

Scilab Textbook Companion for  
Material Science  
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# **Book Description**

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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.

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## Chapter 2

# Atomic structure and electronic configuration

**Scilab code Exa 2.1** Distance of the closest approach alpha particles from the copper nucleus

```
1 //Exam : 2 . 1
2 clc;
3 clear;
4 close;
5 Eg_k=5; //kinetic energy of alpha particles (in MeV)
6 Eg_K=5*(10^6)*1.6*(10^-19); //kinetic energy of alpha
    particles (in J)
7 mv2=2*Eg_K;
8 pi=22/7;
9 phi=180; //firing angle
10 Z=29; //Atomic number
11 e=1.6*(10^-19); //electron charge (in C)
12 Eo=8.85*10^-12; //permittivity of free space
13 d=(Z*e^2/(2*pi*Eo*mv2))*(1+cscd(90))/;
14 disp(d, 'distance of the closest approach alpha
    particles from the copper nucleus (in meter)=');
```

---

**Scilab code Exa 2.2** radius and frequency of an electron in the bohr first orbit in hydrogen atom

```
1 //Exam:2.2
2 clc;
3 clear;
4 close;
5 e=1.6*10^(-19); //electron charge (in C)
6 m=9.1*10^(-31); //mass of electron (in Kg)
7 E_o=8.854*10^(-12); //permittivity of free space
8 h=6.625*10^(-34); //Planck constant
9 n=1; //Orbit number
10 Z=1; //atomic number
11 pi=22/7;
12 r_1=(E_o*h^2)/(pi*m*e^2); //first orbit radius of
    hydrogen atom
13 disp(r_1,'first orbit radius of hydrogen atom (in m)=
    ');
14 Freq=m*(Z^2)*(e^4)/(4*(E_o^2)*(n^3)*h^3); //
15 disp(Freq,'Orbital frequency of electron (in Hz)=');
```

---

**Scilab code Exa 2.3** radius of the second bohr orbit in a singly ionized helium atom

```
1 //Exam:2.3
2 clc;
3 clear;
4 close;
5 Z_1=1; //atomic number for hydrogen
6 n_1=1; //first orbit
7 r_1=0.529; //radius of first orbit of electron for
    hydrogen
```

```

8 Z_2=2; //atomic number for helium
9 n_2=2; //second orbit
10 k=r_1*Z_1/n_1;
11 r_2=k*((n_2)^2)/Z_2; //radius of first orbit of
    electron for helium
12 disp(r_2, 'radius of the second bohr orbit in a
    singly ionized helium atom(in A)=');

```

---

**Scilab code Exa 2.4** Calculate the unit cell dimensions and atomic diameter

```

1 //Exam:2.4
2 clc;
3 clear;
4 close;
5 n_1=1; //first orbit
6 n_2=2; //second orbit
7 n_3=3; //third orbit
8 //E_1=-13.6*(Z^2)/(1^2);
9 //E_2=-13.6*(Z^2)/(2^2);
10 //E_3=-13.6*(Z^2)/(3^2);
11 //E_3-E_1=-13.6*(Z^2)*(-8/9);
12 //E_2-E_1=-13.6*(Z^2)*(-3/4);
13 E_1=-13.6/(1^2); //energy of electron in the first
    bohr orbit of an atom
14 E_2=-13.6/(2^2); //energy of electron in the second
    bohr orbit of an atom
15 E_3=-13.6/(3^2); //energy of electron in the third
    bohr orbit of an atom
16 disp((E_3-E_1)/(E_2-E_1), 'ratio of energy released =
    ');

```

---

**Scilab code Exa 2.5** Calculate the revolutions per second of an electron in the bohr orbit of hydrogen atom

```
1 //Exam:2.5
2 clc;
3 clear;
4 close;
5 m=9.1*10^(-31); //electron mass (in Kg)
6 Z=1; //atomic number
7 e=1.6*10^(-19); //electron charge(in C)
8 E_o=8.25*10^(-12); //permittivity of free space
9 n=1; //first bohr orbit
10 h=6.63*10^(-34); //planck constant
11 R_ps=m*(e^4)/(4*(E_o^2)*(h^3)); //number of
    revolutions per second
12 disp(R_ps,'revolutions per second of an electron in
    the bohr orbit of hydrogen atom=');
```

---

**Scilab code Exa 2.6** orbital frequency of an electron in the first bohr orbit in a hydrogen atom

```
1 //Exam:2.6
2 clc;
3 clear;
4 close;
5 n=1; //first bohr orbit
6 Z=1; //atomic number
7 m=9.1*10^(-31); //electron mass in Kg.
8 e=1.6*10^(-19); //electron charge(in C)
9 E_o=8.85*10^(-12); //permittivity of free space
10 h=6.63*10^(-34); //planck constant
11 v_n=m*(Z^2)*(e^4)/(4*(E_o^2)*(h^3)*(n^3)); //orbital
    frequency of an electron in the first bohr orbit
    in a hydrogen atom
12 disp(v_n,'orbital frequency of an electron in the
```

---

```
first bohr orbit in a hydrogen atom( in Hz)=') ;
```

---

**Scilab code Exa 2.7** kinetic energy potential energy and total energy of an electron

```
1 //Exam :2 .7
2 clc;
3 clear;
4 close;
5 m=9.11*10^-31; //mass of electron (in Kg)
6 Z=1; //atomic number
7 n=1; //first bohr orbit
8 E_o=8.854*10^-12; //permittivity of free space
9 h=6.62*10^-34; //planck constant
10 e=1.6*10^-19; //electron charge(in C)
11 E_k=(m*(Z^2)*(e^4))/(8*(E_o^2)*(n^2)*(h^2)); //
    Kinetic energy(in joule)
12 E=E_k/e; //Kinetic energy(in eV)
13 E_t=-13.6*(Z^2/n^2); //Total Energy(in eV)
14 E_p=E_t-E; //Potential energy(in eV)
15 disp(E_t, 'Total energy (in eV)=') ;
16 disp(E, 'kinetic energy (in eV)=') ;
17 disp(E_p, 'potential energy (in eV)=') ;
```

---

**Scilab code Exa 2.8** velocity of an electron in hydrogen atom in bohr first orbit

```
1 //Exam :2 .8
2 clc;
3 clear;
4 close;
5 h=6.626*10^-34; //planck constant
6 E_o=8.825*10^-12; //permittivity of free space
```

```

7 e=1.6*10^-19; //electron charge(in C)
8 n=1; //first bohr orbit
9 Z=1; //atomic number
10 v=Z*(e^2)/(2*E_o*n*h); //velocity of electron in
    hydrogen atom in bohr first orbit
11 disp(v,'velocity of electron in hydrogen atom in
    bohr first orbit(in meter/sec)=');

```

---

**Scilab code Exa 2.9** principal quantum number and wavelengths of radiation in both energies

```

1 //Exam:2.9
2 clc;
3 clear;
4 close;
5 n_1=1; //electron excited from ground state
6 h=6.62*10^-34; //Planck constant
7 c=3*10^8; //speed of light
8 E_o=8.825*10^-12; //permittivity of free space
9 e=1.6*10^-19; //electron charge(in C)
10 m=9.11*10^-31; //mass of electron(in Kg)
11 E_1=10.2; //energy excites the hydrogen from ground
    level(in eV)
12 K=m*e^4/(8*(E_o^2)*(h^2))//in joule
13 K_e=K/e;//in eV
14 //E_1=K_e*((1/n_1^2)-(1/n^2))
15 //1/(n^2)=1/(n_1^2)-E_1/K_e
16 //n^2=1/(1/(n_1^2)-E_1/K_e)
17 n=(1/(1/(n_1^2)-E_1/K_e))^(1/2); //principal quntum
    number when 10.2 eV energy excites electron
18 disp(ceil(n),'principal quntum number when 10.2 eV
    energy excites electron=');
19 W_1=h*c/(E_1*e)*10^10; //wavelength of radiation when
    10.2 eV energy excites electron
20 disp(W_1,'wavelength of radiation when 10.2 eV

```

```

        energy excites electron (in A)=')
21 E_2=12.09; //energy excites the hydrogen from ground
    level (in eV)
22 n_2=(1/(1/(n_1^2)-E_2/K_e))^(1/2); //principal quantum
    number when 12.09 eV energy excites electron
23 W_2=h*c/(E_2*e)*10^10; //wavelength of radiation when
    12.09 eV energy excites electron
24 disp(ceil(n_2), 'principal quantum number when 12.09
    eV energy excites electron=')
25 disp(W_2, 'wavelength of radiation when 12.09 eV
    energy excites electron (in A)=')

