MAE 212-SP 01
HW 6 SOLUTIONS

1.

$$\frac{C_s - C_x}{C_s - C_0} = \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \quad (*)$$

$C_s = 0.90\%$ $\quad x = 0.5 \text{ mm} = 5.0 \times 10^{-4} \text{ m}$

$C_0 = 0.20\%$ $\quad D_{927°C} = 1.28 \times 10^{-11} \text{ m}^2/\text{s}$

$C_x = 0.40\%$ $\quad t = ? \text{ s}$

Substituting the above values in Eq. (*) gives

$$\frac{0.90 - 0.40}{0.90 - 0.20} = \text{erf}\left[\frac{5.0 \times 10^{-4} \text{ m}}{2\sqrt{(1.28 \times 10^{-11} \text{ m}^2/\text{s})(t)}}\right]$$

$$\frac{0.50}{0.70} = \text{erf}\left(\frac{69.88}{\sqrt{t}}\right) = 0.7143$$

Let $\quad Z = \frac{69.88}{\sqrt{t}}$ $\quad$ then $\quad \text{erf } Z = 0.7143$

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We need a number Z whose error function (erf) is 0.7143 From Table 5.1 of the text we find this number by interpolation (see below) to be 0.755:

erf Z	Z
0.7112	0.75
0.7143	x
0.7421	0.80

$$\frac{0.7143 - 0.7112}{0.7421 - 0.7112} = \frac{x - 0.75}{0.80 - 0.75}$$

$$x - 0.75 = (0.1003)(0.05)$$

$$x = 0.75 + 0.005 = 0.755$$

Thus

$$Z = \frac{69.88}{\sqrt{t}} = 0.755$$

$$\sqrt{t} = \frac{69.88}{0.755} = 92.6$$

$$t = 8567 \text{ s} = 143 \text{ min} \blacktriangleleft$$

2.

$$D_{927^\circ C} = 1.28 \times 10^{-11} \text{ m}^2/\text{s}$$

$$\frac{C_s - C_x}{C_s - C_0} = \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$C_s = 0.90\%$ $\quad x = 0.50 \text{ mm} = 5.0 \times 10^{-4} \text{ m}$

$C_0 = 0.20\%$ $\quad D_{927^\circ C} = 1.28 \times 10^{-11} \text{ m}^2/\text{s}$

$C_x = ?\%$ $\quad t = 5 \text{ h} = 5 \text{ h} \times 3600 \text{ s/h} = 1.8 \times 10^4 \text{ s}$

$$\frac{0.90 - C_x}{0.90 - 0.20} = \text{erf}\left[\frac{5.0 \times 10^{-4} \text{ m}}{2\sqrt{(1.28 \times 10^{-11} \text{ m/s})(1.8 \times 10^4 \text{ s})}}\right]$$

$$\frac{0.90 - C_x}{0.70} = \text{erf } 0.521$$

Let $Z = 0.521$. We need to know what the corresponding error function for the Z value of 0.521 is. To determine this number from Table 4.1, we must interpolate the data as shown in the accompanying table.

Z	erf Z
0.500	0.5205
0.521	x
0.550	0.5633

$$\frac{0.521 - 0.500}{0.550 - 0.500} = \frac{x - 0.5205}{0.5633 - 0.5205}$$

$$0.42 = \frac{x - 0.5205}{0.0428}$$

$$x - 0.5205 = (0.42)(0.0428)$$

$$x = 0.0180 + 0.5205$$

$$= 0.538$$

Therefore

$$\frac{0.90 - C_x}{0.70} = \text{erf } 0.521 = 0.538$$

$$C_x = 0.90 - (0.70)(0.538)$$

$$= 0.52\% \blacktriangleleft$$

2

3 Using $D = D_0 e^{-Q/RT}$,

$T_2 = 1000°C + 273 = 1273$ K

$T_1 = 500°C + 273 = 773$ K

and $R = 8.314$ J/(mol K)

$$\frac{D_{1000°C}}{D_{500°C}} = \frac{\exp(-Q/RT_2)}{\exp(-Q/RT_1)} = \exp\left[-\frac{Q}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)\right]$$

$$\frac{7.0 \times 10^{-13}}{1.0 \times 10^{-17}} = \exp\left\{-\frac{Q}{R}\left[\left(\frac{1}{1273\text{ K}} - \frac{1}{773\text{ K}}\right)\right]\right\}$$

$$\ln(7.0 \times 10^4) = -\frac{Q}{R}(7.855 \times 10^{-4} - 12.94 \times 10^{-4}) = \frac{Q}{8.314}(5.08 \times 10^{-4})$$

$$11.16 = Q(6.11 \times 10^{-5})$$

$$Q = 183{,}000 \text{ J/mol} = 183 \text{ kJ/mol} ◀$$

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$$D_{1100°C} = 7.0 \times 10^{-17} \text{ m}^2/\text{s}$$

$$\frac{C_s - C_x}{C_s - C_0} = \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \quad (*)$$

