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Journal

Journal of Applied Physics, 112(043516)

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Publication Date

2012-08-30

Analysis of the “3-Omega” method for substrates and thick films of anisotropic thermal conductivity

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(Received 18 April 2012; accepted 18 July 2012; published online 30 August 2012)

The heat equation in an anisotropic material under sinusoidal excitation is solved in cylindrical-polar coordinates for the geometry conventionally used in the measurement of thermal conductivity by the “3-Omega” method. Although the solution can be carried out in Cartesian coordinates using Fourier transforms, the inverse transforms have to be evaluated numerically. The current method allows us to make contact with, and extend, the analytical results of Cahill and Pohl for isotropic substrates. We find that the 3-Omega method experiment, if performed conventionally, measures the average thermal conductivity in the in-plane and cross-plane directions, for modest anisotropies. An alternate geometry with separate heater and thermometer lines is explored, where the temperature of the thermometer is expected on physical grounds to be selectively sensitive to the in-plane thermal conductivity. The selectivity is quantified using the analytic forms derived for the temperature profile, and the results are verified by finite element method simulations. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4747836>]

I. INTRODUCTION

The 3ω method¹ is a popular technique for the measurement of the thermal conductivity of substrates and thin films. In the conventional 3ω method, a metal line with four contact pads (two outer pads for sourcing current and two inner ones for measuring voltage) is used both as the heat source, through Joule heating by a sinusoidal current source, and as the thermometer, through its temperature coefficient of resistance. The desired thermal properties of the underlying material appear in the third harmonic of the voltage across the inner (voltage) pads, hence the name of the method. For substrates or films thicker than 2–3 times the thermal penetration depth (defined by Eq. (2) of Ref. 2), conductivity can be calculated from the slope of the temperature profile vs. logarithm of the frequency.¹ If the sample consists of a thin film of lower thermal conductivity on a substrate of higher, then in order to extract the thermal conductivity of the thin film alone, it is customary to perform two frequency sweeps, one on the film/substrate and another on the substrate alone. Their difference gives the temperature drop across the thin film alone.^{3,4} For such thin films, varying the heater width (defined as its dimension along the surface of the sample) is a viable means of extracting the anisotropy in the thermal conductivity.¹³

Cahill and Pohl¹ analyzed the 3ω method experiment for isotropic substrates by solving the heat equation in cylindrical-polar coordinates under sinusoidal heat-flux excitation. For thin film characterization, if the film has lower conductivity than the substrate, a commonly used approximation is to treat the film as a simple thermal insulator and to assume purely cross-plane (1D) heat transfer through the film.³ This may be prone to serious error depending on the film thickness and the heater width, due to 2D heat flow in

the film. Reference 5 has analyzed the most general case of multilayer thin films on a semi-infinite substrate, with a diagonal anisotropic thermal conductivity matrix for each layer. The solution is carried out in Cartesian coordinates by taking the Fourier transform in the in-plane direction, and using a transfer matrix approach for the cross-plane direction. The inverse Fourier transform is then evaluated to yield the 2D temperature profile.

Naturally, the method of Ref. 5 is perfectly applicable to the anisotropic-substrate-only case; however, it is not amenable to closed-form solution because the inverse Fourier transform has to be computed numerically. As formulated, it is not applicable to non-planar (e.g., etched) geometries and does not consider the heat capacity of the heater line.⁶ The latter two defects can be remedied by fully numerical solution using the finite element method (FEM).

For substrates, the temperature of the heater-thermometer depends only logarithmically on its width. Varying the heater width has been utilized for substrate anisotropy determination; however, the attempt was restricted to a relatively thin substrate (60 μm) of high anisotropy ratio (0.7) between the in-plane and cross-plane directions.¹⁴ Attempts at extracting anisotropy for thick substrates of smaller anisotropy are easily masked by effects such as interfacial thermal resistance. It is desirable, therefore, to have separate lines for the heater and thermometer. For modest heater-thermometer separation, the temperature profile on the thermometer line is not sensitive to interfacial thermal resistance, as we will demonstrate later.

