Scilab Textbook Companion for Materials Science and Engineering - A First Course by V. Raghavan[1]

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Book Description

Title: Materials Science and Engineering - A First Course

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Scilab numbering policy used in this document and the relation to the above book.

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

AP Appendix to Example(Scilab Code that is an Appednix to a particular Example of the above book)

For example, Exa 3.51 means solved example 3.51 of this book. Sec 2.3 means a scilab code whose theory is explained in Section 2.3 of the book.

Contents

List of Scilab Codes

Chapter 2

Equilibrium and Kinetics

Scilab code Exa 2.1 Calculate the entropy increase

```
1 // Calculate the entropy increase
2 clc
3 del_h = 6.02 // Heat added in kJ/mol
4 t_m = 273.15 // mean temperature in kelvin
5 printf("\n Example 2.1")
6 del_s = del_h*1e3/t_m
7 printf("\n Increase in entropy is %.2f J mol^-1 K^-1
    ",del_s)
```

Scilab code Exa 2.2 Calculation of fraction of atoms with energy equal to or great

```
1 // Calculation of fraction of atoms with energy
     equal to or greater than 1eV at temperatures
2 clc
3 E = 1 // energy in electron volt
4 e = 1.6e-19 // charge on electron
5 k = 1.38e-23 // constant
```

```
6  t1 = 300 // temperature in K
7  t2 = 1500 // temperature in K
8  printf("\n Example 2.2")
9  printf("\n\n Part A:")
10 n_N = exp(-(e/(k*t1)))
11 printf("\n Fraction of atoms with energy equal to or
       greater than 1eV at temperature %d K is %.2e ",
     t1,n_N) // numerical value of answer in book is 2
     e-17
12 printf("\n\n Part B:")
13 n_N = exp(-(e/(k*t2)))
14 printf("\n Fraction of atoms with energy equal to or
       greater than 1eV at temperature %d K is %.2e ",
     t2,n_N) // numerical value of answer in book is
     4.3e4
```

Chapter 3

Crystal Geometry and Structure Determination

Scilab code Exa 3.2 Calculate effective number of lattice point in three cubic spa

```
1 // Calculate effective number of lattice point in
    three cubic space lattice
2 clc
3 sc_n = 1/8 // sharing of one lattice point in a unit
     cell
4 sc_N = 8 // Number of lattice points in Simple cubic
5 bcc_n_e = 1/4// sharing of one edge lattice point in
     a BCC
6 bcc_N_e = 4// Number of edge lattice point in a BCC
7 bcc_n_c  = 1// sharing of one body center lattice
    point in a BCC
8 bcc_N_c = 1// Number of body center lattice point in
     a BCC
9 fcc_n_e = 1/8 // sharing of one corner lattice point
     in a FCC
10 fcc_N_e = 8// Number of corner lattice point in a
    FCC
11 fcc_n_f = 1/2 // sharing of one face center lattice
    point in a FCC
```

```
12 fcc_N_f = 6// Number of face center lattice point in
       a FCC
13 printf("\n Example 3.2 ")
14 sc_net = sc_n*sc_N
15 bcc_net = bcc_n_e*bcc_N_e+bcc_n_c*bcc_N_c
16 fcc_net = fcc_n_e*fcc_N_e+fcc_n_f*fcc_N_f
17 printf("\n Effective number of lattice points are as
      :")
18 printf("\n\n Space lattice \t Abbreviation \t
      Effective number of lattice point in unit cell \n
      ")
19 printf("\n Simple cubic \t\tSC \t\t\t\t %d\n Body
      center cubic\tBCC \t\t\t\t %d\n Face centered
      cubic\tFCC \t\t\t\t %d ",sc_net,bcc_net,fcc_net)
```

Scilab code Exa 3.7 Determine interplanar spacing and miller indices

```
1  //  Determine Interplanar spacing and miller indices
2  clc
3  a = 3.16 // lattice parameter in angstrom
4  l1 = 1 // line number
5  l2 = 2 // line number
6  l3 = 3 // line number
7  l4 = 4 // line number
8  theta1 = 20.3 // angle for line 1
9  theta2 = 29.2// angle for line 2
10 theta3 = 36.7// angle for line 3
11 theta4 = 43.6// angle for line 4
12 n = 1 // order
13 lambda = 1.54 // wavelength in angstrom
14 printf("\n Example 3.7")
15 d1 = lambda/(2*sin(theta1*%pi/180))
16 d2 = lambda/(2*sin(theta2*%pi/180))
```

```
17 d3 = lambda/(2*sin(theta3*%pi/180))
18 d4 = lambda/(2*sin(theta4*%pi/180))
19 x1 = a^2/d1^2
20 x2 = a^2/d2^2
21 x3 = a^2/d3^2
22 x4 = a^2/d4^2 // where x is function of h,k and l
23 printf("\n Interplanar spacing is %.3f angstrom ",
      x1) // answer in book is 2.220 angstrom
24 if  floor(x1) == 2 then
25     printf("\n\n For a^2/d^2 = %d \t Reflection
          plane is {110}",x1)
26 end
27
28 if floor(x2) == 4 then
29         printf("\n For a^2/d^2 = %d \t Reflection
             plane is {200}",x2)
30 end
31
32  if floor(x3) == 6 then
33     printf("\n For a^2/d^2 = %d \t Reflection plane
          is {211}",x3)
34 end
35
36  if floor(x4) == 8 then
37     printf("\n For a^2/d^2 = %d \t Reflection plane
          is {220}",x4)
38 end
```

