Thermal boundary conductance accumulation and interfacial phonon transmission: measurements and theory

Ramez Cheaito,[1,*] John T. Gaskins,[1,*] Matthew E. Caplan,[1] Brian F. Donovan,[1] Brian M. Foley,[1] Ashutosh Giri,[1] John C. Duda,[1,2] Chester J. Szwejkowski,[1] Costel Constantin,[3] Harlan J. Brown-Shaklee,[4] Jon F. Ihlefeld,[4] Patrick E. Hopkins[1,†]

[1]Department of Mechanical and Aerospace Engineering, University of Virginia, Charlottesville, Virginia 22904, USA
[2]Current Address: Seagate Technology, Bloomington, MN 55435, USA
[3]Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807, USA
[4]Electronic, Optical, and Nanomaterials Department, Sandia National Laboratories, Albuquerque, NM 87185, USA

[*] these authors contributed equally to the paper
[†] author to whom correspondence should be addressed, email: phopkins@virginia.edu

This document includes the data plotted in Fig. 3 of the paper, the 4^{th} order polynomial coefficients used for the dispersion curves of aluminum, gold, and silicon, and listings of 3 MATLAB codes used to generate the plots in Figs. 1 and 4 in the paper.

SUPPLEMENTARY TABLE I. Thermal conductivity and thermal boundary conductance values for different metals on Si measured by TDTR. These values are plotted in Fig. 2 of the manuscript.

Metal	Θ (K)	ω_c (Trads^{-1})	κ (Wm^{-1}K^{-1})	h_K (MWm^{-2}K^{-1})
Au[b]	165	29.5	138.0 $\pm$ 11.2	45.8 $\pm$ 1.6
Pt[a]	240	37.7	125.5 $\pm$ 15.4	123.0 $\pm$ 7.3
Pt[b]	240	37.7	121.7 $\pm$ 14.9	150.3 $\pm$ 9.8
Pd[a]	274	44.0	129.5 $\pm$ 16.5	120.9 $\pm$ 11.0
Pd[b]	274	44.0	121.0 $\pm$ 16.9	162.0 $\pm$ 17.4
Au w/2 nm Ti[b, c]	420	47.8	101.2 $\pm$ 12.1	207.0 $\pm$ 14.1
Au w/15 nm Ti[b, c]	420	47.8	107.6 $\pm$ 7.1	170.0 $\pm$ 8.1
Au w/40 nm Ti[a, c]	420	47.8	130.0 $\pm$ 20.0	178.0 $\pm$ 19.0
Al[b]	428	60.0	151.0 $\pm$ 16.6	215.0 $\pm$ 15.5
Ni[a]	450	56.5	137.3 $\pm$ 14.4	197.0 $\pm$ 12.3
Mo[a]	450	51.8	135.0 $\pm$ 9.7	159.0 $\pm$ 7.1
Ru[a]	600	48.7	159.3 $\pm$ 13.1	190.3 $\pm$ 11.6

[a] Metal deposited at Sandia National Labs
[b] Metal deposited at the University of Virginia
[c] Different Si wafer

We use a 4$^{\text{th}}$ order polynomial to express the phonon dispersion in aluminum, gold, and silicon. Thus, $\omega_j(k) = a_j k^4 + b_j k^3 + c_j k^2 + d_j k + e_j$. Where ω_j is the angular frequency, j represents the phonon branch, k is the wavevector, and a_j, b_j, c_j, d_j, and e_j are constants listed in Supplementary Table II.

SUPPLEMENTARY TABLE II. The 4$^{\text{th}}$ order polynomial constant used for the dispersion curves of silicon, aluminum, and gold. LA is longitudinal acoustic, TA is transverse acoustic, LO is longitudinal optical, and TO is trasverse optical.

