Abstract—A least-squares parameter estimation algorithm is designed to extract the thermal conductivity of metallic nanowires using a nanofabricated microelectrothermal test structure. The device is a thermal analog of a bridge circuit, such as is commonly used to measure electrical impedance. A resistive heater is positioned symmetrically between two temperature sensors. A nanowire array extends from the heater to one sensor, unbalancing the bridge temperatures. The least-squares cost function exploits the underlying symmetry of the thermal bridge circuit, reducing sensitivity to parasitic thermal conductances and other uncertain parameters. The algorithm is demonstrated on a series of aluminum nanowire arrays with varying nanowire widths. The results are shown to be consistent with predictions made using the electron thermal transport analogy.

I. INTRODUCTION

Electricity and thermal properties are critical to state-of-the-art nanometer-scale devices. The electrical resistivity ($\rho$) of metallic films is known to rise considerably from bulk values as film thickness decreases [1]. This is generally attributed to reduced grain size [2] and increased influence of surface scattering [3]. Fabrication of nanowires and direct measurement of electrical resistivity has been reported for a number of technologically important materials [4,5] and $\rho$ found to increase rapidly for structures below several hundred nanometers in thickness and width, attributed to even greater impact of surfaces and grains.

Thermal conductivity ($\kappa$) is important in densely packed devices where heat dissipation is critical to reliability. Several studies have established that $\kappa$ decreases in metallic thin films relative to the bulk values [6,7]. There are many techniques for measurement of thin film thermal properties [1,5-10]. In the 3ω technique an AC current is applied to the heater/sample/sensor structure, and a lock-in amplifier used to detect the current or voltage output signal at a particular frequency [1,5,11]. An alternative, taken in this paper, is based on steady state joule heating with DC current excitation [12,13]. Independent of the technique employed, direct measurement of $\kappa$ for nanoscale structures is challenging, since thin films and wires are generally supported by a substrate, and parasitic thermal losses are significant relative to heat conduction through the feature. One indirect method for avoiding this problem is to obtain $\kappa$ by measuring electrical resistivity of the metal nanowire and assuming validity of the Wiedemann-Franz (W-F) law. In general, thermal transport is mediated by electrons and phonons, with the former dominant in metals, and the latter dominant in semiconductors and dielectrics [14]. The W-F law considers only the electronic contribution to $\kappa$, making W-F alone sufficient for calculation of total thermal conductivity only when thermal conduction by phonons is negligible. Recent measurements and calculations suggest that even in metals the phonon contribution can be significant in comparison to the electronic term in thin films and nanowires [15]. Thus a direct measurement technique is preferred over reliance solely on W-F.

A direct method is to perform thermal measurements on suspended films or nanowires [5,8,9,10]. This has the advantage of minimizing parasitic conductances, but is challenging due to fabrication difficulties. In this paper we report on the design and fabrication of a supported microelectrothermal device for direct measurement of thermal conductivity of metallic nanowires. The device is supported on a glass substrate, facilitating fabrication and subsequent processing. As described below, the device is analogous to a bridge circuit used to measure the impedance of electrical components, with the symmetry of the structure used to minimize the effects of parasitic conductance paths.

We construct a detailed electrothermal finite-element (FE) model of the measurement system. FE modeling has been shown to be a reliable tool for analysis of microfabricated thermal measurement systems [13,16,17]. For example, La Spina et al. use FE analysis to characterize the geometry of heat flow through their device [18]. However, FE analysis has not been widely exploited to actively assist in parameter extraction.

In this paper, a least-squares cost function is constructed incorporating the FE model. The FE model is an accurate representation in the immediate vicinity of the nanowires, but does not completely capture the thermal pathways from the device region to the ambient. We show that the cost function may be chosen to complement the features of the bridge circuit, so that the resulting thermal conductivity value is relatively insensitive to these modeling errors. The method developed here is applied to estimate the thermal

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conduction of Al nanowires. Three test cases are studied incorporating three nanowire widths. The thermal conductivities of the nanowires are extracted, and validated by comparison to electrical measurements and calculations based on the electron thermal transport analogy (ETTA), as reported elsewhere [15]. The agreement is excellent.