Scilab code Exa 3.8 Determine structure and lattice parameter of material

```
1 // Determine structure and lattice parameter of
     material
2 clc
```

```
d = 114.6 // diameter of power camera in angstrom
lambda = 1.54 // wavelength in angstrom
s1 = 86
s2 = 100
s3 = 148
s4 = 180
s5 = 188
s6 = 232
s7 = 272
printf("\n Example 3.8")
R = d/2       // Radius
if R==57.3 then
    k = 1/4 // Bragg angle factor
end
a1 = (sin(s1*k*%pi/180))^2
a2 = (sin(s2*k*%pi/180))^2
a3 = (sin(s3*k*%pi/180))^2
a4 = (sin(s4*k*%pi/180))^2
a5 = (sin(s5*k*%pi/180))^2
a6 = (sin(s6*k*%pi/180))^2
a7 = (sin(s7*k*%pi/180))^2
c = 22 // constant to convert into integral number

printf("\n Within experimental error, values are as
   in integral ratio are as: \n %d:%d:%d:%d:%d:%d:%d
   ",ceil(c*a1),ceil(c*a2),ceil(c*a3),ceil(c*a4),
   ceil(c*a5),ceil(c*a6),ceil(c*a7))
printf("\n So, this structure is FCC and material is
    copper with 3.62 angstrom lattice parameter")
```

Chapter 4

Atomic Structure and Chemical Bonding

Scilab code Exa 4.1 Calculate frequency and wavelength of radiation

```
1 // Calculate frequency and wavelength of radiation
2 clc
3 E = 1.64e-18 // energy difference between two states
    in J
4 h= 6.626e-34 // planks constant
5 c = 2.998e8 // speed of light in m/s
6 printf("\n Example 4.1")
7 nu = E/h
8 lambda = c/nu
9 printf("\n Frequency of emitted radiation is %.2e Hz
   ",nu)
10 printf("\n Wavelength of emitted radiation is %.2e m
    \n\t \tor\t\t %d angstrom",lambda,lambda*1e10)//
    answer in book is 1210 angstrom
```

Scilab code Exa 4.3 Reconcile the difference of energy

```
1 // Reconcile the difference of energy
2 clc
3 e_a = 713 // enthalpy of atomization in kJ/mol
4 e_b = 347 // bond energy in kJ/mol
5 a = 4 // total number of atoms in single crystal
     structure
6 b = 2 // number of atoms in a bond
7 printf("\n Example 4.3")
8 k = a/b // effective number of bond per atom
9 e = k*e_b
10 printf("\n %d kJ should be the enthalpy of
     atomization of diamond", e)
11 printf("\n However, %d kJ is very close to %d kJ",e,
     e_a)
```

Scilab code Exa 4.4 Calculation of fraction of hydrogen bonds which breaks during

```
1 // Calculation of fraction of hydrogen bonds which
     breaks during ice melting
2 clc
3 del_h = 6.02 // enthalpy of fusion in kJ/mol
4 n = 2 // number of hydrogen atom in 1 water atom
5 del_b = 20.5 // hydrogen bond energy in kJ/mol
6 printf("\n Example 4.4")
7 f = del_h/(n*del_b)
8 printf("\n Fraction of hydrogen bonds which broken
     is %.2f",f)
```

Chapter 5

Structure of Solid

Scilab code Exa 5.1 Calculate packing efficiency and density of diamond

```
1 // Calculate packing efficiency and density of
     diamond
2 clc
3 n_c = 1/8 // sharing of corner atom in a unit cell
4 N_c = 8 // Number of corner atoms in unit cell
5 n_b = 1 // sharing of body centered atom in a unit
     cell
6 N_b = 4 // Number of body centered atoms in unit
     cell
7 n_f = 0.5// sharing of face centered atom in a unit
     cell
8 N_f = 6// Number of face centered atoms in unit cell
9 a = 1 // let lattice parameter
10 m = 12 // mass of carbon
11 printf("\n Example 5.1")
12 printf("\n Part A:")
13 N = n_c*N_c+n_b*N_b+n_f*N_f // effective number of
     atoms
14 r = a*sqrt(3)/8
15 p_e = N*4/3*%pi*r^3/a^3 // packing efficiency
16
```

```
17 printf("\n Packing efficiency of diamond is %.2f",
     p_e)
18 printf("\n\n Part B:")
19 a = 3.57 // lattice parameter in angstrom
20 d = m*1.66e-27*N/(a*1e-10)^3
21 printf("\n Density of diamond is %d Kg/m^3",d)//
     numerical answer in book is 3500
22 printf("\n Density of diamond is %.1f g/cm^3",d
     /1000)
```

Scilab code Exa 5.3 Calculate the cation to anion ratio for an ideally close packe

```
1 // calculate the c/a ratio for an ideally close
     packed HCP crystal
2 clc
3 a = 1 // let
4 PR = a
5 printf("\ Example 5.3")
6 RT = a/sqrt(3)
7 PT = sqrt(PR^2-RT^2)
8 c_a = 2*PT/PR
9 // Calculations are made on the crystal structure
     drawn in book
10 printf("\n c/a ratio for an ideally close packed HCP
     crystal is %0.3f ",c_a)
```

