Heat transfer from an ultrafast laser heated metal film to a substrate

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1 Introduction

This note describes how to calculate one-dimensional thermal transport from an ultrafast laser excited metal film into a substrate. The laser rapidly ($\approx$ 1 ps) raises the temperature of the film uniformly. The film has been depositied on top of a bulk material, which is initially at a uniform colder temperature. The specific experiments considered are a 70 nm thick Aluminum film sputtered on top of four different bulk semiconducor crystalline wafers: Silicon, Gallium Arsenide, Indium Antimonide, and Germanium. The different thermal properties of these bulk semiconductor materials provide a useful comparitive study. Metal-on-semiconductor devices are important technologically, and we are undertaking a quantituative study of their heat transport using time-resolved x-ray diffraction. This note describes the different transport models which can be used to simulate the results of the diffraction experiments.

2 Classical Treatment

2.1 Perfect thermal contact

These results are taken from Example 10.8 of Hahn and Ozisik, *Heat Conduction* (Wiley, 2012). They consider a one-dimensional, two-layer composite slab with a film of thickness L on top of a semi-infinite bulk material. We will identify the film as region 1 and the bulk as region 2. The layers are presumed to be in perfect thermal contact with region 1 initially at a uniform temperature T_0 (caused by rapid laser energy absorption) and region 2 at zero temperature. The problem is easiest stated using a dimensionless temperature $\theta_i(x,t)$ defined as as

$$\theta_i(x,t) = \frac{T_i(x,t)}{T_0} \qquad i = 1,2 \tag{1}$$

where the index $i = 1, 2$ refers to the film and bulk, respectively. With this transformation, the heat transfer problem is written

$$\frac{\partial^2\theta_1}{\partial x^2} = \frac{1}{\alpha_1}\frac{\partial\theta_1}{\partial t} \qquad in \qquad 0 < x < L,\ t > 0 \tag{2a}$$

$$\frac{\partial^2\theta_2}{\partial x^2} = \frac{1}{\alpha_2}\frac{\partial\theta_2}{\partial t} \qquad in \qquad x > L,\ t > 0 \tag{2b}$$

subject to the boundary conditions

$$\frac{\partial\theta_1}{\partial x}\Big|_{x=0} = 0 \tag{3a}$$

$$\theta_1(x=L,t) = \theta_2(x=L,t) \tag{3b}$$

$$k_1\frac{\partial\theta_1}{\partial x}\Big|_{x=L} = k_2\frac{\partial\theta_2}{\partial x}\Big|_{x=L} \tag{3c}$$

$$\theta_2(x\to\infty,t) \to 0 \tag{3d}$$

and the initial conditions

$$\theta_1(x,t=0) = 1 \qquad in \qquad 0<x<L \tag{4a}$$

$$\theta_2(x,t=0) = 0 \qquad in \qquad L<x<\infty \tag{4b}$$

where k_i are the thermal conductivities and α_i are the thermal diffusivities of region 1 (film) and region 2 (bulk). Using Laplace rransforms, the solution for the temperature distribution in the two-layer medium is

$$\frac{T_1(x,t)}{T_0} = 1 - \frac{1+\gamma}{2}\sum_{n=0}^{\infty}\gamma^n\left\{\text{erfc}\left[\frac{(2n+1)L-x}{2\sqrt{\alpha_1 t}}\right] + \text{erfc}\left[\frac{(2n+1)L-x}{2\sqrt{\alpha_1 t}}\right]\right\} \tag{5a}$$

$$\frac{T_2(x,t)}{T_0} = \frac{1+\gamma}{2}\sum_{n=0}^{\infty}\gamma^n\left\{\text{erfc}\left[\frac{(2nL+\mu(x-L)}{2\sqrt{\alpha_1 t}}\right] - \text{erfc}\left[\frac{(2n+2)L+\mu(x-L)}{2\sqrt{\alpha_1 t}}\right]\right\} \tag{5b}$$