Section II briefly describes the measurement device. Section III presents the complementary data analysis algorithm used to estimate thermal conductivity of the sample. Section IV describes experiments on aluminum nanowires of varying sizes, and discusses the results. Section V examines the parameter estimation scheme in more detail. Some results on sensitivity of least-squares solutions are presented in an Appendix.

II. DEVICE DESIGN, FABRICATION, AND SIMULATION

A resistive heater is placed symmetrically between two resistance temperature detectors (RTDs). An array of metallic nanowires breaks the symmetry, partially bridging the gap between the heater and one RTD, designated the sample sensor, but not the other, which is designated the reference sensor. The purpose of the device is to measure the thermal properties of these nanowires, in particular their thermal conductivity. The electrically conductive arrays must be interdigitated in order to avoid short-circuiting the heater and the sample sensor.

To estimate the thermal conductivity of Al nanowires of three different widths and the same thickness and length, a series of devices is constructed. The heater and RTD structures are gold, the nanowires are aluminum, and the substrate is glass. Figure 1 shows a schematic of the device design, and a false-color scanning electron microscope (SEM) image of the fabricated structure.

The parameter extraction algorithm incorporates a detailed numerical model of the device. We construct a three-dimensional FE simulation using a commercial multiphysics package [19]. The FE model includes two physics domains, using the heat equation to solve for the temperature distribution and Laplace’s equation to solve for the potential and the current. The domains are coupled through the temperature dependence of the electric resistivity, and the joule heating due to current.

In this model, all material and design parameters other than the nanowire thermal conductivity are either directly determined or based on accepted literature values. Table I summarizes the most important material properties. The FE model geometry is customized for each specific device based on high-resolution SEM images, reflecting, for example, the exact position of the nanowire arrays in relation to the heater and RTDs. The simulation also incorporates thermal barriers at material interfaces, particularly between the nanowires and the glass substrate [20]. For the temperature ranges relevant to our experiments, we may assume that thermal conductivities are independent of temperature [14]. Effects of convection and radiation are included in the simulation for completeness, however these are found to be negligible; conduction is the primary mechanism of heat transfer at these length scales and operating temperatures [13]. Far from the device the substrate is assumed to be at ambient temperature. Due to the large size of the substrate compared to the characteristic feature dimension, it is impractical to include the entire substrate in the FE model. A section 100 μm × 100 μm square and 50 μm deep is used. A portion of the mesh is shown in Fig. 2(a). The result from a representative simulation is shown in Fig. 2(b) for the 100 nm wide nanowires. The temperature distribution is asymmetric due to the presence of the nanowires.

### Table I: Primary Material Properties for Device Simulation

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glass substrate $\chi^\phi$</td>
<td>0.96 W/mK</td>
<td>[14]</td>
</tr>
<tr>
<td>Al/glass interface $K^m$</td>
<td>$2.87 \times 10^7$ W/mK</td>
<td>[20]</td>
</tr>
<tr>
<td>Heater/RTD $\rho^f$</td>
<td>$5.19 \times 10^7$ Ωm</td>
<td>measured</td>
</tr>
<tr>
<td>Heater and RTD TCR</td>
<td>0.00152</td>
<td></td>
</tr>
<tr>
<td>Al nanowire $\rho^f$</td>
<td>$7.44 \times 10^7$ Ωm</td>
<td>measured</td>
</tr>
<tr>
<td></td>
<td>$6.05 \times 10^7$ Ωm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$4.77 \times 10^7$ Ωm</td>
<td></td>
</tr>
</tbody>
</table>

* 75, 100 and 150 nm, respectively.

III. ALGORITHM DESIGN AND ANALYSIS

To minimize confusion between electrical and thermal properties, we discuss only electrical resistance and resistivity and thermal conductance and conductivity. The electrical resistances of the heater, sample RTD, and reference RTD are denoted $R_{H}^f$, $R_{S}^f$, and $R_{R}^f$, respectively. These are the measured outputs of the device. The input thermal power dissipated in the heater, $Q_s$, is also measured. Assume that the heater, sample, and reference RTDs are
each at uniform temperature, \( T_{H}, T_{S}, \) and \( T_{R} \), respectively, and let \( T_{0} \) denote the ambient temperature. Figure 3 depicts a lumped thermal circuit model.

