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Finite Element Analysis of the 3ω Method for Characterising High Thermal Conductivity Ultra-Thin Film/Substrate System

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Abstract: The 3ω method is an attractive technique for measuring the thermal conductivity of materials; but it cannot characterise high thermal conductivity ultra-thin film/substrate systems because of the deep heat penetration depth. Recently, a modified 3ω method with a nano-strip was specifically developed for high thermal conductivity thin film systems. This paper aims to evaluate the applicability of this method with the aid of the finite element analysis. To this end, a numerical platform of the modified 3ω method was established and applied to a bulk silicon and an AlN thin-film/Si substrate system. The numerical results were compared with the predictions of theoretical models used in the 3ω method. The study thus concluded that the modified 3ω method is suitable for characterising high thermal conductivity ultra-thin film/substrate systems.

Keywords: thermal conductivity; finite element analysis; 3ω method; ultra-thin film/substrate system

1. Introduction

Thermal management of advanced thin-film/substrate systems plays an important role in their applications [1–6]. In comparison with that of bulk material, the thermal conductivity of a thin-film could be significantly different because of the size effect and microstructural difference [2,3,7]. However, characterising the thermal conductivity of a thin-film is challenging due to the fact that controlling the heat penetration depth in micro-/nano-scale is difficult [8]. Particularly, if the thermal conductivity of a thin-film is relatively high, the measurement becomes more challenging as the heat could penetrate into the specimen fast and deeply [1].

A few methods have been developed for characterising the thermal conductivity of thin-films, including time-domain thermoreflectance (TDTR) method [9], scanning thermal probes [10,11], coherent optical method [12,13], Raman spectroscopy [14–16], and the 3ω method [1,17,18]. The 3ω method has several unique advantages over the others. Firstly, this method is non-destructive and relatively cost-effective [1]. Secondly, the metal-strip element, used in the 3ω method as a heater and a temperature sensor, is merely a fraction of a Celsius degree hotter than the surrounding material. Such low temperature difference makes less undesirable heat loss from the sample and thus increases measurement accuracy [1,17,18]. Thirdly, this method is applicable to in situ characterisation [1,17,18].

In the conventional 3ω method the thermal conductivity of the thin-film should be significantly lower than that of the substrate [1,18]. This is because the amount of the heat that passed through the thin-film and penetrated into the substrate may affect the measurement accuracy of the thin-film thermal conductivity. Recently, Moridi and Zhang et al. [1] proposed a modified 3ω method with a nano-strip to solve this problem. The extremely narrow metal-strip element provides a much better

control of heat penetration depth over the conventional 3ω method. The heat merely penetrates into several microns of the specimen [1]. Moreover, the narrow strip induces a much higher electrical resistance in comparison with the wide strip elements, making it easier to balance the measurement circuit. Although this method has been applied in characterising ultra-thin film/substrate systems [1], the thermal conductivity models used in this method has not been well evaluated yet.

This paper aims to evaluate the applicability of the modified 3ω method for characterising high thermal conductivity ultra-thin film/substrate system with the aid of the finite element analysis. The thermal theoretical models used in 3ω method will be introduced first. Then the finite element model will be established for the modified 3ω method and applied to a bulk silicon and an AlN thin-films/Si substrate system. Finally, the simulation results will be compared with the theoretical predictions.

2. Methods

2.1. Thermal Theory of 3ω Method

In the 3ω method, the thermal conductivity of the underneath material was obtained by coupling the experimental measurements and theoretical model predictions [1]. Figure 1 shows a typical experimental arrangement of the 3ω method. A long and narrow metal-strip element is deposited on the top surface of the specimen and attached to two square contact pads. This metal-strip element functions as a heater and a temperature sensor [1]. The temperature increase ΔT of the specimen surface can be calculated by Reference [1]:

$$\Delta T = \frac{2V_{3\omega}}{V_0\alpha} \quad (1)$$

where V_0 is the applied voltage and $V_{3\omega}$ can be measured in the experiment, and α is the temperature coefficient of electrical resistance. The temperature increase is a function of applied frequency.

Figure 1. Schematic of a typical measurement arrangement of the 3ω method.