where the unitless parameters μ and γ are defined by

$$\mu = \sqrt{\frac{\alpha_1}{\alpha_2}} \tag{6a}$$

$$\beta = \frac{k_1}{k_2}\frac{1}{\mu} \tag{6b}$$

$$\gamma = \frac{\beta-1}{\beta+1}. \tag{6c}$$

2.2 Examples of the classical heat conduction result

We consider a 70 nm Aluminum film directly on top of bulk semiconductors. In addition to calculating the temperature profile evolution in the film and substate, we perform Time-Resolved X-Ray Diffraction (TRXD) calculations to predict the evolution of Bragg reflection lineshapes following laser excitation. For each material, the absorbed laser fluence is kept constant at 1 mJ/cm^2. TRXD measurements are all done for single crystal (001) cut semiconductors at the [004] reflection at an x-ray energy of 10 keV. In these preliminary calculations only the lineshapes, and not the absolute intensiteis of the diffraction profiles are considered, and they are blurred by convolving the results of a dynamical diffraction calculation with a 0.2 millidegree FWHM Gaussian resolution function. The TRXD calculations should be considered still under development and requiring further benchmarking at this time. The temperature profiles are calcualated on a logarithmic time grid stretching from 1 ps to 1 μs.

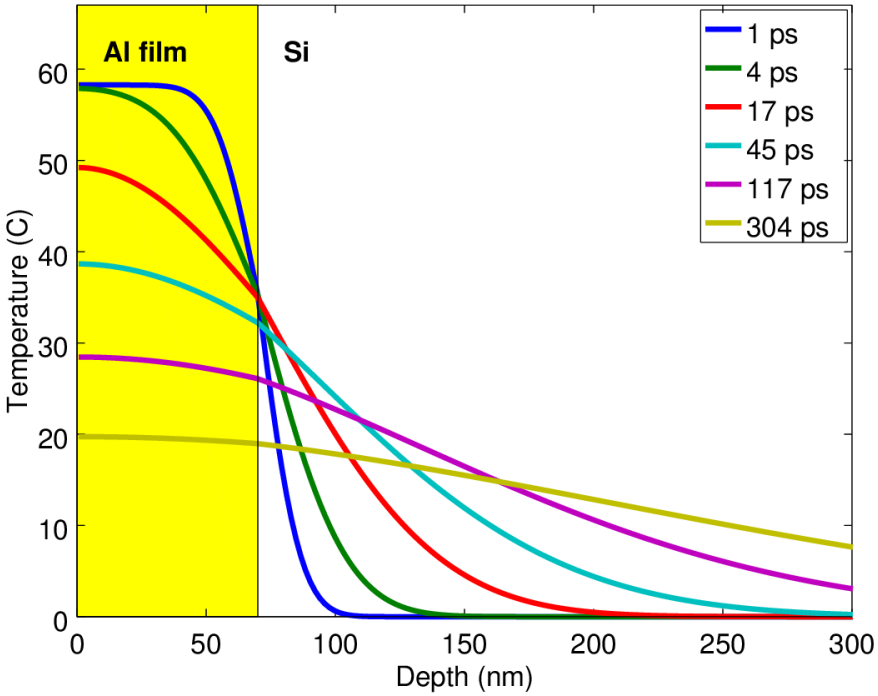

Figure 1: Classical thermal transport result for 70 nm Al on Si.

2.2.1 Aluminum on Silicon

The 70 nm thick Aluminum film received an initial temperature rise of 58.3 deg C. After 1 μs, the average film temperature rise was only 0.4 deg C. The maximum bulk Silicon temperature rise wass 34.0 deg C.