![Fig. 3. Lumped thermal model showing bridge circuit structure.](image)

The thermal circuit is analogous to a Wheatstone bridge, commonly used for precise measurement of electrical impedance. The heat conduction paths from the heater to the reference RTD through the substrate and from the RTD to the ambient are represented by thermal conductances \( K_{0}^{th} \) and \( K_{1}^{th} \), respectively. By symmetry these values also apply to the sample-side RTD in the absence of a sample. The sample provides a parallel path for conduction from heater to sample RTD, represented by thermal conductance, \( K_{2}^{th} \). The thermal paths from the heater direct to ambient, either by convection and radiation at the surface or by conduction through the substrate, are neglected in this model. The actual heat flowing through these paths should be small, based on the small distance between the heater and sensors and the dominance of conduction over convection and radiation at the device length scale and operating temperatures.

For a balanced electrical bridge, the unknown impedance along one arm may be written as a function only of the known impedances in the other three arms. For an unbalanced electrical bridge, the unknown impedance is a function of the drive and bridge potentials as well as the known impedances. The thermal bridge is unbalanced by the sample conductance, where balance means that the sample sensor temperature, \( T_{S} \), is equal to the reference sensor temperature, \( T_{R} \). Denote temperature differentials by \( T_{X} = T_{Y} - T_{Z} \), where \( X \) and \( Y \) may be \( H, R, S, \) or \( 0 \), for the heater, sensor, sample, or ambient, respectively. The thermal analog of the drive potential is the temperature differential \( T_{H0} \), and that of the bridge potential is the temperature differential \( T_{SR} \). The bridge temperature imbalance is related to the driving temperature differential and the lumped thermal conductances by

\[
T_{SR} = \frac{K_{SR}^{th} K_{T}^{th}}{K_{0}^{th} + K_{SR}^{th} + K_{T}^{th}} T_{H0}.
\]

Unlike the usual case for electrical bridge circuits, none of the thermal conductances are known \( a \ priori \). Therefore we rewrite (1) in terms of \( Q \) and the temperature differentials and solve for \( K_{T}^{th} \) to yield,

\[
K_{SR}^{th} (Q, T_{H}, T_{S}, T_{R}, T_{0}) = \frac{T_{SR}}{(Q + T_{R} + T_{0}) T_{H0} T_{ISTHR}}
\]

Expression (2) cannot be used directly to obtain the nanowire thermal conductivity, both because of the approximations implicit in the lumped parameter thermal model and because the nanowire conductivity is not a straightforward function of the sample conductance. However (2) can serve as the basis for a least-squares cost function, and the nanowire thermal conductivity can be estimated by minimizing this function. Contained within the cost function is a detailed FE model of the device, as described above. Many aspects of the device can be captured accurately with such a model, while others, such as the conductance \( K_{0}^{th} \), may be more problematic. It is shown in Section V below that using (2) as the basis for a cost function significantly reduces sensitivity to \( K_{0}^{th} \) (and \( K_{ref}^{th} \)). The remainder of this section details the construction of the cost function.

Measurements of the heater and RTD resistances are made at a series of input power levels \( Q \). We use an overbar, \( \bar{\cdot} \), to denote a measured quantity. The heater, sensor, and reference resistances measured for the \( j^{th} \) input power level are \( \bar{R}_{H,j}^{ref}, \bar{R}_{S,j}^{ref}, \) and \( \bar{R}_{R,j}^{ref} \), respectively. We use a hat, \( \hat{\cdot} \), to denote an estimated quantity. For a given \( Q \), and an estimated parameter vector \( \hat{z} \) the FE simulation predicts the heater and RTD resistances. This map is represented by

\[
\left( \hat{R}_{H,j}^{th}(z), \hat{R}_{S,j}^{th}(z), \hat{R}_{R,j}^{th}(z) \right) = \Phi_{FE}(z, Q_{j}).
\]

Denote the true parameter vector by \( z^{*} \). We will refer to the \( \text{ideal case} \) for which the FE model perfectly predicts the device behavior and for which the measurements are exact with no noise or error. Then (3) will satisfy \( \hat{R}_{X,j}^{th}(z^{*}) = \bar{R}_{X,j}^{ref} \).

