Inversion for Thermal Properties with Frequency Domain Thermoreflectance


ABSTRACT: 3D integration of multiple microelectronic devices improves size, weight, and power while increasing the number of interconnections between components. One integration method involves the use of metal bump bonds to connect devices and components on a common interposer platform. Significant variations in the coefficient of thermal expansion in such systems lead to stresses that can cause thermomechanical and electrical failures. More advanced characterization and failure analysis techniques are necessary to assess the bond quality between components. Frequency domain thermoreflectance (FDTR) is a nondestructive, noncontact testing method used to determine thermal properties in a sample by fitting the phase lag between an applied heat flux and the surface temperature response. The typical use of FDTR data involves fitting for thermal properties in geometries with a high degree of symmetry. In this work, finite element method simulations are performed using high performance computing codes to facilitate the modeling of samples with arbitrary geometric complexity. A gradient-based optimization technique is also presented to determine unknown thermal properties in a discretized domain. Using experimental FDTR data from a GaN-diamond sample, thermal conductivity is then determined in an unknown layer to provide a spatial map of bond quality at various points in the sample.

KEYWORDS: frequency-domain thermoreflectance, thermal boundary conductance, finite element method, gradient-based optimization, heterogeneously integrated microelectronics, GaN-diamond devices

1. INTRODUCTION

Heterogeneous integration (HI) of microelectronic devices allows for an electronic system to be realized by combining integrated circuits with different functions into a single chip. Commonly, this integration occurs through the use of thermocompression bonding of metallic interconnects that can range from tens to hundreds of microns in diameter. These techniques can add residual stress to the system that can impact reliability, and fatigue over time from power cycling the devices can lead to thermomechanical and electrical failures. Data used to screen for manufacturing defects or to characterize the bond quality over time are critically important, as these data can both (a) indicate whether manufacturing processes are of sufficiently high quality and (b) help evaluate physical changes that may occur after the assembly is in use.

To understand how bond quality is affected by fabrication processes as well as assembly operations, more advanced characterization and failure analysis methods are needed. Current techniques such as electron microscopy can provide extensive information about local bond quality at a region of

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interest, but they are destructive and require direct line-of-sight access to the failure region. Methods such as confocal scanning acoustic microscopy offer a picture of debonded regions, but are resolution limited. Recent work has shown that nondestructive evaluation of bond quality can be achieved with high spatial resolution using Brillouin-Mandelstam light scattering spectroscopy to probe energies in acoustic phonons and velocities of Rayleigh acoustic waves at interfaces.

Interrogating the thermal properties of a bump bond offers another interesting alternative to the conventionally used techniques to assess bond quality. For example, the ability of an interface to conduct heat, as measured by a calculated thermal boundary conductance (TBC), can be used as a measure of bond quality. In order to obtain spatially varying information about bond quality, maps of the TBC at boundaries of interest are desirable. Pump–probe thermoreflectance techniques have a previously demonstrated ability to map thermal properties of materials, including rich literature on using time-domain thermoreflectance (TDTR) for thermal conductivity mapping near the surface of a sample, as well as mapping TBC between thin films. In particular, frequency-domain thermoreflectance (FDTR) has been shown to be sensitive to subsurface interfaces located up to hundreds of microns below the surface of semiconductor materials, opening the door to damage detection on scales not possible with TDTR.

To process FDTR data, analytical solutions for time-harmonic temperatures based on Hankel transforms, as well as numerical simulations for cylindrically symmetric geometries, have been successful at determining thermophysical properties. Recent work has combined these techniques to better ascertain depth sensitivity of FDTR. However, more complicated geometries, such as those in HI systems, remain elusive for several reasons. First, with the high frequencies involved (often up to 60 MHz), the finite element method (FEM) requires a highly refined mesh, resulting in many degrees of freedom and an extreme computational burden. Second, even with a capable software infrastructure, defects in a real sample will cause discrepancies between simulation and experiment that may be difficult to understand for irregular geometries. Third, in a geometrically complex system without radial symmetry, each FDTR measurement point can contain information about multiple features simultaneously. Recent work has shown success integrating FEM simulations into conventional fitting routines for FDTR measurements applied to geometries with varying lateral dimensions. Still, separating the effect of each individual feature in a fully 3D geometry presents a significant challenge.