On the other hand, ΔT can be calculated based on a one-dimensional theoretical model [1,18]

$$\Delta T(x) = \frac{P_{\text{rms}}}{l_h \Lambda_{\text{specimen}}} \int_0^\infty \frac{\cos(kx) \sin(kb)}{kb(k^2 + q^2)^{1/2}} dk \quad (2)$$

where x is the distance (in-plane) from the centre of the metal-strip element, $2b$ is the width of metal trip, $\Lambda_{\text{specimen}}$ is the thermal conductivity of the specimen; l_h is the length of the metal strip; P_{rms} is the electrical power applied on the metal strip; $1/q$ is the thermal penetration depth, k is wave number. In the case with an extremely narrow metal strip, the surface temperature increase can be approximated by Reference [1]

$$\Delta T = -\frac{P_{\text{rms}}}{2\pi l_h \Lambda_{\text{specimen}}} (\ln \omega) + c \quad (3)$$

where $\omega = 2\pi f$, and f is the applied frequency, c is a constant. Considering that the slope of $\Delta T - \ln(\omega)$ or curve can be experimentally determined, the thermal conductivity of the specimen can then be obtained.

In the case of the multilayer system, the complex temperature oscillation of the metal strip can be calculated via a two-dimensional multilayer thermal model [1,19]:

$$\Delta T(x) = \frac{-P_{rms}}{\pi l_h \Lambda_{y1}} \int_0^\infty \frac{1}{A_1 B_1} \frac{\sin^2(kb)}{b^2 k^2} dk \quad (4)$$

where

$$A_{i-1} = \frac{A_i \frac{A_{yi} B_i}{A_{yi-1} B_{i-1}} - \tan h(\phi_i - 1)}{1 - A_i \frac{A_{yi} B_i}{A_{yi-1} B_{i-1}} \tan h(\phi_i - 1)}, \quad i = 2 \cdots n, \quad (5)$$

$$B_i = \sqrt{\Lambda_{xyi} k^2 + \frac{i2\omega}{D_{yi}}} \quad (6)$$

$$\phi_i = B_i d_i \quad (7)$$

$$\Lambda_{xy} = \Lambda_x / \Lambda_y \quad (8)$$

where n is the total number of layers including the substrate; subscript i corresponds to the i th layer starting from the top; ω is the angular modulation frequency of the electrical current; subscript y corresponds to the direction perpendicular to the film/substrate interface; d is the layer thickness; D is the thermal diffusivity. Λ_{xy} is the thermal-conductivity anisotropy, defined by the ratio of the in-plane to the cross-plane thermal conductivity of the layers. If the substrate is semi-infinite, then $A_n = -1$ [19]. For a finite thick substrate, A_n depends on the boundary condition at the bottom surface of the substrate. Combining Equation (4) and the temperature increase experimentally determined, one could obtain the unknown thermal conductivities [1].

It should be noted that for both the models simplifications have been used in determining the thermal conductivity of materials. For example, thermal convection on the top surface of the specimen was not considered.

2.2. Finite Element Simulation

Two specimens, a bulk silicon and an AlN thin-films/Si substrate system, were selected for evaluating the above models with the aid of finite element analysis (ABAQUS software package v.6.12-3). Figure 2a shows a two-dimensional model representing a cross-section of the silicon specimen and the Gold (Au) nano-strip (width = 400 nm, thickness = 100 nm). Considering that the specimen size was much larger than that of the nano-strip, only partial specimen was modelled. The finite element model was based on a transient heat conduction equation with an isothermal boundary condition. In particular, the initial temperature of the whole model was set to the room temperature (25 °C). The nano-strip temperature oscillates at a fixed frequency ω and the heat was conducted into the specimen in cylindrical heat flow pattern. The input voltage of the 3ω method was applied to the simulation via an equally calculated surface heat flux. The software was able to calculate the temperature oscillation based on the applied input heat flux and the thermal properties of the underneath material. To investigate the frequency effect, a series of simulations were conducted with different heat inputs oscillated from 100 Hz and 10 kHz.

The material properties of gold and silicon were listed in Table 1 [20–22]. Quad-dominated free mesh control was utilised for the meshing system. Standard linear heat transfer elements of DCC2D4D with a 4-node convection or diffusion quadrilateral and dispersion control were used. Furthermore, a thorough mesh independence study was performed to optimize the mesh size. A typical meshing system is shown in Figure 2b.

