FYS 9n4310
Materials Science of Semiconductors

PROBLEMS

On Crystal structure

PROBLEM 200-1 (Simple calculation on Xtal structure)

a) Assume a Si single-crystal. Calculate the value of the smallest distance between Si atoms.
b) Assume a diamond single-crystal. Calculate the smallest distance between C atoms.

PROBLEM 200-2 (Calculation and visualization Xtal structure, lengthy)

Choose the origo as a lattice point in the Si crystal structure. From the origo we can make lines to the nearest neighbors, the next nearest neighbors and so on. Several atoms will then have the same distance from origo. Sometimes it is said that several atoms are in the same atomic lattice 'shell'

Make a table where you calculate the distance to shells and calculate how many atoms there are in the shell. Use shell number 1 to number 5.
(Hint: can be time consuming, can be solved by programming or by hand)

PROBLEM 200-3 (Calc. and visualization Xtal structure, a..c=simple, d=lengthy)

The semiconductor SiC has many polytypes, which means that it can exist with several different crystal structures. The most common ones are denoted '3C-SiC', '6H-SiC' and '4H-SiC'. 3C-SiC has a so-called Zink Blende crystal structure which is also shared by GaAs. The lattice constant of 3C-SiC is: 0.436 nm.

a) Calculate the nearest Si-C distance in the structure.
b) Calculate the nearest Si-Si distance in the structure.
c) Calculate the nearest C-C distance in the structure.

Create nearest neighbor shells as in problem 2.

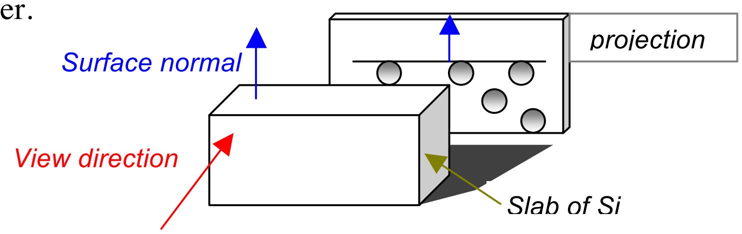
d) Make a table where you calculate the distance to a Si atom around a Si atom and how many Si atoms there are in the shell for shell no 1 to 5.

e) Make a table where you calculate the distance to a C shell around a Si atom and how many C atoms there are in the shell for shell no 1 to 5.

(Hint for d) and e) See Hint for problem 2)

PROBLEM 200-4 (Visualization Xtal structure, projections, intermediate)

Draw a projection of a Si crystal when you look along a given crystal direction – the view direction - and have a certain surface normal. Draw at least 4 unit cells side by side and at least two on top of each other.



a) Look along <100> with <001> normal to the surface
b) Look along <110> with <001> normal to the surface
c) Look along <110> with <-112> normal to the surface

PROBLEM 200-5 (Qualitative on polar semiconductors, easy)

The semiconductors ZnS and GaAs are polar semiconductors. The properties in one direction can be different than those in an opposite direction. In particular, this is true for surface related phenomena like crystal growth and etching; Ga will etch differently on a (111) surface and a (-1 -1 -1) surface. You are supposed to justify that in this problem.

a) Does a (1 1 1) GaAs surface contain As or Ga atoms, or both?
b) Ditto for the (-1 -1 -1) surface.

PROBLEM 200-6 (Calculate stress, order of magnitude, intermediate)

Imagine that we force the unit cell of Ge to occupy the same volume as the unit cell of Si. The Ge is thus deformed and we need to apply a stress (pressure) to maintain this.

a) Calculate the value of the deformation.
b) Calculate the value of the stress.

Hint: $\sigma = F/A$, $E = \sigma / \varepsilon$

PROBLEM 200-7 (Calc., visualization, Xtal surface, easy)

Assume a GaAs crystal with a (100) surface plane. Calculate the areal density (atoms pr sq. cm) of Ga atoms on the surface.

PROBLEM 200-8 (Vacancy defect concentration Si, easy)

a) Calculate the vacancy concentration for intrinsic Si at 1100 °C.
b) Then calculate the equilibrium vacancy concentration at room temperature.

Discuss whether equilibrium is likely at room temperature.
(Intrinsic silicon means in this context that there is an equal concentration of electrons and holes, and this concentration is equal to the so-called intrinsic carrier concentration at the temperature. In practical terms it would mean that it is undoped or low doped)
['Hint' : Calculate this problem, before Problem 9, then possibly reflect on it again]

PROBLEM 200-9 (Defects, Si vacancy charge state, intermediate-easy)

Assume the vacancy in Si can exist in different charge states. Let V* denote a neutral vacancy, V^- denote a negatively charged vacancy. Show that the ratio between the concentration of negatively charged vacancies for the case of n-type conduction and the intrinsic case is equal to the ratio of electron concentration to the intrinsic carrier concentration. That is: show that

$$\frac{\left[V^-\right]}{\left[V^-\right]_i} = \frac{n}{n_i}$$

['Hint': Look at the last equation and rationalize qualitatively why $[V^-]$ increases when n increases. ? Then consider how V* can become V^- and write it down by a chemical reaction formulae. Then, how are the concentration of reactants in a chemical formulae related, and by which law? .]

PROBLEM 200-10 (Xtal growth, easy –difficult)

When you see pictures of the steps from growth to wafers you notice that the crystal is pulled in a specific crystal direction. a) Suggest how this can be accomplished. b) Try to imagine some reasons why you grow the crystal in a particular crystallographic direction. c) Repeat this problem after you have completed the complete course.

PROBLEM 200-11 (Xtal growth, segregation, difficult?)

Derive equation 2.13 in the textbook which give for the surface Cs concentration of a solid during x-tal growth from the melt

$$C_s(x) = kC_0\left(1-x\right)^{k-1}$$

where C_0 is the concentration of dopant atoms in the melt at the onset of growth (x=0) and x is the fraction of the melt that has solidified and k is the segregation coefficient.

PROBLEM 200-12 (Defects, Si vacancy charge state, intermediate-easy)

Assume here the vacancy in Si can exist in 4 different charge states: V+,V*,V-,V= . (positive, neutral, minus, double minus). In the text book is given a relationship between the concentration of neutrals and negatively charged vacancies, equation (2-4)

$\left[V^{-}\right]=\left[V\,*\right]\frac{n}{n_i}\exp\left(\frac{E_i-E_V^{-}}{\mathrm{k}T}\right)$ or with *N* symbols $N_{V^-}=N_V\,\frac{n}{n_i}\exp\left(\frac{E_i-E_{V^-}}{\mathrm{k}T}\right)$

(The subscript 0 in the book means equilibrium). Show or argue that this equation is correct.