Using FEM software optimized for high-performance computing (HPC) clusters in tandem with gradient-based inverse methods can address both computational and geometric challenges. With HPC clusters, simulations with tens to hundreds of millions of degrees of freedom become tractable. Gradient-based inverse methods can then adjust the design parameters for successive simulations. In the case of FDTR, gradient-based methods can be used to adjust an arbitrary number of thermal conductivities and volumetric heat capacities in each simulation. Comparing how the thermal properties have changed in each region of a discretized geometry can then help identify regions of high or low bond quality.

In this work, we develop gradient-based optimization techniques to interpret FDTR data maps and extract TBCs. The remainder of this article is organized as follows. First, we present the governing equations for the FEM simulation of FDTR. Next is a description of the theoretical framework for gradient-based optimization as applied to temperature simulations in the frequency domain with unknown thermophysical properties. We describe the setup and process used to obtain experimental FDTR data, which we use as the input for FEM simulations in the Sierra/SD structural dynamics code coupled with the Rapid Optimization Library to invert for thermophysical properties. Finally, we summarize the work and discuss avenues of further research.

2. GOVERNING EQUATIONS

The governing partial differential equation (PDE) for heat diffusion is

\[ \rho c_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = \dot{q}_v(r, t), \]

where \( r \) is the position, \( t \) is the time, \( T \) is the temperature, \( \rho \) is the density, \( c_p \) is the specific heat capacity, \( k \) is the thermal conductivity, and \( \dot{q}_v \) are volumetric heat sources. Equation 1 is subject to the temperature, heat flux, and convection conditions

\[ T = T_0(r) \text{ on } S_T, \]

\[ -\kappa \frac{\partial T}{\partial n} = \dot{q}_h(t) \text{ on } S_h, \]

\[ -\kappa \frac{\partial T}{\partial n} = h(T - T_\infty) \text{ on } S_h, \]

respectively, where \( T_0 \) is a prescribed temperature on boundary surface \( S_T \), \( \dot{q}_h \) is a prescribed heat flux on boundary surface \( S_h \), \( T_\infty \) is the known temperature of a surrounding convective medium, \( h \) is the heat convection coefficient on boundary surface \( S_h \), and \( \partial T/\partial n \) is the normal component of the temperature gradient on the surface.

For FDTR, only the time-harmonic component of the temperature is relevant. For a time-harmonic temperature with angular frequency \( \omega \), we have

\[ T(r, t) = \frac{1}{2} \hat{T}(r) e^{-i\omega t} + \text{c. c.}, \]

where \( \hat{T} \) is the complex temperature amplitude and c.c. denotes complex conjugate. With the further simplifying assumptions of constant thermal conductivity and adiabatic boundaries except for an applied heat flux, eq 1 becomes

\[ -i \omega \rho c_p \hat{T} - k \nabla^2 \hat{T} = 0 \]

subject to

\[ -\kappa \frac{\partial \hat{T}}{\partial n} = -i \omega \dot{q}_h \text{ on } S_h, \]

\[ -\kappa \frac{\partial \hat{T}}{\partial n} = 0 \text{ otherwise.} \]

Adiabatic boundaries are used because they are most applicable to the experimental samples in which solid materials with high thermal conductivity are surrounded by air with much lower thermal conductivity.

In our formulation of the discretized problem with \( N \) nodes in domain \( \Omega \), we have
\[ \hat{T}(r) = \sum_{i=1}^{N} \hat{T}_i \Psi_i(r), \]

where \( \hat{T}_i \) is the temperature value at node \( i \) and \( \Psi_i \) is the finite element shape function. The discrete weak form can then be written as

\[ g(\hat{T}, p) = [K(p) - i\omega C(p)]\hat{T} - f = 0, \]

where \( p \) is a vector denoting material properties in each portion of the domain, \( K \) and \( C \) are global thermal conductivity and heat capacity matrices, respectively, and \( f \) and \( g \) are generalized forces acting on the boundary of the domain. The thermal conductivity, heat capacity, and generalized forces are written as

\[ K(p) = \int_{\Omega} \kappa(p) \nabla \Psi \cdot \nabla \Psi^T \, d\Omega, \]
\[ C(p) = \int_{\Omega} \rho(p) c(p) \Psi \Psi^T \, d\Omega, \]
\[ f = -\int_{\partial\Omega} \kappa q \cdot n \Psi^T \, dS, \]

where \( q \) and \( n \) are the heat flux and unit normal, respectively, at the boundary \( \partial\Omega \), and \( \Psi \) is the vector of finite element shape functions.