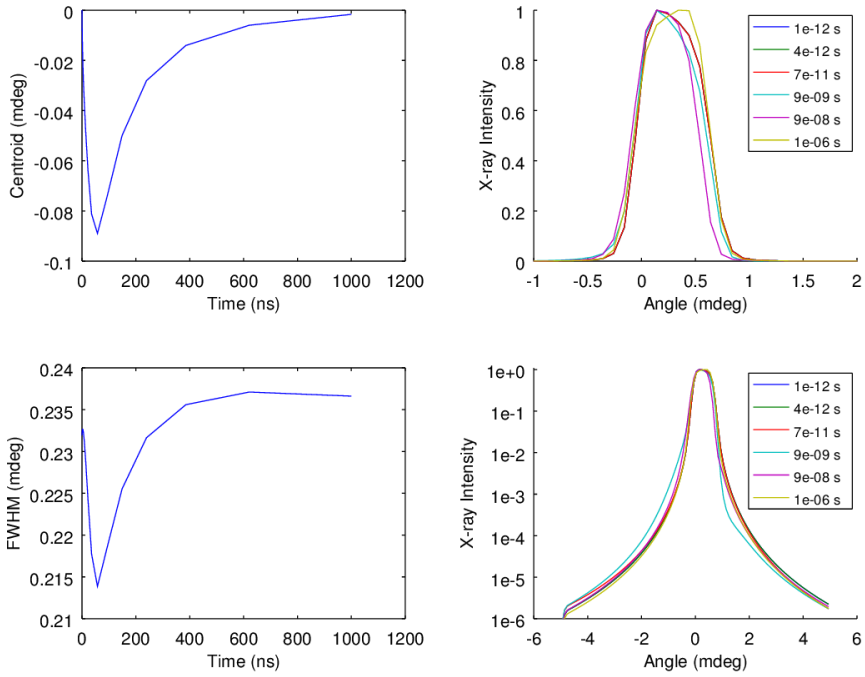

Figure 2: Preliminary TRXD calculations corresponding to classical thermal transport result for 70 nm Al on Si.

2.2.2 Aluminum on Gallium Arsenide

The 70 nm thick Aluminum film received an initial temperature rise of 58.3 deg C. After 1 μs, the average film temperature rise was only 0.6 deg C. The maximum bulk Silicon temperature rise was 39.3 deg C.

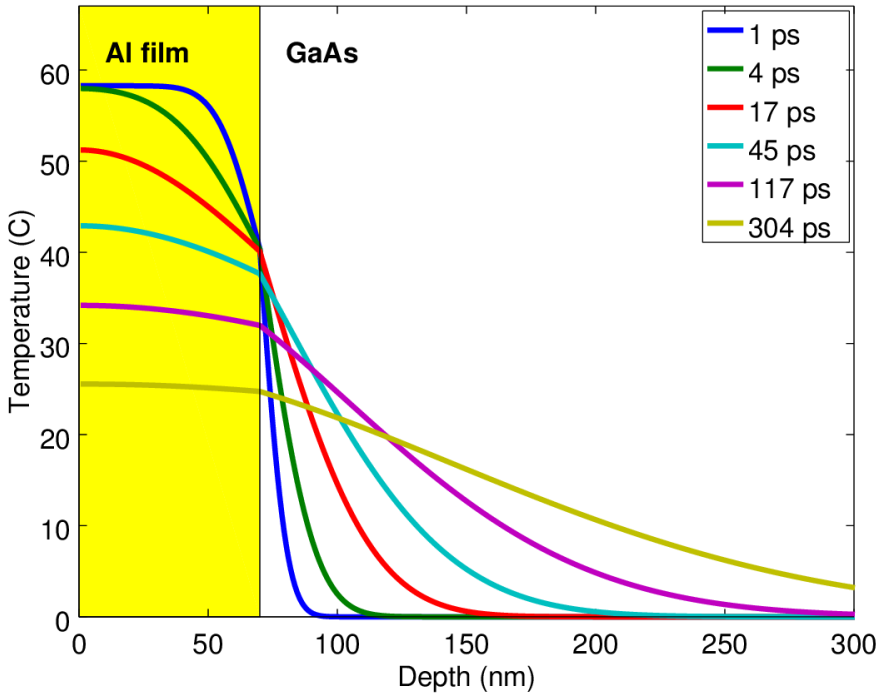

Figure 3: Classical thermal transport result for 70 nm Al on Si.