Material	Branch	a	b	c	d	e
Al	LA	1.20528$\times$ 10^{-27}	-3.54046$\times$ 10^{-17}	1.12452$\times$ 10^{-7}	6.16822$\times$ 10^{3}	0.0
	TA	2.49215$\times$ 10^{-28}	-1.20400$\times$ 10^{-17}	7.64521$\times$ 10^{-8}	3.13157$\times$ 10^{3}	0.0
	TA	2.49215$\times$ 10^{-28}	-1.20400$\times$ 10^{-17}	7.64521$\times$ 10^{-8}	3.13157$\times$ 10^{3}	0.0
Au	LA	1.60988$\times$ 10^{-28}	-5.96185$\times$ 10^{-18}	-5.40549$\times$ 10^{-8}	3.54148$\times$ 10^{3}	0.0
	TA	-1.04516$\times$ 10^{-28}	1.49060$\times$ 10^{-19}	-7.79941$\times$ 10^{-9}	1.59236$\times$ 10^{3}	0.0
	TA	-1.04516$\times$ 10^{-28}	1.49060$\times$ 10^{-19}	-7.79941$\times$ 10^{-9}	1.59236$\times$ 10^{3}	0.0
Si	LA	-5.64528$\times$ 10^{-29}	-2.61150$\times$ 10^{-18}	-1.14000$\times$ 10^{-7}	8.19220$\times$ 10^{3}	0.0
	TA	2.43167$\times$ 10^{-27}	-4.95653$\times$ 10^{-17}	-1.16851$\times$ 10^{-8}	5.51092$\times$ 10^{3}	0.0
	TA	2.43167$\times$ 10^{-27}	-4.95653$\times$ 10^{-17}	-1.16851$\times$ 10^{-8}	5.51092$\times$ 10^{3}	0.0
	LO	4.54697$\times$ 10^{-28}	-5.81431$\times$ 10^{-18}	-1.82201$\times$ 10^{-7}	1.75738$\times$ 10^{2}	9.75592$\times$ 10^{13}
	TO	-2.01331$\times$ 10^{-27}	5.90287$\times$ 10^{-17}	-4.99719$\times$ 10^{-7}	-1.45166$\times$ 10^{2}	9.78423$\times$ 10^{13}
	TO	-2.01331$\times$ 10^{-27}	5.90287$\times$ 10^{-17}	-4.99719$\times$ 10^{-7}	-1.45166$\times$ 10^{2}	9.78423$\times$ 10^{13}

We include listings of the following 3 matlab functions:
TBC_accumulation: generates the plots in Fig. 1 of the paper,
TBC_accumulation_generic_2: generates the plots in Fig. 4 of the paper,
get_omega: computes the phonon dispersion curves for silicon, aluminum, and gold using the 4$^{\text{th}}$ order polynomial values