3. INVERSE METHOD

3.1. Gradient-based Inverse Framework. We formulate the determination of thermal material properties as a PDE-constrained optimization problem to be solved using the adjoint method.\(^{31}\) The problem is written as

\[ \min_{\hat{T}, p} \mathcal{J}(\hat{T}, p), \]

subject to \( g(\hat{T}, p) = 0, \)

where \( \hat{T} \) is the state vector containing real and imaginary parts of the temperature, \( p \) denotes the inverse parameters, \( g \) is given by eq 10, and \( \mathcal{J} \) is the objective function. To solve the inverse problem, we define the Lagrangian functional \( \mathcal{L} \) as\(^ {32}\)

\[ \mathcal{L}(\hat{T}, p, w) : = \mathcal{J} + w^T g, \]

where \( w \) is a vector of Lagrange multipliers. From eq 16, the first-order optimality conditions are found to be

\[ \mathcal{L}_{\hat{T}} = \frac{\partial \mathcal{J}}{\partial \hat{T}} + g^T w = 0, \]
\[ \mathcal{L}_p = \frac{\partial \mathcal{J}}{\partial p} + g^T w = 0, \]
\[ \mathcal{L}_w = g = 0, \]

where subscripted variables indicate derivatives with respect to those variables. \textit{Equation 19} simply restates the forward problem, which is solved at each iteration of the inverse problem to obtain an updated objective function value. The adjoint solution \( w \) is found by solving eq 17, the gradient \( \mathcal{L}_p \) is found from eq 18, and both \( w \) and \( \mathcal{L}_p \) are used to determine material properties for the next iteration. The process is repeated until the objective function has been minimized, or the iterative changes in material properties become very small.

When the PDE constraint is satisfied for the design variables \( p \), the implicit function theorem can be used to condense the objective function to depend only on the design variables.\(^ {33}\)

Then, \( \mathcal{J}(p) \equiv \mathcal{J}[\hat{T}(p), p] \) is equivalent to \( \mathcal{L}_p \) and eq 18 can be written as

\[ \mathcal{J}_p = g^T + \frac{\partial \mathcal{J}}{\partial p}. \]

Differentiating the transpose of eq 10 with respect to the inverse parameters and substituting into eq 20 yields

\[ \mathcal{J}_p = \hat{T}^T(K(p) - i\omega C(p))w + \frac{\partial \mathcal{J}}{\partial p}. \]

When the thermal conductivity \( \kappa \) and heat capacity \( \rho c_p \) are allowed to vary element-wise in the discretized domain, the quantities \( K_p \) and \( C_p \) can be written for each element as

\[ K_p = \nabla \Phi_i \cdot \nabla \Phi_i = \frac{\kappa c_i}{\rho c_p}, \]
\[ C_p = \nabla \Phi_i \cdot \nabla \Phi_i = \frac{C_{c_i}}{(\rho c_p)}, \]

where \( N_e \) is the number of elements with unknown material properties.

3.2. Phase-Only Objective Function. A typical inverse problem may use data from many different points in a domain, with the objective function \( \mathcal{J} \) defined through differences between computed and measured data at each point via the \( L^2 \)-norm

\[ \mathcal{J} = \frac{1}{2} \sum_{n=1}^{N} (u_n^c - u_n^m)^2, \]

where \( N \) is the number of points and superscripts \( c \) and \( m \) refer to computed and measured data, respectively. For data resulting from multiple frequencies and multiple independent experiments, eq 25 can be summed to give

\[ \mathcal{J}_{tot} = \sum_{\ell=1}^{N_f} \sum_{i=1}^{N_e} \mathcal{J}^\ell_{ui}, \]

where \( N_f \) is the number of frequencies and \( N_i \) is the number of experiments.