```

---

**Scilab code Exa 2.13** Weight of copper atom and weight of one proton

```

1 //Exam:2.13
2 clc;
3 clear;
4 close;
5 At_w=63.54; //atomic weight of copper
6 N=6.023*10^23; //avogadro's number
7 W_a=At_w/N; //weight of one atom(in gm)
8 W_p=W_a/63; //weight of one proton(in gm)
9 disp(W_a, 'weight of one atom(in gm)=');
10 disp(W_p, 'weight of one proton(in gm)=');

```

---

**Scilab code Exa 2.15** percentage of Si in Copper silicide

```

1 //Exam:2.15
2 clc;
3 clear;
4 close;
5 Atw_Cu=63.54; //atomic weight of copper
6 Atw_Si=28.09; //atomic weight of silicon

```

```
7 // 5 atoms of copper working in Cu_5_Si
8 Tw_Cu=5*Atw_Cu;//total weight of copper used in
copper silicide
9 Tw_Si=Atw_Si;//total weight of silicon used in
copper silicide
10 Percentage=(Tw_Si/(Tw_Cu+Tw_Si))*100;//percentage of
Si in Copper silicide
11 disp(Percentage,'percentage of Si in Copper silicide
(Cu_5_Si)=')
```

---

# Chapter 3

## Crystal Geometry Structure and Defects

**Scilab code Exa 3.10** Find the angle Between normals to the planes

```
1 //Exam:3.10
2 clc;
3 clear;
4 close;
5 // Miller indices of plane
6 h_1=1;
7 k_1=1;
8 l_1=1;
9 h_2=1;
10 k_2=2;
11 l_2=1;
12 angle=acosd((h_1*h_2+k_1*k_2+l_1*l_2)/(((h_1^2+k_1
    ^2+l_1^2)^(1/2))*( (h_2^2+k_2^2+l_2^2)^(1/2))) );
13 disp(angle,'angle Between normals to the planes
(111) and (121)(in degrees)=');
```

---

**Scilab code Exa 3.11** Determine the packing efficiency and density of sodium chloride

```
1 //Exam:3.11
2 clc;
3 clear;
4 close;
5 r_Na=0.98; //Radius of Na+(in A)
6 r_Cl=1.81; //Radius of Cl-(in A)
7 a=2*(r_Na+r_Cl); //Lattice parameter (in A)
8 pi=22/7;
9 V_i=4*(4/3)*pi*((r_Na^3)+(r_Cl^3)); //Volume of ions
    present in unit cell
10 V_u=a^3; //Volume of unit cell
11 Apf=V_i/V_u; //Atomic packing fraction
12 Ef_p=(Apf)*100; //Packing efficiency (in %)
13 AM_sodium=22.99; //Atomic mass of sodium (in amu)
14 AM_chlorine=35.45; //Atomic mass of chlorine (in amu)
15 M_1=4*(AM_sodium+AM_chlorine)*1.66*10^(-27); //Mass
    of the unit cell
16 a_1=a*10^(-10); //Lattice parameter (in meter)
17 V_u1=(a_1)^3;
18 Density=M_1/V_u1;
19 disp(Ef_p, 'Packing efficiency of sodium chloride (in
    %)=');
20 disp(Density, 'density of sodium chloride (in Kg/m3)='
    );
```

---

**Scilab code Exa 3.12** Calculate the unit cell dimensions and atomic diameter

```
1 //Exam:3.12
2 clc;
3 clear;
4 close;
```

```

5 Density=2.7; // (in g/cm^3)
6 n=4;
7 m=26.98; //atomic weight of Al
8 N_a=6.023*10^(23); //avogadro number
9 a=((n*m/(Density*N_a))^(1/3)); //Lattice parameter (in
Cm)
10 A=a*10^(8); //Lattice parameter (in A)
11 disp(A, 'radius (in A)=');
12 r=A/(2*1.414); //radius for fcc structure
13 disp(2*r, 'Diameter (in A)=');

```

---

**Scilab code Exa 3.13** Calculate the interplaner distance

```

1 //Exam:3.13
2 clc;
3 clear;
4 close;
5 r=1.245; //radius of nickel (in A)
6 a=4*r/(2)^(1/2); //Lattice constant (in A)
7 //Miller indices of plane 200
8 h_1=2;
9 k_1=0;
10 l_1=0;
11 //Miller indices of plane 111
12 h_2=1;
13 k_2=1;
14 l_2=1;
15 d_200=a/((h_1^2)+(k_1^2)+(l_1^2))^(1/2);
16 d_111=a/((h_2^2)+(k_2^2)+(l_2^2))^(1/2);
17 disp(d_200, 'interplaner distance of (200) plane of
nickel crystal (in A)=');
18 disp(d_111, 'interplaner distance of (111) plane of
nickel crystal (in A)=');

```

---

**Scilab code Exa 3.14** Find the number of atoms per mm<sup>2</sup>

```
1 //Exam:3.14
2 clc;
3 clear;
4 close;
5 a=3.03*10^(-7); //lattice constant(in mm)
6 N_100=1/(a^2); //Number of atoms in the (100) plane
                  of a simple cubic structure
7 N_110=0.707/(a^2); //Number of atoms in the (110)
                  plane of a simple cubic structure
8 N_111=0.58/(a^2); //Number of atoms in the (111)
                  plane of a simple cubic structure
9 disp(N_100,'Number of atoms in the (100) plane of a
      simple cubic structure(in per mm^2)=');
10 disp(N_110,'Number of atoms in the (110) plane of a
      simple cubic structure(in per mm^2)=');
11 disp(N_111,'Number of atoms in the (111) plane of a
      simple cubic structure(in per mm^2)=');
```

---

**Scilab code Exa 3.15** Determine the planer density of Ni

```
1 //Exam:3.15
2 clc;
3 clear;
4 close;
5 r=1.245*10^(-7); //Radius of the Ni atom(in mm)
6 NA_100=1+(1/4)*4; //Numbers of atom in (100) plane
7 a=4*r/(2)^(1/2); //Lattice constant(in mm)
8 Area=a^2;
9 P_density=NA_100/Area;
```

```
10 disp(P_density, 'the planer density of Ni (in atoms  
per mm^2)=');
```

---

**Scilab code Exa 3.16** Calculate the planar atomic densities of planes

```
1 //Exam:3.16  
2 clc;  
3 clear;  
4 close;  
5 N_a1=4*(1/4)+1; //Number of atoms contained in (100)  
plane  
6 r=1.75*10^(-7); //radius of lead atom (in mm)  
7 a_1=2*2^(1/2)*r; //edge of unit cell in case of  
(100) plane  
8 PD_100=N_a1/(a_1^2); //Planar density of plane (100)  
9 N_a2=4*(1/4)+2*(1/2); //Number of atoms contained in  
(110) plane  
10 a_21=4*r; //top edge of the plane (110)  
11 a_22=2*2^(1/2)*r; //vertical edge of the plane (110)  
12 PD_110=N_a2/(a_21*a_22); //Planar density of plane  
(110)  
13 N_a3=3*(1/6)+3/2; //Number of atom contained in (111)  
plane  
14 Ar_111=4*(3^(1/2))*r^2; //area of (111) plane  
15 PD_111=N_a3/Ar_111; //Planar density of plane (111)  
16 disp(PD_100, 'Planar density of plane 100(in atoms/mm  
^2)=');  
17 disp(PD_110, 'Planar density of plane 110(in atoms/mm  
^2)=');  
18 disp(PD_111, 'Planar density of plane 111(in atoms/mm  
^2)=');
```

---

**Scilab code Exa 3.17** Calculate the linear atomic densities of planes

```

1 //Exam:3.17
2 clc;
3 clear;
4 close;
5 N_a1=(1/2)+1+(1/2); //Number of diameters of atom
    along (110) direction
6 a=3.61*10^(-7); //lattice constant of copper in mm
7 L_d1=2^(1/2)*a; //length of the face diagonal in case
    of (110) direction
8 p_110=N_a1/L_d1; //linear atomic density along (110)
    of copper crystal lattice (in atoms/mm)
9 N_a2=(1/2)+(1/2); //Number of diameters of atom along
    (111) direction
10 L_d2=3^(1/2)*a; //length of the face diagonal in case
    of (111) direction
11 p_111=N_a2/L_d2; //linear atomic density along (110)
    of copper crystal lattice (in atoms/mm)
12 disp(p_110,'linear atomic density along (110) of
    copper crystal lattice (in atoms/mm)=');
13 disp(p_111,'linear atomic density along (111) of
    copper crystal lattice (in atoms/mm)=');