listed in Supplementary Table II. This function is called by the two other functions.

```
function TBC_accumulation(Metal,T,lw,fs,pts)
% This function calculates the thermal boundary conductance accumulation
% function for metal on silicon using a complete dispersion in both the
% metal and silicon

% The function generates 2 plots:
% The first plot (not in the paper) is the dispersion curves for metal
% on Si where we use a 4th order polynomial fit for the complete dispersion
% in both metal and Si. Metal and silicon dispersions are defined by the
% function get_omega given in the supplementary materials.
%
% The second plot reproduces the 6 plots in Figure 1 of the paper:

% The syntax is TBC_accumulation(Metal, T, lw, fs,pts) where
% Metal: string that can be either 'Al' or 'Au'
% T: the temperature in Kelvins
% lw: the line width of generated plots
% fs: the the fontsize of plot labels
% pts: number of points for the calculation

% copyright to RAMEZ CHEAITO (rc3qf@virginia.edu)
% University of Virginia, Charlottesville, VA 22903
% December 25th 2014

if ~nargin
% parameters used if no argumets were entered
% the default is Aluminum on Si at 296 K
    Metal = 'Al';           % options are Al or Au
    T = 296;                % Temperature
    lw = 2;                 % plots linewidth thickness
    fs = 10;                % plots labels fontsize
    pts = 800;
end

% constants
h = 1.054571726e-34;    % planck's constant
Kb = 1.3807e-23;        % boltzmann constant9

% define complete Silicon dispersion
a_Si = 0.543e-9;                    % silicon lattice constant
kSi = linspace(10,2*pi/a_Si,pts);  % wavevector in Si
wSi = get_omega(kSi,'Si');    % get_omega is a nested function
                                    % that returns Si disperion
wLA = wSi(:,1);    % longitudinal acoustic frequency branch
wTA = wSi(:,2);    % Transverse acoustic frequency branch
                   % we ignore optical modes in Silicon

% define metall dispersion
switch Metal
    case 'Al'
        am = 0.405e-9;   % lattice constant in Aluminum
        km = linspace(10,2*pi/am,pts); % wavevector in metal
        wm = get_omega(km,'Al');
        wLA_m = wm(:,1)';
        wTA_m = wm(:,2)';
    case 'Au'
```

```
        am = 4.08e-10;  % lattice constant in Gold
        km = linspace(10,2*pi/am,pts);
        wm = get_omega(km,'Au');
        wLA_m = wm(:,1)';
        wTA_m = wm(:,2)';
    case 'Si'
        am = 0.543e-9;  % lattice constant in Gold
        km = linspace(10,2*pi/am,length(kSi));
        wm = get_omega(kSi,'Si');
        wLA_m = wm(:,1)';
        wTA_m = wm(:,2)';
end

% customize all wavevectors to make the metal longitudinal frequency the
% common frequency axes for all calculations
kSiLA_TA = interp1(wTA,kSi,wLA_m); kSiLA_TA(isnan(kSiLA_TA))=0;
kSiLA_LA = interp1(wLA,kSi,wLA_m); kSiLA_LA(isnan(kSiLA_LA))=0;
kmTA = interp1(wTA_m,km,wLA_m); kmTA(isnan(kmTA))=0;
kmLA = km;

% transmition coefficient
zetta = (2*kSiLA_TA.^2 + kSiLA_LA.^2)./(2*kSiLA_TA.^2 + kSiLA_LA.^2+ ...
    2*kmTA.^2 + kmLA.^2);

% spectral TBC: Longitudinal and Transverse
hLAs = (1/(8*pi^2)).*h^2.*wLA_m.^2.*kmLA.^2.*zetta.*exp(h.*wLA_m./(Kb.*T))...
    ./(Kb.*T.^2.*(exp(h.*wLA_m./(Kb.*T))-1).^2);
hTAs = (1/(8*pi^2)).*h^2.*wLA_m.^2.*kmTA.^2.*zetta.*exp(h.*wLA_m./(Kb.*T))...
    ./(Kb.*T.^2.*(exp(h.*wLA_m./(Kb.*T))-1).^2);