However, the temperature throughout the domain is unknown in FDTR. Instead, we only have an aggregate measurement of the temperature through the probe beam, which can be described via the surface integral

\[ H = \int_S T(r) e^{-2i(\omega t - k_0 r)}/w_0 \, dS, \]

where \( r \) is the center of a Gaussian probe beam with beamwidth \( w_0 \). The discrete form of the surface integral is

\[ H = \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} \hat{T}(r_{ij}) e^{-2i(\omega t - k_0 r_{ij})}/w_0 (\Delta S)_{ij}, \]

where \( N_i \) is the number of nodes on the discretized measurement surface, \( N_j \) is the number of surface Gauss points associated with node \( j \), \( r_{ij} \) is the position of Gauss point \( ij \), and \( (\Delta S)_{ij} \) is the area associated with Gauss point \( ij \).
In the case where temperature phase lag is considered alone and temperature amplitude information is discarded—frequently true of FDTR measurements—a phase-only objective function is needed. The phase-only objective function $J$ for a single experiment can be defined as

$$J(\hat{T}) = \frac{1}{2} \sum_k \left[ (\cos \phi_{k}^m - \cos \phi_{k}^c)^2 + (\sin \phi_{k}^m - \sin \phi_{k}^c)^2 \right],$$

(29)

where $\phi_{k}^m$ and $\phi_{k}^c$ are the measured and computed phase values, respectively, for each frequency $k$. The computed terms in eq 29 are

$$\cos \phi_{k}^c = \mathfrak{R}(H_k)/|H_k|,$$

$$\sin \phi_{k}^c = \mathfrak{I}(H_k)/|H_k|,$$

(30)

where $\mathfrak{R}$ and $\mathfrak{I}$ denote real and imaginary part, respectively, and $|H_k|$ is the amplitude of the temperature integral.

Adjoint calculations require the derivative of the objective function with respect to the discrete state variable $\hat{T}_i$, written as

$$\frac{\partial J}{\partial \hat{T}_i} = \sum_k \left( \Delta \cos \phi_{k} \frac{\partial \cos \phi_{k}^c}{\partial \hat{T}_i} + \Delta \sin \phi_{k} \frac{\partial \sin \phi_{k}^c}{\partial \hat{T}_i} \right),$$

(31)

where $\Delta \cos \phi_{k}$ and $\Delta \sin \phi_{k}$ are defined as

$$\Delta \cos \phi_{k} = \cos \phi_{k}^m - \cos \phi_{k}^c,$$

$$\Delta \sin \phi_{k} = \sin \phi_{k}^m - \sin \phi_{k}^c.$$

(32)

The real and imaginary parts of $\partial J / \partial \hat{T}_i$ are then

$$\Re\left(\frac{\partial J}{\partial \hat{T}_i}\right) = \sum_k \left( \frac{1}{|H_k|^2} \Re(H_k) \Delta \cos \phi_{k} + \frac{\Re(H_k) \Im(H_k)}{|H_k|^3} \Delta \sin \phi_{k} \right) \frac{\partial H_k}{\partial \hat{T}_i},$$

$$\Im\left(\frac{\partial J}{\partial \hat{T}_i}\right) = \sum_k \left( \frac{1}{|H_k|^2} \Im(H_k) \Delta \cos \phi_{k} + \frac{\Re(H_k) \Im(H_k)}{|H_k|^3} \Delta \sin \phi_{k} \right) \frac{\partial H_k}{\partial \hat{T}_i},$$

(34)

and $\partial H_k / \partial \hat{T}_i$ is written as

$$\frac{\partial H_k}{\partial \hat{T}_i} = \psi(\tau) \exp^{-2i(k\hat{T}_i - \omega \hat{T}_i)} \left(\Delta S\right)_k.$$

(35)

With $\partial J / \partial \hat{T}_i$ known, the adjoint solution $\mathbf{w}$ can be obtained from eq 17.

4. EXPERIMENTAL DESIGN

Exercising the inverse method described in Section 3 requires data from FDTR experiments. In this work, a wide-bandwidth FDTR system is used to periodically heat a sample using a pump beam with frequency $f_{\text{pump}} = 1$ kHz to 60 MHz and beam radius $w_{\text{pump}} = 3.46 \mu m$ [blue Gaussian in Figure 1a]. The heat dissipates into the sample with a thermal penetration depth $\delta_{\text{th}}$ written as

$$\delta_{\text{th}} \approx \frac{\kappa}{\sqrt{\rho C_{\text{p}} f_{\text{pump}}}}.$$

(36)