PROBLEM 200-13 (Phase diagrams, GaAs MBE, easy (=book 2-4))

During GaAs MBE there is a strong tendency to form droplets of Ga on the surface of the GaAs. They are clearly linked to oval defects observable in a microscope. They constitute a serious problem to fabrication of devices. Without necessarily identifying the reasons for the defect discuss with the help of the phase diagram (Fig. 2.2) how you could a) avoid these droplets b) find out something about their origin c) explain why thermodynamics favor the formation of droplets.

PROBLEM 200-14 (Phase diagrams, Solid solubility, easy (=book 2.5))

A process technology that has gained a great interest recent years is rapid thermal annealing, which we also will cover later. The process allows the wafers that may contain a high doping concentration of dopant atoms to be heated to high temperature very rapidly, minimizing dopant diffusion. Try to explain the desirability of such a process in the light of a discussion of solid solubility and phase diagrams.

PROBLEM 200-15 (Segregation, X-tal growth, easy)=book2.14)

A melt for use in a Czochralski crystal grower contains 0.1 atomic percent P in Si. Assume the well-mixed approximation and calculate the dopant concentration when 10% of the x-tal is pulled, when 50 % of the crystal is pulled and 90 % of the x-tal is pulled

PROBLEM 200-16 (X-tal growth, -easy)

Why does Bridgeman growth tend to have higher impurity content than LEC.

PROBLEM 200-17 (X-tal growth, - intermediate)

We consider Czochralski crystal growth of Si. In describing the heat flow during growth, assign the following symbols; *L*: latent heat of fusion, k_L=thermal conductivity of liquid Si, k_S: thermal conductivity of solid Si, *m*: mass of solidified Si, (grown x-tal), *N*: density of solid, *A*: areal cross section, *r*: radius of growing crystal.

a) Set up an expression for the amount of Si solidified per unit time d*m*/d*t* based upon the heat balance during growth. Consider the heat released in solidification, heat flowing out of the melt and flow into the crystal.

Let the pulling rate of the crystal be denoted v_P. It is given by

$$v_P = \frac{dm}{dt}\frac{1}{AN}$$

We want to find the maximum pulling rate $v_{P.\max}$ we can have at the same time as fulfilling the heat balance. This max rate should occur when there is no net heat transferred from the liquid to the growth zone. The heat that is transferred to the Si crystal will be lost by i)radiation loss from the surface, ii) convection loss (when done in Ar ambient) iii) conduction through the neck. Assume mechanism i) dominates.

b) Show that the max pull rate is given by

$$v_{p.\max} = \frac{1}{LN}\sqrt{\frac{2\sigma\varepsilon k_m T_m^5}{3r}}$$

where k_m is the thermal conductivity at the melting temperature Tm, σ is Stefan Bolzmann's constant, ε is the emissivity of the Si solid r is the radius of the crystal.

c) Calculate the value of the max pull rate for the case of 6 inch diameter wafer. Use $L = 430$ cal/g, ε=0.55, k_m=0.048 cal s^{-1} cm^{-1} K^{-1}

d) Verify if the assumption that radiation loss dominates over convection is justified by looking up the needed parameters.

PROBLEM 200-18 (=2.12 book, X-tal growth, doping - intermediate)

A Czochralski growth process is begun by inserting 1000 moles of pure Si and 0.01 mole of pure As in the crucible. For this boule the maximum permissible doping concentration is 10^{18} cm^{-3}. What fraction, X, of the boule is usable?

PROBLEM 200-19 (≈2.13 book, X-tal growth, doping - intermediate)

In an attempt to form a heavily doped p-type boule of Si, a Czochralski growth process is run in which the initial melt concentration of boron (B) was 1.5 atomic %. Assume the solidification temperature 1400 °C, and that the boule cooled rapidly after solidification.

a) What is the solubility of B at this temperature?

b) What fraction of the boule must be pulled (i.e. solidified) before the concentration of the boron in the solid will begin to exceed the solid solubility of boron in silicon?

c) What is the concentration (in percent) of boron in the liquid at this point, assuming that the liquid has a uniform concentration.

d) Make a plot of the concentration of B in the Si crystal , Cs, vs the fraction solidified, X. Also include the case that the melt was 2.5% and 3.7%. Set off the solid solubility in the same plot.

e) What qualitative modification to the solution would we have if the concentration in the liquid were not constant?

PROBLEM 200-20 (Si CZ X-tal growth, oxygen- easy)
The oxygen content of a Si crystal usually decreases from the seed towards the bottom of the crystal.
Explain why! - please!

PROBLEM 300-1 (Diffusion, Electrical field, intermediate)

We will estimate the electrical field between an ionized donor atom and a negatively charged vacancy, and its effect upon diffusion. Assume a Si crystal at 1000 °C. The donor atom and vacancy will interact by Coulomb forces. We will calculate the corresponding electrical field for different separations of the vacancy and the donor. Make suitable simplifying assumptions. We aim at an order of magnitude estimation. Call d_0 the nearest neighbor distance.

a) Calculate the electric field when the donor and vacancy is separated by 10 d_0, 4 d_0, and 2 d_0.

Assume that the activation energy for atomic jumps necessary for the vacancy to diffuse (make a jump) is 2 eV if we ignore the electrical field. Make a simple choice for the shape of the potential along a jump path for a vacancy.

b) Calculate how much the activation energy will change with an electrical field when the vacancy –donor separation is 10, 4 and 2 d_0.

c) At the same separations calculate the ratio between the probability for the vacancy to jump towards the donor and that for jumping away.

d) From the above, discuss correlations between donor and vacancies and its influence on diffusion of a donor.

PROBLEM 300-2 (3-2 book, Diffusion, using Fairs model, plot, intermediate)

Construct a semi-log plot using Table 3.2 and 3 contributions to the diffusivity of phosphorous as a function of temperature from 700 ..1100 °C. ! Please!
Assume the concentration C of phosphorous is 10^{19} cm^{-3}
.
PROBLEM 300-3 (Diffusion, understanding Fairs model, intermediate)

Consider the diffusivity as denoted in Fairs diffusion model for diffusion of dopant atoms in Si.

a) Define stringently each symbol.
b) Explain the equation.