Scilab code Exa 5.4 find the size of largest sphere that can fit into a tetrahedra

```
// find the size of largest sphere that can fit into
    a tetrahedral void
clc
r = 1 // let
a = 3/4
printf("\n Example 5.4")
pt = 2*sqrt(2/3)*r
s = a*pt-r // size of sphere
printf("\n Size of largest sphere that can fit into
   a tetrahedral void is %.3fr",s)
```

Scilab code Exa 5.5 Find critical radius ratio for triangular coordination

```
// find critical radius ratio for triangular
   coordination
clc
theta = 60 // angle in degree
printf("\n Example 5.5")
r_c_a = (2/3*2*sin(theta*%pi/180))-1 // ratio
   calculation
printf("\n Critical radius ratio for triangular
   coordination is %0.3f ",r_c_a)
```

Scilab code Exa 5.6 Calculate density of MgO

```
// Calculate density of MgO
clc
r_mg = 0.78 // radius of magnesium cation in
   angstrom
```

```
r_o = 1.32 // radius of oxygen anion in angstrom
n = 4 // effective number of unit cell
m_o = 16 // mass of oxygen
m_mg = 24.3 // mass of magnesium
printf("\n Example 5.6")
a = 2*(r_mg+r_o)// lattice parameter
d = (m_o+m_mg)*1.66e-27*n/(a*1e-10)^3// density
printf("\n Density of MgO is %d Kg/m^3",d) // answer
    is 3610 kg/m^3
printf("\n Density of MgO is %0.2f g/cm^3",d/1000)
```

Chapter 6

Crystal Imperfection

Scilab code Exa 6.1 Find equilibrium concentration of vacancies in metals at given

```
1 // Find equilibrium concentration of vacancies in
     metals at given temperature
2 clc
3 t1 = 0 // temperature in kelvin
4 t2 = 300 // temperature in kelvin
5 t3 = 900// temperature in kelvin
6 R = 8.314 // universal gas constant
7 del_hf_al = 68 // Enthalpy of formation of aluminium
      crystal in KJ
8 del_hf_ni = 168 // Enthalpy of formation of nickel
     crystal in KJ
9 printf("\n Example 6.1")
10
11 printf("\n Equilibrium concentration of vacancies of
      aluminium at %dK is 0",t1)
12 n_N = exp(-del_hf_al*1e3/(R*t2))
13 printf("\n Equilibrium concentration of vacancies of
      aluminium at %dK is %.2e",t2,n_N) // answer in
     book is 1.45e-12
14 n_N = exp(-del_hf_al*1e3/(R*t3))
15 printf("\n Equilibrium concentration of vacancies of
```

```
    aluminium at %dK is %.2e",t3,n_N) // answer in
    book is 1.12e-4
16
17 printf("\n\n Equilibrium concentration of vacancies
    of Nickel at %dK is 0",t1)
18 n_N = exp(-del_hf_ni*1e3/(R*t2))
19 printf("\n Equilibrium concentration of vacancies of
    Nickel at %dK is %.2e",t2,n_N)
20 n_N = exp(-del_hf_ni*1e3/(R*t3))
21 printf("\n Equilibrium concentration of vacancies of
    Nickel at %dK is %.2e",t3,n_N) // answer in book
    is 1.78e-10
```

Scilab code Exa 6.2 Compute the line energy of dislocation

```
1 // Compute the line energy of dislocation
2 clc
3 a = 2.87 // lattice parameter in angstrom
4 b= 2.49 // magnitude of burgers vector in angstrom
5 G = 80.2 // shear modulus in GN
6 printf("\n Example 6.2")
7 E = G*1e9*(b*1e-10)^2*1/2
8 printf("\n Line energy of dislocation is %.2e J m^-1
   ",E)
```

Scilab code Exa 6.4 Calculation of down climb of crystal on heating

```
1 // calculation of down climb of crystal on heating
2 clc
```

```
3 a = 1e10// total number of edge dislocation
4 N = 6.023e23 // Avogadro number
5 R = 8.314 // Universal gas constant
6 t1 = 0 // initial temperature in K
7 t2 = 1000 // Final temperature in K
8 del_hf = 100 // Enthalpy of vacancy formation in KJ
9 d = 2 // length of one step in angstrom
10 v = 5.5e-6 // volume of one mole crystal
11 printf("\n Example 6.4")
12 n = N*exp(-(del_hf*1e3)/(R*(t2-t1)))/v
13 k = 1/(d*1e-10) // atoms required for 1 m climb
14 b = n/(k*a)// average amount of climb
15 c = b*d*1e-10
16
17 printf("\n Average down climb of crystal is %.2em",c
   )
```

Scilab code Exa 6.5 Calculate surface energy of copper crystal of type 111

```
1 // Calculate surface energy of copper crystal of
     type {111}
2 clc
3 E = 56.4 // bond energy in KJ
4 N_a = 6.023e23 // Avogadros number
5 n = 12 // number of bonds
6 m = 3 // number of broken bonds
7 N = 1.77e19 // number of atoms in copper crystal of
     type {111} per m^2
8 printf("\n Example 6.5")
9 b_e = 1/2*E*1e3*n/N_a // bond energy per atom
10 e_b = b_e*m/n // energy of broken bond at surface
11 s_e = e_b*N // surface enthalpy of copper
12 printf("\n Surface enthalpy of copper is %0.2f J m
```

```
    ^-2",s_e)
13 printf("\n Surface enthalpy of copper is %d erg cm
    ^-2",s_e*1e3)
14 // Answer in book is 2490 erg cm^-2
```