In this work, we solve the anisotropic heat equation in cylindrical-polar coordinates under sinusoidal heat-flux excitation and derive the temperature profile throughout the solid. With some work, this profile gives a formula that closely parallels the original result of Cahill and Pohl, if the heater and thermometer are identical.^{1,14} We then use the derived temperature profile to examine the important case of

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separate heater and thermometer lines and show selective sensitivity of the temperature of the thermometer line to the in-plane thermal conductivity. We will briefly formulate a frequency-domain FEM for the 3ω problem and demonstrate the validity of our analytical expressions by means of FEM simulations.

II. ANALYTICAL FORMS FOR THE TEMPERATURE PROFILE IN ANISOTROPIC SUBSTRATES

Fig. 1 shows a schematic of the problem geometry. A metal heater line of width w_{heater} is used to pump heat into the sample, and either the same metal line or another line of width w_{therm} at a distance D away from the heater is used to measure the temperature. The thermometer line is parallel to the heater and their separation (typically $100\ \mu\text{m}$) is much smaller than their lengths (typically 1-4 mm) in order to apply 2D heat-flow models. The coordinate system is (r, θ) in cylindrical coordinates and (x, y) in Cartesian, with the usual relationship between the pairs of variables. The heat equation is

$$\nabla \cdot (\hat{K} \cdot \nabla \bar{T}) = C_v \frac{\partial \bar{T}}{\partial t}. \quad (1)$$

Here and henceforth, we shall use normal font for scalars and bold font for vectors. The gradient symbol, however, will be written in normal font. A caret will signify a tensor or matrix. A bar on top will represent explicit time dependence of the form $e^{j2\omega t}$. The thermal conductivity tensor $\hat{K}$ can be represented by a 2×2 matrix, assumed diagonal.

$$\hat{K} = \begin{bmatrix} k_x & 0 \\ 0 & k_y \end{bmatrix}. \quad (2)$$

C_v is the volumetric specific heat capacity and $\bar{T}$ is the temperature at any point in the solid as a function of time. Let $k_x = k$ be the “in-plane” thermal conductivity. Furthermore, we define the anisotropy ratio η by

$$\eta = \frac{k_y}{k_x} = \frac{k_y}{k}. \quad (3)$$

Equations (1)–(3) give

$$k \left(\frac{\partial^2 \bar{T}}{\partial x^2} + \eta \frac{\partial^2 \bar{T}}{\partial y^2} \right) = C_v \frac{\partial \bar{T}}{\partial t}. \quad (4)$$

We now execute the following change of variables on Eq. (4)

$$x \rightarrow x', \quad y \rightarrow \sqrt{\eta} y', \quad (5)$$

thus getting the following differential equation,

$$k \left(\frac{\partial^2 \bar{T}}{\partial x'^2} + \frac{\partial^2 \bar{T}}{\partial y'^2} \right) = C_v \frac{\partial \bar{T}}{\partial t}. \quad (6)$$

For harmonic excitation at frequency 2ω , in steady-state, $\bar{T} = T e^{j2\omega t}$ and Eq. (6) reduces to

$$\left(\frac{\partial^2 T}{\partial x'^2} + \frac{\partial^2 T}{\partial y'^2} \right) = q^2 T, \quad (7a)$$

where

$$q = \sqrt{\frac{j2\omega C_v}{k}}. \quad (7b)$$

$|1/q|$ is the characteristic length-scale over which the temperature amplitude decays to zero along the surface of the sample. Equation (7) has the series solution

$$T(r', \theta') = \sum_{n=0,2,\dots} A_n K_n(qr') (e^{-jn\theta'} + B_n e^{jn\theta'}), \quad (8)$$

which is in terms of the cylindrical system corresponding to (x', y') . Here, K_n is the modified Bessel function of the second kind, of order n . The modified Bessel functions of the first kind are excluded since they diverge as $r \rightarrow \infty$. A_n and B_n are as-yet undetermined expansion coefficients. n must be an even integer because the temperature profile must be the same for $\theta = \theta' = \pi$ as it is for $\theta = \theta' = 0$. n can be further restricted to non-negative integers because negative integers do not give linearly independent solutions.

