Instructions

This document contains the Project assignment for the course ME-469 Nanoscale Heat Transfer.

In the following you find three problems that require a combination of analytical, numerical and coding approaches to be solved.

For some projects there is some supplementary material to read. This is detailed in the text of the problem and the material is made available in Moodle (see the Project Section).

We recommend using Matlab and COMSOL as preferred softwares but we will accept other tools as well (e.g. Mathematica, Abaqus, Ansys). For accessing these tools you can also use the *Virtual Desk Infrastructure - VDI* provided by EPFL.

This is a **group work**. Each group (2/3 people) is expected to submit:

a) a written report detailing the analytical solutions and the major results of the numerical/coding parts. Program codes should be added in Appendix.

b) well-commented code files (e.g. Matlab) that can be run by the TAs for grading purposes

c) numerical modelling files (e.g. COMSOL), without solution to reduce the storage volume, that can be run by the TAs with an appropriate software for grading purposes

The **deadline** for the submission of the Project Assignment is 10.04.2024 **at** $23:59h$ **CET**

Problem 1: Measuring the Thermal Conductivity

Prerequisites: basic heat transfer knowledge. The solutions can be tackled from Week 1

Measuring the thermal conductivity of thin-films or nanoscale objects (e.g. nanowires) is a very challenging tasks. A number of methods has been developed to achieve this goal. In the following you are asked to model analytically and numerically one very common method called **membrane method for thin-film thermal conductivity measurements.**

It consists in creating a freestanding film (i.e. a membrane) by removing part of the substrate, as shown in Figure 1. A thin-film heater is deposited at the center of the membrane. A thin layer of electrical insulator (such as SiO_2 or Si_3N_4) is used between the film and the heater if the film itself is electrically conducting. The substrate temperature is assumed to be uniform (alternatively, another temperature sensor can be deposited at the edge of the film and the substrate). Thermal conductivity along the film can be measured but one must be very careful to address various factors that may affect the final results.

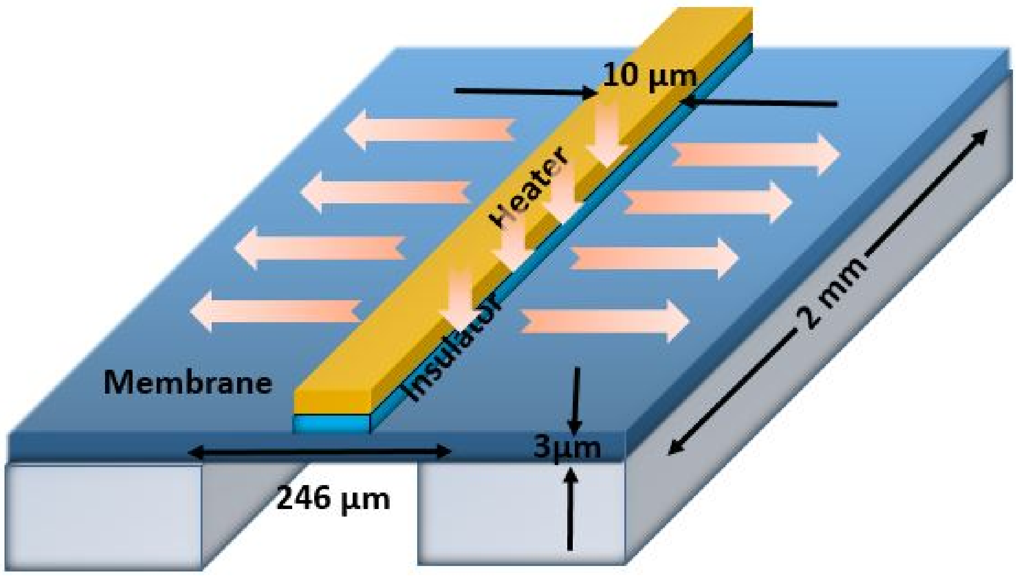

Figure 1: Schematic of the thin-film thermal conductivity measurement. The arrow indicates the direction of heat flux from the heater and then along the membrane. One can assume that the part of the membrane in contact with the substrate is in thermal equilibrium with the substrate.