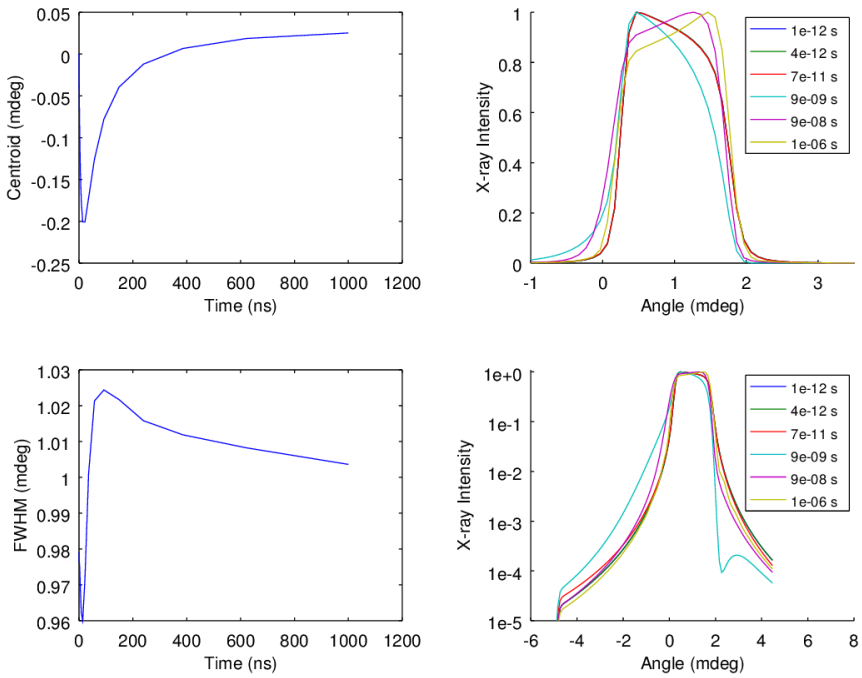

Figure 4: Preliminary TRXD calculations corresponding to classical thermal transport result for 70 nm Al on GaAs.

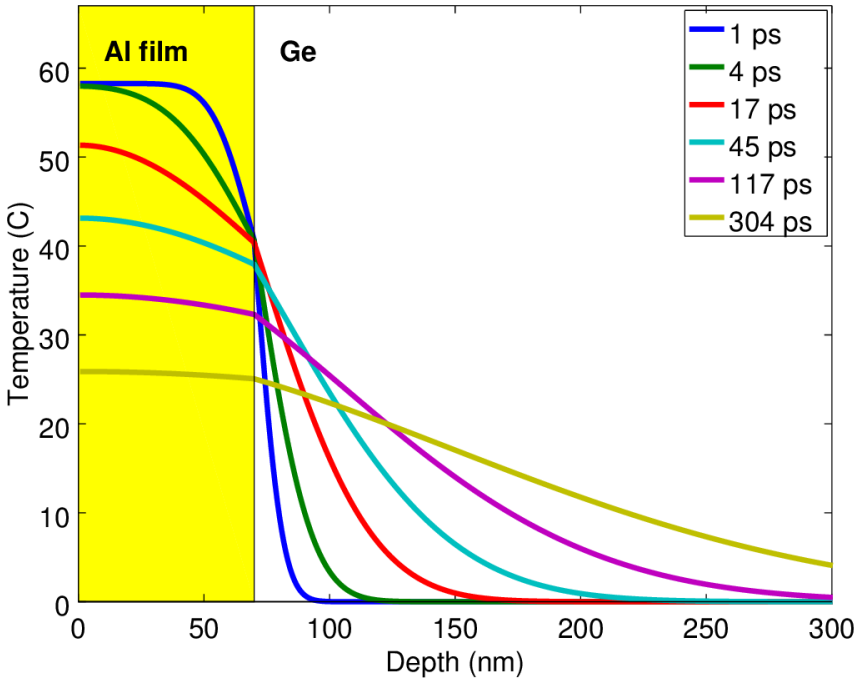

Figure 5: Classical thermal transport result for 70 nm Al on Si.

2.2.3 Aluminum on Germanium

The 70 nm thick Aluminum film received an initial temperature rise of 58.3 deg C. After 1 μs, the average film temperature rise was only 0.6 deg C. The maximum bulk Germanium temperature rise was 39.6 deg C.