Converting back to the original coordinate system,

$$T(r, \theta) = \sum_{n=0,2,\dots} A_n K_n \left(qr \sqrt{1 + \left(\frac{1}{\eta} - 1 \right) \sin^2 \theta} \right) \times \left(e^{-jncos^{-1} \left(\cos \theta / \sqrt{\cos^2 \theta + \frac{\sin^2 \theta}{\eta}} \right)} + B_n e^{jncos^{-1} \left(\cos \theta / \sqrt{\cos^2 \theta + \frac{\sin^2 \theta}{\eta}} \right)} \right). \quad (9)$$

In order to determine the coefficients of the series expansion, we need to make contact with the problem under study. We will first prove that $A_n = 0$ for $n \neq 0$. (For the case of isotropic substrates ($\eta = 1$) treated by Ref. 1, cylindrical symmetry automatically ensures this, but our problem lacks cylindrical symmetry and the reasoning is more subtle.) We will then connect A_0, B_0 to the heater power.

FIG. 1. Problem geometry.

FIG. 2. Closed semi-cylindrical volume for applying the Gauss-Ostrogradsky theorem.

To do so, we consider a semi-cylindrical region Γ of vanishingly small radius b around an infinitesimally narrow segment of the heater strip (Fig. 2); let the boundary of the region be divided into two parts: the upper flat surface Ω' and the cylindrical surface Ω . Let $\mathbf{n}$ be the outward normal to the cylindrical surface Ω . Inside the semi-cylinder, there is no heat generation, and the heat equation reads $\nabla \cdot \bar{\mathbf{F}} = -C_v \frac{\partial T}{\partial t}$, where $\bar{\mathbf{F}}$ is the heat-flux.

Ignoring the heat capacity of the metal heater line itself, the net power entering the semi-cylinder through Ω' is equal to the power $\Delta \bar{P} = \Delta P e^{j2\omega t}$ generated within the

strip. Let L be the length of the heater line. Applying the Gauss-Ostrogradsky theorem to the heat equation, and dropping the explicit time dependence $e^{j2\omega t}$ throughout leads to

$$-\Delta P - \int_{\Omega} \mathbf{n} \cdot (\bar{\mathbf{K}} \cdot \nabla T) d\Omega = -LC_v \int_{\rho=0}^b \rho d\rho \int_{\theta=0}^{\pi} j2\omega T d\theta. \quad (10)$$

Looking first at the surface integral,

$$\int_{\Omega} \mathbf{n} \cdot (\bar{\mathbf{K}} \cdot \nabla T) d\Omega = \lim_{b \rightarrow 0} Lb \int_{\theta=0}^{\pi} \mathbf{n} \cdot (\bar{\mathbf{K}} \cdot \nabla T) d\theta. \quad (11)$$

We note here two important features of Eq. (11). First, had $\bar{\mathbf{K}}$ been isotropic, as in the original treatment of Ref. 1, the integral over θ would have been trivial, since $\mathbf{n}$ would always be parallel to $\bar{\mathbf{K}} \cdot \nabla T$, and the integrand independent of θ . Our problem requires numerical or analytical evaluation of the θ integral. Second, in the limit that $b \rightarrow 0$, ∇T cannot diverge faster than $1/b$. It is this last condition that will exclude modified Bessel functions of order higher than 0 from the series Eq. (9).

Using $\mathbf{n} = i\cos\theta + j\sin\theta$ and the appropriate expressions for the partial derivatives of T in cylindrical coordinates, we obtain

$$\int_{\Omega} \mathbf{n} \cdot (\bar{\mathbf{K}} \cdot \nabla T) d\Omega = \lim_{b \rightarrow 0} L \int_{\theta=0}^{\pi} \left(kb \frac{\partial T}{\partial b} (\cos^2\theta + \eta \sin^2\theta) + k \frac{\partial T}{\partial \theta} (\eta - 1) \cos\theta \sin\theta \right) d\theta, \quad (12)$$

$T(b, \theta)$ is given by the series Eq. (9) and $\frac{\partial T}{\partial b}$ here means the radial derivative of T evaluated at b . Note that $K_n(z) \propto 1/z^n$ for $|z| \ll 1$ and n a positive integer.⁷ Thus, the right-hand side of Eq. (12) diverges for all $n \neq 0$. Therefore in Eq. (9), we must have $A_n = 0$ for all $n \neq 0$, and only the zeroth order modified Bessel function survives.