PROBLEM 300-4 (=book 3.4, Stress high concentration, easy..difficult)
The book says stress is a high concentration effect that was not discussed in the book. Here we consider As as doping atoms in Si. The book says As is much larger than Si. When high concentration of As are incorporated in the lattice, it creates strain. Discuss qualitatively how this stress may affect the diffusivity of As. Make educated guesses weather it goes up or down with the stress, and try to justify it.
This is easy to start to discuss. It is very difficult to know your guesses are right.

PROBLEM 300-5 (Diffusion, electrical field enhancement difficult/tricky)

Consider the diffusion of dopant atoms, diffusing in from the surface and creating a concentration profile with a gradient. That will create an electrical field. Since the dopant atoms are assumed to have shallow levels they will be fully ionized at a temperature where they diffuse. Because of this charge, they will be influenced by the electrical field giving an enhancement to the diffusion. We can then write the flux of atoms as

$$J = -D(1+\eta)\frac{\partial C}{\partial z} \quad \text{[eq1]}$$

where z is depth, η is the electrical field enhancement, and the rest have their usual meaning. For simplicity we consider just diffusion and flux by one vacancy charge state, which we assume is irrelevant for the problem
a) Derive equation [eq1] (Hint: see lecture notes).
b) Show that the parameter η will have a value between 0 and 1.
Hint: 1) See lecture notes. 2) Show you can write η as

$$\eta = \frac{C(z)\left(\frac{\partial n(z)}{\partial z}\right)}{n(z)\left(\frac{\partial C(z)}{\partial z}\right)}$$

Info: Several textbooks and review articles show a solution to b) by assuming local charge neutrality. That is formally incorrect, and should be considered a bad idea since it is the deviation from local charge neutrality that gives the electrical field. But by doing so, for extrinsic diffusion $n >> n_i$, they arrive at

$$\eta = \frac{C(z)}{\sqrt{C(z)^2 + 4n_i^2}}$$

, which obviously have a value between 0 and 1. The value range is correct, but the derivation is not.

c) Discuss very briefly whether the results would be principally different if we consider interstitial diffusion,

PROBLEM 300-6 (=3.12 in book 3rd Ed; As diffusion doping in Si , intermediate)

A pre-deposition of As in Si is carried out with the following parameters: time 10 min, temperature 1100 °C. Assume that the surface concentration reaches the solubility limit. Following the pre-deposition, there will be a drive-in diffusion for 24 h at 1000 °C. Use equation (3.23?) in the book to predict the maximum carrier concentration. How does this compare to the solid solubility limit at 1000 °C? Explain the distinction between solid solubility and Equation (3.23?).

PROBLEM 300-7 (=3.9 in book 3rd Ed; P diffusion doping in Si , intermediate)

Si wafers with bulk p=type doping concentration of 10^{17} cm^{-3} are diffusion doped with P (Phosphorous). A pre-deposition step is carried out at 1000 °C for 20 min. Assume that the solid solubility was reached at the surface. The surface of the wafer was sealed and a a 1100 °C drive in diffusion was carried out. Find the drive in time necessary to give a junction depth of 4 μm. What is the surface concentration after the drive-in? It is highly recommended that you in addition to solving the problem by analytical expressions found in the text book also simulate the process with tools available at http://nanohub.org
(You may use “Process Lab : Concentration-Dependent Diffusion”)

PROBLEM 300-8 (=3.7 in book 3rd Ed; B diffusion doping in Si , intermediate)

For scaled down CMOS devices, there is a large interest in forming so-called shallow p-n junctions, i.e. the junction depth is small. Assume you have access to an ion implanter with exceptional small energy for boron implants in Si. You implant a dose of $5x10^{15}$cm^{-2} and ultra-shallow. The surface of the wafer is sealed and the wafer is annealed at 1000 °C for 10 sec. Assume intrinsic diffusion and find

a) The final junction depth if the substrate doping is 10^{17} cm^{-3}
b) Find the final concentration of B at the surface.
c) Can you compare your calculations with simulations at http://nanohub.org
(You may use “Process Lab : Concentration-Dependent Diffusion”)

PROBLEM 300-9 (=3.14 in book 3rd Ed; B diffusion in SiO_2 , intermediate)

For CMOS devices, there is often a desire to create Boron doped poly-Si gates. That is a B doped poly crystalline Si film as a gate on top of the gate oxide. Assume here a 10 nm gate oxide. Assume also that the B concentration in the oxide close to the poly-Si/SiO_2 interface is constant at $C_s = 10^{21}$ cm^{-3}. For the proper operation of the device (minimal shift of turn on voltage) it is required that the maximum amount B diffused into the substrate is less that $Q_{Tmax}=3x10^{11}$ cm^{-2}. Use table 3.4 to estimate the dose of B atoms that enter the semiconductor after 4 hr at 1000 C. Will this anneal produce unacceptable threshold shift?

PROBLEM 300-10 (=3.13 in book 3rd Ed; CV measurement of ??)

Assume that a wafer is uniformly doped. If a Schottky contact is formed on the surface, what would the C-V curve look like? Plot it in a convenient/optimum way for this question: What information can you obtain from it?

PROBLEM 300-11 (Diffusion – std. easy)

Assume diffusion of a p-type dopant from the surface in an n-type doped substrate with concentration C_{sub}.

a) If possible, derive an expression for the junction depth when the diffusion profile is described by the conditions applicable to the idealized case yielding an erfc type distribution for predeposition.

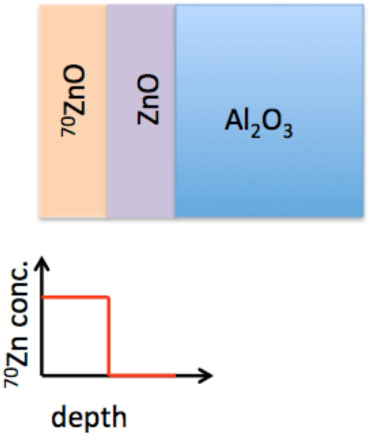
Assume a surface solid solubility of C_S=5x10^{20} cm^{-3} for an erfc distribution. Assume a substrate doping C_{sub} of 5x10^{15} cm^{-3}and a diffusivity of 5x10^{-15} cm^{-2}s^{-1} (which is close to that of B in Si at 900 °C).