Scilab code Exa 6.6 Compute the angle at the bottom of groove of a boundary

```
1 // Compute the angle at the bottom of groove of a
    boundary
2 clc
3 Gamma_gb = 1 // let, energy of grain boundary
4 Gamma_s = 3* Gamma_gb// energy of free surface
5 printf("\n Example 6.6")
6 theta = 2*acos(1/2*Gamma_gb/Gamma_s)
7 printf("\n Angle at the bottom of groove of a
    boundary is %d degrees.",ceil(theta*180/%pi))
```

Chapter 7

Phase Diagram

Scilab code Exa 7.1 Find degrees of freedom of a system of two components

```
1 // Find degrees of freedom of a system of two
     components
2 clc
3 c = 2 // number of components
4 printf("\n Example 7.1")
5 for n = 1:4
6     p = (c-1) +2 // Total variables
7     f = c-n+2 // degree of freedom
8     printf("\n\n Degree of freedom for two
         components when \n number of phases is %d is
         %d",n,f)
9 end
```

Scilab code Exa 7.2 Find minimum number of component in system

```
1 // Find minimum number of component in system
2 clc
```

```
3 p = 4 // number of phases of system
4 f = 0 // number of degree of system
5
6 printf("\n Example 7.2")
7 C = f+p-1 // components number
8 printf("\n Minimum number of components in system is
    %d",C)
```

Scilab code Exa 7.3 Calculate amount of pure water that can be extracted from sea

```
1 // Calculate amount of pure water that can be
   extracted from sea water
2 clc
3 L = 23.3 // % composition of L
4 a = 3.5 // concentration of Nacl in sea water
5 ice = 0 // % composition of ice
6 printf("\n Example 7.3")
7 f_ice = (L-a)/(L-ice)
8 printf("\n Fractional amount of pure water that can
   be extracted from sea water is %0.2f",f_ice)
```

Scilab code Exa 7.5 Calculate proeutectoid ferrite and eutectoid ferrite in 6 tent

```
1 // Calculate proeutectoid ferrite and eutectoid
   ferrite in 0.6% steel
2 clc
3 a = 0 // limiting value
4 b = 0.8 // limiting value
5 c = 0.6 // percentage composition of carbon
```

```
f = 0.88 // fraction of ferrite in a eutectoid steel
printf("\n Example 7.5")
f_pro_alpha = (b-c)/(b-a)
f_perlite = 1 - f_pro_alpha
f_eut = f*f_perlite
printf("\n Composition of proeutectoid ferrite is %0
   .2f",f_pro_alpha)
printf("\n Composition of eutectoid ferrite is %0.2f
   ",f_eut)
```

Chapter 8

Diffusion in Solids

Scilab code Exa 8.1 Calculate the rate at which hydrogen escapes through the walls

```
1 // calculate the rate at which hydrogen escapes
     through the walls of the steel tank
2 clc
3 t = 5 // thickness in mm
4 c = 10 // concentration
5 D = 1e-9 // diffusion coefficient
6 printf("\n Example 8.1")
7 j  = D*c/(t*1e-3)
8 printf("\n Outward flux is %.0e kg m^-2 s^-1",j)
```

Scilab code Exa 8.2 Calculate maximum time till which material can be kept at 550

```
1 // Calculate maximum time till which material can be
     kept at 550 degree Celsius
2 clc
3 D_0 = 0.24e-4 // diffusion coefficient
4 Q = 121e3
```

```
R = 8.314// Universal gas constant
T = 550 // temperature in Celsius
k = 0.2 // thickness of pure Al sheet in mm
d = 0.1 // penetration depth in mm
c_x = 0.4 // concentration in percentage
A  = 2 // Constant in percentage
B = 2// Constant in percentage
printf("\n Example 8.2")
x = d-k
D_cu_al = D_0*exp(-Q/(R*(T+273)))
k = (A-c_x)/B
if k ==0.8 then
    z = 0.9 // from table
end
t = (x*1e-3)^2/(z^2*4*D_cu_al)// time in sec

printf("\n Material can be kept at %d degree Celsius
    for nearly %d minute",T,t/60)// answer in book
   is 100 min
```

Scilab code Exa 8.3 Calculate minimum depth up to which post machining is to be do

```
// Calculate minimum depth up to which post
   machining is to be done
clc
D_0 = 0.7e-4 // diffusion coefficient
Q = 157 // Energy in kJ mol^-1, considered from
   table 8.2
R = 8.314// Universal gas constant
T = 950 // temperature in Celsius
c2 = 0.8 // concentration in percentage
cs = 0 // concentration in percentage
c_x = 0.6// concentration in percentage
```

```
10 t = 4 // time in hours
11 a = 1 //let
12 printf("\n Example 8.3")
13 A = cs
14 B = c2-cs
15 D = D_0*exp(-Q*1e3/(R*(T+273)))
16 k = erf(((A-c_x)/B))*-1
17 if k >0.7 then
18     if k<0.712 then
19             z = 0.81 // from table
20     end
21
22 end
23 x = z*2*sqrt(D*t*3600)
24
25 printf("\n Depth up to which machining is required
      is nearly %.2f mm",x*1e3)
26 // numerical value of answer in book is 0.75
```