The volume integral on the RHS of Eq. (10) vanishes for finite frequencies because the zeroth-order modified Bessel function can be proved to satisfy the following condition, for any constant $a \neq 0$:

$$\lim_{b \rightarrow 0} \int_{\rho=0}^b K_0(a\rho) \rho d\rho = 0. \quad (13)$$

We thus arrive at the following equation for the temperature profile, and this profile when used in Eq. (10) gives finite surface and volume integrals:

$$T(r, \theta) = C_0 K_0 \left(qr \sqrt{1 + \left(\frac{1}{\eta} - 1 \right) \sin^2 \theta} \right). \quad (14)$$

Here, $C_0 = A_0(1 + B_0)$. Equation (14) shows that in the anisotropic case, the contours of constant temperature-amplitude around the heater are no longer circles, but instead are

slightly elongated (contracted) in the direction normal to the surface for $\eta > 1$ ($\eta < 1$). The constant C_0 can be determined by substituting Eq. (14) into Eqs. (10)–(13). However to the best of our knowledge, the integral over θ in Eq. (12) cannot be evaluated in closed form and approximations are necessary. For convenience, we define the quantity ε as

$$\varepsilon = \left(\frac{1}{\eta} - 1 \right). \quad (15)$$

For anisotropic ratios η not too different from 1, $|\varepsilon|^2 \ll 1$; we may thus expand Eq. (14) in a Taylor series around $qr \ll 1$ and truncate it at the leading order in ε , to obtain

$$T(b, \theta) \sim C_0 (K_0(qb) + \frac{qb}{2} \varepsilon K'_0(qb) \sin^2 \theta), \quad (16)$$

where $K'_0(qb) \equiv \frac{dK_0(qr)}{d(qr)}$ evaluated at $r = b$.

Using the asymptotic form⁷ of $K_0(qb)$ for $qb \ll 1$, we get

$$T(b, \theta) \sim C_0 \left(-\ln \left(\frac{qb}{2} \right) - 0.577 - \frac{1}{2} \varepsilon \sin^2 \theta \right) \quad (17)$$

Substituting Eq. (17) in Eq. (12), evaluating the integral over θ , and using Eqs. (10) and (13), we get

$$C_0 = \frac{\Delta P}{\pi L k} \cdot \frac{2}{\eta + 1} \cdot \frac{1}{1 - \frac{(\eta-1)^2}{4\eta(\eta+1)}}. \quad (18)$$

Equations (14) and (18) give the temperature amplitude profile due to an infinitesimally wide line source for anisotropy ratios not too different from 1. If the heater and thermometer lines are the same, the extension to a finite width almost exactly mirrors that of Ref. 2; only $\frac{P}{\pi L k}$ therein is replaced by the RHS of Eq. (18) and q is evaluated corresponding to the in-plane thermal conductivity (Eq. (7b)). Accordingly, under the condition $w_{\text{heater}} \ll |1/q|$, the measured temperature in phase with the applied power is given by

$$T_{\text{meas}}^{\text{phase}} = \frac{P}{\pi L k} \cdot \left(\frac{2}{\eta + 1} \right) \cdot \frac{1}{1 - \frac{(\eta-1)^2}{4\eta(\eta+1)}} \left(\frac{1}{2} \ln \frac{k}{C_v (w_{\text{heater}}/2)^2} + a - \frac{1}{2} \ln(2\omega) \right), \quad (19)$$

where $a = 0.923$ in theory and P is given by V_{rms}^2/R , where V_{rms} is the RMS voltage applied to the heater line of resistance R . In practice, Ref. 4 notes that $a = 1.05$ fits experiment better; this may need to be adjusted for different substrates. This uncertainty makes the slope of $T_{\text{meas}}^{\text{phase}}$ vs. $\ln(\omega)$ a better indicator of the thermal conductivity. This procedure also eliminates errors due to interface thermal resistance, which gives a frequency-independent contribution to the measured temperature.

Eq. (19) has some interesting consequences. It tells us that for anisotropic thick films and substrates, the 3ω experiment, if performed conventionally, measures the quantity

$$\tilde{k} = k \cdot \left(\frac{\eta + 1}{2} \right) \cdot \left(1 - \frac{(\eta - 1)^2}{4\eta(\eta + 1)} \right). \quad (20)$$

When $\eta = 1$, $\tilde{k} = k$ as required. Also, neglecting $(\eta - 1)^2$, $\tilde{k} = k \cdot (\eta + 1)/2 = (k_x + k_y)/2$. The conventional 3ω experiment (slope of the in-phase temperature vs. logarithm of frequency), when performed on an anisotropic substrate, measures the average thermal conductivity in the in-plane and cross-plane directions, a fact confirmed by finite-element simulations (Fig. 3). The determination of each of these components, however, is tricky; the only other knob available in Eq. (19) is w_{heater} and the dependence on this parameter is merely logarithmic. The above expression for $\tilde{k}$ is accurate to within 5% over a large range in anisotropic ratios, between 0.6 and 1.7.