hTAs(isnan(hTAs)) = 0; hLAs(isnan(hLAs)) = 0;

% total spectral TBC, Transvere modes are degenerate
htots = hLAs + 2*hTAs;

% spectral temperature derivative of phonon flux
q1s = htots./zetta; q1s(isnan(q1s)) = 0;

% Un-normalized TBC accumulation h_tot_acc and un-normalized accumulation
% of the temperature derivative of phonon flux q1_acc
htot_acc = cumtrapz(wLA_m,htots);
hLA_acc = cumtrapz(wLA_m,hLAs); % TBC accumulation of longitudinal branch
hTA_acc = cumtrapz(wLA_m,hTAs); % TBC accumulation of one transverse branch
q1_acc = cumtrapz(wLA_m,q1s);

% --------------------------- plotting ----------------------------------
figure(1) % plot dispersion
plot(-km,wLA_m,'--',-km,wTA_m,':',kSi,wLA,'--',kSi,wTA,':','Linewidth',lw)
set(gca,'FontSize',fs)
ylabel('Angular Frequency \omega (rad s^{-1})','Fontsize',fs)
xlabel('Wavevector k (m^{-1})','Fontsize',fs)
title('Dispersion Curves')
legend(' Metal LA',' Metal TA',' Silicon LA',' Silicon TA')

figure(2)
suptitle(sprintf('%c%c on Silicon \n\n',Metal))
subplot(2,3,2)
% un-normalized TBC accumulation function
plot(wLA_m./1e12,htot_acc./1e6,'Linewidth',lw)
ylabel('h_{K}(\omega_{\alpha}) (MW m^{-2}K^{-1})','Fontsize',fs)
```

```
xlabel('\omega_{\alpha} (Trad s^{-1})','Fontsize',fs)
title('Fig.1b','Fontsize',fs)
subplot(2,3,1)
% normalized TBC accumulation
plot(wLA_m./1e12,htot_acc./max(htot_acc),'Linewidth',lw)
xlabel('\omega(\alpha) (Trad s^{-1})','Fontsize',fs)
ylabel('\alpha_K(\omega_{\alpha})','Fontsize',fs)
title('Fig.1a','Fontsize',fs)
subplot(2,3,3)
% accumulation of the temperature derivative of phonon flux
plot(wLA_m./1e12,q1_acc./max(q1_acc),'Linewidth',lw)
xlabel('\omega_{\alpha} (Trad s^{-1})','Fontsize',fs)
ylabel('\alpha_{qT}(\omega_{\alpha})','Fontsize',fs)
title('Fig.1c','Fontsize',fs)
subplot(2,3,4)
% transmission coefficient
plot(wLA_m./1e12,zetta,'Linewidth',lw)
xlabel('\omega (Trad s^{-1})','Fontsize',fs)
ylabel('\zeta(\omega)','Fontsize',fs)
title('Fig.1d','Fontsize',fs)
subplot(2,3,5)
% spectral TBC
plot(wLA_m./1e12,htots./1e5,'Linewidth',lw)
ylabel('Spectral h_K(\omega) (\times 10^5 W s m^{-2}K^{-1} rad^{-1})','Fontsize',fs)
xlabel('\omega (Trad s^{-1})','Fontsize',fs)
title('Fig.1e','Fontsize',fs)
subplot(2,3,6)
% temperature derivative of phonon flux
plot(wLA_m./1e12,q1s./1e-5,'Linewidth',lw)
ylabel('\partial q_1/\partial T(\omega)(\times 10^{-5}W m^{-2}K^{-1})','Fontsize',fs)
xlabel('\omega (Trad s^{-1})','Fontsize',fs)
title('Fig.1f','Fontsize',fs)
end
```

```
function output= TBC_accumulation_generic_2(am,wLA_max,wTA_max,T,lw,fs,pts,plot_flag)
% This function mimics the thermal boundary conductance accumulation for
% metal on silicon using a sine-type dispersion in metal and complete
% dispersion in silicon

% The function output a 4 column matrix storing the frequency vector, the
% unnormalized Kapitza accumulation, The normalized Kapitza accumulation
% the normalized accumulation of the phonon flux in the metal

% The code also generates a plot of the normalized and un-normalized
% thermal boundary conductance accumulation function and the accumulation
% of the temperature derivative of phonon flux in the metal side

% The syntax is TBC_accumulation_generic(am,wLA_max,wTA_max,T,lw,fs) where
% am: the metal lattice constant
% wLA_max and wTA_max: the max cutoff frequencies of the longitudinal
% and transverse acoustic branches in metal, respectively
