is proposed in this article. HFSS software is used to simulate the influence of structural parameters such as axial length ratio, height, dielectric layer thickness, and TSV spacing on the transmission characteristics of elliptic cylinder TSV model, and the relative optimal solution of each geometric parameter is obtained. Then, the influence of temperature change on the transmission characteristics of elliptic cylinder TSV is studied. This article provides a reference for the optimal design of TSV structure.

### 2 | NOVEL ELLIPTIC CYLINDRICAL TSV

The structure of the proposed elliptical cylindrical TSV in GS mode is shown in Figure 1. In order to study the influence of axial length ratio, height, dielectric layer thickness, and TSV spacing on the transmission characteristics of TSV, $a$ and $b$ are, respectively, used to represent the semi-minor axis and semi-major axis of the elliptical surface of TSV, $h_{TSV}$ is the height of TSV structure, $r_{ox}$ is the thickness of SiO$_2$ dielectric layer, $\omega_{ox}$ is the thickness of intermetallic dielectric layer, and $L_{TSV}$ is the distance between TSV. The TSV conductive material is filled with Cu. The dielectric isolation layer is SiO$_2$, and the bottom is n-type doped Si substrate, and the doping concentration is expressed by $N_D$. The effect of the bias voltage on the Cu–SiO$_2$–Si MOS structure is represented by the change of the width of the depletion region, which is expressed by $r_{dep}$.

The manufacturing process of elliptical cylindrical TSV is as follows: the through hole is produced by deep reactive ion etching (DRIE), and a closed blind hole at the bottom is formed. Then an insulating layer is deposited on the side wall of the through hole by plasma-enhanced chemical vapor deposition (PECVD) to avoid leakage between the conductor and the surrounding silicon substrate. Metal adhesive layer, barrier layer, and seed layer were deposited by metal-organic chemical vapor deposition (MOCVD). Then, copper metal is electroplated in the TSV through hole as the conductor material of TSV interconnection. Finally, the silicon wafer was thinned by chemical mechanical polishing (CMP).

In terms of stress distribution of elliptic cylindrical TSV, according to Reference 18, compared with cylindrical TSV, the
maximum von Mises stress of both are concentrated at the bottom of TSV, and their stress size and distribution are almost the same. It should be noted that when preparing elliptic cylindrical TSV, the influence of structural parameters on the thermo-mechanical stability of TSV structure should be fully considered. According to Reference 27, it can be seen that preparing TSV with aspect ratio (the ratio of TSV height to semi-major axis length) greater than 8 is conducive to relieving the thermal stress of TSV, and the design of TSV with aspect ratio of 1.0~5.0 should be reduced. For TSVs with the same depth width ratio, the thermal stress distribution is more uniform when the hole spacing is more than 1.6 times of the hole diameter (the semi-major axis length of elliptic cylindrical TSV). Increasing the thickness of insulating layer and preparing smooth scallop sidewall are conducive to improve the reliability of TSV.

According to the state-of-art technology, the initial simulation values of the device structure parameters and physical parameters are shown in Table 1.

### Table 1: Geometric parameters

| Geometric parameter | Symbol | Value |
|---------------------|--------|-------|
| The height of TSV   | \( h_{TSV} \) | 60 \( \mu \)m |
| TSV spacing         | \( L_{TSV} \) | 20 \( \mu \)m |
| The elliptical surface of semi-minor axis length | \( a \) | 2.5 \( \mu \)m |
| The elliptical surface of semi-major axis length | \( b \) | 7.5 \( \mu \)m |
| Thickness of SiO\(_2\) dielectric layer | \( r_{ox} \) | 0.4 \( \mu \)m |
| Doping concentration of TSV substrate | \( N_D \) | \( 6 \times 10^{16} \) cm\(^{-3}\) |

3 | THE INFLUENCE OF GEOMETRIC PARAMETERS ON ELLIPTIC CYLINDRICAL TSV

3.1 | The influence of the axial length ratio of elliptic cylindrical TSV on transmission characteristics

The axial length of elliptic cylindrical TSV corresponds to the radius of cylindrical or conical TSV, and its size affects the distribution density of TSV, and the change of axial length also affects the transmission characteristics of elliptic cylindrical TSV. In this article, the simulation is completed at 300 K at room temperature.