Scilab code Exa 8.4 Calculate time required to get required boron concentration

```
1 // Calculate time required to get required boron
     concentration
2 clc
3 D = 4e-17 // diffusion coefficient
4 c1 = 0
5 cs = 3e26
6 c_x = 1e23 // number of atoms
7 x = 2e-6 // depth in m
8 printf("\n Example 8.4")
9 A = cs
10 B = cs - c1
11 k = (A-c_x)/B
```

```
12 if k >0.99966 then
13     if k< 0.9997 then
14         z = 2.55 // from table
15     end
16 end
17 t = x^2/(z^2*4*D)// time in sec
18
19 printf("\n Time required to get required boron
   concentration is %d sec",t)// answer in book is
   3845 sec
```

Scilab code Exa 8.5 Calculate ratio of cross sectional areas

```
1 // Calculate ratio of cross sectional areas
2 clc
3 r = 10 // radius in mm
4 t = 4 // thickness in angstrom
5 printf("\n Example 8.5")
6 r = 2*%pi*r*1e-3*t*1e-10/(%pi*(r*1e-3)^2)
7 printf("\n Ratio of cross sectional areas is %.0e ",
   r)
```

Chapter 9

Phase Transformation

Scilab code Exa 9.1 Calculate the critical free energy of nucleation of ice from w

```
1 // Calculate the critical free energy of nucleation
     of ice from water and critical radius
2 clc
3 del_t1 = 0// temperature difference in degree
     Celsius
4 del_t2 = -5 // temperature difference in degree
     Celsius
5 del_t3 = -40 // temperature difference in degree
     Celsius
6 del_h = 6.02 // enthalpy of fusion in kJ/mol
7 T_m = 273 // mean temperature
8 Gamma = 0.076 // energy of ice water interface in J
     /m^2
9 v = 19 // molar volume of ice
10 printf("\n Example 9.1")
11 printf("\n Part A")
12 printf("\n At del_t = %d, there is no supercooling.
     So there is no critical radius",del_t1)
13 printf("\n\n Part B")
14 del_f = 16/3*%pi*(Gamma)^3*T_m^2/((del_h*1e3*1e6/v)
     ^2*del_t2^2)
```

```
15 r = 2*T_m*Gamma/(-del_h*1e3*1e6/v*del_t2)
16 printf("\n Critical free energy of nucleation is %.1
   eJ",del_f)
17 printf("\n Critical radius is %d angstrom",ceil(r*1
   e10))
18 printf("\n\n Part C")
19 temp_r = del_t3/del_t2
20 del_f_ = del_f/temp_r^2
21 r_ = r/temp_r
22
23  printf("\n Critical free energy of nucleation is %
    .1eJ",del_f_)
24 printf("\n Critical radius is %d angstrom.", ceil(r_
   *1e10))
```

Scilab code Exa 9.2 Calculate the change in delta f required to increase nucleatio

```
1 // Calculate the change in del_f required to
   increase nucleation rate
2 clc
3 T= 300 // temperature in kelvin
4 R = 8.314 // universal gas constant
5 k = 2.303 // conversion factor
6 a1 = 1e42
7 a2 = 1e6 // nucleation rate
8 a3 = 1e10 // nucleation rate
9 printf("Example 9.2")
10 I1 = (log10(a1)-log10(a2))*k*R*T // exponent factor
11 I2 = (log10(a1)-log10(a3))*k*R*T// exponent factor
12 del_f = I1-I2 // difference
13 a = 10^(log10(a3)-log10(a2))
14
15 printf("\n  A change of %d KJ mol^-1 energy is
```

```
    required to increase nucleation factor from \n %
    .0e m^-3 s^-1 to %.0e m^-3 s^-1 ",ceil(del_f/1
    e3),a,a3)
```

Scilab code Exa 9.4 Calculate delta f of heterogeneous as a fraction of delta f of

```
1 // Calculate del_f_het as a fraction of del_f_homo
2 clc
3 Gamma_alpha_del = 0.5 // in J m^-2
4 Gamma_alpha_beta = 0.5 // in J m^-2
5 Gamma_beta_del = 0.01 // in J m^-2
6
7 printf("\n Example 9.4")
8 theta = acos((Gamma_alpha_del -Gamma_beta_del)/
    Gamma_alpha_beta)
9 del_f_ratio = 1/4*(2-3*cos(theta)+(cos(theta))^3)
10
11
12 printf("\n del_f_het is %0.4fth fraction of
    del_f_homo.",del_f_ratio)
```

Scilab code Exa 9.6 Calculate the free energy change during recrystallization

```
1 // Calculate the free energy change during
    recrystallization
2 clc
3 mu = 45.5e9
4 b = 2.55e-10
5 n1 = 1e9 // initial dislocation density
```

```
n2 = 1e13 // final dislocation density
printf("\n Example 9.6")
E = 1/2*mu*b^2*n2
del_g = E // as difference between initial and final
    dislocation energy is four order magnitude
printf("\n Free energy change during
   recrystallization is %d J m^-3",-del_g)
// Numerical value of answer in book is 14800
```