Part I - Analytical Analysis

a) Derive an expression for determining the thermal conductivity of the film, given the power input to the heater, the temperature rise of the heater, the temperature of the substrates and the geometries, under the following assumptions: (1) heat conduction is one-dimensional, (2) heat losses along the film are negligible (no convection nor radiation), and (3) the thermal resistance of the insulating film is negligible.

b) For a 3 µm thick silicon film/membrane, the thermal conductivity at room temperature is $145 W m^{-1} K^{-1}$. The measured temperature rise of the heater is 2K. Given the geometries in Figure (1), and using $w = 10\mu m$, $2L = 246\mu m$, estimate how much power input is needed.

c) For the silicon thermal conductivity measurement, an insulating layer must be placed between the heater and the silicon film for electrical isolation. Assuming a 200nm thick SiO_2 film with a thermal conductivity of $1.2 \mathrm{W m^{-1} K^{-1}}$ is used, estimate what thermal conductivity you will get if the thermal resistance of the SiO_2 layer is taken into account in analyzing the experimental data, based on the power input condition given in (b).

d) Now, consider heat losses along the film. The combined heat transfer coefficient due to convection and radiation is $10 Wm^{-2}K^{-1}$. For the silicon membrane example given in (b), determine how much additional power input is needed as a result of this heat loss. Assume, that the ambient temperature is 298K which is the same as the substrate temperature(i.e, $T_s = T_\infty = 298K$).

Part II - Numerical Model

To get an understanding of the limitations of the analytical model, you now need to build a numerical model of the thin-film thermal conductivity set-up. For the numerical modelling we recommend COMSOL and the following instructions are based on this software. Nonetheless, you can also use ANSYS or Abaqus.

To familiarize yourself with the approach, read *Problem1-Reading1-COMSOLmodel.pdf* uploaded on Moodle in the Project Section. Pay particular attention to the discussion about the mesh size.

a) Under the following assumptions: (1) heat conduction is one-dimensional, (2) heat losses along the film are negligible (no convection nor radiation), you can build a 2D cartesian model including only the solid. Take special care in defining the appropriate boundary conditions and perform a mesh independency test. Use this model to solve case b) and c) defined in Part I. Compare the results of the analytical and numerical models.

b) Now use your 2D model to study how the geometrical parameters of the system (i.e. membrane thickness d, membrane length L and ratio of heater size and membrane size w/L) affect the sensitivity of your thermal conductivity measurement. For example, introduce a variation in the thermal conductivity Δk of the membrane and observe how much the power input needs to change to achieve the same temperature variation of the heater. **Note:** In the 2D model you probably set a temperature boundary condition at the edges on the membrane. As the ratio of the heater to the membrane size increases, is this a valid boundary condition? Verify!

c) Compare the results of your analysis with the analytical model. Does your analytical model fail under certain conditions?

d) Use your 2D model to compare to case c). Furthermore, vary the thickness of SiO_2 and determine when it is no longer negligible.

e) Update your 2D model and include convection using the combined heat transfer coefficient of part d). Next, vary the combined convection coefficient and determine for which value its effect must be taken into account.

f) In the analytical analysis and the 2D models we completely ignored the heat loss along the heater which has a relatively high thermal conductivity. Now build a 3D model of the heater under the assumption of negligible convection. As you can see in Figure (1) the heater has a length of $L_{heater} = 2mm$. Assuming that the heater thickness is t=200nm and the material is gold with a thermal conductivity of $315Wm^{-1}K^{-1}$, determine the heat loss along the heater to the substrate. How does the heat loss along the heater changer as its length L_{heater} is changed?