III. THE CASE OF SEPARATE HEATER AND THERMOMETER LINES

We consider using a thermometer line of width w_{therm} separated from the heater by a distance D as shown in Fig. 1. Equation (14) with $\theta = 0$, together with Eq. (18) gives the surface-response due to an infinitesimal source. The temperature measured on the thermometer line due to the power pumped in using a heater of finite width can be derived by

FIG. 3. FEM simulations of the temperature oscillation amplitude in phase with the applied power, as a function of the frequency ω , for two different combinations of inplane and cross-plane conductivities. Both combinations have the same average conductivity. Input power = 1 W, $L = 1$ cm, and $w_{\text{heater}} = 20 \mu\text{m}$. The slopes of the graphs are nearly identical, as predicted by Eq. (20), and the intercepts differ by $\sim 3\%$.

convolving this response over the heater width, followed by averaging over the thermometer line. The resulting temperature on the thermometer line is given by

$$T_{\text{meas}} = \frac{P}{\pi L \tilde{k} w_{\text{therm}} w_{\text{heater}}} \cdot \int_{x=-w_{\text{heater}}/2}^{w_{\text{heater}}/2} \int_{\tau=-w_{\text{therm}}/2}^{w_{\text{therm}}/2} K_0(q(D + \tau - x)) d\tau dx, \quad (21)$$

where $\tilde{k}$ is given by Eq. (20). Equation (21) is the general result; the integrals may always be evaluated numerically, and in some cases analytical solutions are possible, as outlined in the Appendix. Note that q in the integrand makes T_{meas} a frequency-dependent, complex quantity. Also, note that the only approximations in Eq. (21) are $|\varepsilon|^2 \ll 1$ leading to Eq. (16), and of course 2D heat flow (i.e., neglect of end effects due to finite heater/thermometer length).

We verified Eq. (21) independently by comparing it with numerical simulations of the heat equation based on the finite element method, which is discussed in Sec. IV. Fig. 4 shows that the equation is correct. Fig. 4 also shows two important features of the thermometer temperature component in phase with the applied power. First, with the cross-plane thermal conductivity set to 9 W/m-K, changing the in-plane thermal conductivity from 9 to 11 W/m-K resulted in a 37% increase in the temperature sensed by the thermometer. Second, with the in-plane thermal conductivity set to 9 W/m-K, the temperature as a function of frequency, at low frequencies between 50 and 150 Hz, is nearly independent of the cross-plane thermal conductivity, with the latter varied between 9 and 11 W/m-K. The parameters of the simulation were $D = 100 \mu\text{m}$, $L = 1$ cm, $w_{\text{heater}} = w_{\text{therm}} = 20 \mu\text{m}$ (please see Fig. 1) and volumetric heat capacity $C_v = 2.74 \text{ J/cm}^3\text{-K}$. The time-averaged input power to the heater, $P = V_{\text{rms}}^2/R$

FIG. 4. FEM simulations show that Eq. (21) is accurate and that the temperature component in phase with the applied power is highly and selectively sensitive to the in-plane thermal conductivity for low frequencies. Parameters: input power = 1 W, $L = 1$ cm, $D = 100$ μm , $w_{\text{therm}} = w_{\text{heater}} = 20$ μm , and volumetric heat capacity $C_v = 2.74$ J/cm³-K.

was set to 1 W. The significant differences between the cases $(k_x, k_y) = (9, 11)$ W/m-K and $(k_x, k_y) = (11, 9)$ W/m-K stand in sharp contrast to the results of conventional 3ω sweeps (Fig. 3), which do not discriminate between the two cases since both have the same average conductivity.