Chapter 10

Elastic Anelastic and Viscoelastic Behaviour

Scilab code Exa 10.1 Estimate Youngs modulus of material

```
1 // Estimate youngs modulus of material
2 clc
3 n = 1
4 m = 9
5 A = 7.68e-29 // Constant having unit J m
6 r_0 = 2.5e-10 // bonding distance in m
7 printf("\n Example 10.1")
8 B = A*r_0^8/9
9
10 Y = (90*B/(r_0)^11-2*A/(r_0)^3)/r_0
11
12 printf("\n Youngs modulus of material is %d GN m
   ^-2",Y/1e9)
```

Scilab code Exa 10.2 Calculation of stress in fibers

```
// Calculation of stress in fibers
clc
Y_f = 440
Y_m = 71
sigma_total= 100 // total load
printf("\n Example 10.2")
r = Y_f/Y_m
sigma_f = r*(sigma_total/0.7)/(1+r*3/7)
printf("\n Part A:")
printf("\n When load is applied parallel to fiber
    then, stress in fiber is %d MN m^-2",sigma_f)

printf("\n\n Part B:")
printf("\n When load is applied perpendicular to
    fiber then, stress in fiber and matrix is same i.
    e. %d MN m^-2",sigma_total)
```

Scilab code Exa 10.3 Estimate diffusion coefficient

```
// Estimate diffusion coefficient
clc
t_r = 100 // relaxation time in s
d = 2.5 // distance in angstrom
printf("\n Example 10.3")
f = 1/t_r // jump frequency
D = (d*1e-10)^2*f
printf("\n Diffusion coefficient is %.2e m^2 s^-1",D
    )
```

Chapter 11

Plastic Deformation and Creep in Crystalline Materials

Scilab code Exa 11.2 Calculate the stress required to move the dislocation at give

```
1 // Calculate the stress required to move the
     dislocation at given temperature
2 clc
3 b = 2 // burger vector in angstrom
4 v = 20*b^3 // activation volume
5 tau_pn = 1000 // P-N stress of crystal in MNm^-2
6 k = 1.38e-23 // physical constant
7 t1 = 0 // temperature in K
8 t2 = 100// temperature in K
9 t3 = 300// temperature in K
10 t4 = 500// temperature in K
11 printf("\n Example 11.2")
12 printf("\n\n Part A:")
13 T = t1
14 tau_app = tau_pn - 40*k*T/(v*1e-30)
15 printf("\n The stress required to move the
     dislocation at temperature %dK is %d MNm^-2",T,
     tau_app)
16 printf("\n\n Part B:")
```

```
17 T = t2
18 tau_app = tau_pn - 40*k*T/(v*1e-30*1e6)
19 printf("\n The stress required to move the
      dislocation at temperature %dK is %d MNmˆ-2",T,
      tau_app)
20 printf("\n\n Part C:")
21 T = t3
22 tau_app = tau_pn - 40*k*T/(v*1e-30*1e6)
23 if tau_app<0 then
24     printf("\n Stress to be applied is zero")
25     printf("\n The stress required to move the
          dislocation at temperature %dK entirely
          overcome by thermal fluctuations", T)
26 end
27 printf("\n\n Part D:")
28 T = t4
29 tau_app = tau_pn - 40*k*T/(v*1e-30*1e6)
30 if tau_app<0 then
31     printf("\n Stress to be applied is zero")
32     printf("\n The stress required to move the
          dislocation at temperature %dK entirely
          overcome by thermal fluctuations", T)
33 end
```

Scilab code Exa 11.3 Calculate the dislocation density in copper

```
1 // Calculate the dislocation density in copper
2 clc
3 mu = 44 // shear modulus of copper in GN mˆ-2
4 b = 2.55 // burgers vector in angstrom
5 tau = 35 // shear stress in MN mˆ-2
6 printf("Example 11.3")
7 l = mu*1e9*b*1e-10/(tau*1e6)
```

```
8 rho = 1/l^2
9
10 printf("\n Dislocation density in copper is %.1e m
   ^-2",rho)
11 // Answer in book is 1e12 m^-2
```

Scilab code Exa 11.4 Find the yield stress for a grain size of ASTM 9

```
1 //  Find the yield stress for a grain size of ASTM 9
2 clc
3 sigma1 = 120 // initial yield strength of material
   in MNm^-2
4 sigma2 = 220 // Final yield strength of material in
   MN m^-2
5 d1 = 0.04 // initial diameter in mm
6 d2 = 0.01 // final diameter in mm
7 n = 9 // astm number
8 printf("Example 11.4")
9 k = (sigma2-sigma1)*1e6/(1/sqrt(d2*1e-3)-1/sqrt(d1*1
   e-3))
10 sigma_i = sigma1*1e6 -k/sqrt((d1*1e-3))
11 d = 1/sqrt(2^(n-1)*1e4/645)
12 sigma_y = sigma_i+k*(d*1e-3)^(-0.5)
13
14 printf("\n Yield stress for a grain size of ASTM 9
   is %d MN m^-2",ceil(sigma_y/1e6))
```

Scilab code Exa 11.5 Estimate the change in yield strength

```
// Estimate the change in yield strength
clc
n1 = 1e6 // initial number of particles
n2 = 1e3 // final number of particle
printf("\n Example 11.5")
k = (n1/n2)^(1/3)
printf("\n Yield strength would have decreased to
   %d%% of its initial value.",100/k)
```