The surface temperature $T_{\text{surf}}$ changes as a result of heat dissipation, depending on $\delta_{\text{th}}$ and therefore on both the sample thermal properties and $f_{\text{pump}}$. To improve the thermoreflectance signal, the sample is typically coated in a metallic transducer layer that enables $T_{\text{surf}}$ to be monitored by a continuous wave probe beam [green Gaussian in Figure 1a] with a beam radius $w_{\text{probe}} = 2.75 \mu m$. In this study, the green and blue lasers are coaxially aligned. The modulated surface temperature due to laser pumping modifies the surface reflectance and therefore the reflected probe signal, which phase-lags the incident excitation by $\theta$. The phase lag can be quantified through subtraction of the system’s phase accumulation.

FDTR is often implemented as a characterization method to extract thermal properties of a sample. Experimentally, the method involves...
By sweeping \( f_{\text{pump}} \) measuring \( \theta( f_{\text{pump}}) \) and fitting \( \theta( f_{\text{pump}}) \) to the frequency-domain heat diffusion equation evaluated in a radially symmetric geometry to extract thermal properties of interest.\(^{35,36}\) By raster-scaning the sample underneath the FDTR microscope, hyperspectral 3-dimensional data cubes are obtained to relate the depth-dependent thermal properties of the sample to lateral spatial coordinates.

In this work, the sample of interest consists of bulk gallium nitride (GaN) bonded to commercial diamond (Diamond Foundry) through a thermal compression bond. Prior to bonding, the GaN and diamond are coated in an e-beam evaporated TiAu film (5 nm/120 nm). The film-coated surfaces are cleaned in a PlasmaTherm RIE chamber using Ar plasma at 100 W for 30 seconds. The film sides of each die are brought into close contact and lightly pressed together to evacuate the majority of the air from between the surfaces. The die pair is then loaded into an EVG wafer bonder and subjected to a 2 kN force bond for 15 seconds at room temperature to promote a cold weld of the gold surfaces. The GaN is then thinned and polished to a thickness of \( d_2 \approx 5 \mu m \) [see Figure 1a].\(^{37}\) Finally, FDTR is used to quantify \( G_2 \) with the TBC indicating the interface quality.

Figure 1b presents a hyperspectral FDTR \( \theta \)-data cube of the GaN-diamond material system. At each \( x, y \)-pixel, an FDTR measurement in the range of \( f_{\text{pump}} = 1 \) kHz to 60 MHz is obtained for depth-dependent thermal characterization. For example, at 60 MHz the Au transducer layer is predominantly sensed, while at 1 kHz, FDTR penetrates approximately 100 \( \mu m \) into the diamond substrate. Clear spatial variations in the FDTR \( \theta \)-data cube correspond to a spatially varying thermal system. Minimal variation at 1 kHz (\( \delta_\theta > 0.1 \) mm) suggests that the diamond layer is spatially invariant, and minimal variation above 1.5 MHz (\( \delta_\theta = 3.3 \) \( \mu m \)) suggests that the Au/GaN layers are only slightly spatially variant. Conversely, \( \theta( f_{\text{pump}}) \) between 39 and 736 kHz shows a thermal feature, most clearly seen at \( f_{\text{pump}} = 170 \) kHz (\( \delta_\theta = 9.7 \) \( \mu m \)) as shown in Figure 1c, which looks through the GaN-diamond interface. Spatial variations of nearly 5\% are seen at length scales of approximately 10 \( \mu m \). Here, \( \theta \) values closer to zero (i.e., red regions) indicate better thermal transport and vice versa for more negative values. Thus, FDTR is capturing thermal defects at the GaN-diamond bond.

Figure 2a provides FDTR data extracted from an unbonded point and a bonded region shown in Figure 1c. The spatial variation observed is clearly isolated between \( f_{\text{pump}} = 9 \) kHz and 1 MHz suggesting that the effect is subsurface. In fact, the value of \( f_{\text{pump}} \) that senses at the GaN-diamond interface (approximately 5 \( \mu m \) below the surface) at one \( \delta_\theta \) is approximately 25 kHz from eq 36, which is within the frequency range where the suspected bonded and unbonded differences arise.