$C_s = 10^{24}$ atoms/m³ $\quad x = ?$m (depth at which $C_x = 10^{22}$ atoms/m³)

$C_x = 10^{22}$ atoms/m³ $\quad D_{1100°C} = 7.0 \times 10^{-17}$ m²/s

$C_0 = 0$ atoms/m³ $\quad t = 3 \text{ h} = 3 \text{ h} \times 3600 \text{ s/h} = 1.08 \times 10^4$ s

Substituting the above values into Eq. (*) gives

$$\frac{10^{24} - 10^{22}}{10^{24} - 0} = \text{erf}\left[\frac{x\text{ m}}{2\sqrt{(7.0 \times 10^{-17} \text{ m}^2/\text{s})(1.08 \times 10^4 \text{ s})}}\right]$$

$$1 - 0.01 = \text{erf}\left(\frac{x\text{ m}}{1.74 \times 10^{-6}\text{ m}}\right) = 0.99$$

Let $\quad Z = \dfrac{x}{1.74 \times 10^{-6}\text{ m}}$

Thus $\quad \text{erf } Z = 0.99 \quad$ and $\quad Z = 1.82$

(from Table 4.1 using interpolation). Therefore

$$x = (Z)(1.74 \times 10^{-6}\text{ m}) = (1.82)(1.74 \times 10^{-6}\text{ m})$$

$$= 3.17 \times 10^{-6}\text{ m} ◀$$

Note: Typical diffusion depths in silicon wafers are of the order of a few micrometers (i.e., about 10^{-6} m), while the wafer is usually several hundred micrometers thick.

5.

Derive expressions for the Burger's vectors in terms of the lattice parameter, a, for FCC and BCC materials For copper (an FCC material with $a = 0\ 1278$ nm) calculate the magnitude and direction of the Burger's vector

A Burgers vector is defined on a slip plane in a slip direction (see class notes).

- FCC Crystal
  Slip directions: $< \bar{1}10 >$, which are the directions of Burgers vectors
  Magnitude: $b = 2r$ and from sketch, $4b^2 = a^2 + a^2$, thus $b = \frac{a}{\sqrt{2}}$.
  Unit vector in $< \bar{1}10 >$ direction: $\frac{<\bar{1}10>}{\sqrt{2}}$.
  Thus $\boxed{\mathbf{b} = \pm\frac{a}{2} < \bar{1}10 >}$
- BCC Crystal
  Slip directions: $< 111 >$ which are the directions of the Burgers vectors
  Magnitude. Still $b = 2r$, but $4b^2 = 2a^2 + a^2 \Rightarrow b = \frac{\sqrt{3}}{2}a$
  Unit vector in $< 111 >$ direction: $\frac{<111>}{\sqrt{3}}$

  Thus: $\boxed{\mathbf{b} = \pm\frac{a}{2} < 111 >}$

  Application. Copper, FCC crystal, $a = 0.1278$ nm.
  Magnitude: $b = \frac{a}{\sqrt{2}} = 0.0904$ nm
  Direction: $< \bar{1}10 >$
  $\mathbf{b} = \pm 0.0639 < \bar{1}10 >$

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A molybdenum (Mo) crystal has a Burger's vector of length 0 272 nm If the lattice parameter, a, of Mo is 0 314 nm, determine its crystal structure (i e. FCC, BCC or HCP ?)

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From Exercise 1:

FCC . $b = \frac{a}{\sqrt{2}}$
BCC . $b = \frac{\sqrt{3}}{2}a$

Let us calculate $\frac{b}{a}$ for a molybdenum: $\frac{b}{a} = \frac{0\ 272}{0\ 314} = 0\ 866$.