Figure 2. (a) Finite element model of the Au nano-strip and Si specimen, and (b) the corresponding mesh used in the simulation.

To obtain the minimum feasible model size, numerical analyses were performed on different specimen sizes to remove any possible boundary effects. Moreover, heat convection was applied on the specimen top surface. According to the literature, the heat transfer coefficient for natural convection on a plane wall is between 5 and 25 W m⁻² K [23]. Comparing the modelling results with and without natural convection on the top surface, it was found that a slight change (less than 5%) of temperature was observed near the top surface. Here, the most conservative assumption (i.e., 25 W m⁻² K), where the heat transfer has the highest coefficient of natural convection, was applied to the model.

A simulation model was further established for a high thermal conductivity thin-film/substrate system. As shown in Figure 3, the model consists of a nano-strip (width = 400 nm, thickness = 100 nm), an AlN thin-film (thickness = 5 µm) and the Si substrate. Similar to the previous model, the simulation was a transient heat conduction model with an isothermal boundary condition. Considering that the thickness of AlN thin-film was too small and its thermal conductivity was too high, a higher frequency range 30–100 kHz was investigated for this system. The mesh and boundary size studies were performed to obtain the optimum mesh and model size. The material properties were applied based on the experimental characterisation in this study and the thermal properties available in the literature (Table 1). The numerical model did not take into account any interface thermal resistance between the layers (perfect bonding condition), to match with the theoretical conditions. Considering that the effect of interface thermal resistance (ITR) cannot be avoided in the experiment, we carried out further finite element analysis including the effect of AlN/Si interface thermal resistance (1.796×10^{-9} m² K/W, in Reference [1]).

Figure 3. Finite element model of the Au nano-strip, AlN thin film and Si substrate.

Table 1. Material properties of Au, Si and AlN [20–22].

Material	Λ (W/m·K)	ρ (kg/m ³)	C_p (J/kg·K)
Au	318	19300	129
Si	142	2330	710
AlN	285	3260	740

3. Results and Discussion

3.1. Bulk Silicon

Figure 4a shows a typical temperature increase (ΔT) profile of the nano-strip center with a heat input oscillation frequency of 2000 Hz. Here only a short period of time from 0.02 to 0.025 s was presented. To observe the gradual temperature increase/decrease of the nano-strip, each temperature oscillation period has been divided into 40 sub-steps. As shown in the figure, the ΔT of the nano-strip oscillates from 0.005 to 0.06 °C. Its average value is about 0.03 °C. Figure 4b shows the changes of the averaged ΔT from the beginning to 0.1 s. In the beginning ΔT increased very quickly and then gradually approached to a stable value of 0.34 °C. The results demonstrate that the modified 3ω method with nano-strip reaches a stabilised condition after some time (i.e., about 0.04 s), which is necessary for a reliable 3ω method measurement [1].

Figure 4. (a) A typical temperature increase profile of the nano-strip center ($f = 2000$ Hz). (b) The average temperature increase of the nano-strip center versus the simulation time.

Figure 5 shows a typical heat penetration pattern within the bulk silicon specimen in one heating oscillation cycle ($f = 2000$ Hz). The time interval between each image is $T/8$ (0.0625 ms). The insets of Figure 5 show the corresponding time within a heating oscillation cycle. At the beginning of the cycle the temperature increases as the input heat going up, and the heat penetrates gradually into the specimen, as shown in Figure 5a,b. The maximum temperature reaches a peak value at $T/4$ (Figure 5b) and then decreases. Meanwhile, the temperature gradient in the specimen also decreases, evidenced by the lessening of the temperature contour lines. This is due to the decrease of heat input at the top surface and the heat conductance. After $3T/4$, temperature gradient starts to increase again with increasing heat input and finally the cycle finishes and the next cycle starts. Figure 6 shows a typical variation of ΔT from the top surface of the specimen down into the underneath material along the model center line. Near the top surface, ΔT decreases very fast in a small distance of 50 nm and then approached to zero gradually, proving that the penetration depth of the modified 3ω method is very small.