For further insight, the FDTR data can be fit to the radially symmetric heat diffusion equation in the frequency domain. The thermal properties of the Au transducer layer are determined via FDTR calibration of the same layer on SiO\(_2\) and confirmed by a four-point probe.\(^{38}\) The analysis begins with the unbonded point data, where the measurement is sensitive to \( G_1, \kappa_G, d_G, \) and \( G_2.\) Fitted values for these parameters, including uncertainties,\(^{39}\) are \( G_1 = 66.5 \pm 4.4 \text{ MW/m}^2 \text{K}, \kappa_G = 119 \pm 9.5 \text{ W/m}^\circ \text{K}, d_G = 4840 \pm 180 \text{ nm}, \) and \( G_2 = 3.84 \pm 0.23 \text{ MW/m}^2 \text{K}.\) These values are shown in Table 1. Here, the value of \( G_2 \) indicates a poor thermal interface (i.e., an unbonded interface). The ability of FDTR to extract each parameter for the unbonded interface analysis can be confirmed by inspecting the sensitivity curves\(^{38}\) shown in Figure 2b. We find that the peak sensitivities for all four parameters are above the system noise floor (~0.2\%) and are centered at distinct, well-separated frequencies: \( S_\kappa = 8.2\% \) at 3.3 MHz, \( S_\kappa = 5.4\% \) at 420 kHz, \( S_{d_G} = 15.3\% \) at 46 MHz, and \( S_{\delta_\theta} = 2.7\% \) at 62 kHz.

We now move to the bonded region data given the known thickness \( d_2 \) from the unbonded interface analysis. Fitting yields values of \( G_1 = 78.6 \pm 5.4 \text{ MW/m}^2 \text{K}, \kappa_G = 124 \pm 9.3 \text{ W/m}^\circ \text{K}, \) and \( G_2 = 100 \text{ MW/m}^2 \text{K},\) corresponding to a good thermal bond. These values are listed in Table 2. FDTR sensitivity over a bonded region changes, as shown in Figure 2c. Here, \( S_\kappa \) and \( S_{\delta_\theta} \) have strong and unique sensitivities, while those of \( S_{d_2} \) and \( S_{\delta_\theta} \) overlap near 300 kHz: \( S_{d_2} = 3.8\% \) at 295 kHz, \( S_{\delta_\theta} = 15.3\% \) at 46 MHz, and \( S_{\delta_\theta} = 1.0\% \) at 330 kHz. While simultaneous fitting for \( d_2 \) and \( G_2 \) does not result in a converged fit, fixing \( d_2 \) based on the unbonded point analysis enables estimation of \( G_2.\) We conservatively estimate that the well-bonded value for \( G_2 \) is above

![Figure 2](https://www.acsami.org)

**Figure 2.** (a) FDTR data extracted from the hyperspectral data cube from the bonded region and unbonded point shown in Figure 1c. The data are then fit to the radially symmetric, frequency-domain heat diffusion equation based on the parameters shown in Tables 1 and 2. (b) Sensitivity curves generated for the unbonded fitted values in Table 1, indicating that FDTR has good sensitivity to \( G_2, G_1, d_2, \) and \( \kappa_G.\) (c) Sensitivity curves generated for the bonded fitted values in Table 2, indicating that FDTR has good sensitivity to \( G_2, G_1, \) and \( \kappa_G \) when \( d_2 \) is fixed at the unbonded value.

| Table 1. Unbonded Model Parameters (Fitted Parameters Bolded) |
| --- | --- | --- | --- | --- |
| material | \( \rho C^0_p [\text{MJ/m}^2\text{K}] \) | \( \kappa [\text{W/m}^\circ\text{K}] \) | \( d [\text{nm}] \) | \( G [\text{W/m}^2\text{K}] \) |
| Au (i = 1) | 2.48\(^{39a}\) | 188\(^a\) | 134\(^a\) | 66.5 \pm 4.4 |
| GaN (i = 2) | 2.52\(^{39b}\) | 119 \pm 9.5 | 4840 \pm 180 | 3.84 \pm 0.23 |
| diamond (i = 3) | 1.73\(^{31c}\) | 2500 \(^b\) | 5 \times 10\(^{1c}\) | |

\(^{a}\)Fitted from SiO\(_2\) calibration samples. \(^{b}\)Fitted from bulk diamond sample. \(^{c}\)Manufacturer specification.