Part III - Discussion

Discuss the following aspects:

a) Based on the previous analytical/numerical analysis, what are the advantages and limitations of the membrane-based, thin-film thermal conductivity measurement method?

b) What other methods have been developed to measure the thermal conductivity of thin films?

c) How can these approaches be adapted to the measurement of the thermal conductivity of other nano-sized materials, in particular nanowires? Do you envision specific challenges?

Problem 2: Electron Transport Across an Interface and Heterostructures

Prerequisites: electron wavefunction, band structure. The solution can be tackled from Week 2

When a wave, be it electron, photon or phonon wave, reaches a boundary, it gets reflected and refracted. Quantum tunneling is a phenomenon in which particles penetrate a potential energy barrier with a height greater than the total energy of the particles. The phenomenon is interesting and important because it violates the principles of classical mechanics. Quantum tunneling is important in a wide range of applications, such as the **scanning tunneling microscope(STM)**, and **tunnel diode**. For example in STM, the scanning tip moves along the surface and the tunneling-electron current between the tip and the surface is registered at each position. The amount of the *current depends on the probability of electron tunneling from the surface to the tip, which, in turn, depends on the elevation of the tip above the surface.* Hence, at each tip position, the distance from the tip to the surface is measured by measuring how many electrons tunnel out from the surface to the tip. This method can give an unprecedented resolution of about 0.001 nm, which makes it possible to see individual atoms on the surface.

Part I - Electron reflection

As shown in the figure, an electron with energy E moving from left to right encounters a potential barrier of height δ. The electron wave can be reflected or transmitted.

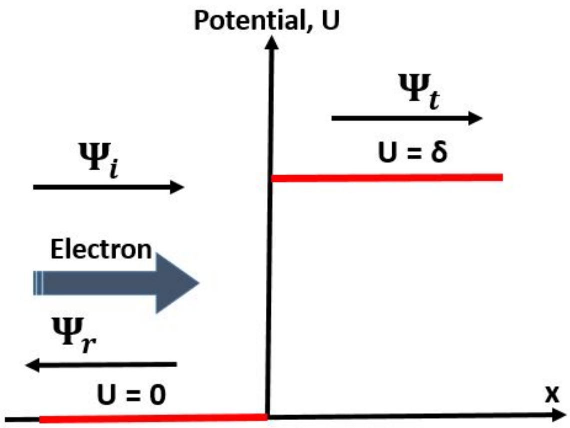

Figure 2: The incident, reflected and transmitted wave barrier with height δ

a) Show that the proper forms of the incoming, reflected, and transmitted wave functions are:

$$\Psi_i = Aexp[-i(\omega t - k_1 x)]$$

$$\Psi_r = Bexp[-i(\omega t + k_1 x)]$$

$$\Psi_t = Cexp[-i(\omega t - k_2 x)]$$

respectively, where

$$k_1 = \sqrt{\frac{2mE}{\bar{h}^2}} \; and \; k_2 = \sqrt{\frac{2m(E-\delta)}{\bar{h}^2}}$$

and A, B, c are constants to be determined from the interface conditions at x=0.

b) At the interface $x = 0$, the wavefunctions and its first derivative must be continuous, derive the expressions for $\frac{B}{A}$ and $\frac{C}{A}$

c) The reflectivity R is defined as the ratio of the reflected particle flux divided by the incoming particle flux, and similarly for transmissivity T.

$$R = \frac{J_r}{J_i} \text{ and } T = \frac{J_t}{J_i}$$

Derive the expressions for **R** and **T**.

d) For $E = 1.2eV$ and $\delta = 1eV$, calculate the electron reflectivity and transmissivity.

e) For $E = 1eV$ and $\delta = 1.2eV$,show that the transmissivity T is zero,and also show that Ψ_t is not zero. This non-zero wave function that does not carry a material flux is called an evanescent wave.