Figure 2 shows the curve of S-parameter changing with frequency under different axial length ratio in HFSS simulation. The semi-minor axis length \( a \) of the TSV elliptical surface is fixed at 2.5 \( \mu \)m, and the corresponding semi-major axis length \( b \) of the TSV elliptical surface is 5.0, 7.5, 10.0, 12.5, and 15.0 \( \mu \)m respectively. At this time, the ratio of semi-minor axis length and semi-major axis length of corresponding elliptical surface is 1/2, 1/3, 1/4, 1/5, and 1/6, respectively. The corresponding other structural parameters are shown in Table 1, and remain unchanged.

The simulation results show that when the ratio of axis length decreases gradually, the return loss \( S_{11} \) of the elliptic cylindrical TSV simulated in Figure 2A decreases gradually in 0~50 GHz, and the amplitude of the decrease is smaller. In Figure 2B, the insertion loss \( S_{21} \) of the elliptic cylindrical TSV increases gradually in the frequency range. At low frequency, the coupling effect of parasitic parameters can be ignored, and the variation of TSV characteristics with size mainly depends on the impedance change caused by the change of TSV cross-sectional area. The reduction of the axial length ratio increases the relative cross-sectional area of the TSV, thereby reducing the impedance, which is beneficial to TSV transmission. When the frequency increases to a certain value, the return loss increases and the insertion loss decreases. This is because the decrease of axis length ratio increases the internal current flowing through Cu and decreases the parasitic resistance. With the increase of TSV axis length ratio, the total inductance decreases, the relative area of capacitance increases, and the relative spacing between TSVs decreases, which leads to the increase of depletion layer capacitance and SiO\(_2\) capacitance. Because the substrate conductance plays a leading role, even if the resistance and inductance of TSV decrease, the increase of substrate conductivity will make the overall transmission performance of TSV worse. Therefore, for elliptic cylindrical TSV, the ratio between the semi-minor axis and the semi-major axis should be reduced as much as possible. For this article, when the values of the semi-minor axis and the semi-major axis of the
elliptical surface are 2.5 and 15.0 μm, that is, the ratio of the axis length is 1/6 and the transmission performance of TSV is the best.

3.2 The influence of the height of elliptic cylindrical TSV on transmission characteristics

The change of TSV height has an influence on each parasitic parameter. In the manufacturing field, the height of TSV also affects the thickness of chip stack, and the thinner chip thickness will affect the thermal stress reliability of TSV. In order to study the influence of the height change of elliptic cylinder TSV on its transmission characteristics, the following simulation is completed at 300K.

Based on the study of the ratio of the axis length of the elliptic cylindrical TSV, the ratio of the better solution is 1/6. The axis length ratio is fixed unchanged, and the height values of the elliptic cylindrical TSV are selected as 50, 60, 70, 80, and 90 μm, respectively. The remaining structural parameters are shown in Table 1.

The simulation results are shown in Figure 3. The results show that the insertion loss $S_{21}$ decreases and the return loss $S_{11}$ increases with the increase of height in 0 ∼ 50 GHz. When the height increased gradually, each parasitic parameter increased in direct proportion with the height. The contact area between TSV and SiO₂ increases with the increase of height. The external inductance of TSV is positively correlated with the height of TSV, while the dielectric capacitance $C_{IMD} = \pi \varepsilon_{ox} w_{ox}/\cosh^{-1}(L_{TSV}/2ab)$ is independent of the height. Except for the substrate capacitance, the increase of other parasitic parameters makes the transmission characteristics of TSV worse. This demonstrates that the increase of height is not conducive to the signal transmission of TSV. Generally speaking, the transmission characteristics of elliptic cylindrical TSV become worse with the increase of height. Therefore, the height of TSV should be reduced as much as possible in the manufacturing process of TSV.