| Table 2. Bonded Model Parameters (Fitted Parameters Bolded) |
| --- | --- | --- | --- | --- |
| material | \( \rho C^0_p [\text{MJ/m}^2\text{K}] \) | \( \kappa [\text{W/m}^\circ\text{K}] \) | \( d [\text{nm}] \) | \( G [\text{W/m}^2\text{K}] \) |
| Au (i = 1) | 2.46\(^{39a}\) | 188\(^a\) | 134\(^a\) | 78.6 \pm 5.4 |
| GaN (i = 2) | 2.52\(^{39b}\) | 124 \pm 9.3 | 4840 | >100 |
| diamond (i = 3) | 1.73\(^{31c}\) | 2500 \(^b\) | 5 \times 10\(^{1c}\) | |

\(^{a}\)Fitted from SiO\(_2\) calibration samples. \(^{b}\)Fitted from bulk diamond sample. \(^{c}\)Manufacturer specification.
100 MW/m²·K given FDTR’s sensitivity to the GaN-diamond interface at 5 μm thickness. It should be noted that $G_i > 100$ MW/m²·K is maintained when propagating uncertainty in $\delta_i$ through the fitting analysis. However, the precise quantification of this value requires a more detailed uncertainty analysis that will be discussed in future work.

5. RESULTS

5.1. Inversion of Point Measurement Data. With the FDTR phase data described in Section 4, our first goal is to verify the inversion algorithm. The phase data are obtained from a 200 μm by 200 μm specimen and includes 20,000 measurement points at 16 frequencies. Each of the measurement points may be considered a separate experiment, and we can use as many as necessary to formulate the objective function with eqs 26 and 29 for the region of interest. The finite element mesh used to model FDTR is the stadium geometry shown in Figure 3 with a major axis of 280 μm, a minor axis of 240 μm, and layer thicknesses from top to bottom of 130 nm, 5 μm, 100 nm, and 100 μm. A more refined central region with characteristic lateral dimension $h \approx 1$ μm and a coarser surrounding region with $h \approx 16$ μm result in 55,825 quadratic hexahedral elements for a total of 231,537 nodes.

We select three of the 20,000 measured points for verification. The points are chosen from relatively homogeneous regions in the phase data, showing little variation from the surrounding points. This choice allows for the use of a separate mesh for each data point, with homogeneous thermal properties in the unknown layer and $N_i = 1$ for each inversion. The first location is chosen over a region that appears well bonded with thermal properties of the unknown block assumed to be the same as those in the GaN layer. The close agreement between simulated and measured data supports this assumption (location 1 in Figure 4). Then, since the measurements at the second and third points differ from the phase data for a well bonded layer, we infer thermal properties of the unknown layer by minimizing the phase objective function using a line-search-based quasi-Newton method with bound constraints on the thermal properties. The inferred thermal conductivities are 1.784 W/(m·K) for the second point (location 2 in Figure 4) and 0.472 W/(m·K) for the third point (location 3 in Figure 4). Converted to TBC = $\kappa L$, where $L$ is the thickness of the unknown layer, the TBCs are 17.84 and 4.72 MW/m²·K, respectively. Since the unknown block is very thin, the specific heat in the unknown layer has no apparent effect on the simulated phase data. Close agreement between the simulated and measured data suggests a bond of intermediate quality at the second location and poor quality at the third location.

5.2. Inversion of Line Measurement Data. In some areas of the measured sample, the approximation of locally homogeneous thermal properties appears inappropriate due to lateral variations in the measured phase values. To probe one such area, we choose a region showing larger phase variation and use measurements along a 1D line to infer unknown material properties. To accurately model the phase variation, we use a heterogeneous model in which thermal properties are allowed to vary spatially (i.e., element by element) in the unknown layer of the mesh. Examining the map in Figure 1c, we select a 40 μm line from $(x, y) = (60, 120)$ to $(100, 120)$ and use measurements at evenly spaced points along this line. This line is chosen because
there is a clear variation in the x-direction and much less in the y-direction. We use the same FEM mesh and inversion algorithm as those in Section 5.1. However, we now invert using data from all points along the line simultaneously, with the phase measurements extending from 20 μm left of the center to 20 μm right of the center on the top surface of the geometry in Figure 3.