Similar sensitivity results were obtained for thermal conductivities close to 1 W/m-K. With the in-plane thermal conductivity held constant at 0.9 W/m-K, increasing the cross-plane conductivity from 0.9 to 1.1 W/m-K resulted in a maximum increase of 9.5% in the temperature sensed by the thermometer. With the cross-plane thermal conductivity held constant at 0.9 W/m-K, increasing the in-plane value from 0.9 to 1.1 W/m-K resulted in a much larger (43%) increase in the sensed temperature. Once again, FEM simulations reproduced the results of Eq. (21). The rest of the physical parameters was the same as before, namely $D = 100$ μm , $L = 1$ cm, $w_{\text{heater}} = w_{\text{therm}} = 20$ μm , and $C_v = 2.74$ J/cm³-K.

Equation (21) seems to show a strong dependence on w_{heater} and w_{therm} , suggesting high sensitivity to errors in measuring these quantities. However, the double integrals make this dependence rather weak in most cases. It is in fact proved in the appendix that if $w_{\text{therm}} \ll D$ and $w_{\text{heater}} \ll D$, the dependencies vanish. For thermal conductivities of the order of 10 W/m-K, with $D = 100$ μm and $w_{\text{therm}} = w_{\text{heater}} = 20$ μm , a 10% error in the heater and thermometer widths results in 0.6% error in the sensed temperature at 50 Hz, and the error remains <1% even at a separation D as low as 30 μm . The errors become smaller as w_{therm} and w_{heater} decrease, due to the conditions mentioned above being satisfied more closely. However for thermal conductivities of the order of 1 W/m-K, errors of 10% in the widths result in $\sim 5\%$ error in the temperature with $D = 30$ μm , $w_{\text{therm}} = w_{\text{heater}} = 20$ μm . By increasing D to 100 μm , we can reduce this sensitivity to 0.25%. Thus, the sensitivity to the heater and thermometer widths is highest for low substrate thermal conductivities and small heater-thermometer separations.

IV. FREQUENCY-DOMAIN FEM FORMULATION OF THE GENERAL 3ω METHOD PROBLEM

The FEM is the reformulation of a partial differential equation as a variational equation, following which a solution is sought within a subspace spanned by a finite set of basis functions. The variational equation is converted into a matrix equation whose solution generates exactly that function within the chosen subspace which is closest to the actual solution in a least-squares sense (Ref. 8, pp. 24–25).

Reference 9 uses the finite-volume method to solve the heat equation in the time-domain with a sinusoidal heat source term to obtain the temporal response of the system and propagates the solution to steady state. Our approach is to solve the heat equation in the frequency domain instead, so as to directly obtain the in-phase and quadrature components of temperature oscillation without any post-processing. Thus, we do not capture the transients, which are anyway discarded. Heat generation is explicitly included, using a 500 nm thick Pt heater line whose thermal conductivity and heat capacity are known to be 70 W/m-K¹⁰ and 2.84 J/cm³-K.¹¹ Reference 12 demonstrates the validity of this approach by comparing the results of simulation to an experimental standard 3ω sweep on a material of known thermal conductivity, strontium titanate.

In the Fourier domain, the heat equation with a source term, upon separating real and imaginary parts leads to a system of two coupled PDEs,

$$\nabla \cdot (\hat{K} \cdot \nabla T_{Re}) = -2\omega C_v T_{Im} - Q, \quad (22a)$$

$$\nabla \cdot (\hat{K} \cdot \nabla T_{Im}) = 2\omega C_v T_{Re}. \quad (22b)$$

Here, $\bar{T} = T e^{j\omega t}$ is the steady-state temperature profile and $T = T_{Re} + jT_{Im}$, where T_{Re} and T_{Im} are the in-phase and quadrature components of temperature oscillation. The power density $Q = P/(w_{\text{heater}} t_{\text{heater}} L)$, where t_{heater} is the heater thickness, $P = V_{\text{rms}}^2/R$ as before, and Q is non-zero only within the heater. The phase of the temperature is referenced to the applied power; thus, the imaginary part of Q is 0 in Eq. (22b). Using the FEM discretization procedure, the pair of Eqs. (22) is rewritten as a single matrix equation having the form

$$\begin{bmatrix} \hat{S} & 2\omega \hat{M} \\ -2\omega \hat{M} & \hat{S} \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix} = [B] \quad (23)$$

where $\hat{S}$ and $\hat{M}$ are the so-called “stiffness” and “mass” matrices (Ref. 8, pp. 149–150). $\hat{S}$ and $\hat{M}$ are constructed from the basis functions, the thermal conductivity tensor, and the heat capacity. If N is the number of grid points, T_1 and T_2 are $N \times 1$ arrays containing T_{Re} and T_{Im} evaluated at the grid points. The first N rows of B are constructed from the power density Q , and the next N rows are zero since Eq. (22b) has no source term. Eq. (23) is a $2N$ by $2N$ matrix equation, N being the number of grid points. By solving Eq. (23) using the usual linear algebraic methods, we can directly obtain the in-phase and quadrature components of temperature

