TERM-PROJECT GUIDELINES:

Instructor: Seong Hyuk Lee
April 23, 2012

1. **Two-individual projects:** All the students will have three different term-projects in this class. Individual project (not a group project): two subjects will be assigned to all the students who should submit the reports for these projects on schedule. (Delivery: program (in-house code made by oneself) and reports)

2. **Group project**: at first, find your partner and make your group. The subject should be picked by the students based upon their own personal interest (or based on research they are currently doing) However, if your group fails to find it, the instructor may assign the problem. Any of commercial codes can be used in conducting your subject.
    i. Make your topic or subject for simulation (delivery: one page descriptions for your problem): this will be presented in my class for 15 min.
    ii. For each class, we will open the progress meeting every week for feedback.
    iii. Finally, all the groups should submit the final reports before final exam. and the final presentation for evaluation will be made. (deliveries: data files and final report (MS WORD)

Term-Project #1. (due 7th, May 2012)

<Phonon Thermal Conduction Problem>

A. Mathematical Representation

The analytical model for the thermal conduction which can be varied with the phonon group velocity has been established. Understanding thermal properties of nanostructures is very crucial and phonon behavior regarding thermal transport in solids is very similar to that of radiation heat transfer. Using Casimir limit, thermal conductivity can be expressed as

$$k = k_{Bulk}\left[1 + \Lambda_0 / \Lambda_{BS}\right]^{-1}, \tag{1}$$

where Λ_0 represents the phonon mean free path (MFP) in bulk materials. To get the thermal conductivity, we have to know the behavior of Λ_{BS} on the basis of the framework of Casimir's theory (BS method). First, inner and outer intensities of thermal energy can be expressed as

$$\begin{aligned} I_i(r_i, z_R) &= -4\pi r_i \int_{r_i}^{r_e} E(r, r_i, \theta_{C1}, z_R) r dr \\ I_e(r_i, r_e, z_R) &= -4\pi r_e \int_{r_i}^{r_e} E(r, r_e, \theta_C, z_R) r dr \end{aligned} \tag{2}$$

where the corresponding energy intensity involved in the above equations can be obtained by

$$E(r_1, r_2, \theta, z) = \int_0^{\theta} \frac{z(r_2 - r_1 \cos u)}{\left[r_1^2 + r_2^2 - 2r_2 r_1 \cos u + z^2\right]} du \tag{3}$$

Figure 1 (as shown below) shows the cylindrical coordinate basically is used for the expressions.

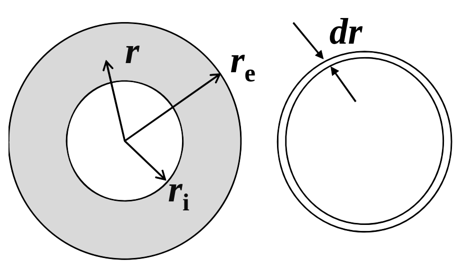

Fig. 1 The schematic of the cylindrical materials.

In addition, some definitions should be noted as follows:

$$\begin{aligned} \theta_{C1} &= \cos^{-1}(r_i / r), \\ \theta_{C2} &= \cos^{-1}(r_i / r_e), \\ \theta_C &= \theta_{C1} + \theta_{C2}, \end{aligned} \tag{4}$$

The final expression of the mean free path can be obtained as follows:

$$\Lambda_{BS}(r_i, r_e) = 2\Pi(r_i, r_e) / \left(r_e^2 - r_i^2\right). \tag{5}$$

The above equation includes the following relationship showing the integration in the *z* direction (using cylindrical coordinate system)

$$\Pi(r_i, r_e) = \left(\frac{3}{4}\pi^2\right)\int_0^{\infty}\left[I_i(r_i, z_R) + I_e(r_i, r_e, z_R)\right] z_R dz_R \tag{6}$$

For comparison, the following approximated solutions would be useful.

$$\Lambda_{BS,Approx.}(r_i, r_e) \cong 2\frac{r_e^2 + r_i^2 + r_e r_i}{\left(r_e + r_i\right)}\left[1 - \left(\frac{r_i}{r_e}\right)^P\right]. \tag{7}$$

where *p* means an adjustable parameter which can be controlled to match your results.