The temperatures \( T_{X} \) are not measured directly, but must be inferred from the electrical resistance of the heater and RTDs. This is done using a calibration function,

\[
\Theta_{X}(\bar{R}_{X,j}^{ref}) = T_{ref} \frac{\hat{\theta}_{X}^{th} - \hat{\theta}_{X,j}^{th}}{\hat{\theta}_{X,j}^{th}}.
\]

(4)

\( T_{ref} \) is a fixed reference temperature. The temperature coefficient of resistance (TCR) of the heater and the two RTDs, \( \hat{\theta}_{X} \) and a calibration parameter, \( \hat{\theta}_{X,j}^{ref} \), are fit based on calibration data. If the temperature of each component is uniform, as in the calibration experiment, then \( \Theta_{X} = T_{X} \). When the temperatures are not uniform, \( \Theta_{X} \) is an average value. Then (2) may be evaluated using (4), the FE simulation, and the parameter estimate \( \hat{z} \). To signify the dependence on the parameter estimate we denote this function by \( \hat{R}_{SR,j}^{th} \);

\[
\hat{R}_{SR,j}^{th}(z) = \frac{\hat{\theta}_{SR}^{th}(Q_{j}, T_{H}, \Theta_{H}(\bar{R}_{H,j}^{ref}(z)), \Theta_{S}(\bar{R}_{S,j}^{ref}(z)), \Theta_{R}(\bar{R}_{R,j}^{ref}(z)), T_{0}))}{\hat{\theta}_{SR,j}^{th}}.
\]

Alternatively, (2) may be evaluated using (4) and the measured resistances. To signify that it is solely dependent on the measurements, we denote this function by \( \hat{R}_{SR,j}^{th} \);

\[
\hat{R}_{SR,j}^{th}(\bar{R}_{H,j}^{ref}, \bar{R}_{S,j}^{ref}, \bar{R}_{R,j}^{ref}) =
\]

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The corresponding weighted least-squares cost function is

\[ J_K(z) = \sum_j w_j \left( \frac{\rho_{\text{samp},j}(z) - \rho_{\text{samp},j}(R_{R_{\text{h},j}}, R_{S_{\text{j},j}}, R_{R_{\text{j},j}})}{\rho_{\text{samp},j}(R_{R_{\text{h},j}}, R_{S_{\text{j},j}}, R_{R_{\text{j},j}})} \right)^2 \]  

(7)

where the weight \( w_j \) is the inverse of the variance of \( \rho_{\text{samp},j} \), computed by propagation of the variance in the resistance measurements through (6).

It may not be immediately clear that (7) is a suitable cost function for estimating \( \kappa_{\text{nw}} \). Here we briefly show that for the ideal case of perfect model and measurements, \( z^* \) minimizes \( J_K \). This follows from the fact that \( J \) is positive semidefinite, and that for the ideal case \( J_K(z^*) = 0 \). The first property is obvious from the definition. For the second property, note that in the ideal case \( \rho_{\text{samp},j}(z^*) = \rho_{\text{samp},j} \), implying that \( \Theta_K\left(R_{R_{\text{h},j}}, R_{S_{\text{j},j}}, R_{R_{\text{j},j}}\right) = 0 \), and therefore that \( \rho_{\text{samp},j}(z^*) = \rho_{\text{samp},j} \left( R_{R_{\text{h},j}}, R_{S_{\text{j},j}}, R_{R_{\text{j},j}} \right) \). We expect that the cost function will change continuously with small measurement and modeling errors, so the non-ideal case \( J_K \) should have a minimum near \( z^* \).

### IV. EXPERIMENTS AND DATA ANALYSIS

Heater drive currents \( I_{\text{p}} \) of 2.0, 2.5, and 3.0 mA were applied, and the corresponding drive voltage measured. The sample and reference RTD voltage differentials were measured for a 100 \( \mu \)A probe current. The ambient temperature \( T_0 \) was measured at the probe station chuck. From this measurement set can be derived the total heater joule heating, and the electrical resistance of the heater and sensors. The probe current value was chosen to allow an accurate resistance measurement (\( \pm 0.01 \) \( \Omega \)) while avoiding substantial self-heating (< 0.1 \( \degree C \)). The resistance measurement uncertainty of 0.01 \( \Omega \) is propagated through (6) to obtain the weights in (7).