Figure 5 shows measurement locations and a 2D cross section of inferred thermal conductivity values around the measurement line with black dots representing the locations of the point measurements. Inferred thermal conductivity along the measurement line is shown in Figure 6a for two different measurement spacings: sparse ($N_e = 11$ measurement points, solid line) and dense ($N_e = 41$ measurement points, dashed line). Inversion results show that there are three distinct areas of thermal conductivity: less than 1 W/m·K (unbonded), greater than 10 W/m·K (bonded), and 1–10 W/m·K (partially bonded). Converted to TBC, these values are less than 10 MW/m²·K, greater than 100, and 10–100 MW/m²·K. These ranges agree with the values reported in Tables 1 and 2, as well as with values reported in existing literature. While deviations exist in the partially bonded regions, the inversions using sparse and dense measurement data show good agreement, suggesting an accurate inversion.

We observe that due to the choice of a 1D line for the measured data, the thermal conductivity in Figure 5 shows a high degree of symmetry but that the material properties vary significantly off the measurement axis. For a more complete 2D map of thermal material properties, we would need a grid of measurement points and a correspondingly larger domain for the FEM mesh. Thermal property inversion over larger domains warrants further study. In addition, note that from the pixelation shown in Figure 5, the number of unknown material properties is significantly greater than the number of measurement points. This discrepancy could result in overfitting due to the inverse problem being underconstrained. Further research is needed to determine the effect of “smoothing” the material properties such that no pixel is independent of its surroundings, which would likely provide a more physically accurate picture of the thermal conductivity in the unknown layer.

Finally, we compare with the results from a locally homogeneous assumption as in Section 5.1 using the same 1D line segment but considering the phase at each point independently from the others, and we invert for the material properties in the entire layer instead of element by element. Inversion results are shown in Figure 6b. Comparing with Figure 6a, we observe that the locally homogeneous inversion does not effectively differentiate between unbonded and partially bonded regions. Specifically, the locally homogeneous inversion settles at a thermal conductivity around 1 W/m·K for all locations on the line past 10 μm, suggesting that it underperforms in unbonded areas.

6. CONCLUSIONS

We have presented a formulation to determine unknown thermal material properties using phase data from FDTR. Furthermore, we have demonstrated the use of large-scale gradient-based optimization in selecting material properties for several test cases using measured data from an actual FDTR.

Figure 6. (a) Thermal conductivity distribution along the measurement line using heterogeneous model inversion using dense (dashed line) and sparse data (solid line). (b) Thermal conductivity distribution along the measurement line using a locally homogeneous inversion.
experiment. While the test cases shown in this work are relatively simple, the same techniques can be readily applied to more complicated questions about bond quality.

As mentioned in Section 5, one avenue for further research is to use phase data from a larger region of the sample. The two inversion examples in this work were selected for testing purposes due to their lower computational burden: single-point measurements over relatively homogeneous regions and measurement points along a line to capture variation in a single direction. An important next step is to use a grid of phase measurements to obtain a 2D map of unknown thermal properties. While gradient-based optimization allows for an arbitrary number of unknown thermal properties without a corresponding increase in computational overhead, it is not without challenges. First, the method described in Section 3.1 does not necessarily find the globally optimal solution to the inverse problem. Material property changes alter the system matrices in the FEM simulation, resulting in a nonconvex optimization with local minima. Second, each new measurement point represents another experiment, and hence, an additional forward solve that must be performed before the next iteration of thermal properties can be selected. The Sierra/SD code is written for use on high-performance computing (HPC) clusters, which can facilitate many additional simulations, even for more refined meshes. Still, the use of hundreds or thousands of measurement locations will increase the time needed to arrive at a full thermal property map, especially as we examine bond quality in larger regions of interest.

Another issue worth investigating is the effect of “smoothing” the thermal properties of the unknown layer. Variation in the thermal properties of the unknown layer is necessary to accurately represent the sample, which is unlikely to have large regions of uniform bond quality. However, since the elements in the FEM mesh are artificial, allowing each to be completely independent of its surroundings may allow for nonphysical checkerboard patterns. In addition, with many more material parameters than measurement points, the problem may be under-constrained, resulting in a map of thermal properties that is not unique. Further work is needed to choose an appropriately sized parameter that results in more physically reasonable damage patterns while capturing the typical feature size of lower quality bonds.

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**Notes**

The authors declare no competing financial interest.

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