```

---

### Scilab code Exa 3.18 Find lattice constant

```

1 //Exam:3.18
2 clc;
3 clear;
4 close;
5 A=55.8; //atomic weight of Fe
6 n=2; //number of atoms per unit cell
7 N=6.02*10^(26); //Avogadro's number
8 p=7.87*10^3; //density of Fe (in kg/m^3)
9 a=((A*n/(N*p))^(1/3))*10^10; //Value of lattice
    constant
10 disp(a,'Value of lattice constant (in A)=');

```

---

**Scilab code Exa 3.19** Find the numbers of atoms per unit cell

```
1 //Exam:3.19
2 clc;
3 clear;
4 close;
5 a=2.9*10^(-10); //lattice parameter (in m)
6 A=55.8; //atomic weight of Fe
7 N=6.02*10^(26); //Avogadro's number
8 p=7.87*10^3; //density of Fe (in kg/m^3)
9 n=(a^3)*N*p/A; //Numbers of atoms per unit cell
10 disp(floor(n), 'Numbers of atoms per unit cell=');
```

---

**Scilab code Exa 3.20** Calculate the line energy of disslocation in bcc iron

```
1 //Exam:3.20
2 clc;
3 clear;
4 close;
5 a=2.87*10^(-10); //lattice parameter for bcc iron
6 b=a*(3^(1/2))/2; //Magnitude of burgers vector
7 u=80*10^9; //shear modulus
8 E=(1/2)*u*b^2; //line energy of disslocation
9 disp(E, 'line energy of disslocation (in J/m)=');
```

---

**Scilab code Exa 3.22** Calculate the number of vacancies

```
1 //Exam:3.22
2 clc;
```

```

3 clear;
4 close;
5 N=6.023*10^23; // avogadro number
6 T=1000; // absolute temperature
7 R=8.314; // constant
8 H_f=100*1000; // enthalpy of formation of vacancies (in
J/mol)
9 n=N*exp(-(H_f)/(R*T)); //number of vacancies created
during heating (in per mol)
10 V=5.5*10^(-6); //volume of 1 mole of the crystal in m
^3
11 n_1=n/V; //number of vacancies created during heating
(in per m^3)
12 disp(n_1, 'number of vacancies created during heating
(in per m^3)=');

```

---

**Scilab code Exa 3.23** Calculate the surface energy of copper

```

1 //Exam:3.23
2 clc;
3 clear;
4 close;
5 //bond energy per atom of copper=bond energy per
bond*numbers of bond per atom*(1/2)
6 A=56.4*1000; //
7 N=6.023*10^23; // avogadro number
8 n_1=12; // numbers of bond per atom
9 n_2=3; // bonds broken at the surface
10 E=A*n_1/(2*N); // Energy of total bonds
11 E_b=E*(n_2/n_1); // Energy of broken bonds on surface
12 disp(E_b, 'E_b');
13 n_a=1.77*10^19; // no. of atoms on {111} planes in
copper (in m^-2)
14 E_c=n_a*E_b; // Surface energy (enthalpy) of copper
15 disp(E_c, 'Surface energy (enthalpy) of copper (in J/m

```

$\wedge 2) = ') ;$

---

**Scilab code Exa 3.24** Calculate the equilibrium concentration of vacancies in aluminium

```
1 //Exam:3.24
2 clc;
3 clear;
4 close;
5 H_f=68*1000; //enthalpy of formation of vacancies (in
J/mol)
6 T_1=0; //temp (in K)
7 T_2=300; //temp (in K)
8 R=8.314; //constant
9 n=exp(-H_f/(R*T_2)); //equilibrium concentration of
vacancies in aluminium at 300 K
10 disp(n, 'equilibrium concentration of vacancies in
aluminium at 300 K=') ;
```

---

**Scilab code Exa 3.25** Determine the interplanar spacing

```
1 //Exam:3.25
2 clc;
3 clear;
4 close;
5 Wavelength=1.54*10^(-10); //in meter
6 Angle=20.3; //in degree
7 n=1; //First order
8 d=Wavelength*n/(2*sind(Angle)); //the interplanar
spacing (in Meter)
9 disp(d/(10^-10), 'the interplanar spacing between
atomic plane (in A)=') ;
```

---

**Scilab code Exa 3.26** Calculate the size of unit cell

```
1 //Exam:3.26
2 clc;
3 clear;
4 close;
5 wavelength=0.58; //in Angstrom
6 angle=9.5; //in degree
7 n=1; //First order
8 d_200=wavelength*n/(2*sind(angle)); //interplanar
      spacing(in Angstrom)
9 //Miller indices of plane
10 h=2;
11 k=0;
12 l=0;
13 a=d_200*(h^2+k^2+l^2)^(1/2); //Size of unit cell(in
      Angstrom)
14 disp(a, 'Size of unit cell(in Angstrom)=');
```

---

**Scilab code Exa 3.27** Calculate the Bragg angle

```
1 //Exam:3.27
2 clc;
3 clear;
4 close;
5 //Miller indices of plane
6 h=1;
7 k=1;
8 l=1;
9 wavelength=0.54; //in angstrom
10 a=3.57; //size of a cube
11 n=1;
```

```
12 d_111=a/(h^2+k^2+l^2)^(1/2); //interplanar spacing (in  
Angstrom)  
13 angle=asind(n*wavelength/(2*d_111));  
14 disp(angle,'Bragg angle (in degree)=');
```

---

**Scilab code Exa 3.28** Calculate the bragg reflection index

```
1 //Exam:3.28  
2 clc;  
3 clear;  
4 close;  
5 d=1.181; //  
6 wavelength=1.540; //in angstrom  
7 angle=90; //in degree  
8 n=2*d*sind(angle)/(wavelength); //the bragg  
reflection index  
9 disp(n,'bragg reflection index for BCC crystal=');
```

---

**Scilab code Exa 3.29** Calculate the angle for 3rd order reflection

```
1 //Exam:3.29  
2 clc;  
3 clear;  
4 close;  
5 n_1=1; //1st order reflection index  
6 angle_1=10; //1st order reflection angle  
7 n_3=3; //3rd order reflection index  
8 //sind(angle_1)/sind(angle_3)=n_1/n_3  
9 angle_3=asind(n_3*sind(angle_1)/n_1); //  
10 disp(angle_3,'3rd order reflection angle=')
```

---

**Scilab code Exa 3.30** Obtain the interplanar spacing and miller indices of the reflection plane

```
1 //Exam:3.30
2 clc;
3 clear;
4 close;
5 angle=20.3; //in degree
6 wavelength=1.54; //in angstrom
7 n=1;
8 a=3.16; //lattice parameter in angstrom
9 d=n*wavelength/(2*sind(angle)); //interplanar spacing
10 M_indices=a^2/(d^2);
11 disp(d, 'interplanar spacing of reflection plane');
12 disp(floor(M_indices), 'miller indices of the
    reflection plane');
13 disp((101),(110),(011));
```

---

**Scilab code Exa 3.31** Determine interatomic spacing

```
1 //Exam:3.31
2 clc;
3 clear;
4 close;
5 //Miller indices of plane
6 n=1;
7 h=1;
8 k=1;
9 l=1;
10 angle=30; //in degree
11 wavelength=2; //in angstrom
12 d=n*wavelength/(2*sind(angle)); //interplanar spacing
13 a=d*(h^2+k^2+l^2)^(1/2); //interatomic spacing
14 disp(a, 'interatomic spacing (in angstrom)=');
```

---

# Chapter 4

## Bonds in solid

Scilab code Exa 4.1 distance at which the dissociation occurs

```
1 //Exam:4.1
2 clc;
3 clear;
4 close;
5 r_o=2.8 //interatomic distance in
6 R_o=2.8*10^(-10); //interatomic distance in m
7 u_o=8; //released energy in eV
8 e=1.6*10^(-19); //charge of electron in C
9 U_o=8*e //released energy in Joule
10 A=(5/4)*U_o*(R_o^2); //proportionality constant for
    attraction in J-m2
11 B=A*(R_o^8)/5; //proportionality constant for
    repulsion in J-m2
12 r_c=(110*B/(6*A))^(1/8); //interatomic distance at
    which the dissociation occurs in m
13 F=-(2/r_c^3)*(A-5*B/(r_c^8)); //the force required to
    dissociate the molecule in N
14 disp(A,'proportionality constant for attraction (in
    J-m2)=');
15 disp(B,'proportionality constant for repulsion (in J
    -m2)=');
```

```
16 disp(r_c,'interatomic distance at which the  
dissociation occurs (in m)=');  
17 disp(F,'the force required to dissociate the  
molecule (in N)=');
```