Figure 5. A typical heat penetration pattern within the bulk silicon specimen in one heating oscillation cycle ($f = 2000$ Hz). (a) 0.0625 ms; (b) 0.125 ms; (c) 0.1875 ms; (d) 0.25 ms; (e) 0.3125 ms; (f) 0.375 ms; (g) 0.4375 ms; (h) 0.5 ms.

Figure 6. A typical variation of ΔT from the top surface of the Silicon specimen down into the underneath material.

To evaluate the theoretical prediction of Equation (2), a series of simulations were conducted with different heat inputs oscillated from 100 Hz to 10 KHz. Figure 7 shows the changes of the average temperature increase at the specimen top surface center with input heat oscillation frequency. It is clear that the higher the frequency, the lower the temperature increase. The red dashed line in Figure 7 shows the theoretical prediction made via Equation (2), which agrees very well with the numerical result. It proves that the theoretical model used in the modified 3ω method is suitable for characterising the thermal conductivity of bulk silicon. According to Equation (3), the slope of $\Delta T - \ln(2\pi f)$ can be used to calculate the specimen thermal conductivity $\Lambda_{\text{Specimen}}$, in which P_{rms} is equal to the power of input heat flux, and l_h is the length of the nano-strip (the element thickness in the finite element model). One can obtain that the measured thermal conductivity is 124.8 W/mK, which is similar to the literature value shown in Table 1.

Figure 7. A comparison between the numerical simulation and theoretical prediction results (Equation (2)) on ΔT versus f .

3.2. AlN Thin-Film/Si Substrate

Numerical simulations were conducted for characterising the thermal conductance of the high thermal conductivity AlN thin-film/Si substrate. Figure 8 presents a typical temperature contour profile of the AlN thin-film/Si substrate system during the simulation. As can be seen from the figure, the heat propagation in the thin film is faster than that in the substrate. This is due to the fact that the AlN has a higher thermal conductivity than Si substrate. Figure 9 shows a typical variation of ΔT from the thin-film top surface into the substrate along the model center line. Similar to Figure 6, ΔT decreases very fast in a small distance of 50 nm from the top surface and then approaches zero gradually.

Figure 8. A typical cylindrical temperature increase ($^{\circ}\text{C}$) contour profile of the AlN thin-film/Si substrate system. The thickness of the thin film is 2 μm .

Figure 9. A typical variation of ΔT from the AlN thin-film top surface into the Si substrate.

To evaluate the theoretical prediction of Equation (4), a series of simulations were conducted with different heat inputs oscillated from 30 to 100 kHz. Figure 10 shows the changes of the average temperature increase at the specimen top surface center with input heat oscillation frequency. The red dashed line in Figure 10 shows the theoretical prediction made via Equation (4). Overall, the numerical simulation and the theoretical prediction show a very good agreement with each other, proving that the theoretical model used in the modified 3ω method is suitable for characterising the thermal conductivity of high thermal conductivity thin film/substrate system. The slight difference may due to the strong assumption made in the theoretical model. Figure 10 also presents the simulation results taking account of the AlN/Si ITR effect, which agree very well with the experimental results from Reference [1].

According to Equation (3), the slope of $\Delta T - \ln(2\pi f)$ can be used to calculate the overall thermal conductivity of the AlN thin-film/Si substrate underneath. Given that the thermal conductivity of the Si substrate is $142 \text{ W/m}\cdot\text{K}$, the thermal conductivity of AlN thin-film can be obtained via the implicit Equations (4)–(8). A Matlab code was developed to numerically solve these equations, and the calculated thermal conductivity of the AlN thin-film is $195.3 \text{ W/m}\cdot\text{K}$.

Figure 10. A comparison among the numerical simulation, theoretical prediction, and experimental results on ΔT versus f .

4. Conclusions

This paper evaluated the theoretical models used in a modified 3ω method in characterising the thermal conductivity of materials with the aid of the finite element analysis. Numerical models were established for a bulk silicon and an AlN thin-film/Si substrate system, and a series of simulations were conducted over a wide range of input heat oscillation frequencies. It was found that for both the cases the temperate increase of the specimen top surface center matches very well with the theoretical predictions. This study thus concludes that the modified 3ω method with a nano-strip is suitable for characterising high thermal conductivity ultra-thin film/substrate systems.

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