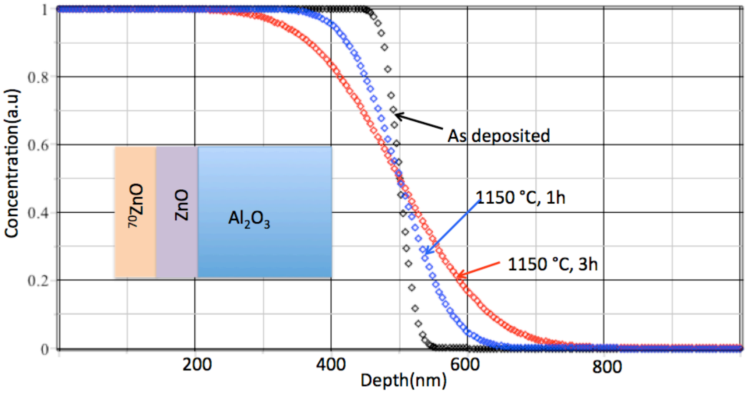
b) Calculate the junction depth and the concentration gradient of the space charge at the junction. (This sometimes enters in the analysis of electrical junction parameters) when the total deposited amount of acceptors is Q_T=10^{14} cm^{-2}

c) Calculate the junction depth after drive-in diffusion for 10, 30, 60 and 120 min. at 900 °C.

PROBLEM 300-12 (Diffusion, general – Diffusion Eq. std. solutions, intermediate)

We will consider a diffusion experiment to measure the self-diffusion of Zn in ZnO.
In the experiment we grow ZnO thin (500 nm) films by molecular beam epitaxy. The Zn is deposited on a substrate (sapphire) by heating Zn in Knudsen cells. We use two different Knudsen cells for Zn. One contains pure Zn with its natural abundance of isotopes, the other is very much enriched in isotope 70. By using shutters in front of the cells this can result in a ZnO film structure that has almost only Zn^{70} in the top of ZnO layer and only 0.6 percent Zn^{70} in the bottom ZnO. Consider the initial Zn concentration shown in the figure below. i.e. assume for simplicity 100% and 0 %t Zn^{70} in the two layers respectively





We measure the concentration profile of ^{70}Zn by SIMS just after growth, see Figure below. Then we anneal the sample at 1150 °C for 1h and 3 h respectively and measure the SIMS profiles. From these measurements, you should determine the self diffusion coefficient of Zn at the temperature!

Hint: The first part of the problem is to find an expression for the concentration profile. Show, or rationalize, that the profile will (approximately) be given by:

$$C(x, t) = \frac{1}{4} N_{ZnO} \operatorname{erfc}\left(\frac{1}{2} \frac{x - x_0}{\sqrt{Dt}} \right)$$

Here x is the depth, t is the time, x_0 is the thickness of the ^{70}ZnO layer and D is the diffusivity. (The approximation is equivalent to assuming the films extending to infinity on each side of x_0, which is OK when the 'inter-diffusion zone' is well separated from the surface or the interface)

PROBLEM 400-1 (Oxidation, Deal Grove model, easy)

Consider the so-called Deal Grove Model for thermal oxidation of Si.
a) Write down all the assumptions in the Deal Grove Model.
b) Derive the familiar expression for the oxide thickness vs. time.

PROBLEM 400-2 (Oxidation , Deal Grove model, easy - difficult)

Si nanostructures with strong confinement have been made from intermediate sized nanostructures by oxidation. For example it has been reported that Si wires with a length of a few μm and a diameter of 10-30 nm can be grown. These can be made into quantum wires by thermal oxidation of Si.

a) Consider a (hypothetical) Si thin plate with thickness 20 nm that is oxidized in dry oxygen at 750 °C. For how long would you need to oxidize to get a 3 nm thick Si crystal plate surrounded by SiO_2?

b) Consider a 20 nm diameter Si rod that is oxidized in dry oxygen at 750 °C. For how long would you need to oxidize to get a 3 nm diameter Si quantum wire? Assume the Deal Groves model, but use cylinder coordinates.

c) Consider a 20 nm diameter Si sphere that is oxidized in dry oxygen at 750 °C. For how long would you need to oxidize to get a 3 nm diameter Si quantum dot? Assume the Deal Groves model, but use spherical coordinates. Assume Deal groves model, but use spherical coordinates.

d) The cases b) and c) will lead to self-limited growth situation. Explain why. Is this self-limiting process fundamentally temperature dependent? –i.e. do we get equally strong self limiting effect at different temperatures, possibly just scaled by the Diffusivity of O_2 in the oxide and the reaction rate constant?

PROBLEM 400-3 (Oxidation , wet and dry, easy-difficult)

a) Express short and precisely what *is* “dry oxidation” and what *is* “wet oxidation” in the context of the physics and chemistry of Si device processing.

   Notice Fig 4.2 gives two experimental curves for the parabolic rate constant B, and similarly Fig 4.3 gives two curves for the linear rate constant B/A. The two curves are to be taken for dry oxidation and wet oxidation respectively. Note that the data for wet oxidation is given for “640 torr”

b) Express short and precisely what this 640 torr may refer to. If you don’t know how wet oxidation is done, try to imagine how it could have been done. At what temperature is the equilibrium pressure above water equal to 640 torr?
   (Hint: Units torr and °C : T=1668.21/(7.96681-log10(P))-228.0);

c) Mention some reasons that could give a parabolic rate constant that is higher for wet oxidation than for dry.

d) Mention some reasons that could give a linear rate constant that is higher for wet oxidation. Discuss the detail that the activation energy is nearly identical for the two oxidation processes.

e) In Example 4.1 is made calculation ‘steam oxidation’. Will this be faster or slower than wet oxidation?

PROBLEM 400-4 (Oxidation , wet and dry, easy-intermediate)

Consider oxidation of intrinsic (100) Si :

a) We oxidize a wafer at 1000 °C in dry oxygen. Calculate how long oxidation time we need to get a 50 nm thick oxide.

b) We oxidize in steam by an inert gas bubbling through steam. The steam has a partial pressure of 640 torr and the wafer is kept at 1050 °C. Calculate the oxidation time to get a 1μm thick oxide.

c) Suggest how we could measure the oxide thickness so-called *in-situ* meaning that the thickness is measured while the oxide film is growing. What corrections would be needed to this measurement to accurately get the oxide thickness of a device.