---

**Scilab code Exa 4.2** Find the repulsive exponent n

```
1 //Exam:4.2  
2 clc;  
3 clear;  
4 close;  
5 r_o=3.14; // nearest neighbour equilibrium distance in  
6 R_o=3.14*10^(-10); // nearest neighbour equilibrium  
distance in m  
7 K=5.747*10^(-11); //compressibility of KCl in m2/N  
8 M=1.748; //Madelung constant  
9 pi=22/7;  
10 E_o=8.854*10^(-12);  
11 q=1.6*10^(-19); //electron charge  
12 n=1+18*(R_o^4)*4*pi*E_o/(K*M*q^2);  
13 disp(n,'repulsive exponent n=');
```

---

**Scilab code Exa 4.3** Find the radius of Cl ion

```
1 //Exam:4.3  
2 clc;  
3 clear;  
4 close;  
5 F_1=3.02*10^(-9); //force of attraction b/w ions of  
Na+ and Cl-  
6 Z_1=+1;  
7 Z_2=-1;
```

```

8 e=1.6*10^(-19);
9 E_o=8.854*10^-12;
10 pi=22/7;
11 r_Na=0.95; //ionic radius of Na+ ion
12 r=(-Z_1*Z_2*e^2/(4*pi*E_o*F_1))^(1/2); //Radius of
    ion in meter
13 R=r/10^(-10); //Radius of ion in Angstrom
14 r_Cl=(R-r_Na); //Radius of Cl- ion in Angstrom
15 disp(r_Cl, 'Ionic Radius of Cl- ion (in Angstrom)=');

```

---

#### Scilab code Exa 4.4 force of attraction between ions

```

1 //Exam:4.4
2 clc;
3 clear;
4 close;
5 Z_1=+2;
6 Z_2=-2;
7 r_Mg=0.65; //radius of Mg++ ion
8 r_S=1.84; //radius of S-- ion
9 r=r_Mg+r_S; //net radius(in Angstrom)
10 R=r*10^(-10); //net radius(in meter)
11 e=1.6*10^(-19);
12 E_o=8.854*10^-12;
13 pi=22/7;
14 F=-Z_1*Z_2*e^2/(4*pi*E_o*R^2); //force of attraction
    between ions(in Newton)
15 disp(F, 'force of attraction between ions(in Newton)=
    ');

```

---

#### Scilab code Exa 4.5 How much net energy is spent in the process

```
1 //Exam:4.5
```

```
2 clc;
3 clear;
4 close;
5 //Na atom requires +5.14 eV of energy. When this
   electron is transferred to a vacant position ,it
   gives back 4.02 eV of energy
6 E_1=+5.14; //in eV
7 E_2=-4.02; //in eV
8 NET_energy=E_1+E_2;//in eV
9 disp(NET_energy , 'Net spent energy in whole process(
   in eV)=')
```

---

**Scilab code Exa 4.6** Estimate the fraction of hydrogen bonds that are broken when ice melts

```
1 //Exam:4.6
2 clc;
3 clear;
4 close;
5 Enthalpy=6.02; //enthalpy of fusion of ice is 6.02 kJ
   /mol
6 E_h=20.5; //Hydrogen bond energy (in kJ/mol)
7 //There are two moles of hydrogen bonds per mole of
   H2O in ice.
8 H_b=Enthalpy/(2*E_h); //the fraction of hydrogen
   bonds that are broken when ice melts
9 disp(H_b , 'fraction of hydrogen bonds that are broken
   when ice melts=')
```

---

# Chapter 5

## Electron Theory of Metals

**Scilab code Exa 5.1** Evaluate the temperature

```
1 //Exam:5.1
2 clc;
3 clear;
4 close;
5 //The probability that a particular quantum state at
   energy E is filled , is given by
6 //f(E) =1/(1+exp(E-E_f)/kT)
7 e=1.6*10^(-19); //charge on the electron
8 dE=0.5*e; //E-E_f in joule
9 //0.01=1/(1+exp(x))
10 //1+exp(x)=100
11 x=log(99);
12 k=1.38*10^(-23); //constant
13 T=dE/(x*k); //temperature
14 disp(ceil(T), 'temperature at which there is one per
   cent probability that a state with an energy 0.5
   eV above the Fermi energy will be occupied by an
   electron (in K)=');
```

---

**Scilab code Exa 5.2** Find the drift velocity of carriers

```
1 //Exam:5.2
2 clc;
3 clear;
4 close;
5 n=10^19; //electrons per m^3
6 V=0.017; //applied voltage
7 d=0.27*10^-2; //distance with material
8 e=1.602*10^-19; //in coulomb
9 m=9.1*10^-31; //mass of an electron (in kg)
10 conductivity=0.01; //in mho.m^-1
11 E=V/d; //Electric field (in V/m)
12 v=(conductivity*E/(n*e))*10^2; //drift velocity of
   carriers (in meter/sec)
13 disp(v, 'drift velocity of carriers (in meter/sec)=');
```

---

**Scilab code Exa 5.3** Find the conductivity of copper at 300K

```
1 //Exam:5.3
2 clc;
3 clear;
4 close;
5 T=300; //Temperature (in Kelvin)
6 t=2*10^-14; //time (in sec)
7 V_c=8.9; //volume of 63.54gm of copper (in cc)
8 Aw_c=63.54; //Atomic weight of copper (in a.m.u)
9 e=1.6*10^(-19);
10 m=9.1*10^-31;
11 N_a=6.023*10^23; //avogadro's number
12 n=(N_a/(Aw_c/V_c))*10^6; //Number of electrons per m
   ^3
13 conductivity=(e^2)*n*t/m; //conductivity of copper at
   300K (in mho/m)
14 disp(conductivity, 'conductivity of copper at 300K (in
```

mho/m)=') ;

---

**Scilab code Exa 5.4** Find the mobility of conduction electron

```
1 //Exam:5.4
2 clc;
3 clear;
4 close;
5 t=10^(-14); //mean free time between the collisions (
    in second)
6 e=1.6*10^-19;
7 m=9.1*10^-31;
8 Mobility=e*t/m; //in m^2/V-s
9 disp(Mobility , 'mobility of conduction electron (in m
    ^2/V-s)=') ;
```

---

**Scilab code Exa 5.5** Find the mobility of conduction electron and drift velocity

```
1 //Exam:5.5
2 clc;
3 clear;
4 close;
5 n=6*10^23; //conduction electron per m^3
6 conductivity=6.5*10^7; //in mho/m
7 E=1; //electric field intensity (in V/m)
8 e=1.6*10^-19;
9 m=9.1*10^-31;
10 Mobility=conductivity/(n*e); //in m^2/V-s
11 v=Mobility*E; //drift velocity (in m/sec)
12 disp(Mobility , 'mobility of conduction electron (in m
    ^2/V-s)=') ;
13 disp(v , 'drift velocity (in m/sec)=') ;
```

---

**Scilab code Exa 5.6** Find the number of free electrons and also calculate mobility of electrons

```
1 //Exam:5.6
2 clc;
3 clear;
4 close;
5 d=10.5; // density of silver (in gm/cc)
6 At_w=107.9;
7 e=1.6*10^-19;
8 conductivity=6.8*10^5; //in mho/centimeter
9 N=6.023*10^23;
10 n=N*d/At_w; //number of free electrons
11 Mobility=conductivity/(n*e); //mobility of electrons(
    in cm^2/V-s);
12 disp(n,'number of free electrons=');
13 disp(Mobility,'mobility of electrons (in cm^2/V-s)' );
;
```

---

**Scilab code Exa 5.7** maximum velocity of an electron in a metal and mobility of electrons

```
1 //Exam:5.7
2 clc;
3 clear;
4 close;
5 E_f=3.75; //Fermi energy (in eV)
6 e=1.602*10^-19;
7 W_f=e*E_f; //fermi energy in joules
8 t=10^-14; //mean free time between the collisions (in
    second)
```

```

9 m=9.1*10^-31; //mass of electron
10 v_f=(2*W_f/m)^(1/2); //maximum velocity of an
    electron in a metal(in m/s)
11 mobility=e*t/m; //mobility of electrons(in m^2/V-s)
12 disp(v_f,'maximum velocity of an electron in a metal
    (in m/s)=');
13 disp(mobility,'mobility of electrons (in m^2/V-s)=')