% T: the temperature in Kelvins
% lw: the line width of generated plots
% fs: the fontsize of plot labels
% pts: number of points to generate the plot

% the silicon dispersions are defined by the function get_omega given in
```

```
% the supplementary materials

% copyright to RAMEZ CHEAITO (rc3qf@virginia.edu)
% University of Virginia, Charlottesville, VA 22903
% December 25th 2014

cd(fileparts(mfilename('fullpath')))

if ~nargin
    % if no arguments entered then use Aluminum for side 1
    am = 0.405e-9;          % Aluminum Lattice constant
    wLA_max = 60.38e12;     % Aluminum Longitudinal cutoff frequency
    wTA_max = 36.4e12;      % Aluminum Transverse cutoff frequency
    T = 296;                % Temperature in Kelvin
    pts = 800;
    lw = 2;                 % plots linewidth thickness
    fs = 10;                % plot labels fontsize
    plot_flag = 1;
end
pp = wTA_max/wLA_max;  % ratio of transverse to longitudinal cutoffs
km = linspace(10,2*pi/am,pts);  % wavevector in metal

% constants
h = 1.054571726e-34;    % planck's constant
Kb = 1.3807e-23;        % boltzmann constant

% define complete Silicon dispersion
a_Si = 0.543e-9;    % silicon lattice constant
kSi = linspace(10,2*pi/a_Si,pts);
wSi = get_omega(kSi,'Si'); % get_omega is a function that returns disperion
wLA = wSi(:,1);            % we ignore optical branches
wTA = wSi(:,2);

% define cutoff frequency vector
wLAc = linspace(10,wLA_max,pts);

% preallocate
htot_acc = zeros(length(wLAc),1);
hLA_acc = htot_acc; hTA_acc = htot_acc; q1_acc = htot_acc;

for ii = 1:length(wLAc) % loop over the cutoffs frequencies
    % define sine dispersion in metal for each cutoff frequency
    wLA_m = wLAc(ii)*sin(km*am./4);
    wTA_m = pp*wLAc(ii)*sin(km*am./4);

    % customize silicon dispersion to make metal LA branch the common
    % frequency vector for all calculations
    kSiLA_TA = interp1(wTA,kSi,wLA_m); kSiLA_TA(isnan(kSiLA_TA))=0;
    kSiLA_LA = interp1(wLA,kSi,wLA_m); kSiLA_LA(isnan(kSiLA_LA))=0;
    kmTA = interp1(wTA_m,km,wLA_m); kmTA(isnan(kmTA))=0;
    kmLA = km;

    % transmition coefficient
    Gam = (2*kSiLA_TA.^2 + kSiLA_LA.^2)./(2*kSiLA_TA.^2 + kSiLA_LA.^2+...
        2*kmTA.^2 + kmLA.^2);

    % spectral Thermal boundary conductance
    hLAs = (1/(8*pi^2)).*h^2.*wLA_m.^2.*kmLA.^2.*Gam.*...
        exp(h.*wLA_m./(Kb.*T))./(Kb.*T.^2.*(exp(h.*wLA_m./(Kb.*T))-1).^2);
```

```
    hTAs = (1/(8*pi^2)).*h^2.*wLA_m.^2.*kmTA.^2.*Gam.*...
        exp(h.*wLA_m./(Kb.*T))./(Kb.*T.^2.*(exp(h.*wLA_m./(Kb.*T))-1).^2);
    hTAs(isnan(hTAs)) = 0; hLAs(isnan(hLAs)) = 0;
    %-------------------------------------------------------------------------
    htots = hLAs + 2*hTAs; %(TA branch is degenerate)

    % temperature derivative of q1 (del q/del T)
    q1s = htots./Gam; q1s(isnan(q1s)) = 0;
    % TBC "accumulation"
    htot_acc(ii) = trapz(wLA_m,htots);
    hLA_acc(ii) = trapz(wLA_m,hLAs);
    hTA_acc(ii) = trapz(wLA_m,hTAs);
    q1_acc(ii) = trapz(wLA_m,q1s);
end
wLAc = wLAc';
output = [wLAc htot_acc htot_acc./max(htot_acc) q1_acc];
% ---------------------------- plotting ----------------------------------
if plot_flag
figure(1)

subplot(1,2,1)
% un-normalized Kapitza accumulation function, same as Fig.4a
plot(wLAc./1e12,htot_acc./1e6,'LineWidth',lw)
ylabel('h_K(\upsilon_1(\omega_{max}))  (MW m^{-2}K^{-1})','Fontsize',fs)