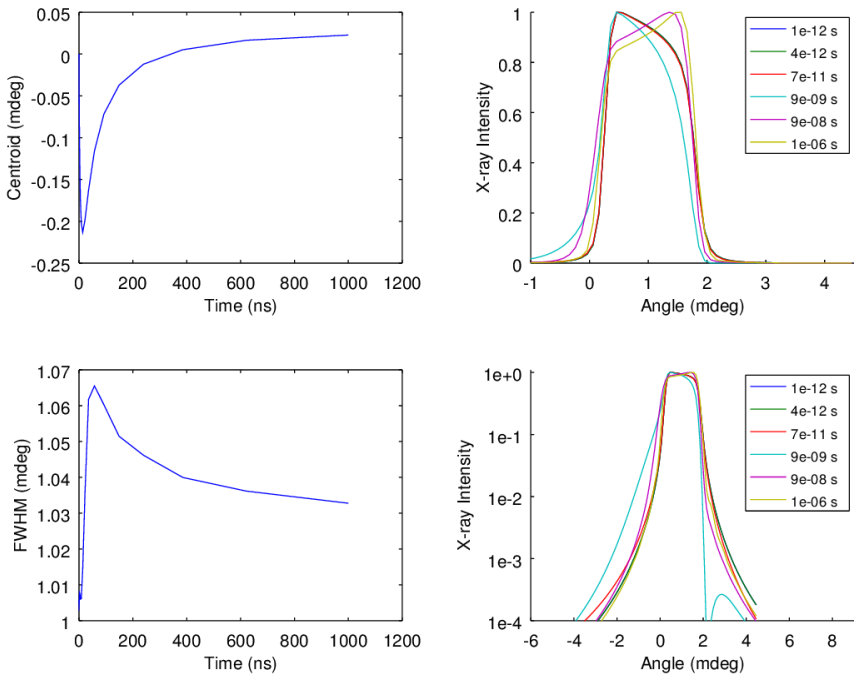

Figure 6: Preliminary TRXD calculations corresponding to classical thermal transport result for 70 nm Al on Ge.

2.2.4 Aluminum on Indium Antimonide

The 70 nm thick Aluminum film received an initial temperature rise of 58.3 deg C. After 1 μs, the average film temperature rise was only 1.2 deg C. The maximum bulk Indium Antimonide temperature rise was 47.3 deg C.

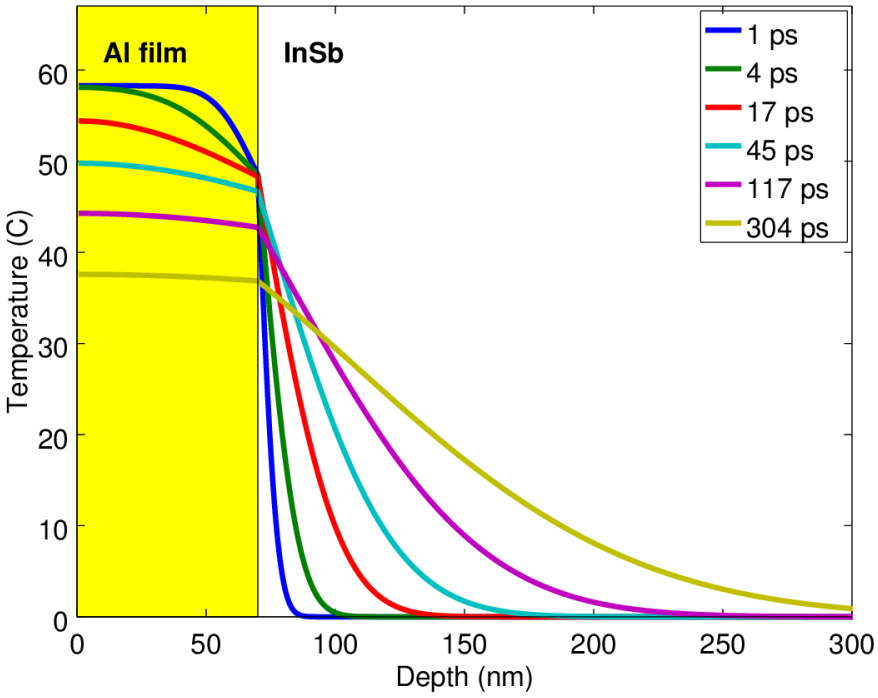

Figure 7: Classical thermal transport result for 70 nm Al on Si.