Hence, $\boxed{\text{molybdenum is a BCC crystal}}$

$\underline{\underline{7}}$

(a) For a BCC metal,

$$\sqrt{3}\,a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{3}} R$$

$$\left.\begin{array}{l} |b|_{110} = \sqrt{2}\,a = \sqrt{2}\,\frac{4}{\sqrt{3}}\,R \\ \text{But } |b|_{111} = 2R \end{array}\right\} \Rightarrow$$

$$|b|_{110} = \sqrt{\frac{2}{3}}\;2\,|b|_{111} \quad \text{or} \quad \frac{|b|_{110}}{|b|_{111}} = 2\sqrt{\frac{2}{3}}$$

Finally: $\left(\frac{|b|_{110}}{|b|_{111}}\right)^2 = 4\,\frac{2}{3} = \underline{\underline{2.67}}$

(b) $|b|_{100} = a = \frac{4R}{\sqrt{3}} = \frac{2\,|b|_{111}}{\sqrt{3}}$ or

$$\frac{|b|_{100}}{|b|_{111}} = \frac{2}{\sqrt{3}}$$

Finally: $\left(\frac{|b|_{100}}{|b|_{111}}\right)^2 = \frac{4}{3} \approx \underline{\underline{1.33}}$

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8 $a[110] \rightarrow \frac{a}{2}[111] + \frac{a}{2}[11\bar{1}]$

For the above reaction to take place, the energy of the $a\langle 110\rangle$ dislocation must be greater than the sum of the energies of the two $\frac{a}{2}\langle 111\rangle$ dislocations. Since the energy of a dislocation is proportional to b^2, we require:

$$a^2[1^2+1^2+0^2] > 2\left(\frac{a^2}{4}[1^2+1^2+1^2]\right)$$

or

$$2a^2 > \frac{3}{2}a^2$$

The reaction is therefore energetically favorable.

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9 You are designing a turbine engine part made of an FCC single crystal. By using the Schmid law, determine the τ_c necessary for the part to have a uniaxial yield strength of 200 MPa in the [331] crystallographic direction?

Let us determine the Schmid factor of a FCC crystal pulled in the [331] direction.

Slip Systems		(111) $[\bar{1}10]$	(111) $[0\bar{1}1]$	(111) $[10\bar{1}]$	$(\bar{1}11)$ $[110]$	$(\bar{1}11)$ $[01\bar{1}]$	$(\bar{1}11)$ $[101]$	$(1\bar{1}1)$ $[110]$	$(1\bar{1}1)$ $[011]$	$(1\bar{1}1)$ $[10\bar{1}]$	$(\bar{1}\bar{1}1)$ $[1\bar{1}0]$	$(\bar{1}\bar{1}1)$ $[011]$	$(\bar{1}\bar{1}1)$ $[101]$
Tensile	$\cos\phi$	$\frac{7}{\sqrt{57}}$	$\frac{7}{\sqrt{57}}$	$\frac{7}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{-5}{\sqrt{57}}$	$\frac{-5}{\sqrt{57}}$	$\frac{-5}{\sqrt{57}}$
Axis	$\cos\lambda$	0	$\frac{-2}{\sqrt{38}}$	$\frac{2}{\sqrt{38}}$	$\frac{6}{\sqrt{38}}$	$\frac{2}{\sqrt{38}}$	$\frac{4}{\sqrt{38}}$	$\frac{6}{\sqrt{38}}$	$\frac{4}{\sqrt{38}}$	$\frac{2}{\sqrt{38}}$	0	$\frac{4}{\sqrt{38}}$	$\frac{4}{\sqrt{38}}$
[331]	M	0	$\frac{-14}{19\sqrt{6}}$	$\frac{14}{19\sqrt{6}}$	$\frac{6}{19\sqrt{6}}$	$\frac{2}{19\sqrt{6}}$	$\frac{4}{19\sqrt{6}}$	$\frac{6}{19\sqrt{6}}$	$\frac{4}{19\sqrt{6}}$	$\frac{2}{19\sqrt{6}}$	0	$\frac{-20}{19\sqrt{6}}$	$\frac{-20}{19\sqrt{6}}$

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The Schmid factor is thus $\frac{20}{19\sqrt{6}}$ (tensile test in [331] direction).

So $\boxed{\tau_c = MY = \frac{20}{19\sqrt{6}} \times 200 = 86 \text{ MPa}}$