Heater and sensor electrical resistance are related to temperature by the TCR of gold, \( a_{\text{Al}} \) which is constant over the temperature range of interest. Because the TCR of the gold film may differ from the bulk value, the calibration is performed using complete devices in a thermostated DI water bath over a temperature range from 22\( \degree C \) to 70\( \degree C \). The calibration is of the form (5). Linear regression is used to fit the value of \( \rho_{\text{Al}} \), which is the same for all components, and of \( \rho_{\text{Al}} \), which is the resistance of the specific component at the calibration reference temperature \( T_{\text{ref}} \).

While the function \( \Theta_K \) gives the component temperature only under the conditions of uniform component temperature, the calibrated value of \( \rho_{\text{Al}} \) is valid even if the temperature is nonuniform. Thus the value of \( \rho_{\text{Al}} \) determined in the calibration step is used in the FE device model. We obtain \( \rho_{\text{Al}} = 0.00152 \) K\(^{-1}\). The maximum drive current of 3.0 mA corresponds to temperature rises of \( \approx 100 \degree C \) for the heater and \( \approx 50 \degree C \) for the sensors.

The least-squares algorithm of Section III is applied to find \( z^* \)—here a scalar containing only the nanowire thermal conductivity, \( \kappa_{\text{nw}} \)—for Al nanowires having thickness of 100 nm and widths of 75, 100, and 150 nm. Equation (7) is minimized in a straightforward manner using the Matlab function \( \text{fminbnd} \) [21], with initial \( \kappa_{\text{nw}} \) estimate set to the bulk value. Because we have assumed in our model that the thermal conductivities are independent of temperature, each \( \rho_{\text{samp},j}(z) \) is independent of \( \rho_{\text{Al}} \), and so for each nanowire width we write \( \rho_{\text{samp},j} \). Figure 4 shows the value of \( \rho_{\text{samp},j}(z^*) \) compared to the \( \rho_{\text{samp},j} \left( R_{R_{\text{h},j}}, R_{S_{\text{j},j}}, R_{R_{\text{j},j}} \right) \) for the 100 nm nanowire. Error bars for the \( \rho_{\text{samp},j} \) are standard deviations corresponding to the resistance measurement accuracies propagated through (6). The simulation is consistent with the derived measurements to within experimental error. We note that the variances are large for low drive current, due to small temperature rises and correspondingly small changes in RTD resistance. Figure 5(b) shows the corresponding optimal estimates of \( \kappa_{\text{nw}} \) for the 75, 100, and 150 nm wide nanowires, which are 105, 115, and 140 W/mK respectively. The value of \( \kappa \) for bulk Al is 237 W/mK.

The chi-squared (\( \chi^2 \)) test [22] may be applied to the linearized least-squares problem near the optimal value, to evaluate whether the fit obtained by minimizing (7) is consistent with the model (5). A p-value is computed by integrating the probability density function associated with the \( \chi^2 \) distribution from the minimal cost function value \( J_K(z^*) \) to \( \chi^2 \) \( \rightarrow \) \( \infty \). The integral takes values from zero to one. Intermediate p-values, for example between 0.1 and 0.9, are consistent with a valid model. Very low p-values close to zero indicate that the model does not fit the data, while very high p-values close to one suggest that the model may be over-parameterized [22]. For the 100 nm nanowire case we have a p-value of 0.77, consistent with a valid model. The uncertainty in the least-squares \( \kappa_{\text{nw}} \) estimate may then be found from (A3), which gives \( \pm 3.2 \) W/mK.