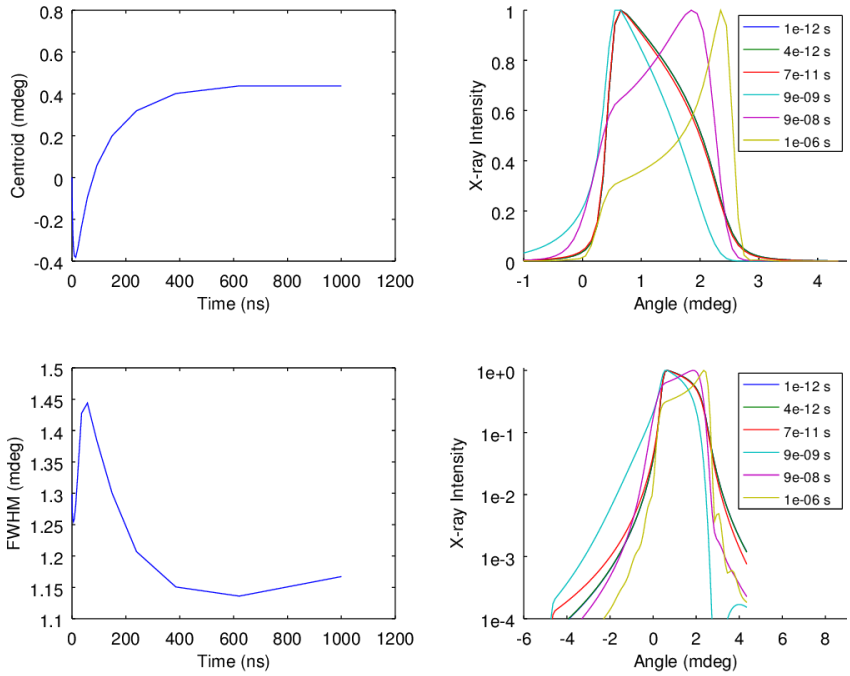

Figure 8: Preliminary TRXD calculations corresponding to classical thermal transport result for 70 nm Al on InSb.

2.3 Imperfect thermal contact

This section will explore corrections to the classical treatment due to imperfect thermal contact between the film and substrate. In particular, the "Diffusive Mismatch Model" can be used to correct the classical heat conductivity values by applying a locally quantum model of heat flow.

3 Microscopic Treatment

Considerable recent interest in this problem at the 10 - 100 nm lengthscales has been motivated by the semiconductor fabrication techniques working at these dimensions. The classical treatment given above, even including corrections for interfaces, is known to be insufficient since the phonon mean free path, Λ, can be comparable to these dimensions. This section will explain a simple one-dimensional Lattice Boltzman Model (LBM) to treat heat flow as a phonon transport problem.