```

---

**Scilab code Exa 5.8** Calculate the velocity of an electrons at fermi level

```

1 //Exam:5.8
2 clc;
3 clear;
4 close;
5 E_f=2.1; //fermi energy (in eV)
6 e=1.602*10^-19;
7 m=9.1*10^-31;
8 W_f=e*E_f; //fermi energy in joules
9 v_f=(2*W_f/m)^(1/2); //velocity of an electrons at
    fermi level(in m/sec)
10 disp(v_f,'velocity of an electrons at fermi level(in
    m/sec )')

```

---

**Scilab code Exa 5.9** Estimate the mean path of free electrons in pure copper

```

1 //Exam:5.9
2 clc;
3 clear;
4 close;
5 t=10^-9; //collision time(in seconds)
6 E_f=7; //fermi energy(in eV)
7 e=1.6*10^-19;

```

```
8 m=9.1*10^-31;
9 W_f=E_f*e; //fermi energy(in joules)
10 v_f=(2*W_f/m)^(1/2); //velocity of an electrons at
    fermi level(in m/sec)
11 P=v_f*t; //Mean free path(in meter)
12 disp(P, 'Mean free path(in meter)=')
```

---

**Scilab code Exa 5.10** Find the conductivity of copper

```
1 //Exam:5.10
2 clc;
3 clear;
4 close;
5 N_a=6.023*10^23;
6 V_c=8.9; //volume of 63.54gm of copper(in cc)
7 Aw_c=63.54; //Atomic weight of copper(in a.m.u)
8 n=(N_a/(Aw_c/V_c))*10^6; //Number of electrons per m
    ^3
9 e=1.6*10^-19;
10 m=9.1*10^-31;
11 t=2*10^-14; //collision time
12 conductivity=n*(e^2)*t/m; //conductivity of copper
13 disp(conductivity, 'conductivity of copper(in ohm^-1/
    m)=');
```

---

# Chapter 6

## Photoelectric Effect

**Scilab code Exa 6.1** kinetic energy of electrons ejected from the surface

```
1 //Exam :6 . 1
2 clc;
3 clear;
4 close;
5 h=6.62*10^-34;
6 c=3*10^8;
7 e=1.6*10^-19;
8 Wavelength_1=2300*10^-10;
9 W=h*c/Wavelength_1; //Work function
10 Wavelength_2=1800*10^-10;
11 E_in=h*c/Wavelength_2;
12 E=E_in-W; //kinetic energy of the ejected electron (in
   Joules)
13 E_1=E/e; //kinetic energy of the ejected electron (in
   eV)
14 disp(E_1, 'kinetic energy of the ejected electron (in
   eV)=');
```

---

**Scilab code Exa 6.2** Calculate the threshold frequency and the corresponding wavelength

```
1 //Exam:6.2
2 clc;
3 clear;
4 close;
5 h=6.625*(10^(-34)); //Planck's constant (in m2*kg/s)
6 c=3*10^8; //speed of light (in m/s)
7 e=1.602*10^-19; //electron charge (in coulomb)
8 W=2.3; //work (in eV)
9 W_1=W*e; //work (in joules)
10 v_o=W_1/h; //threshold frequency (in Hz)
11 Wavelength=(h*c/W_1)/10^(-10); //Wavelength in
    Angstrom
12 disp(v_o,'threshold frequency (Hz)=');
13 disp(Wavelength,'Wavelength (in Angstrom)=');
```

---

**Scilab code Exa 6.3** Calculate the threshold frequency and the work function of metal

```
1 //Exam:6.3
2 clc;
3 clear;
4 close;
5 h=6.625*(10^(-34)); //Planck's constant (in m2*kg/s)
6 c=3*10^8; //speed of light (in m/s)
7 e=1.602*10^-19; //electron charge (in coulomb)
8 wavelength=6800*10^-10; //wavelength of radiation
9 v_o=c/wavelength; //frequency
10 W=h*v_o; //Work function
11 disp(v_o,'threshold frequency (in Hz)=')
12 disp(W,'work function of metal (in joule)=')
```

---

**Scilab code Exa 6.4** Calculate the photons emitted by lamp per second

```
1 //Exam:6.4
2 clc;
3 clear;
4 close;
5 h=6.625*(10^(-34)); //Planck's constant (in m2*kg/s)
6 c=3*10^8; //speed of light (in m/s)
7 L_r =150*8/100; //Lamp rating (in joule)
8 wavelength=4500*10^-10; //in meter
9 W=h*c/wavelength; //work function
10 N=L_r/W; //number of photons emitted by lamp per
    second
11 disp(N, 'number of photons emitted by lamp per second
    =' )
```

---

**Scilab code Exa 6.5** Determine the region of electrons spectrum

```
1 //Exam:6.5
2 clc;
3 clear;
4 close;
5 h=6.6*(10^(-34)); //Planck's constant (in m2*kg/s)
6 c=3*10^8; //speed of light (in m/s)
7 e=1.6*10^-19; //electron charge (in coulomb)
8 W=2.24; //work function (in eV)
9 W_1=W*e; //work function (in joule)
10 v=(W_1/h)*10^-10; //frequency
11 wavelength=c/v; //region of electrons spectrum is
    less than (in angstrom)
12 disp(wavelength, 'region of electrons spectrum is
    less than (in angstrom) ')
```

---

**Scilab code Exa 6.6** Calculate the photons emitted by radio receiver

```
1 //Exam:6.6
2 clc;
3 clear;
4 close;
5 h=6.625*(10^(-34)); //Planck's constant (in m2*kg/s)
6 c=3*10^8; //speed of light (in m/s)
7 P_o=10*10^3; //Power of radio receiver (in Watt)
8 v=440*10^3; //Operating frequency
9 E=h*v; //Energy of each electron
10 N=P_o/E; //Number of photons emitted/sec
11 disp(N, 'Number of photons emitted/sec by radio
    receiver=')
```

---

**Scilab code Exa 6.7** wavelength of light which can just eject electron from tungsten and from barrium

```
1 //Exam:6.7
2 clc;
3 clear;
4 close;
5 W_t=4.52; //Work function for tungesten (in eV)
6 W_b=2.5; //Work function for barrium (in eV)
7 h=6.62*(10^(-34)); //Planck's constant (in m2*kg/s)
8 c=3*10^8; //speed of light (in m/s)
9 e=1.6*10^-19; //electron charge (in coulomb)
10 W_T=W_t*e; //Work function for tungesten (in Joule)
11 W_B=W_b*e; //Work function for barrium (in Joule)
12 Wavelength_T=(h*c/W_T)*10^10; //wavelength of light
    which can just eject electron from tungsten
```

```
13 Wavelength_B=(h*c/W_B)*10^10; //wavelength of light  
    which can just eject electron from barrium  
14 disp(Wavelength_T , 'wavelength of light which can  
    just eject electron from tungsten(in Angstrom)=')  
15 disp(Wavelength_B , 'wavelength of light which can  
    just eject electron from barrium(in Angstrom)=')
```

---

# Chapter 7

## Diffusion in Solids

**Scilab code Exa 7.1** find the time required for carburization

```
1 //Exam:7.1
2 clc;
3 clear;
4 close;
5 D=1.28*10^(-11); //diffusion coefficient of carbon in
                     given steel in m2/s
6 c_s=0.9; //Surface concentration of diffusion element
            in the surface
7 c_o=0.2; //Initial uniform concentration of the
            element in the solid
8 c_x=0.4; //Concentration of the diffusing element at a
            distance x from the surface
9 x=0.5*10^(-3); //depth from the surface in m
10 //((c_s-c_x)/(c_s-c_o))=erf(x/(2*(D*t)(1/2)))
11 t=(x/(2*erfinv((c_s-c_x)/(c_s-c_o))*D^(1/2)))^2; //
            time required for carburization (in sec)
12 disp(t,'time required for carburization (in sec)=');
```

---

**Scilab code Exa 7.2** time required

```

1 //Exam:7.2
2 clc;
3 clear;
4 close;
5 D=4*10^(-17); // diffusion coefficient of carbon in
     given steel in m2/s
6 c_s=3*10^26; //Surface concentration of boron atoms
     in the surface
7 c_1=0; //Initial uniform concentration of the element
     in the solid
8 c_x=10^23; //Concentration of the diffusing element
     at a distance x from the surface
9 x=2*10^(-6); //depth from the surface in m
10 //((c_s-c_x)/(c_s-c_1))=erf(x/(2*(D*t)^(1/2)))
11 a=erfinv((c_s-c_x)/(c_s-c_1));
12 disp(a, '==')
13 t=(x^2/(D*4*(2.55)^2)); //time required to get a
     boron content of 1023 atoms per m3 at a depth of
     2 micro meter
14 disp(t, 'time required to get a boron content of 1023
     atoms per m3 at a depth of 2 micro meter(in sec)
     ==');
15 disp((c_s-c_x)/(c_s-c_1));
16 T=(x/(2*(2.55)*D^(1/2)))^2;
17 disp(T, '==')