The results obtained above are compared to values predicted by the electron thermal transport analogy (ETTA),
as follows: The electrical conductivity of the nanowires is measured, as shown in Fig. 5(a), and the Boltzmann transport equation is used to predict the dependence of the electrical conductivity on nanowire size by adjusting the grain boundary electron reflectivity parameter, $R$. The resulting value of $R$ is found to be consistent with literature values, and the fit, as shown in Fig. 5(a), is excellent. Next, the Wiedemann-Franz law is used in conjunction with bulk thermal and electrical properties of Al to obtain the electronic component of the nanowire thermal conductivity. Finally, the phonon component of the nanowire thermal conductivity is computed based on the Boltzmann transport equation [23]. The $\kappa_{nw}$ curve in Fig. 5(b) is the sum of the two terms. Further details of the ETTA-based analysis are reported elsewhere [15]. Agreement with the values obtained by the bridge device and least-squares parameter estimation algorithm is excellent.

V. COMPARISON OF COST FUNCTIONS

An obvious approach to estimating an optimal value for $\kappa_{nw}$ is to minimize the cost function

$$J_R(z) = \sum_j \left[ w_{S,j} (\hat{R}_{S,j}^e(z) - \bar{R}_{S,j}^e)^2 + w_{R,j} (\hat{R}_{R,j}^e(z) - \bar{R}_{R,j}^e)^2 \right]$$

where $z$ is $\kappa_{nw}$ and the weight $w_{X,j}$ is the inverse of the variance of $\bar{R}_{X,j}^e$. As desired, $J_R \geq 0$, and $J_R(z^*) = 0$ for the ideal case.

We proceed as in Section IV, minimizing (8) for the 100 nm wide nanowire case. Again we calculate the $p$-value associated with the $\chi^2$ test. However $J_R^*$ is much larger than $J_R^*$, and the corresponding $p$-value is less than $10^{-4}$, indicating that the observed measurements are improbable based on the FE model. We attribute the problems with estimating $\kappa_{nw}$ using $J_R$ to higher sensitivity to unmodeled parameters, as is now discussed.

We use (A6) to compute the sensitivity of the estimate of $\kappa_{nw}$ to three parameters that are potentially poorly known. The FE model described in Section II for the 100 nm nanowires is used. We set $z = [\kappa_{nw}, s, T_0, h]^T$. Here the scaling parameter $s$ determines the portion of the substrate in the FE model, where the dimensions of the modeled substrate are $2 \times 1 \mu m \times 2 \times 1 \mu m \times 1 \mu m$. Nominal $s$ is 50, but this choice is arbitrary. The ambient reference temperature $T_0$ is measured at the probe station chuck, and may differ in the glass substrate, which is a poor thermal conductor. The convective heat transfer coefficient at the device surface is $h$. The actual value of $h$ is poorly known, but 10 is a reasonable nominal choice [24]. These parameters all affect $K_0$, the conductance from the sensors to ambient, to which $J_R$ should be naturally insensitive. Cost function (7) exploits this insensitivity, while (8) does not. Sensitivity to errors in these parameters is found from (A6) for both (7) and (8). Table II gives the resulting sensitivities.

<table>
<thead>
<tr>
<th>s (\mu m)</th>
<th>T_0 (°C)</th>
<th>h (W/mK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal</td>
<td>50</td>
<td>22</td>
</tr>
<tr>
<td>Perturbed</td>
<td>55</td>
<td>32</td>
</tr>
<tr>
<td>$S_{s,h}$</td>
<td>9.427</td>
<td>36.3</td>
</tr>
<tr>
<td>$S_{s,K}$</td>
<td>0.531</td>
<td>0.265</td>
</tr>
<tr>
<td>$S_{s,h}/S_{s,K}$</td>
<td>0.056</td>
<td>7.3×10^{-3}</td>
</tr>
</tbody>
</table>

To compute $X$, each parameter is perturbed separately, with the others held at their nominal values.

*Both $J_R$ and $J_p$ are insensitive to $h$, and a large perturbation is needed for a detectable effect.

VI. CONCLUSIONS

We have demonstrated a method for design, fabrication, and analysis of supported microelectrothermal structures for making accurate measurements of thermal properties of conducting nanowires. The important problem of parasitic conductance through the substrate is addressed using a thermal bridge circuit in combination with a complementary least-squares parameter estimation scheme. A least-squares cost function is constructed incorporating a FE model of the operating device. The cost function may be chosen to complement the features of the bridge circuit, so that the
resulting thermal conductivity value is relatively insensitive to modeling errors. This has several advantages, including that the areas of the wafer far from the device need not be carefully modeled, saving effort in the modeling phase and reducing computational time during the optimization.