xlabel('\omega_{max} (Trad s^{-1})','Fontsize',fs)
title('Fig.4a','Fontsize',fs)
hold on
subplot(1,2,2)
% plot the normalized TBC accumulation and normalized
% accumulation of the temperature derivative of phonon flux
% this is the inset of Fig.4a
plot(wLAc./1e12,htot_acc./max(htot_acc),wLAc./1e12,q1_acc./max(q1_acc),'LineWidth',lw)
xlabel('\omega_{max} (Trad s^{-1})','Fontsize',fs)
legend('\alpha_{K}(\upsilon_1(\omega_{max}))','\alpha_{qT}(\upsilon_1(\omega_{max}))')
title('The inset of Fig.4a','Fontsize',fs)
end
end
```

```
function W = get_omega(k,metal)
% returns a matrix storing the different frequency branches
% of a the dispersion curve of Silicon, Aluminum, or Gold
% the function defines a 4th order polynomial and evaluates this polynomial
% at an input wavevector

% syntax is: W = get_omega(k,metal)
% k is the wavevector,
% metal is a string that can take 'Al', 'Au' or 'Si'
% W is a matrix storing the omega of the different branches of the
% dispersion curve

% copyright to RAMEZ CHEAITO (rc3qf@virginia.edu)
% University of Virginia, Charlottesville, VA 22903
% July 27th 2014

    switch metal
        case 'Al'
            aLA = 1.2052819309e-27;
```

```
        bLA = -3.5404650479e-17;
        cLA = 1.1245207530e-7;
        dLA = 6.1682297866e+03;
        eLA = 0.0000000000e+00;
        LA = [aLA bLA cLA dLA eLA];
        % Transverse Acoustic
        aTA = 2.4921580928e-28;
        bTA = -1.2040018850e-17;
        cTA = 7.6452184964e-08;
        dTA = 3.1315719768e+3;
        eTA = 0;
        TA = [aTA bTA cTA dTA eTA];

        % Define omega vectors
        wLA = polyval(LA,k);
        wTA = polyval(TA,k);

        W = [wLA' wTA'];

    case 'Au'
        aLA = 1.6098894832e-28;
        bLA = -5.9618545015e-18;
        cLA = -5.4054943024e-08;
        dLA = 3.5414888665e+03;
        eLA = 0;
        LA = [aLA bLA cLA dLA eLA];
        % Transverse Acoustic
        aTA = -1.0451675944e-28;
        bTA = 1.4906054087e-19;
        cTA = -7.7994150409e-09;
        dTA = 1.5923675002e+03;
        eTA = 0;
        TA = [aTA bTA cTA dTA eTA];

        % Define omega vectors
        wLA = polyval(LA,k);
        wTA = polyval(TA,k);

        W = [wLA' wTA'];

    case 'Si'
        aLA = -5.6452828338e-29;
        bLA = -2.6115041869e-18;
        cLA = -1.1400043744e-7;
        dLA =  8.1922093105e3;
        eLA = 0;
        LA = [aLA bLA cLA dLA eLA];
        % Transverse Acoustic
        aTA = 2.4316751480e-27;
        bTA = -4.9565315956e-17;
        cTA = -1.1685174315e-8;
        dTA = 5.5109223649e3;
        eTA = 0;
        TA = [aTA bTA cTA dTA eTA];
        % Longitudinal Optical
        aLO = 4.5469793226e-28;
        bLO = -5.8143150642e-18;
        cLO = -1.8220185964e-7;
        dLO = 1.7573815528e2;
```

```
            eLO = 9.7559229984e13;
            LO = [aLO bLO cLO dLO eLO];
            % Transverse Optical
            aTO = -2.0133132500e-27;
            bTO = 5.9028704760e-17;
            cTO = -4.9971917015e-7;
            dTO = -1.4516668251e+2;
            eTO = 9.7842368802e+13;
            TO = [aTO bTO cTO dTO eTO];
            % Define omega vectors
            wLA = polyval(LA,k);
            wTA = polyval(TA,k);
            wLO = polyval(LO,k);
            wTO = polyval(TO,k);

            W = [wLA' wTA' wLO' wTO'];

    end

end
```