3.3 The influence of the dielectric layer thickness of elliptic cylindrical TSV on transmission characteristics

The elliptic cylindrical TSV is studied in this article. SiO₂ is used as the isolation layer between Cu and Si, and the thickness is less than 0.5 μm. The thickness of the dielectric layer directly affects the MOS capacitance in the oxide layer and the depletion layer capacitance in the substrate. Therefore, the substrate capacitance and conductivity of TSV are closely related to the thickness of the dielectric layer, while the parasitic resistance and parasitic inductance of TSV are not closely related to the thickness of the dielectric layer. The influence of dielectric layer thickness on transmission characteristics of TSV is studied at room temperature of 300 K.
Based on the study of the axial length ratio and height of elliptic cylindrical TSV, the better solutions of axial length ratio and height are 1/6 and 50 μm, respectively, and the two parameters are fixed. Then the SiO$_2$ thickness of the dielectric layer is 0.1, 0.2, 0.3, 0.4, and 0.5 μm, respectively, and the corresponding other structural parameters remain unchanged as shown in Table 1.

The simulation results are shown in Figure 4. The results show that when the thickness of dielectric layer increases gradually, within the range of 0 ~ 50 GHz, the insertion loss $S_{21}$ of the elliptic cylindrical TSV increases and the transmission characteristics become better; the return loss $S_{11}$ decreases continuously, and the amplitude of the decrease increases at high frequency, which has a more serious impact on the transmission of TSV signal. When the dielectric layer thickness of TSV increases, the depletion layer capacitance in the substrate increases, the MOS capacitance in the oxide layer decreases, and the substrate conductivity increases. With the decrease of total capacitance and the increase of impedance, the coupling effect between TSV and ground is reduced. The increase in capacitance enhances the transmission characteristics of the elliptic cylindrical TSV, and the increase in conductance makes the transmission characteristics of TSV weaker. Although the conductivity plays a leading role, the transmission characteristics of TSV become better because the thickness of SiO$_2$ has little effect on the substrate conductivity. Therefore, when the thickness of the dielectric layer SiO$_2$ is 0.5 μm, it has relatively good transmission characteristics in 0 ~ 50 GHz.
3.4 The influence of the spacing of elliptic cylindrical TSVs on transmission characteristics

The spacing between elliptic cylindrical TSVs affects the distribution density of TSV. Based on the study of the geometric parameters such as TSV axis length ratio, height, and dielectric layer thickness, the optimized values are $1/6$, $50\,\mu\text{m}$, and $0.5\,\mu\text{m}$, respectively. Meanwhile, the TSV spacing is 20, 25, 30, and $35\,\mu\text{m}$, and the following simulations are completed under the condition of $300\,\text{K}$.

The simulation results are shown in Figure 5. The results show that when the TSV spacing increases, the S-parameter changes slightly at low frequency, that is, the TSV spacing has little effect on the transmission performance of TSV at low frequency, and the density of TSV array can be increased. At high frequency, the insertion loss $S_{21}$ of elliptic cylindrical TSV increases with the increase of spacing, while the return loss $S_{11}$ decreases. This is because the increase of the spacing will weaken the mutual parasitic effect between the elliptic cylindrical TSVs, and the interaction between TSVs will be reduced, which is conducive to the transmission of TSV. Therefore, increasing TSV spacing as much as possible under the condition of fulfilling the chip and process constraints is conducive to improving the transmission characteristics of TSV. In Figure 5, when the distance between the elliptic cylindrical TSVs is $35\,\mu\text{m}$, the transmission performance of the TSV is better.

3.5 Parameter optimization of elliptic cylindrical TSV

The transmission performance of TSV depends on its structure type and geometric parameters. The TSV structures previously studied are mostly cylindrical or conical, and different structures of TSV need to be studied to obtain the best performance. Based on the above simulation research on the axis length ratio, height, thickness of dielectric layer, and TSV spacing of elliptic cylindrical TSV, the relative better solution of geometric structure parameters can be obtained. Due to the complex influence among geometric parameters in real process, it is difficult to obtain the optimal solution of a certain TSV structure. In this article, through the optimization and simulation of the geometric structure parameters of the elliptic cylindrical TSV, the relative optimal structural dimensions are obtained:

The values of the semi-minor axis length and the semi-major axis length of the TSV elliptical surface are, respectively, $2.5$ and $15.0\,\mu\text{m}$, that is, the axis length ratio is $1/6$, the height is $50\,\mu\text{m}$, the dielectric layer thickness is $0.5\,\mu\text{m}$, and the spacing of TSV is $35\,\mu\text{m}$.

