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

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1 Introduction

2 Classical Treatment

2.1 Perfect thermal contact

These results are taken from Example 10.8 of Hahn and Ozisik, *Heat Conduction* (Wiley, 2012). The consider a two-layer composite slab with one semi-infinite layer as shown in Fig. XXX. 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 and region 2 at zero temperature. Define a dimensionless temperature $\theta_i(x,t)$ as

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

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

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

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

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

2.2.1 Aluminum on Silicon

2.2.2 Aluminum on Gallium Arsenide

2.2.3 Aluminum on Germanium

2.2.4 Aluminum on Indium Antimonide

2.3 Diffusive Mismatch Correction

2.4 Acoustic Mismatch Correction

3 Microscopic Treatment

Consider the same problem as in the previous section, but determine the second order energy correction. You may leave your answer in the form of a summation.

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
```