FIG. 5. Boundary conditions for the FEM formulation of the general 3ω problem. P.D. refers to the power density generated in the Joule heater, and $F.n$ is the heat flux through the indicated surfaces. The sense (thermometer) line is optional.

oscillation. The method is capable of handling arbitrary 2D geometries with multiple layers, with arbitrary material properties for each layer. Fig. 5 shows the boundary conditions used; heat loss through convection and radiation is neglected, and the bottom surface is set to $T = 0 + j0$. One restriction on our current FEM implementation is that $\bar{K}$ be symmetric; however, it need not be diagonal.

As mentioned earlier, the main advantage of this formulation over that of Ref. 9 is that the frequency response is calculated directly, which makes it easier to run a large number of frequencies in one simulation. Also, no ODE solution is required for time-stepping. The disadvantage is that the matrix size is quadrupled. This was inconsequential for 2D simulations, but might cause problems in extension to three dimensions if one wishes to account for end effects due to the finite heater length. The advantages of FEM over the Fourier-transform approach of Ref. 5 are the applicability to non-planar geometries, the consideration of the heat capacity of the heater line, and the applicability to a broader range of $\bar{K}$ matrices. As derived, the method of Ref. 5 applies only to diagonal matrices, while the FEM can handle off-diagonal elements in the thermal conductivity matrix. The MATLAB[®] source code for the 2D frequency-domain FEM implementation is available from the authors upon request.

A brief discussion of end effects due to the finite heater length is in order here. Reference 9 has analyzed the problem numerically in cylindrical-polar coordinates for the case of infinitesimally narrow heater lines and has identified large $|Lq|$ as one condition for end effects to minimally impact the accuracy of the measurement. For $L = 4$ mm, the error due to finite length is $<1\%$ even for a material of large thermal conductivity (Si, 148 W/m-K) and at a low frequency (10 Hz).⁹ For finite heater widths between $w_{heater} = 10 - 30 \mu\text{m}$, we have found no variation in the measured thermal conductivity of Si when $L = 1$ mm, suggesting $L > 30[D + (w_{heater} + w_{therm})/2]$ as a plausible condition for neglecting errors due to finite L/D . However, 3D FEM simulations need to be conducted to confirm this expectation.

FIG. 6. FEM simulation of (a) the standard one-wire 3ω sweep, and (b) the temperature oscillation amplitude in phase with the applied power for the case of separate heater and thermometer lines, with and without accounting for interfacial thermal resistance. Panel (b) shows no sensitivity to the interface, whereas (a) shows a discernible effect.

V. THE EFFECT OF INTERFACIAL THERMAL IMPEDANCES

We will use the finite element method to prove our last remaining claim in the Introduction, namely the insensitivity of the thermometer temperature to interfacial thermal resistances if separate heater and thermometer lines are utilized. The geometry of the simulation is the same as in Sec. III, namely $D = 100 \mu\text{m}$, $L = 1$ cm, $w_{heater} = w_{therm} = 20 \mu\text{m}$. The substrate volumetric heat capacity was chosen as $C_v = 2.74 \text{ J/cm}^3\text{-K}$ and the thermal conductivity to be $(k_x, k_y) = (11, 9) \text{ W/m-K}$. The interfacial thermal resistance was modeled as a 100 nm thick SiO_2 film (conductivity 1.1 W/m-K, heat capacity $1.94 \text{ J/cm}^3\text{-K}$) between each metal line and the substrate. Fig. 6(a) shows a $\sim 6\%$ deviation in amplitude when the heater and thermometer lines are the same. In contrast, Fig. 6(b) shows that the temperature responses with and without accounting for the interfaces are virtually indistinguishable. Physically, this is expected because the heat flux is approximately perpendicular to the interface below the heater and approximately parallel to the interface beneath the thermometer. Thus, there is a temperature drop across the substrate-thermometer interface in Fig. 6(a) and none in Fig. 6(b). FEM simulations also prove insensitivity to the

interfacial thermal impedance when separate heater and thermometer lines are used, for substrate thermal conductivities of the order of 1 W/m-K.