As shown in Figure 6, the S-parameters pre-optimized and optimized are compared in $0 \sim 50\,\text{GHz}$. The structural parameters pre-optimized are listed in Table 1. The simulation results show that the transmission characteristics are significantly improved than before. Compared with the S-parameters pre-optimized in Table 1, the structural parameters...
of the optimized elliptic cylindrical TSV have decreased axial length ratio, decreased height, increased dielectric layer thickness, and enhanced TSV spacing. The return loss $S_{11}$ is reduced from about $-33$ dB pre-optimized to about $-49$ dB optimized. The less the return loss $S_{11}$ is, the less the signal which is reflected back to the source is, so the transmission performance is better. The insertion loss $S_{21}$ increases from about $-0.67$ dB pre-optimized to about $-0.35$ dB optimized. The larger this value is, the higher the transmission efficiency of TSV is.

In order to compare the transmission characteristics of the optimized elliptic cylindrical TSV with the cylindrical, conical and coaxial TSV structures in Reference 16 in the GS mode, this article sets the structure parameters of the above three types of TSVs as follows: The height and spacing of the cylindrical TSV are, respectively, 50 and 35 $\mu$m and the radius is 6 $\mu$m. The cylindrical TSV and the optimized elliptic cylindrical TSV have almost the same cross-sectional area and volume. The height and spacing of the conical TSV are, respectively, 50 and 35 $\mu$m, the radius is 8.6 $\mu$m, and the sidewall inclination angle is 85°. The conical TSV and the optimized elliptic cylindrical TSV have almost the same volume. The structural dimensions of the elliptic cylindrical TSV remain unchanged after the above optimization. The geometrical dimensions of the coaxial TSV are set to be the same as the cylindrical TSV. In addition, SiO$_2$ with low permittivity is used as the dielectric layer of elliptic cylindrical, cylindrical, and conical TSV, which is consistent with the dielectric layer material of coaxial TSV in Reference 16.

The simulation results in Figure 6 show that the elliptic cylindrical TSV proposed in this article has better transmission characteristics in 0 $\sim$ 50 GHz than the traditional cylindrical, conical, and coaxial TSV. Compared with the above three types of TSV, the insertion loss $S_{21}$ of elliptic cylindrical TSV is larger, and the return loss $S_{11}$ is smaller, which indicates that the optimized transmission characteristics of elliptic cylindrical TSV are more conducive to signal transmission.

As shown in Figure 7, the proposed elliptic cylindrical TSV has the same cross-sectional area as the traditional cylindrical TSV. In terms of TSV array layout, under the condition of using the same substrate area, more elliptic cylindrical TSV structures can be arranged horizontally, which can greatly improve the array density and chip integration of TSV.

## 4 | TEMPERATURE CHARACTERISTICS OF ELLIPTIC CYLINDRICAL TSV

The rise in temperature affects the transmission characteristics of TSV. Based on the above research on the geometric parameters of the elliptic cylindrical TSV, the optimized structural dimensions are selected: the semi-minor axis length and semi-major axis length of the elliptical surface are, respectively, 2.5 and 15.0 $\mu$m, that is, the axis length ratio is 1/6, the height is 50 $\mu$m, the thickness of the dielectric layer is 0.5 $\mu$m, and the TSV spacing is 35 $\mu$m. Then the following simulation is completed in 300 $\sim$ 400 K.
The temperature change mainly affects the majority carrier density $n_0$ of the substrate in the elliptic cylindrical TSV. When the temperature rises, the majority carrier density in substrate continues to increase. The insertion loss $S_{21}$ of the TSV decreases at low frequency and increases at high frequency while the return loss $S_{11}$ increases at low frequency and decreases at high frequency. Therefore, when the temperature increases, the transmission characteristics of elliptic cylindrical TSV are poor at low frequency and better at high frequency.