B. TERM-PROJECT: INDIVIDUAL PROJECT

In Sec. A, we know that thermal conductivity consists of bulk property and additional property which is associated with the wave-like feature (radiation characteristics) from the small scale viewpoint. To get the final solution of thermal conductivity, we have to solve Eq. (5) to get the final solution with the use of Eqs. (2)~(4), and (6).

- **a)** Make your in-house code (made by yourself) for getting thermal conductivity.
- **b)** Plot the calculated thermal conductivity for different the inner radius r_i ranging from 10 nm to 200 nm at the fixed value of r_e (=1000 nm).
- **c)** Make the comparison of your calculation with approximated solutions, as shown in Eq. (7), with using $p = 1$.

<Delivery> your own source code (FORTRAN, C++, MATLAB are available) and your report stored in MS-WORD format.

Term-Project #2. (due 30th, May 2012)

<1D Transient Conduction Problem>

Heat transfer analysis of a metal-dielectric thin film heated by the lamp

We may think a metal-dielectric thin film structure which consists of Au film and SiO2 substrate with different thicknesses. A lamp was used to heat the film surfaces, and in bulk phenomena, we assume that thermal conduction is based on Fourier' law. In this project, we are trying to develop an in-house code which can estimate transient energy transport characteristics which are happening inside the structure. Let us first think about the two-layer structure including Au film and SiO2 substrate as shown below.

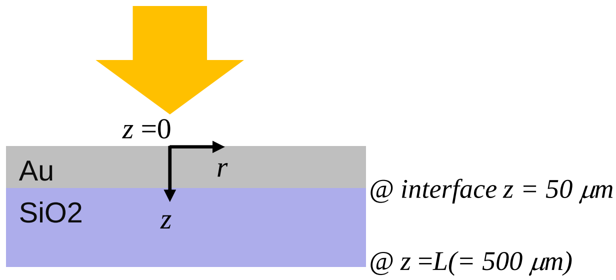

Fig. 1. A two-layer structure with Au film deposited on the SiO2 substrate.

Using the conventional 1-D Fourier law, the following 1D transient conduction equation can be established.

$$\frac{\partial}{\partial t}(\rho C_P T) = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + S \, , \tag{1}$$

where k and C_P represents the thermal conductivity and the heat capacity which are varied with temperature. Initial temperature is 300 K and for the source term, it is assumed that a constant temperature of 930 K was maintained on the top surface for simplicity. However, at the bottom surface exposed to ambient environment. (i.e., standard atmospheric condition is assumed), such an appropriate boundary condition regarding convective heat transfer should be considered. At this point, suitable assumptions are needed. Additionally, the thermal properties such as thermal conductivity and heat capacity are no longer constants, i.e. functions of temperature. Thus, variation of thermal properties with temperature should be considered to solve this problem. In particular, the interfacial boundary conditions should be implemented in the developed code.

B. TERM-PROJECT: Individual project

All the students should find detailed ways to solve this problem under suitable assumptions from the literature survey. By considering a) variation of thermal properties, b) interfacial condition between two layers, and c) appropriate boundary conditions at the bottom surface, therefore, you should do the followings:

- **a)** Make your in-house code (made by) for getting thermal conductivity
- **b)** Plot the spatial distribution of temperature inside the structure with respect to time
- **c)** Compare the numerical schemes for discretization: explicit, Crank-Nicolson, fully-implicit
- **d)** Compare the results with and without considering variation of thermal properties

```
!Modules should be placed at the beginning of the Main Program.
        MODULE VARIABLES
        INTEGER, PARAMETER :: N=81,M=81
        LOGICAL :: HORIZONTAL=.TRUE.
        REAL, DIMENSION (N,M) :: T      !temperature
! You can define other variables here
!.......................................
!.......................................
       END MODULE VARIABLES
!----------------------------------------------------------------

!----------------------------------------------------------------
        MODULE AE_ARRAYS
! N=number of nodes along x-axis (including boundary nodes)
! M=number of nodes along y-axis (including boundary nodes)
        USE VARIABLES, ONLY : N,M
        REAL, DIMENSION (N,M) :: AE,AW,AS,AN,AP,SU,SP
        END MODULE AE_ARRAYS
!-----------------------------------------------------------------

!-------------------------------------------------------------------------
!Main program comes here:
PROGRAM CFD
!..................................
!..................................
CALL TDMA_SOLVER(T,MAXIT)
!..................................
!..................................
END PROGRAM CFD
!-------------------------------------------------------------------

!-----------------------------------------------------------------
SUBROUTINE TDMA_SOLVER(X,MAXIT)
!This subroutine performs horizontal (along x-axis) or vertical (along y-axis) sweeps
!along lines for solving 2-dimensional problems using TDMA
!X= required solution
!MAXIT=Maximum iterations (number of sweeps)
USE VARIABLES, ONLY : N,M,HORIZONTAL
REAL,DIMENSION(N,M) :: X
DO ITER=1,MAXIT
IF(HORIZONTAL)THEN
CALL HSWEEP(X)
HORIZONTAL=.FALSE.
ELSE
CALL VSWEEP(X)
HORIZONTAL=.TRUE.
ENDIF
END DO
END SUBROUTINE TDMA_SOLVER
!-------------------------------------------------------------------

!-----------------------------------------------------------------------
SUBROUTINE HSWEEP(X)
!This subroutine performs horizontal sweeps for solving 2-D problems along
!horizontal lines
USE AE_ARRAYS
REAL,DIMENSION(N,M) :: X
REAL,ALLOCATABLE :: A(:),B(:),C(:),D(:),X1(:)
ALLOCATE(A(N),B(N),C(N),D(N),X1(N))
DO J=2,M-1
DO I=2,N-1
A(I)=AW(I,J)
```

```
D(I)=-AP(I,J)
C(I)=AE(I,J)
B(I)=-(SU(I,J)+(AS(I,J)*X(I,J-1))+AN(I,J)*X(I,J+1))
END DO
CALL TDMA(A,C,D,B,X1,N)
DO I=2,N-1
X(I,J)=X1(I)
END DO
END DO
DEALLOCATE (A,B,C,D,X1)
END SUBROUTINE HSWEEP
!------------------------------------------------------------------------------

!------------------------------------------------------------------------------
SUBROUTINE VSWEEP(X)
!This subroutine performs horizontal sweeps for solving 2-D problems along
!vertical lines
USE AE_ARRAYS
REAL,DIMENSION(N,M) :: X
REAL,ALLOCATABLE :: A(:),B(:),C(:),D(:),X1(:)
ALLOCATE(A(M),B(M),C(M),D(M),X1(M))
DO I=2,N-1
DO J=2,M-1
A(J)=AS(I,J)
D(J)=-AP(I,J)
C(J)=AN(I,J)
B(J)=-(SU(I,J)+(AW(I,J)*X(I-1,J))+AE(I,J)*X(I+1,J))
END DO
CALL TDMA(A,C,D,B,X1,M)
DO J=2,M-1
X(I,J)=X1(J)
END DO
END DO
DEALLOCATE (A,B,C,D,X1)
END SUBROUTINE VSWEEP
!--------------------------------------------------------------------

!----------------------------------------------------------------------
SUBROUTINE TDMA(A,C,D,B,X1,K)
!This subroutine solves 1-dimensional problems along a line.
! A(:) contains left diagonal elements
! D(:) contains diagonal elements
! C(:) contains right diagonal elements
! B(:) right hand side vector
! X1(:) required solution
REAL,DIMENSION(K) :: A,B,C,D,X1
DO I=3,K-1
E=A(I)/D(I-1)
D(I)=D(I)-(E*C(I-1))
B(I)=B(I)-(E*B(I-1))
END DO
X1(K-1)=B(K-1)/D(K-1)
DO I=K-2,2,-1
X1(I)=(B(I)-(C(I)*X1(I+1)))/D(I)
END DO
END SUBROUTINE TDMA
!--------------------------------------------------------------------------
```