f) Plot the expressions for **R** and **T** as a function of barrier height δ

g) **Top Mark Question** In the above case, we have taken the barrier width to be infinite. How will the expressions for reflected and transmitted wave change if we have a barrier width of finite width. For instance the barrier width in the figure below is **2a** and barrier height is V_0. Derive and plot the expressions for **R** and **T** in this case as a function of: i) Barrier height, and ii)barrier width

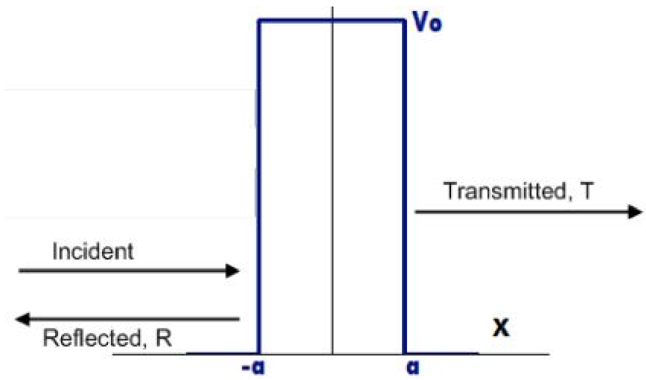

Figure 3: Potential barrier of finite width

Part II - Schottky Diode

When two different materials get in contact, their Fermi levels need to align. This occurs through charge redistribution at the interface. In particular, when a metal makes a contact with a semiconductor, two situations can occur: the formation of an Ohmic contact or the formation of a Schottky contact. While the first result in a resistive contact with a linear voltage/current relationship, the latter case give rise to a diode behavior, i.e. a device which exhibit an asymmetric current/voltage curve.