Chapter 12

Fracture

Scilab code Exa 12.1 Estimate fracture strength

```
1 // Estimate fracture strength
2 clc
3 c = 2 // crack of half length in micro meter
4 Y = 70 // youngs modulus in GN m^-2
5 Gamma = 1 // specific surface energy
6 printf("\n Example 12.1")
7 sigma_f = sqrt(2*Gamma*Y*1e9/(%pi*c*1e-6))/1e6
8 r = Y*1e3/sigma_f
9 printf("\n Fracture strength of %d MN m^-2 is 1/%dth
    of youngs modulus. ",ceil(sigma_f),ceil(r
   /100)*100)
10 printf("\n Thus Griffiths criterion bridges the gap
   between the \n observed and ideal strengths of
   brittle material")
```

Scilab code Exa 12.2 Estimate the brittle fracture strength at low temperatures

```
// Estimate the brittle fracture strength at low
   temperatures
clc
Gamma = 1.5// specific surface energy in J/m^2
Y = 200 // Youngs modulus in GN/m^2
c = 2 // half length of crack

printf("\n Example 12.2")
sigma_f = sqrt(2*Gamma*Y*1e9/(%pi*c*1e-6))

printf("\n Brittle fracture strength at low
   temperatures is %d MNm^-2 ",sigma_f/1e6)// answer
    in book is 310MNm^-2
```

Scilab code Exa 12.3 Estimate the temperature at which the ductility of brittle tr

```
// Estimate the temperature at which the ductility
   of brittle transition occurs at given strain
   rates
clc
Gamma = 2// specific surface energy in J/m^2
Y = 350 // Youngs modulus in GN/m^2
c = 2 // half length of crack
de_dt1 = 1e-2 // strain rate
de_dt2 = 1e-5 // strain rate
printf("\n Example 12.3")
printf("\n Part A:")
sigma_f = sqrt(2*Gamma*Y*1e9/(%pi*c*1e-6))
sigma_y = sigma_f/1e6
T = 173600/(sigma_y-20.6-61.3*log10(de_dt1))//
   temperature calculation

printf("\n Transition temperature for strain rate %
```

```
    .0e s^-1 is %d K",de_dt1,T)// answer in book is
    300 K
printf("\n\n Part B:")

T = 173600/(sigma_y-20.6-61.3*log10(de_dt2))//
    temperature calculation

printf("\n Transition temperature for strain rate %
    .0e s^-1 is %d K",de_dt2,T)// answer in book is
    230 K
// Solution in book for two parts is divided into
    three parts
```

Chapter 13

Oxidation and Corrosion

Scilab code Exa 13.2 Calculation of required quantity of magnesium

```
1 // Calculation of required quantity of magnesium
2 clc
3 j = 15 // current density in mA m^-2
4 m = 0.0243 // molar mass of magnesium
5 F = 96490 // farad charge
6 n = 2 // charge on ion
7 t = 10 // time in years
8 printf("\n Example 13.2")
9 a = m*j*1e-3*(t*365*24*3600)/(n*F)
10 printf("\n Amount of magnesium required is %0.1f kg
   m^-2",a)
```

Chapter 14

Conductors and Resistors

Scilab code Exa 14.1 Calculate energy difference

```
// Calculate energy difference
clc
n_x1 = 1 // atomic level
n_y1 = 1// atomic level
n_z1 = 1// atomic level
n_x2 = 2// atomic level
L = 10 // lattice parameter in mm
h = 6.626e-34 // plank constant
m_e = 9.109e-31 // mass of electron in kg
printf("\n Example 14.1")
E1 = h^2*(n_x1^2+n_y1^2+n_z1^2)/(8*m_e*(L*1e-3)^2)
E2 = h^2*(n_x2^2+n_y1^2+n_z1^2)/(8*m_e*(L*1e-3)^2)
E = E2-E1 // energy difference
printf("\n Energy difference is %.2e J ",E)
```

Scilab code Exa 14.2 Calculate conductivity of copper at 300 K

```
// Calculate conductivity of copper at 300 K
clc
tau = 2e-14 // collision time of electron in s
e = 1.602e-19 // charge on electron
m_e = 9.1e-31 // mass of electron in kg

printf("\n Example 14.2")
n = 6.023e23*8960/0.06354

sigma= n*e^2*tau/m_e
printf("\n Conductivity of copper at 300 K is %.1e
   ohm^-1 m^-1 ",sigma)
```

Scilab code Exa 14.3 Estimation of resistivity due to impurity scattering of 1 per

```
// Estimation of resistivity due to impurity
   scattering of 1% of Nickel in copper lattice
clc
r_cu = 1.8e-8 // resistivity of pure copper in ohm-m
r_Ni_cu = 7e-8 //resistivity of copper 4% Ni in ohm-
   m
per1 = 4//impurity in percent
per2 = 1 // impurity in percent
printf("\n Example 14.3")
r = (r_Ni_cu-r_cu)*per2/per1 // resistivity of
   copper 1% Ni in ohm-m
printf("\n Resistivity due to impurity scattering of
    1 %% of Nickel in copper lattice is %.1e ohm-m",
   r)
```