```

---

**Scilab code Exa 7.3** find the constant of the equation and activation energy

```

1 //Exam:7.3
2 clc;
3 clear;
4 close;
5 t_1=736; //Temperature in C
6 t_2=782; //Temperature in C

```

```

7 T_1=t_1+273; //Temperature in K
8 T_2=t_2+273; //Temperature in K
9 D_1=2*10^(-13); //Coefficient of diffusion at T_1 (in
m2/s)
10 D_2=5*10^(-13); //Coefficient of diffusion at T_2 (in
m2/s)
11 k=1.38*10^(-23); //in J/K
12 //log(d_1)=log(d_o)-E/(k*T_1)
13 //log(d_2)=log(d_o)-E/(k*T_2)
14 E=(log(D_1)-log(D_2))/((1/(k*T_1))-(1/(k*T_2))); //
15 disp(E, 'activation energy(in J)=');
16 D_o=2*10^(-13)/exp(E/(k*T_1));
17 disp(D_o, 'constant of the equation(in m2/s)=')
18 t_4=500; //Temperature in C
19 T_4=t_4+273; //Temperature in K
20 D_4=D_o*exp(E/(k*T_4)); //diffusion coefficient at
500 C
21 disp(D_4, 'diffusion coefficient at 500 C (in m2/s)='
)

```

---

**Scilab code Exa 7.4** approximate time that will produce same diffussion at 500 C

```

1 //Exam:7.4
2 clc;
3 clear;
4 close;
5 D_500=4.8*10^(-14); //Diffusion coefficient for
copper in aluminimium at 500*C(in m2/s)
6 D_600=5.3*10^(-13); //Diffusion coefficient for
copper in aluminimium at 600*C(in m2/s)
7 t_600=10; //time of diffussion at 600*C(in Hours)
8 //D_500*t_500=D_600*t_600
9 t_500=D_600*t_600/D_500; //time of diffussion at 500*
C

```

```
10 disp(t_500,'Time at 500*C that will produce the same  
diffusion as in 600*C(in Hours)=');
```

---

# Chapter 8

## Mechanical Properties of Materials and Mechanical Tests

**Scilab code Exa 8.1** Determine the fracture strength

```
1 //Exam:8.1
2 clc;
3 clear;
4 close;
5 Y=180*10^9; //Young's modulus of a certain material(
    in N/m^2)
6 E=1.8; //true surface energy (in J/m^2)
7 c=(5/2)*10^-6; //Crack (in meter)
8 pi=3.14;
9 F_strength=(2*Y*E/(pi*c))^(1/2);
10 disp(F_strength*10^-6, 'fracture strength (in MN/m^2)=
    ');
```

---

**Scilab code Exa 8.2** true stress and strain with engineering stress and strain

```

1 //Exam:8.2
2 clc;
3 clear;
4 close;
5 d_o=12.7; // tensile test specimen diameter (in mm)
6 d=12; // tensile test specimen diameter after load (in
      mm)
7 P=76*10^3; //load (in N)
8 pi=22/7;
9 A_o=(pi/4)*(d_o^2); //Initial area of cross section (
      in mm^2)
10 A=(pi/4)*(d^2); //area of cross section after load of
      76 kN
11 E_stress=P/A_o; //engineering stress
12 T_stress=P/A; //true stress
13 T_strain=log(A_o/A); //true strain
14 E_strain=exp(T_strain)-1; //engineering strain
15 disp(E_stress,'engineering stress (in N/mm^2)=');
16 disp(T_stress,'true stress (in N/mm^2)=');
17 disp(E_strain,'engineering strain=');
18 disp(T_strain,'true strain=');

```

---

**Scilab code Exa 8.3** Determine the fracture strength

```

1 //Exam:8.3
2 clc;
3 clear;
4 close;
5 Y=210*10^9; //Young's modulus of a certain material(
      in N/m^2)
6 E=10; //true surface energy (in J/m^2)
7 c=(100/2)*10^-6; //Crack (in meter)
8 pi=3.14;
9 F_strength=(2*Y*E/(pi*c))^(1/2);
10 disp(F_strength,'fracture strength (in Newton/m^2)=')

```

;

---

**Scilab code Exa 8.4** Find the resultant elongation

```
1 //Exam:8.4
2 clc;
3 clear;
4 close;
5 l_o=305*10^-3; //length of copper piece(in meter)
6 E=110*10^9; //surface energy
7 stress=276*10^6; //in Pa
8 dl=stress*l_o/E; //resultant elongation(in meter)
9 disp(dl*10^3, 'resultant elongation(in mm)=');
```

---

**Scilab code Exa 8.5** Compute the strain hardening exponent

```
1 //Exam:8.5
2 clc;
3 clear;
4 close;
5 T_stress=415; //True stress (in Megapascal)
6 T_strain=0.10; //True strain
7 K=1035; //(in Megapascal)
8 n=(log(T_stress)-log(K))/log(T_strain); //
9 disp(n, 'Strain hardening exponent for an alloy=')
```

---

# Chapter 9

## Alloys Systems Phase Diagrams and Phase Transformations

**Scilab code Exa 9.1** Find the percentage of proeutectoid ferrite

```
1 //Exam:9.1
2 clc;
3 clear;
4 close;
5 //Fulcrum is at 0.5% carbon
6 //from lever rule
7 Pro_f=((0.80-0.5)/(0.80-0.0))*100; // % Proeutectoid
    ferrite
8 Pea_f=100-Pro_f; // % Pearlite ferrite
9 disp(Pro_f ,'% Proeutectoid ferrite=');
10 disp(Pea_f ,'% Pearlite ferrite=');
```

---

**Scilab code Exa 9.2** Degrees of freedom of a system of two components

```
1 //Exam:9.2
2 clc;
```

```

3 clear;
4 close;
5 N=2;
6 C=2;
7 //F=C-P+N
8 P_1=1;
9 P_2=2;
10 P_3=3;
11 P_4=4;
12 F_1=C-P_1+N;
13 F_2=C-P_2+N;
14 F_3=C-P_3+N;
15 F_4=C-P_4+N;
16 disp(F_1,'Degrees of freedom for 1 phase=');
17 disp(F_2,'Degrees of freedom for 2 phases=');
18 disp(F_3,'Degrees of freedom for 3 phases=');
19 disp(F_4,'Degrees of freedom for 4 phases=');

```

---

**Scilab code Exa 9.3** Find the minimum number of components in the system

```

1 //Exam:9.3
2 clc;
3 clear;
4 close;
5 P=4; //Number of phases exhibit by a material
6 F=0; //Minimum degrees of freedom
7 //modified form of the phase rule F=C-P+1
8 C=F+P-1; //minimum number of components in the system
9 disp(C,'the minimum number of components in the
    system=')

```

---

# Chapter 10

## Heat Treatment

**Scilab code Exa 10.1** Determine the grain diameter of an ASTM Number 8

```
1 //Exam:10.1
2 clc;
3 clear;
4 close;
5 N=8; //ASTM grain size number
6 n=2^(N-1); //Number of grains per inch square at a
               magnification
7 N_1=n*100*100; //Number of grains per inch square
                   without magnification
8 N_2=N_1/(25.4)^2; //Number of grains per mm square
                   without magnification
9 A_a=1/(N_2); //Average area of each grain(in mm^2)
10 D=(A_a)^(1/2); //Average grain diameter(in mm)
11 disp(D, 'Average grain diameter(in mm)=')
```

---

# Chapter 11

## Deformation of Materials

**Scilab code Exa 11.1** Determine the value of critical resolved shear stress

```
1 //Exam:11.1
2 clc;
3 clear;
4 close;
5 h_1=1;
6 k_1=1;
7 l_1=1;
8 //Miller indices of slip plane
9 h_2=1;
10 k_2=-1;
11 l_2=1;
12 //Miller indices of stress plane
13 h_3=1;
14 k_3=1;
15 l_3=0;
16 //Miller indices of slip direction
17 A=(h_1*h_2+k_1*k_2+l_1*l_2)/(((h_1^2+k_1^2+l_1^2)
    ^^(1/2))*((h_2^2+k_2^2+l_2^2)^(1/2))); //Value of
    cos(x) where x =angle between slip plane and
    stress plane
18 B=(h_1*h_3+k_1*k_3+l_1*l_3)/(((h_1^2+k_1^2+l_1^2)
```

```


$$^{(1/2)} * ((h_3^2 + k_3^2 + l_3^2)^{(1/2)}) ; // Value of$$

cos(y) where y = angle between slip direction and
stress direction
19 C = (1 - A^2)^{(1/2)} ; // Value of sin(x)
20 stress = 3.5 ; // Applied Stress in MPa
21 T_cr = stress * A * B * C ; // Critical resolved shear stress (
    in MPa)
22 disp(T_cr, 'Critical resolved shear stress (in MPa)=')
;