Appendix: Parameters

Appendix: Code

The most recent and up to date code should be obtained from `https://github.com/elandahl/dynamical-diffraction/tree/TRXD/strain_functions`. This code listing is for reference only.

```
% thermalFilm.m
% Classical strain model for a thin Aluminum film on a semiconductor
% Presumes that the temperature rise on the film is uniform and instantaneous
% and that the thermal contact is perfect
% A more sophisticated model with better Physics (e.g. AMM, DMM) will be needed!
% Also, does not include nanoscale phenomena (e.g. phonon mean free path)
% Also, no acoustic propogation is included.  This could be called later.
% Model: see p. 429 (Sec. 10.7) of Hahn, "Heat Conduction" 3rd edition
% Aluminum properties are hard coded
% Semiconductor properties looked up in sample.dat, which is required
% First written by Eric Landahl, 12.28.2016
% Revised by EL 1.9.2017
% Usually called by TRXD.m
%
%% INPUTS:
%   crystal     determines x-ray and strain properties, chosen from:
%     GaAs
%     Si
%     Ge
%     InSb
%   fluence     absorbed laser fluence in mJ/cm^2
%   time        a vector of times to be calculated in seconds
%   max_depth   usually 5*Lext, Lext is the x-ray extinction length in meters
%% OUTPUTS:
%   longitudinal    longitudinal strain, size = length(time_out) x length(z)
%   transverse      transverse strain, size = length(time_out) x length(z)
%   sheer           sheer strain, size = length(time_out) x length(z)
%   z               a vector of depths in meters
%   time_out        a vector of times returned in seconds, not the same as time_in
%
%% NOTE: The strain will be calculated out to time_in(end) however the time-steps
%        are chosen for convenience and accuracy in evaluating the strain.
%        time_in is NOT usually equal to time_out
%        therefore the strain must be interpolated temporally after calling this
%        function
%
%% NOTE ALSO: Three strain components are returned, but usually only longitudinal
%             is non-zeros
%
%% TYPICAL USAGE
%
% [st1 st2 st3 time_out z] = thermalFilm ('Si', 1, (1e-10:2e-10:1e-8), 1e-5);
```

```
%
function [longitudinal trans sheer time_out z]=thermalFilm(crystal,fluence,time_in,max_depth)

% Remesh time
  time = time_in;
  % In this simple model, there is no penalty for calculating many timepoints
  % so the given array of timepoints is used.

% Aluminum film properties.  "1" refers to the film
  L = 70e-9; % Film thickness in m
  C1 = 904; %Specific heat of film in J/(kg K)
  rho1 = 2712; % Film density in kg/m^3
  k1 = 204; % Film thermal conductivity in W/(m K)
  alpha1 = 8.418E-5; % Film thermal diffusivity in m^2/s

% Load substrate properties.  "2" referes to the substrate
  load sample.dat;
  ID = find(strcmp({sample.name}, crystal)==1);
  alpha_t = sample(ID).thermalExpansion.val; % 1/K
  alpha2 = sample(ID).thermalDiffusion.val; % cm^2/s
  alpha2 = alpha2 / 10000; % convert from cm^2/s to m^2/s
  k2 = sample(ID).thermalConductivity.val; % W/(cm K)
  k2 = k2 * 100; % Convert from W/(cm K) to W/(m K)
  C2 = sample(ID).specificHeat.val; % J/(g K)
  C2 = C2 * 1000; % Convert from J/(g K) to J/(kg K)
  rho2 = sample(ID).massDensity.val; % g/cm^3
  rho2 = rho2 * 1000; % Convert from g/cm^3 to kg/m^3


  %% Temporary for troubleshooting: make the sampe all semiconductor
%  rho1 = rho2;
%  k1 = k2;
%  C1 = C2;

% Calculate initial temperature rise
  fluence = fluence*10; % Convert from mJ/cm^2 to J/m^2
  T0 = fluence/(L * C1 * rho1); % Initial temperature rise in film
  fprintf('A %d nm thick Aluminum film gives a temperature rise of %.1f K.\n',L*1e9,T0)

% Unitless parameters (see Hahn, "Thermal Conductivity", Eqs. 10-135 and 10-138)
  mu = sqrt(alpha1/alpha2);
  beta = (k1/k2)/mu;
  gamma = (beta - 1)/(beta + 1);

% Spatial grid
  num_depths = 10000;  % number of depth points z to be calculated
  dz = max_depth/num_depths;
  z = dz:dz:max_depth;
```

```
% Meshgrid for calculation speed & ease
  [Time Z] = meshgrid(time,z); % Time and Z are 2D, time and z are 1D

% Calculate temperature profile in bulk
  max_n = 100; % number of terms in series expansion, default 100
  T2a = 0.*Time.*Z; % each term gets added to this, starts at zero
  for n = 0: max_n  % Series expansion solution of heat equation
    T2b = erfc((2*n*L + mu*Z)./(2*(sqrt(alpha1*Time)))); % temporary
    T2c = erfc(((2*n + 2)*L + mu*Z)./(2*sqrt(alpha1*Time))); % temporary
    T2a = T2a + (gamma^n) * (T2b - T2c); % temporary, adding up
  end
  T2 = T0 * (1/2) * (1 + gamma) * T2a; % Temperature at all z and time

% Film calculations are not needed except to check conservation of energy
% Calculate temperature profile in film.  zz and ZZ are the film depths
  dzz = L/100; % Choose 100 depth points in the film by default
  zz = dzz:dzz:L;
  [Time ZZ] = meshgrid(time,zz);
  T1a = 0.*Time.*ZZ;
  for n = 0:max_n
    T1b = erfc(((2*n + 1)*L - ZZ)./(2*sqrt(alpha1*Time)));
    T1c = erfc(((2*n + 1)*L + ZZ)./(2*sqrt(alpha1*Time)));
    T1a = T1a + (gamma^n) * (T1b + T1c);
  end
  T1 = T0 - T0 * (1/2) * (1 - gamma) * T1a; % Temperature in film
  T1_end = mean(T1(:,end)); % Average temperature at final timepoint
  fprintf('After %.1f ns, the average film temperature rise is only %.1f deg C.\n', ...
  time(end)*1e9,T1_end);
  fprintf('The maximum bulk %s temperature rise is %.1f deg C.\n',crystal, ...
  max(max(T2)));

% Calculate heat in film
% Q = integral dzz of rho*C*T
%  Q1 = trapz(ZZ,T1*rho1*C1);
%  Q2 = trapz(Z,T2*rho2*C2);
%  Q1 = Q1/10; % convert from J/m^2 to mJ/cm^2
%  Q2 = Q2/10; % convert from J/m^2 to mJ/cm^2


% Calculate strains in bulk
  longitudinal = alpha_t.*T2'; % Strain is thermal expansion coeff times temperature
  trans =0.*T2'; % No transverse strain
  sheer = 0.*T2'; % No sheer strain
  time_out = time;

% Outputs not needed for TRXD

save thermalFilmOut.m; % Save all variables for future use
```

```
end
```