PROBLEM 400-5 (RT, rapid thermal oxidation, computer calcs)

Rapid thermal oxidation is a treatment sometimes made for creating thin oxides. The Si wafer is heated up by lamps, allowing fast temperature ramping and thus better control of short durations than what an oxidation furnace allows. Since one is interested in thin oxides it means one operates in a regime where the Deal Grove model does not apply and does not work well. A model with more success at short time is due to Massoud. The oxide thickness, *x,* can in the model be written as.

$$x = -\frac{A}{2} + \sqrt{\left(\frac{A}{2}\right)^2 + B \cdot t + M_1\left(1 - \exp\left(-\frac{t}{\tau_1}\right)\right) + M_2\left(1 - \exp\left(-\frac{t}{\tau_2}\right)\right) + M_0}$$

Where A and B has similar function as in the Deal Grove model and the two exponentials disappear for thick oxides. The constants M_1, M_2 and M_0 are determined by the initial oxide thickness x_i according to :

$$M_0 = x_i^2 + Ax_i, \qquad M_1 = K_1\tau_1, \qquad M_2 = K_2\tau_2$$

The parameters are temperature dependent and have temperature dependencies as follows:

$$K_1 = K_1^0 \exp\left(-\frac{E_{K_1}}{\mathrm{k}T}\right), \qquad K_2 = K_2^0 \exp\left(-\frac{E_{K_2}}{\mathrm{k}T}\right), \qquad \tau_1 = \tau_1^0 \exp\left(-\frac{E_{\tau_1}}{\mathrm{k}T}\right), \qquad \tau_2 = \tau_2^0 \exp\left(-\frac{E_{\tau_2}}{\mathrm{k}T}\right)$$

$$B = C_B \exp\left(-\frac{E_B}{\mathrm{k}T}\right), \qquad B/A = C_{B/A} \exp\left(-\frac{E_{B/A}}{\mathrm{k}T}\right),$$

The parameters have the following values

K_1^0	$[\mathrm{nm}^2\,\mathrm{min}^{-1}]$	2.48×10^{11}
E_{K_1}	$[eV]$	2.18
K_2^0	$[\mathrm{nm}^2\,\mathrm{min}^{-1}]$	3.72×10^{11}
E_{K_2}	$[eV]$	2.28
τ_1^0	[min]	4.14×10^{-6}
E_{τ_1}	$[eV]$	1.38
τ_2^0	[min]	2.71×10^{-7}
E_{τ_2}	$[eV]$	1.88

C_B	$[\mathrm{nm}^2\,\mathrm{min}^{-1}]$	1.70×10^{11}
E_B	[eV]	2.22
$C_{B/A}$	$[\mathrm{nm} \cdot \mathrm{min}^{-1}]$	7.35×10^{6}
$E_{B/A}$	[eV]	1.76

(NB the values for B og B/A are to be used for T<1000 °C)

a)Assume oxidation at 950 °C, Find how long the rapid thermal processing needs to be to get an oxide with thickness 10 nm.

b) Calculate what corrections you would need to make to this thickness if you ramped the temperature from 500 °C with a ramp rate of 200 °C/min, held it at 900 °C for 10 s and then ramped down to 500 with an exponential decay T (t)=T_{950} exp (-t/τ) with τ = 60 s.

PROBLEM 400-6 (4.17 in book 3rd Ed, oxide characterization)

A thermal oxide thickness is measured both by the use of a Nanospec and by measuring the accumulation capacitance. The results are found to to differ by 20 %, even though the same wafer was used for each measurement. Give three possible errors that might account for the discrepancy.

PROBLEM 400-7 (4.11 in book 3rd Ed, oxide growth rates, Deal Grove parameters)

Assume that negatively charged O_2- has exactly twice the diffusion coefficient in SiO_2 as neutral O_2 (due to a field aided term) but 10 times the reactivity at the surface, with exactly the same activation energy for the reaction rate coefficient (is that reasonable?) We have a source of 1 atm of O_{2-}. We want a thickness of 100 nm and do oxidation at 1000 °C. If there is no initial oxide, how long should the oxidation be done? Is the oxidation in the linear regime, the parabolic regime, or between?

PROBLEM 400-8 (4.7 in book 3rd Ed, oxide growth rates, Deal Grove parameters)

A gate oxide is grown in a 640 Torr of water vapor at 1000 °C. The oxide is grown on a bare (100) Si wafer. The oxidation time is 2 min.
a) Assuming the tau is zero, use the Deal Grove model to predict the oxide thickness that would be grown.
b) When the process is run, the oxide thickness is actually found to be 60 nm but the oxidation rate after 2 min agrees with the B/A ratio. Fin the value of tau that should be used for these process conditions to take into account the rapid growth regime.

PROBLEM 400-9 (4.8 in book 3rd Ed, oxide growth rates, Deal Grove parameters)

An oxidation of a bare Si wafer is to be done in one atmosphere of dry O_2 at 1000 °C. The desired thickness for this oxide is 400 Å
a) Find the time needed for this oxidation if one ignores rapid growth effects
b) Find the time needed for this oxidation taking into account rapid growth effects

PROBLEM 400-10 (4.12 in book 3rd Ed, why grow oxide high T)

For submicron MOSFETs, it is often necessary to grow very thin oxide of order of 10 nm or thinner. Although process control is very difficult due to the short oxidation times involved, it is preferable to grow these oxides at high temperatures. Explain why!

PROBLEM 500-1 (5.1 in book 3rd Ed, Ion implantation, Ranges)

A 30 keV implant of ^{11}B is done into bare Si. The dose is 10^{12} cm^{-2}.

a) What is the depth of the peak of the implanted profile?
b) What is the concentration at this depth?
c) What is the concentration at a depth of 300 nm?
d) The measured concentration is found to be an order of magnitude larger than the value predicted in part c), although the profile agrees with answers a) and b). Give a possible explanation, assuming that the measured value is correct.

PROBLEM 500-2 (5. 2 in book 3rd Ed, Ion Implantation Ranges)

A particular Si device needs to have an implant of boron with a peak at a depth of 0.3 μm and a peak concentration of 10^{17} cm^{-3}. Determine the implant energy and dose that should be used for this process. Find the as-implanted junction depth if the substrate is n-type with a concentration of 10^{15} cm^{-3}.

PROBLEM 500-3 (5.3 in book 3rd Ed, Ion Implantation Ranges)

P is implanted into Si. The implant parameters are: dose=10^{15}cm^{-2},energy=150 keV

a) Find the depth of the peak concentration and the value of the peak concentration.
b) If the Si wafer originally had a uniform boron doping concentration of 10^{16} cm^{-3}, find the depth(s) at which the B concentration equals the P concentration.