```

---

### Scilab code Exa 11.3 Find the yield stress

```

1 //Exam:11.3
2 clc;
3 clear;
4 close;
5 D=0.002; //Grain diameter (in mm)
6 d=D*10^(-3); //Grain diameter (in m)
7 K=0.63; //Constant (in MNm^(-3/2))
8 sigma_i=80; //in MNm^-2
9 sigma_y=sigma_i+K*d^(-1/2); //Yield stress for a
    polycrystalline alloy
10 disp(sigma_y, 'Yield stress for a polycrystalline
    alloy (in MN/m^2)');

```

---

### Scilab code Exa 11.4 Find the yield stress

```

1 //Exam:11.4
2 clc;
3 clear;
4 close;
5 sigma_y1=120; //primary yield strength of
    polycrystalline material (in MN*m^-2)

```

```

6 sigma_y2=220; //increased yield strength of
    polycrystalline material(in MN*m^-2)
7 d_1=0.04*10^(-3); //primary grain diameter(in meter)
8 d_2=0.01*10^(-3); //grain diameter after decreasing(
    in meter)
9 //sigma_y1=sigma_i+K*(d_1)^(-1/2)
10 //sigma_y2=sigma_i+K*(d_2)^(-1/2)
11 //putting the values and solving the equation
12 K=(220-120)/((d_2^(-1/2))-((d_1^(-1/2)))); //constant
    (in MN*m(-3/2))
13 sigma_i=sigma_y1-K*(d_1)^(-1/2); //in MN*m^-2
14 d=1/((10^4)*(256/645))^(1/2); //grain diameter for
    grain size ASTM 9(in mm)
15 D=d*10^(-3); //grain diameter for grain size ASTM 9(
    in meter)
16 sigma_y=sigma_i+K*(D)^(-1/2); //Yield stress for a
    polycrystalline alloy for grain size ASTM 9(in MN
    *m^-2)
17 disp(ceil(sigma_y), 'Yield stress for a
    polycrystalline alloy for grain size ASTM 9(in MN
    *m^-2)= ');

```

---

# Chapter 12

## Oxidation and Corrosion

**Scilab code Exa 12.1** Find the distance at which magnesium anode capable of giving 2MA

```
1 //Exam:12.1
2 clc;
3 clear;
4 close;
5 D=320*10^-3; //in meter
6 L=1; //in meter
7 A=%pi*D*L; //Surface area in meter^2
8 l=ceil (200/A);
9 disp(l,'the distance at which magnisium anode
    capable of giving 2MA (in meters)=');
```

---

**Scilab code Exa 12.2** Quality of magnesium required per square meter of the hull surface

```
1 //Exam:12.2
2 clc;
3 clear;
```

```
4 close;
5 W=0.0243; //1 mole of magnesium weight (in Kg)
6 C=2*96490; //used charge (in A-s)
7 A=15*10^(-3); //current density (in A/metre2)
8 t=10; //time (in years)
9 T=10*365*24*3600; //time (in sec)
10 //amount of magnesium required =charge required per
    m2 of hull surface for a design life of 10 years
    /(used charge for anode)
11 Mg_required=W*A*T/C; //magnesium required per square
    meter of the hull surface for a design life of 10
    years
12 disp(Mg_required, 'magnesium required per square
    meter of the hull surface for a design life of 10
    years (in Kg/m2)=');
```

---

# Chapter 13

## Thermal and Optical Properties of Materials

**Scilab code Exa 13.1** Maximum temperature to which the rod may be heated without exceeding a compressive stress

```
1 //Exam:13.1
2 clc;
3 clear;
4 close;
5 alpha=20*10^(-6); //linear coefficient of thermal
                     expansion per C
6 Sigma=-(172); //compressive stress MPa
7 T=20; //Temprature at which rod is stress free(in C
         )
8 E=100*10^3; //modulus of elasticity (in MPa)
9 T_f=T-(Sigma/(alpha*E)); //maximum temperature the
                           rod may be heated without exceeding a compressive
                           stress of 172 MPa
10 disp(T_f, 'maximum temperature(in C) the rod may be
          heated without exceeding a compressive stress of
          172 MPa=');
```

---

# Chapter 14

## Electrical and Magnetic Properties of Materials

**Scilab code Exa 14.1** Calculate the resistance of an aluminium wire

```
1 //Exam:14.1
2 clc;
3 clear;
4 close;
5 l=100; //length of wire
6 p=2.66*10^(-8); //resistivity
7 A=3*10^(-6); //cross sectional area
8 R=p*l/A; //resistance of an aluminium wire
9 disp(R,'resistance of an aluminium wire(in Ohm)=');
```

---

**Scilab code Exa 14.2** Resistivity of a copper alloy containing 1 atomic percent nickel and 3 atomic percent silver

```
1 //Exam:14.2
2 clc;
3 clear;
```

```

4 close;
5 R_Cu=1.56; // Resistivity of pure copper (in micro-ohm-
cm)
6 R_CuNi = 4.06; // Resistivity of Cu containing two
atomic percent (in micro-ohm-cm)
7 R_Ni=(R_CuNi-R_Cu)/2; // Increase in resistivity due
to one atomic % Ni
8 R_CuAg= 1.7; // resistivity of copper , containing one
atomic percent silver (in micro-ohm-cm)
9 R_Ag=R_CuAg-R_Cu; // Increase in resistivity due to
one atomic % Ag
10 R_CuNiAg=R_Cu+R_Ni+3*R_Ag; // Resistivity of copper
alloy containing one atomic percent Ni and 3
atomic percent Ag
11 disp(R_CuNiAg,' Resistivity of copper alloy
containing one atomic percent Ni and 3 atomic
percent Ag(in micro-ohm-cm)=')

```

---

**Scilab code Exa 14.3** Find the resistivity due to impurity scattering per percent of Ni in the Cu lattice

```

1 //Exam:14.3
2 clc;
3 clear;
4 close;
5 R_Cu=1.8*10^(-8); // resistivity of pure copper at
room temperature
6 R_CuNi=7*10^(-8); // resistivity of Cu 4% Ni alloy at
room temperature
7 R_Ni=(R_CuNi-R_Cu)/4; // resistivity due to Impurity
scattering per % of Ni
8 disp(R_Ni,' resistivity due to impurity scattering
per percent of Ni in the Cu lattice (in ohm-meter)
= ')

```

---

**Scilab code Exa 14.4** Calculate the relative dielectric constant of a barium titanate crystal

```
1 //Exam:14.4
2 clc;
3 clear;
4 close;
5 C=10^(-9); //capacitance (in F)
6 d=2*10^(-3); //distance of separation in a parallel
    plate condenser
7 E_o=8.854*10^(-12); //dielectric constant
8 A=(10*10^(-3))*(10*10^(-3)); //area of parallel plate
    condenser
9 //C=E_o*E_r*A/d
10 E_r=C*d/(E_o*A); //Relative dielectric constant
11 disp(ceil(E_r), 'Relative dielectric constant of a
    barium titanate crystal')
```

---

**Scilab code Exa 14.5** Calculate the polarization

```
1 //Exam:14.5
2 clc;
3 clear;
4 close;
5 q=1.6*10^(-19); //charge (in C)
6 d_1=0.06 //shift of the titanium ion from the body
    centre (in )
7 d_2=0.08 //shift of the oxygen anions of the side
    faces (in )
8 d_3=0.06 //shift of the oxygen anions of the top and
    bottom face (in )
```

```

9 D_1=d_1*10^(-10); // shift of the titanium ion from
the body centre (in m)
10 D_2=d_2*10^(-10); // shift of the oxygen anions of the
side faces (in m)
11 D_3=d_3*10^(-10); // shift of the oxygen anions of the
top and bottom face (in m)
12 U_1=4*q*D_1; // dipole moment due to two O2 ions on
the four side faces (in C-m)
13 U_2=2*q*D_2; // dipole moment due to one O2 on top
and bottom (in C-m)
14 U_3=4*q*D_3; // dipole moment due to one Ti4+ ion at
body centre (in C-m)
15 U=U_1+U_2+U_3; // Total dipole moment (in C-m)
16 V=4.03*((3.98)2)*10^(-30); // volume (in m3)
17 P=U/V; // polarization the total dipole moments per
unit volume
18 disp(P, 'polarization (in C/m2)=');
19 disp(U, '==')