VI. SUMMARY AND CONCLUSIONS

We have derived a closed-form expression for the temperature response of an anisotropic material under sinusoidal heat-flux excitation and used it to relate the result of the standard 3ω measurement to the average thermal conductivity of the material in the in-plane and cross-plane directions. We have further shown that having separate heater and thermometer lines enhances the sensitivity to the in-plane thermal conductivity. We have developed a frequency-domain FEM formulation of the problem, and verified our analytical results by comparing them to fully numerical solutions. We have used FEM simulations to show that interfacial thermal resistances do not impact the measured temperature for the case of separate heater and thermometer lines.

In principle, Eq. (19) can be used to determine the average thermal conductivity in the two directions, and Eq. (21) to obtain the in-plane component. In practice, in order to use these results in the measurement of anisotropy, one has to take cognizance of certain other factors. At 100 μm heater-thermometer separation, a comparison of Figs. 3 and 4 shows that the temperature signal is more than an order of magnitude weaker than in the standard single-line situation, for the same applied heating power. A smaller separation will help, but at the expense of decreased sensitivity to the in-plane conductivity. The weak signals may necessitate the use of more sophisticated instrumentation than needed for the standard 3ω method, e.g., cleaner current sources both for heating and for sensing the temperature.

ACKNOWLEDGMENTS

We wish to thank Rachel Koltun (Materials Department, U.C. Santa Barbara) for helpful discussion. This work was supported by the Center for Energy Efficient Materials, an

Energy Frontier Research Center funded by the US Department of Energy, Office of Basic Energy Sciences, under Award No. DE-SC0001009.

APPENDIX: A CLOSED-FORM SOLUTION FOR THE MEASURED TEMPERATURE FOR THE CASE OF SEPARATE HEATER AND THERMOMETER LINES

Equation (21) gives the temperature profile on a thermometer line located parallel to, and a distance D from, the heater line. The integration variable τ goes over the thermometer width and x over the heater width. In the special case where $|1/q| \ll D \ll L$ (the heater-thermometer distance is large compared to the thermal penetration depth but smaller than the wire lengths—the latter condition ensuring that these 2D models are valid) the temperature-amplitude profile is approximated using the asymptotic properties of the modified Bessel function, by

$$T_{meas} = \frac{P}{\sqrt{2Lk}w_{heater}q} \int_{x=-w_{heater}/2}^{w_{heater}/2} (1/w_{therm}) \times (erf(\sqrt{q(D + (w_{therm}/2) - x)}) - erf(\sqrt{q(D + (w_{therm}/2) - x)})) dx \quad (A1)$$

where $erf(z)$ is the error function;

$$erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt. \quad (A2)$$

For $w_{therm} \ll D$ which is a reasonable assumption,

$$T_{meas} = \frac{P}{\sqrt{2Lk}w_{heater}q} \times \int_{x=-w_{heater}/2}^{w_{heater}/2} d/dz(erf(\sqrt{q(D + z - x)})) \Big|_{z=0} dx, \quad (A3)$$

$$T_{meas} = \frac{P}{\sqrt{2\pi Lk}w_{heater}} \int_{x=-w_{heater}/2}^{w_{heater}/2} \frac{e^{-q(D-x)}}{\sqrt{q(D-x)}} dx = \frac{P}{\sqrt{2Lk}q} \left(\frac{erf(\sqrt{q(D + (w_{heater}/2))}) - erf(\sqrt{q(D - (w_{heater}/2))})}{w_{heater}} \right). \quad (A4)$$

Finally by means of a similar manipulation we obtain,

$$T_{meas} = \frac{P}{\sqrt{2\pi Lk}} \sqrt{\frac{1}{qD}} e^{-qD}. \quad (A5)$$

A simple analytic expression can thus be derived for the temperature response under certain conditions, namely $w_{therm} \ll D$, $w_{heater} \ll D$ and $|1/q| \ll D \ll L$. This result can also be derived by setting $q(D + \tau - x) \sim qD$ in the integrand of Eq. (21), and then using the asymptotic form⁷ of $K_0(z)$ for large $|z|$.

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