PROBLEM 500-6 (5.6 in book 4th Ed, Ion Implantation Ranges, multilayers)

A MOSFET threshold voltage adjust implant is done through a gate oxide of 15 nm. The implanted species are boron ions at 30 keV. Estimate the fraction of boron implanted in the oxide. (You may have to use the approximation that $x \ll R_p$ for the Gaussian)

PROBLEM 500-7 (5.7 in book 4th Ed, Ion Implantation Ranges)

A mass spectrometer as described in textbook chapter 5 is used for element extraction in an implanter. Calculate the magnetic field necessary to extract silicon (mass 28) if the extraction potential is 20 kV an the radius of curvature of the analyzer is 30 cm. Explain why one might also see some N2 in the implanted profile if the source cabinet has a small vacuum leak.

PROBLEM 600-1 (6.1 in book 4th Ed, Rapid thermal annealing)

Undoped Si ia nearly transparent for photons with energies close to or less than the bandgap(1.1eV). Assume that a wafer is transparent for $\lambda > 1$ µm. If the wafer is heated with a tungsten-halogen lamp operating at 2000 K, what fraction of the incident energy is transmitted through the wafer? Would GaAs absorb more or less of the energy? Why?

PROBLEM 600-3 (6.3 in book 4th Ed, Rapid thermal annealing)

Large diameter wafers are difficult for RTP at high temperature without the occurrence of thermoplastic induced slip at the edge of the wafer. Describe the reasons for this slip. If the slip is more pronounced after high temperature raps, what does this tell you about the radiation pattern at the surface of the wafer?

PROBLEM 800-1 (Pattern transfer, resists , easy)

What are the main general advantages and weaknesses of positive and negative resist respectively. Also explain why (qualitatively and in particular which properties of the resist is playing a part in this)

PROBLEM 900-1 (e-beam lithography = 9.2 in book, easy)

If one examines the Monte Carlo results for an e-beam exposure shown in Fg. 9.10, some of the scattering events involve scattering angles (the angle between the incident and outgoing velocity vector) of greater than 90 °. Explain briefly why this is seen far more often in e-beam lithography than in ion implantation.

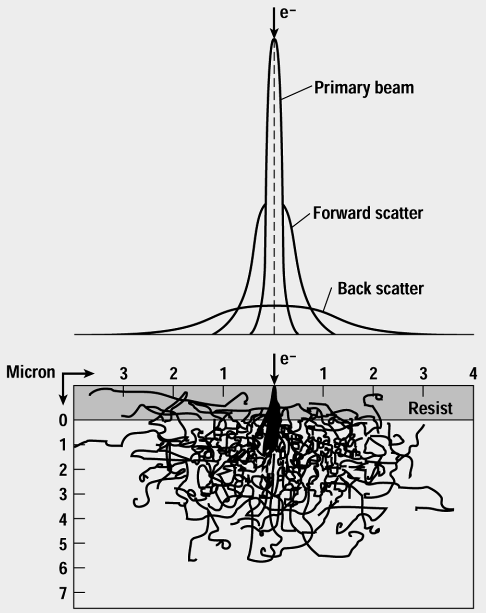


Figure 9.10 Monte Carlo simulation of electron trajectories during an EBL exposure. The upper curve indicates the forward and backscattered components of the beam *(after Hohn, reprinted by permission, SPIE).*

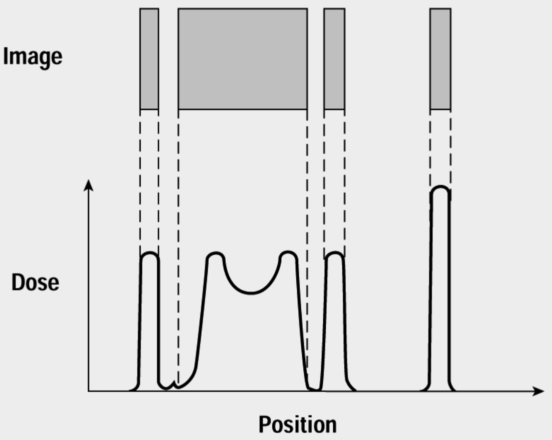


Figure 9.11 Small and large figures to be patterned with EBL requires position-dependent dosage to compensate for proximity effects.

PROBLEM 900-2(x-ray lithography= 9.5 in book, easy)

A proximity X-ray mask is made up of tungsten-absorbing patterns on a silicon nitride membrane. If the membrane heats 10 °C during exposure and the field size is 2.5 cm on a side, how much can the field be distorted due to thermal expansion? Using approximation that the maximum allowable distortion is about one-fourth the minimum feature size, what is the maximum temperature rise allowable on the mask if the minimum feature size is 0.1 μm?

PROBLEM 1400-1 (CVD epi-growth of Si =14.1 in book, easy)

A silicon epitaxial growth process is attempted with a chamber temperature of 1050 °C. and as flows of 200 sccm $SiCl_4$ and 100 sccm of Si_2H_6. Assume that the mixture attains chemical equilibrium. What is the super-saturation in the chamber? Will these conditions grow an epitaxial layer or etch? If the temperature is increased to 1300 °C, by what percentage would you expect the growth (or etch) rate to increase or decrease?

.

PROBLEM 1400-2 (CVD growth of Si =14.2 in book, easy)

Starting with equation 14.1, derive equation 14.2.

$$F = h_g\left(C_g - C_s\right) = k_s C_0 \qquad (14.1)$$

$$R = \frac{k_s h_g}{k_s + h_g}\frac{C_g}{N} \qquad (14.2)$$

PROBLEM 1400-3 (CVD growth mechanisms, easy, tedious (=14.3.in book))

Consider CVD growth and the limiting processing in the CVD growth of Si and the simple growth model by Deal described in the book arriving at equation (14.2)

$$R = \frac{k_s h_g}{k_s + h_g}\frac{C_g}{N}$$

for the growth rate R, where N is the density of Si ($5\text{x}10^{22}$ cm^{-3}) divided by the number of Si atoms in the growth molecule (the gas molecule) . C_g is the concentration of the gas, k_s is the surface reaction rate and h_g is the mass transport factor of gas molecules across the stagnant gas layer. Assume the reaction rate is given by

$$k_s = k_0 \exp\left(-\frac{E_g}{\mathrm{k}T}\right)$$

Assume that h_g is independent upon temperature and that $C_g=10^{15}$ cm^{-3} at all temperatures. Figure 14.8 in the book is shown below