Chapter 15

Semiconductors

Scilab code Exa 15.1 Calculate intrinsic carrier density

```
1 // Calculate intrinsic carrier density
2 clc
3 rho = 3000 // resistivity in ohm m
4 mu_e = 0.14
5 mu_h = 0.05
6 e = 1.602e-19 // charge on electron
7 printf("\n Example 15.1")
8 sigma = 1/rho
9 n = sigma/((mu_e+mu_h)*e)
10 printf("\n Intrinsic carrier density is %.3e m^-3",n
   )
```

Chapter 16

Magnetic Materials

Scilab code Exa 16.1 Calculate the net magnetic moment per iron atom in crystal

```
1 // Calculate the net magnetic moment per iron atom
     in crystal
2 clc
3 a = 2.87 // lattice parameter in angstrom
4 n = 2 // number of atoms per unit cell
5 m = 1750 // Saturation magnetization in kAmˆ-1
6 mu = 9.273e-24 // bohr magneton
7 printf("\n Example 16.1")
8 m_atom = m*1e3*(a*1e-10)^3 /n
9 mu_b = m_atom/mu
10
11 printf("\n Net magnetic moment per iron atom in
     crystal is %.3e Amˆ2",m_atom)
12 printf("\n In unit of mu_b, Net magnetic moment per
     iron atom in crystal is %.1f ",mu_b)
```

Scilab code Exa 16.2 Comparison of saturation temperatures

```
// Comparison of saturation temperatures
clc
t1 = 0 // temperature in kelvin
t2 = 300 // temperature in kelvin
m_net_Gd = 7 // net magnetic moment of gadolinium
m_net_Co = 1.7 // net magnetic moment of cobalt
t_c_Gd = 289 // curie temperature for Gd
printf("\n Example 16.2")
printf("\n Part A:")
if m_net_Gd> m_net_Co then
printf("\n At %d K, Net magnetic moment of
   gadolinium i.e. %d is greater than net magnetic
   moment of cobalt i.e. %.1f ",t1,m_net_Gd,m_net_Co
   )
printf("\n So, Gd will have higher saturation
   magnetization")
end
printf("\n\n Part B:")
if t_c_Gd<t2 then
    printf("\n At temperature %d K, Gd is above its
       curie temperature of %dK",t2,t_c_Gd)
    printf("\n Gd will be paramagnetic at %d K and
       will have negligible magnetization\n as
       compared to Co, which has higher curie
       temperature",t2)
end
```

Scilab code Exa 16.4 Calculation of hysteresis loss

```
// Calculation of hysteresis loss
clc
v = 0.01 // volume in m^3
x = 1e-4 // axis intercept
```

```
y = 1e2 // axis intercept
a = 60000 // Hysteresis loop area
f = 50 // frequency in Hz
printf("\n Example 16.4")
e = x*y*a // Energy loss in one loop
E = e*v // energy loss in core in one cycle
P = E*f // Power loss
printf("\n Power loss due to hysteresis is %d W",P)
```

Scilab code Exa 16.5 Calculation of eddy current loss at normal voltage and freque

```
// Calculation of eddy current loss at normal
   voltage and frequency
clc
Total1 = 2300 // total iron loss in W at 440 V and
   50 Hz
Total2 = 750 // total iron loss in W at 220 V and 25
    Hz
printf("\n Example 16.5")
W_e = 1/2*(Total1-2*Total2)
printf("\n Eddy current loss at normal voltage and
   frequency is %dW",4*W_e)
```

Chapter 17

Dielectric Materials

Scilab code Exa 17.1 Calculation of relative dielectric constant

```
1 // calculation of relative dielectric constant
2 clc
3 l= 10// length of capacitor in mm
4 b = 10 // width of capacitor in mm
5 d = 2 // distance of separation in mm
6 c = 1e-9 // capacitance in farad
7 epsilon_0 = 8.85e-12 // permittivity of free space
8 printf("\n Example 17.1")
9 epsilon_r = c*d*1e-3/(epsilon_0*l*1e-3*b*1e-3)
10
11 printf("\n Relative dielectric constant is %d",
   epsilon_r)
```

Scilab code Exa 17.2 Calculate the polarization of a BaTio3 crystal

```
1 // calculate the polarization of a BaTio3 crystal
2 clc
```

```
Ti_shift= 0.06 // shift of TI ion in angstrom
O_shift = 0.06 // shift of oxygen ion of side face
    in angstrom
o_shift = 0.08 //shift of oxygen ion of top and
    bottom faces in angstrom
O_charge  = 2 // unit charge on oxygen ion of side
    face
o_charge  = 2 // unit charge on oxygen ion of top
    and bottom faces
Ti_charge  = 4 // unit charge on titanium ion
n_O = 2 // number of oxygen ion of side face
n_o = 1 // number of oxygen ion of top and bottom
    face
n_Ti = 1 // number of titanium ion
e = 1.6e-19 // amount of one unit charge in coulomb
printf("\n Example 17.2")
p_Ti = n_Ti*Ti_charge *e*Ti_shift*1e-10
p_O = n_O*O_charge*e*O_shift*1e-10
p_o = n_o*o_charge*e*o_shift*1e-10
Total = p_Ti+p_O+p_o
P = Total/(4.03*3.98^2*1e-30)
printf("\n Polarization of BaTiO3 crystal is %.2f Cm
    ^-2 ", P)
```