```

---

**Scilab code Exa 14.6** Find net magnetic moment per iron atom in the crystal

```

1 //Exam:14.6
2 clc;
3 clear;
4 close;
5 V=((2.87)3)*10^(-30) //Volume of unit cell of BCC
iron (in m3)
6 N=2 //Number of atoms in the unit cell
7 M=1750*103; //saturation magnetization of BCC Iron A
/m
8 M_Net=V*M*(1/N) //net magnetic moment per atom
9 Bohr_magneton=9.273*10^(-24); //Bohr_magneton (
magnetic moment) in A/m2
10 M_moment=M_Net/Bohr_magneton; //The magnetic moment (

```

```
    in units of U_B)
11 disp(M_moment,'The magnetic moment (in units of U_B)
=');
```

---

**Scilab code Exa 14.7** Calculate the saturation magnetization and the saturation flux density

```
1 //Exam:14.7
2 clc;
3 clear;
4 close;
5 p=8.90*10^6; //density of nickel in gm/m3.
6 N_A=6.023*10^23; //Avogadro's number atoms/mol
7 At_w=58.71; //Atomic weight of Ni in gm/mol
8 N=p*N_A/At_w; //number of atoms/m3
9 U_B=9.273*10^(-24); //Bohr_magneton
10 M_s=0.60*U_B*N; //saturation magnetization
11 pi=22/7;
12 U_o=4*pi*10^(-7); //magnetic constant
13 B_s=U_o*M_s; //Saturation flux density
14 disp(M_s,'the saturation magnetization=');
15 disp(B_s,'Saturation flux density=');
```

---

**Scilab code Exa 14.8** Calculate the saturation magnetization

```
1 //Exam:14.8
2 clc;
3 clear;
4 close;
5 //Each cubic unit cell of ferrous ferric oxide
//contains 8 Fe2+ and 16 Fe3+ ions and
6 n_b=32; //
7 U_B=9.273*10^(-24); //Bohr_magneton
```

```
8 a=0.839*10^(-9); //the unit cell edge length in m
9 V=a^3; //volume(in m3)
10 M_s=n_b*U_B/V; //the saturation magnetization
11 disp(M_s,'the saturation magnetization=');
```

---

**Scilab code Exa 14.9** Calculate eddy current loss at the normal voltage and frequency

```
1 //Exam:14.9
2 clc;
3 clear;
4 close;
5 //hysteresis loss (Ph) and the induced emf loss (Pe)
//are proportional to the frequency
6 //Pe is proportional to the square of the induced
//emf (Pe)
7 //Pe + Ph = 750 W (at 25 Hz)
8 //4Pe + 2Ph = 2300 W(at 50Hz)
9 //solving equation
10 P_e=800/2; //induced emf loss
11 I_d=4*P_e; //The eddy current loss at the normal
//voltage and frequency
12 disp(I_d,'The eddy current loss at the normal
//voltage and frequency (in W)=');
```

---

# Chapter 15

## Semiconductors

**Scilab code Exa 15.1** Find the conductivity and resistivity of a pure silicon crystal

```
1 //Exam:15.1
2 clc;
3 clear;
4 close;
5 U_n=1350 // mobility of electron in cm2/volt-sec
6 U_h=480 // hole mobility in cm2/volt-sec
7 Sigma=1.072*1010 //density of electron hole pair per
cc at 300 K for a pure silicon crystal
8 e=1.6*10-19; //charge on the electron in C
9 Sigma_i=Sigma*e*(U_n+U_h); //Conductivity of pure
silicon crystal
10 p_i=1/(Sigma_i); //Resistivity of silicon crystal in
Ohm-cm
11 P_i=p_i*10-2; //Resistivity of silicon crystal in
Ohm-m
12 disp(Sigma_i,'Conductivity of pure silicon crystal(
in mho/cm)=');
13 disp(P_i,'Resistivity of silicon crystal (in Ohm-m)=
');
```

---

**Scilab code Exa 15.2** Find the resistivity at room temperature

```
1 //Exam:15.2
2 clc;
3 clear;
4 close;
5 U=1200; //electron mobility in cm2/Volt-sec
6 e=1.6*10^(-19); //charge on the electron in C
7 n=10^13; //concentration of phosphorus
8 sigma=U*e*n; //conductivity of crystal in mho/cm
9 p_i=1/sigma; //resistivity of silicon wafer if all
    donor atom are active
10 disp(p_i,'resistivity of silicon wafer if all donor
    atom are active(in ohm-cm)=');
```

---

**Scilab code Exa 15.3** Find the resistance of an intrinsic germanium rod

```
1 //Exam:15.3
2 clc;
3 clear;
4 close;
5 U_n=3900 //mobility of electron in cm2/volt-sec
6 U_h=1900 //hole mobility in cm2/volt-sec
7 n_i=2.5*10^13; //concentration of electron
8 u_n=U_n*10^(-4); //mobility of electron in m2/volt-
    sec
9 u_h=U_h*10^(-4); //hole mobility in m2/volt-sec
10 e=1.6*10^(-19); //charge on the electron in C
11 Sigma_i=n_i*e*(u_n+u_h)*10^6; //Conductivity
12 p_i=1/(Sigma_i); //resistivity of intrinsic germanium
    rod
13 l=1*10^(-2); //length of germanium rod in m
```

```
14 w=1*10^(-3); //width of germanium rod in m
15 t=1*10^(-3); //thick of germanium rod in m
16 A=w*t; //Area of cross section in m2
17 R=p_i*1/A; //Resistance of an intrinsic germanium rod
    in Ohm
18 disp(R/10^3, 'Resistance of an intrinsic germanium
    rod (in K-Ohm)=');
```

---

**Scilab code Exa 15.4** Obtain density relation in P type material

```
1 //Exam:15.4
2 clc;
3 clear;
4 close;
5 N_a=1.1*10^20; //acceptor density in atoms/m3
6 n_i=2.5*10^19; //concentration of majority carrier
    per m3
7 n_p=(n_i^2)/N_a; //intrinsic density
8 R=n_p/n_i; //Ratio of n_p and n_i
9 disp(R, 'n_p/n_i=');
```

---

# Chapter 16

## Superconductivity and Superconducting Materials

**Scilab code Exa 16.1** Energy gap in electron volts and Calculate the wavelength of a photon

```
1 //Exam:16.1
2 clc;
3 clear;
4 close;
5 T_c=4.2; // critical temperature of mercury
6 k=1.4*10^(-23); //
7 E_g=3*k*T_c; //energy gap (in Joule)
8 e=1.6*10^(-19); //charge on the electron
9 E=E_g/e; //energy gap (in electron volt)
10 h=6.6*10^(-34) // in J-s
11 c=3*10^8; //in m/s
12 wavelength=h*c/E_g; //wavelength of a photon (in m)
13 disp(E,'energy gap (in electron volt)=');
14 disp(wavelength,'wavelength of a photon (in m)=');
```

---

# Chapter 18

## Composites

**Scilab code Exa 18.1** Calculate the modulus of elasticity

```
1 //Exam:18.1
2 clc;
3 clear;
4 close;
5 E_f=69; //modulus of elasticity in GPa
6 V_f=40/100; //Volume of glass fibres %
7 E_m=3.4; //modulus (in GPa)
8 V_m=60/100; //Volume of polyester resin %
9 E_cl=E_m*V_m+E_f*V_f; //modulus of elasticity (in Gpa
    )
10 disp(ceil(E_cl), 'modulus of elasticity (in Gpa)=');
```

---

**Scilab code Exa 18.2** Elastic modulus when the stress is applied perpendicular to the direction of the fibre alignment

```
1 //Exam:18.2
2 clc;
3 clear;
```

```
4 close;
5 E_f=69; //modulus of elasticity in GPa
6 V_f=40/100; //Volume of glass fibres %
7 E_m=3.4; //modulus (in GPa)
8 V_m=60/100; //Volume of polyester resin %
9 E_cl=E_m*E_f/(E_m*V_f+E_f*V_m); //modulus of
    elasticity when the stress is applied
    perpendicular to the direction of the fibre
    alignment(in Gpa)
10 disp(E_cl,'modulus of elasticity when the stress is
    applied perpendicular to the direction of the
    fibre alignment(in Gpa)=');
```

---