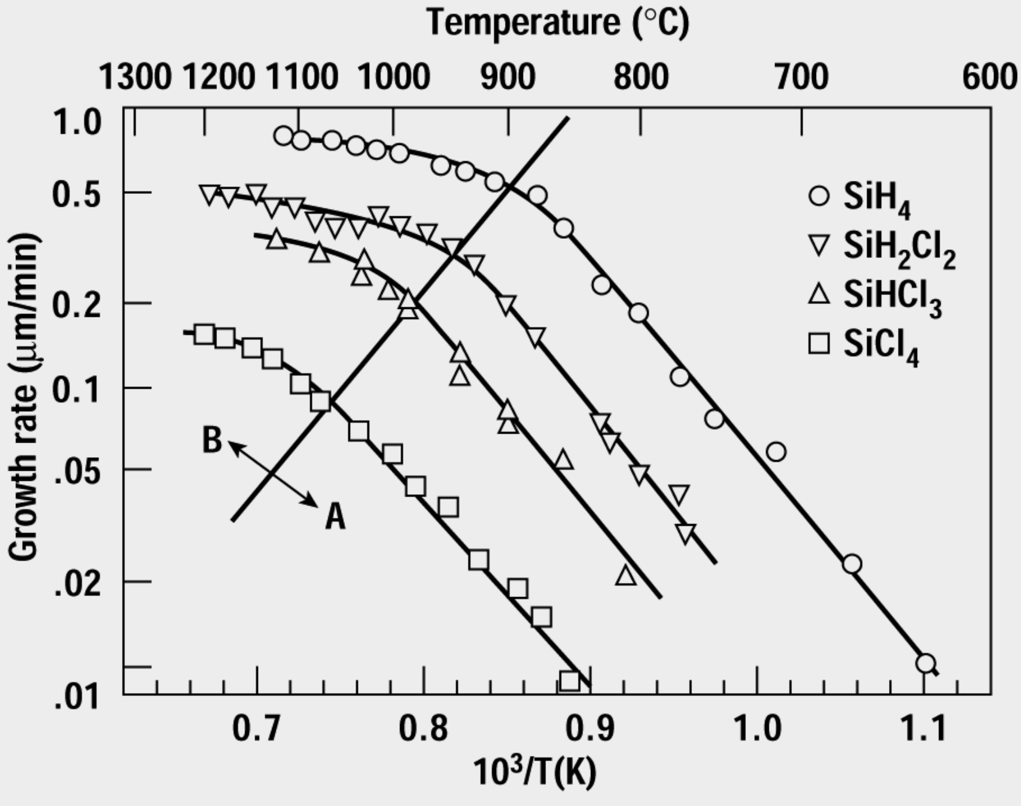


Figure 14.8 Arrhenius behavior of a variety of silicon-containing growth species *(after Eversteyn, reprinted by permission, Philips).*

With the use of this figure and the model do the following

a) Identify, for each molecule, the approximate temperature where the growth becomes mass transport limited.
b) Find for each molecule h_g
c) Find for each molecule k_0 and E_a

PROBLEM 1400-4 (Si epi growth, surface, easy(=14.4 in book))

An epitaxial growth chamber has a background O_2 pressure of 2x10-5 torr. What would be the minimum annealing temperature to ensure a Si-stable surface if only the background gases are present? Alternatively, one can flow H_2, which contains 5 ppb of O_2. If this gas flushes the chamber of its background contaminants, what would be the minimum annealing temperature be at 760 torr of H_2. ?

PROBLEM 1400-5 (Si CVD epitaxi, 14.5 in book)

Explain why the growth rate curve shown in Fig 14.5 in the book and reproduced below becomes negative.

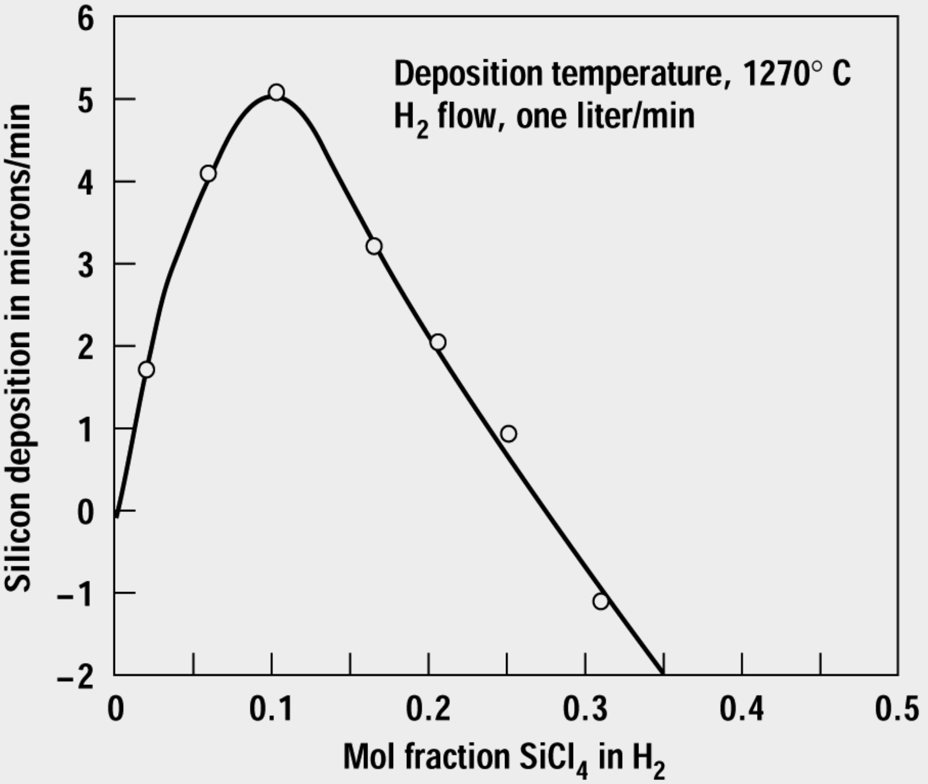


Figure 14.6 Growth rate as a function of the $SiCl_4$ flow. At high concentrations, the chlorine in the chamber leads to etching *(after Theuerer, reprinted by permission of the publisher, The Electrochemical Society).*

PROBLEM 1400-6 (Si epi-growth at low temp, 14.6 in book)

Over the years several alternatives to the standard CVD epi-growth of Si has emerged which allows epitaxial growth at lower temperatures.
Try to discuss why there is a desire to do so, and repeat this problem at the end of the course.
Some hints/relevant sub-questions: Why low temperature growth would be desirable. Then why do you really use a high temperature at all? Check out Fig. 14.8 to determine the time needed to grow 1 μm epi Si at 800, 900, 1000 and 1100 °C. Find the diffusion length sqrt(Dt) for As at these temperatures.