The simulation results are shown in Figure 8. By analyzing the influence factors of temperature and majority carrier density in substrate, respectively, the interaction between them is explained. When the majority carrier density in TSV substrate increases, the width of depletion region $r_{dep}$ will be changed, which will affect the capacitance of depletion region and substrate conductivity of TSV. Specifically, the increase of temperature will increase the resistivity of the copper conductor of TSV and reduce the width of depletion zone of TSV, which will increase the inductance, capacitance, and resistance of TSV, and weaken the transmission characteristics of TSV. At the same time, it will reduce the substrate conductivity, which is conducive to the signal transmission of TSV. With the increase of frequency, the contradiction between the effect of temperature and substrate concentration on the transmission performance of TSV reaches equilibrium at about 5 GHz. Before this frequency point, the resistance and inductance are the main factors affecting the transmission performance of TSV, so the transmission characteristics are poor affected by temperature. When the frequency continues

**FIGURE 7** Comparison of transverse arrangement of traditional cylindrical TSV and elliptic cylindrical TSV

**FIGURE 8** S-parameter variation with frequency of elliptic cylindrical TSV under temperature change. (A) S11, (B) S21
to increase, the main factors at high frequency are the conductivity and capacitance of TSV substrate, so the transmission characteristics become better affected by the substrate concentration.

5 | CONCLUSION

In this article, a novel elliptic cylindrical TSV structure model is proposed. Based on this model, the effects of axial length ratio, height, dielectric layer thickness, and spacing on the transmission characteristics of the elliptic cylindrical TSV are studied by using the single variable method. The simulation results show that the transmission characteristics of TSV are enhanced when the ratio of axial length is reduced, the height is reduced, the thickness of dielectric layer is increased, and the TSV spacing is increased. After the simulation and analysis of a certain geometric parameter, the better solution of the parameter is obtained, and then the better solution of other parameters is obtained by fixing the parameter value. Finally, the better solution of each geometric parameter is combined to form the optimized elliptic cylindrical TSV structure, and the transmission characteristics of TSV are significantly improved. Compared with the traditional cylindrical TSV, conical TSV, and coaxial TSV, it is shown that the elliptic cylindrical TSV has better transmission performance. Meanwhile, the temperature characteristics of the elliptic cylindrical TSV are simulated. The results indicate that the transmission characteristics of the elliptic cylindrical TSV are poor at low frequency and better at high frequency when the temperature is increased. The results of this article provide a reference for the optimal design of TSV structure.

However, the 3D structures of the elliptic cylindrical TSV proposed in this article are ideal, and the possible fabrication errors in the actual art are not discussed and studied. The TSV models established in this article are based on simulation software such as HFSS, and there is no research on the preparation and testing of structural models in reality. In the next work, it is necessary to further improve and consider the fabrication art, and complete the analysis of its fabrication art and test.

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The authors have no conflict of interest relevant to this article.

AUTHOR CONTRIBUTIONS

Wenbo Guan: Conceptualization (lead); data curation (lead); formal analysis (lead); investigation (lead); methodology (lead); resources (equal); software (lead); validation (lead); visualization (lead); writing – original draft (lead); writing – review and editing (lead). Hongliang Lu: Conceptualization (lead); data curation (lead); formal analysis (lead); investigation (lead); methodology (lead); project administration (lead); resources (equal); software (equal); supervision (lead); validation (lead); visualization (lead); writing – original draft (supporting); writing – review and editing (supporting). Yuming Zhang: Conceptualization (supporting); data curation (supporting); formal analysis (supporting); funding acquisition (supporting); investigation (supporting); methodology (supporting); project administration (supporting); resources (supporting); software (supporting); supervision (supporting); validation (supporting); visualization (supporting); writing – original draft (supporting); writing – review and editing (supporting).

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