The method has been applied to the measurement of thermal conductivity in a series of Al nanowires of varying dimension. The results have been shown to be consistent with Boltzmann transport equation computations of phonon thermal conductivity in Al combined with ETTA-based predictions of the electronic contribution to the total thermal conductivity.

APPENDIX

Consider a set of $n$ measurements $\tilde{y} = [\tilde{y}_1, \tilde{y}_2, ..., \tilde{y}_n]^T$, and a model $\tilde{f}(z) = [\tilde{f}_1(z), \tilde{f}_2(z), ..., \tilde{f}_n(z)]^T$ that predicts the measurements based on a parameter vector $z = [z_1, z_2, ..., z_m]^T$. Define the vector of residuals, $\tilde{r}(z) = \tilde{y} - \tilde{f}(z)$. Now consider a nonlinear least-squares cost function,

$$J(z) = \sum w_i \tilde{r}_i^2(z) = \tilde{r}^T(z)W\tilde{r}(z).$$

(A1)

Write $\lambda = \sqrt{\lambda_i}$, $A = \text{diag} \{\lambda_1, \lambda_2, ..., \lambda_n\}$, and let $f(z) = \Lambda\tilde{f}(z)$. $\tilde{y} = \Lambda\tilde{x}$, and $r(z) = f(z) - \tilde{y}$. Then $J(z) = r(z)^T r(z)$. The optimal parameter value $z^*$ minimizes $J(z)$.

A necessary condition for $z^*$ to be a local minimum is that for any nearby $z$,

$$X^TX(z^* - z) = X^T(\tilde{y} - f(z))$$

where $X = \partial f/\partial z)|_{z^*}$. Abbreviating $\hat{\varepsilon} = z^*-z$ and $\hat{\varepsilon} = \tilde{y} - f(z)$, (A2) has solution $\hat{\varepsilon} = X^T \hat{\varepsilon}$, where $X^T$ is the Moore-Penrose pseudo-inverse of $X$ [25]. Then the optimal value $z^* = z + X\hat{\varepsilon}$. We partition $p = [p^T_-, p^T_+]^T$, where the elements of $z_+$ are the parameters of interest for estimation, and the elements of $z_-$ are model parameters that are neglected in the minimization scheme. We are concerned with uncertainty in the estimate of $z_+$ due to two factors, namely uncertainty in the measurements $\hat{\varepsilon}$ and uncertainty in the unmodeled parameters $z_-$. Partition $X$ as $X = [X_+, X_-]$, following the partition of $z$. That is, $X = \partial f/\partial z_+$, and $X = \partial f/\partial z_-$. We assume that $X_+^T X_+$ is invertible.

Solving the equation for $\hat{\varepsilon}$ gives

$$\hat{\varepsilon}_+ = X_+ (\hat{\varepsilon} - X_+ \hat{\varepsilon}_-).$$

(A3)

The variance $\Sigma_{\varepsilon}^2$ in $\hat{\varepsilon}_+$ due to the variance $\Sigma_{\varepsilon}^2$ in $\hat{\varepsilon}$ is [26],

$$\Sigma_{\varepsilon}^2 = (X_+^T X_+)^{-1} X_+^T \Sigma_{\varepsilon}^2 X_+ (X_+^T X_+)^{-1}$$

(A4)

We handle the term due to $\hat{\varepsilon}_-$ differently, because we assume that we do not know the variance in these parameters. We compute instead $S_{ij}$, the sensitivity of the estimate of the $j$th element of $\hat{\varepsilon}_+$ to the $k$th element of $\hat{\varepsilon}_-$. From (A3), we write the error in the estimate of $\hat{\varepsilon}_+$ due to errors in $\hat{\varepsilon}_-$:

$$e = X \cdot \hat{\varepsilon}_+,$$

$$S_{jk} = [X_+ X_-]_{(j,k)}.$$

(A5)

(A6)

REFERENCES