PROBLEM 1400-7 (Si CVD epi, 14.7 in book)

Consider Si CVD epitaxi. In the present case a gas consisting of 5% $SiCl_4$ in H_2 is used. The substrate temperature is 1100 C. Calculate the super-saturation for this case. Will growth or etching result?

PROBLEM 1400-8 (14.8 in book)

Why isn’t halide transport used for silicon epitaxial growth?

PROBLEM 1400-9 (Heteroepi, 14.9 in book)

What is commensurate, incommensurate and pseudomorphic growth in the context of epitaxial growth? In particular what are the differences? Try to describe advantages and limitations of each.

PROBLEM 1400-10 (Hetero epi, 14.10 in book)

The growth of GaAs on Si, has some advantages. What might that be? Hetero-epitaxi with Si as a substrate has been extended to other materials than GaAs. Among these are InP , CdTe and HgCdTe. For each discuss what merits may be involved. If you would extend it to other/new materials, what would you need to find out to determine whether it would be technically feasible to grow the material epitaxially on Si?

PROBLEM 1400-11 (14.11 in book)

See text in 3rd edition.

PROBLEM 1500-1(ohmic contacts, easy)
We will make a simple ohmic contact for p-type Si for laboratory use, that is, we want to perform electrical measurements, which require an ohmic contact and where the influence of this upon the measurement result is minimal. We assume the influence is at a minimum when the contact resistance is the smallest. We have the choice of evaporating Al or Pt. Which metal would give the least contact resistance? Give a short explanation. (You may use textbook chapter 15 as reference)

PROBLEM 1500-2*(Schottky barriers, intermedium)
We consider a Schottky barrier to n-Si. Let the donor concentration be 10^{15} cm^{-3} and the temperature 22 °C. Without image force reduction, the barrier height is 0.75 eV.
a) Calculate how large the reduction in the barrier height is due to image force lowering for an applied bias of 0V.
b) Calculate the distance from the metallurgical junction to the maximum of the electron potential energy.
c) Repeat the calculations for a) and b) for an applied bias of 0.2 V in the forward direction.

PROBLEM 1500-3*(Thin films, easy)
When we evaporate a thin metal film on a substrate, the film will be poly-crystalline. The film will consist of many crystallites. It is possible to find out how large are these grains. One popular method for doing so is X-ray diffraction. In the X-ray diffraction method, the film is exposed to a parallel beam of monochromatic X-rays. Each crystallite – every grain- will contribute to the intensity in the diffraction pattern, which we in principle takes a picture of. The diffraction pattern can be viewed as an addition of Fourier transforms of all the grains. For a polycrystalline film the diffraction pattern will consist of rings of a certain width. The width tells about the grain size and is the most widespread method for measuring the grain size.
a) Explain why the width of the intensity in a ring tells about the grain size.
b) What does the ratio of the intensity of different rings tell?

PROBLEM 1500-4(Ohmic contacts)
We will estimate the value of the specific contact resistance for a particular contact to Si: We have a donor concentration of 2E18cm^{-3} and have a metal contact of NiSi with a barrier height of 0.68 eV. The specific contact resistance is defined as R_c=(diff(J, V))$^{-1}$ where J is the current density (It is usual, albeit confusing, to say resistance pr area)

a) Calculate an estimate for the value (and units) of the specific contact resistance.
b) Calculate the resistance if the area of the contact is 1x1μm
c) Assume that you measure the total resistance from the contact, including the contact resistance and the resistance of a wafer that is 500 μm thick and has a similar back contact with an area of 75 cm^2. What is the total resistance?

PROBLEM 1500-5(Thin film inter-diffusion, Silicides, easy)
Diffusion will be involved in a reaction between a metal and a semiconductor to form silicide. Assume the metal Ni deposited onto Si. Heat treatment will induce a planar layer of Ni_2Si between Ni and Si. The thickness of the Ni_2Si layer increases with annealing time. This is due to diffusion. (For convenience and as a suggestion how to easy answer the questions below we can notate the development of different layers as follow, with the surface to the right:
Si/Ni -> Si/$SiNi_2$/Ni

In an experiment we use radioactive metal atom labeling in order to study the diffusion mechanisms. Assume that we deposit 50 nm inactive Ni, then deposit 5 nm radioactive Ni*. Schematically we can notate the structure as 'Si/Ni/Ni*' where the surface is to the right. We can measure how Ni* is distributed after diffusion by measuring the activity after successive short ion etches of the material. Assume for simplicity that the diffusivity of Ni in Ni is small.

a) Sketch how the radioactive Ni* will distribute if the diffusion proceeds by grain boundary diffusion of Ni.

b) Sketch how the radioactive Ni* will distribute if the diffusion proceeds by grain boundary diffusion of Si.

c) Sketch how the radioactive Ni* will distribute if the diffusion proceeds by lattice diffusion of Ni.

d) Sketch how the radioactive Ni* will distribute if the diffusion proceeds by lattice diffusion of Si.

PROBLEM 1500-6(Thin film interdiffusion)

Grain boundary diffusion is important in thin films. The diffusivity is given by as $D_0\exp(-E_a/kT)$ where D_o is the pre-exponential constant and E_a an activation energy. Which will have the largest value, you think, the diffusivity for grain boundary diffusion or that for lattice diffusion? Tell briefly why.

Will lattice diffusion or grain boundary diffusion dominate atomic transport in the film at high temperatures (say close to the melting point)

PROBLEM 1500-7(Thin film interdiffusion)

The grain size in a thin film will depend upon various parameters(surprise!) Assume that we deposit a film of Ta (tantalum) and one film of In (indium) using the same deposition rate (0.3 nm/sec) onto a substrate at room temperature. Which film will yield the largest grains? Explain your reasoning. (Hint: Check the melting temperatures of the metals, try to explain what it has to do with the matter, without rigorous mathematical deductions)

PROBLEM 1500-8(Schottky barriers)

A p-type Si Schottky diode can be used for an IR detector. The response will vanish at a certain wavelength. Make a rough estimate of how far into the infrared (maximum wavelength) a p-Si/Pt Schottky diode can be used.