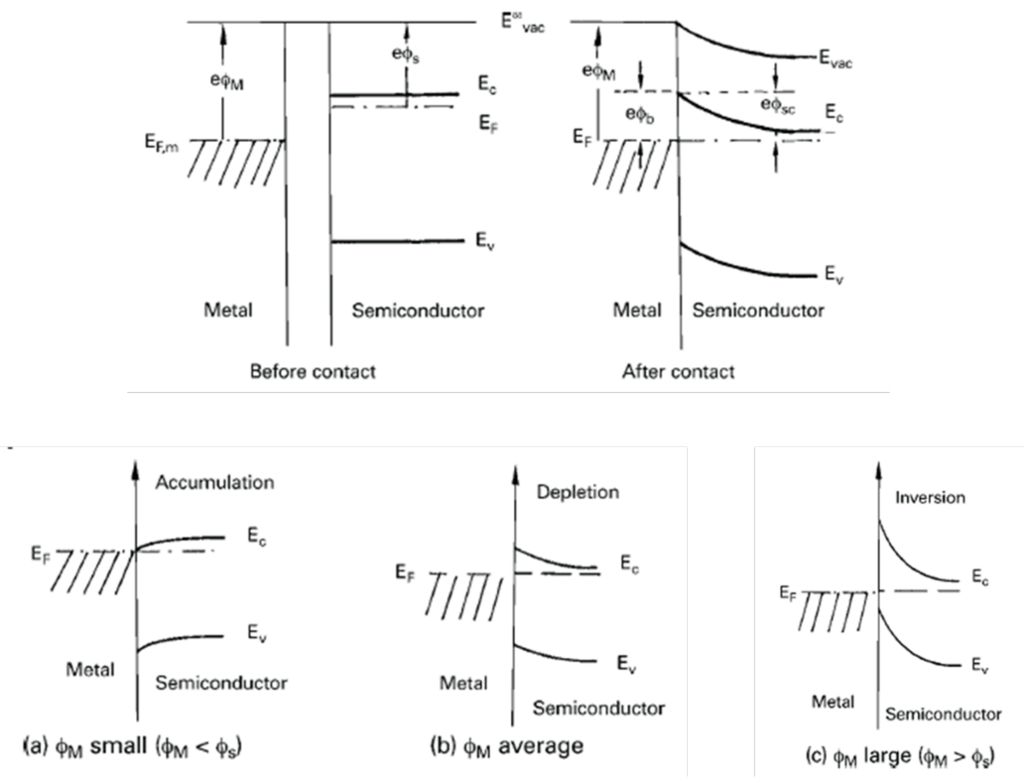

Figure 4: Top) Energy-band diagrams of metal-semiconductor contacts before/after physical contact. Bottom) Metal/semiconductor band alignment as a function of the metal work function (Φ_M) with respect to that of the Semiconductor (Phi_S) leading to an Ohmic contact (a) a Schottky contact (b) a Schottky contact with inversion layer (c).

Considering the properties provided in the Table below, and assuming an ideal metal/semiconductor interface, calculate the Fermi level $E_F(eV)$, the depletion layer width W_D, the electric field $E(x)$ and the conduction band profile $E_c(x)$ as a function of the voltage $V = [-2 : 2](V)$ for the following range of doping levels ($N_D = [1e^{15} : 1e^{18}](cm^{-3})$) and Schottky barrier heights $\phi_B = [0.2 : 1](eV)$.

Material	$E_g(eV)$	ϵ_r	N_C
Silicon	1.12	12	$2.78E19$
Germanium	0.663	16	$1.04E19$

Table 1: Semiconductor Properties

Top Mark Question: plot the current-voltage curve of the Schottky Diode for one of the cases calculated above.

Problem 3- Transfer Matrix Method

Prerequisites: wave equations. The solution can be best tackled from Week 4

Calculating the light transmission and reflection coefficient of multilayer structures is very important. For example, this is critical to design multilayer solar cells consisting of a stack of diverse cells (See *Energy Environ. Sci., 2009, 2, 174-192*). Materials in each cells are optically designed so that they selectively absorb different wavelengths of the sunlight spectrum. In order to maximize the total efficiency of the solar cell energy conversion, it is crucial to know how much energy is absorbed, transmitted or reflected between each cells at given material parameters(thickness, refractive index, etc.)

A very versatile approach to calculate the transmission and reflection coefficients of a multilayer structure is to use the **Transfer Matrix Method**. Read the pdf file *Problem4-Reading1-TMM.pdf* in the Project section on Moodle to find out about this method. Then do the following:

a) Develop a transfer matrix method code to find the reflectivity and transmitivity of single film shown in Figure 5. Plot the reflectivity and transmitivity as a function of the film thickness at the normal incidence of 500nm wavelength photon. Refractive index of the film is 2.5 and assume vacuum on both sides.

b) Figure 6 is a Bragg reflector, which is made of two alternating thin film layers. Develop a transfer matrix method to calculate the reflectivity of the multilayer for normal incident and for a photon energy range $1.2eV - 4.1eV$. Plot the reflectivity for different number of layer pairs: 2,5,10,20. The refractive index of the two layers is $n_1 = 3$ and $n_2 = 3.5$, respectively. The thickness is $d_1 = 41.7nm$ and $d_2 = 35.2nm$, respectively. Again, assume vacuum on both sides.

c) For the case of 5 pairs, analyze the effect of d_1 and d_2, respectively. Also discuss the effect of the difference between the refractive indexes of the two materials.

Figure 5: A single film.

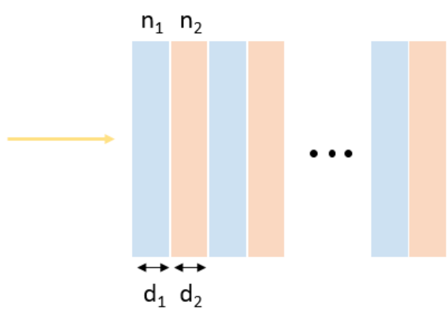

Figure 6: A Bragg reflector consist of two alternating layers.