Lecture 10-14:

Crystal defects in metals: vacancy, interstitial, substitutional, free energy of mixing, dislocation (elementary concepts only), edge / screw dislocation, partial dislocation, stacking fault, dislocation lock, dislocation pile up, Hall Petch relation, grain boundary structure

Questions:

1. FCC crystals have more packing density than BCC crystal yet why solubility of carbon in FCC form of iron is higher than in its BBC form?
2. What is the effect of temperature on concentration of vacancy?
3. If the ratio of iron ions to oxygen ions is 0.994 in FeO, what fraction of Fe sites are filled with Fe^{3+} ions? What is the ratio of Fe^{3+} to O^{2-} ions?
4. What are the major differences between an edge & screw dislocation? Which of these can cross slip?
5. There is a dislocation lying along $[\bar{1}01]$ in a fcc crystal. Its Burgers vector is $\frac{a}{2}[0\bar{1}1]$. What type of dislocation is it? Determine its slip plane.
6. Find out the ratio of elastic stored energy of an edge dislocation to that of a screw. Assume energy of the core to be negligible.
7. What is the hydrostatic stress (or strain) field around a screw dislocation?
8. What is the hydrostatic stress field of an edge dislocation?
9. Assume that dislocations are arranged in an array in three dimensions described as a cubic lattice. If average number of dislocations intersecting a plane is ρ /unit area show that the average distance between two dislocations is proportional to √ (1/ρ).
10. Dislocation density of annealed metal is $10^{12}\ m^{-2}$. Find out elastic stored energy per unit volume.
11. Elastic stored energy / unit length of an edge dislocation is given by $E^e = \frac{Gb^2}{4\pi(1-\nu)} ln\left(\frac{r}{r_0}\right)$. Does this mean it can approach infinity as r becomes very large?
12. What is the difference between a kink and a jog? An edge dislocation crosses another dislocation which is perpendicular to the slip plane. Show with neat diagram the effect of such an interaction.
13. A perfect dislocation moving on plane $(11\bar{1})$interacts with another moving on$(1\bar{1}\bar{1})$. What are the different reactions possible? Which of these are Lomer locks?
14. On what planes can a screw dislocation having Burgers vector $\frac{a}{2}[111]$could move in a BCC crystal? What will be the slip plane if it were an edge dislocation?
15. An fcc crystal is pulled along [123]. What is the possible combination of glide plane & direction? Estimate the force on the mobile dislocation if applied tensile stress is 100MPa & lattice parameter = 0.36nm.
16. What is the force acting on a dislocation ***b*** [010] lying along [100] if the applied stress is given by$\begin{bmatrix} 0 & 0 & 0 \\ 0 & \sigma_{22} & 0 \\ 0 & 0 & 0 \end{bmatrix}$? Will this help it to glide?

17. An edge dislocation moving on a crystal plane stops at an obstacle. A second dislocation having the same Burgers vector & lying on the same plane approaches the same on application of a shear stress of magnitude 140MPa. Estimate the distance of separation if E = 210GPa, Poisson ratio = 0.3 & lattice parameter = 0.362nm. What will be the distance between the two if they were screw dislocation?

18. A dislocation is pinned between two obstacles spaced 1micron apart. What will be the magnitude of stress to bow the dislocation into a semi circle? Hence estimate its yield strength. Given G = 100 GPa, Burgers vector = 0.25nm

19. Nickel sheet is being rolled at room temperature in a rolling mill (diameter = 50cm, rpm = 200). Initial thickness is 20mm and thickness after rolling 10mm. Estimate average strain rate, energy that will be stored in material if final dislocation density is $10^{11}/cm^2$, total energy / unit volume spent during rolling (assume flow stress = 300MPa), adiabatic temperature rise if specific heat = 0.49J/g/K

20. Iron (a = 0.286nm and G = 70GPa) is deformed to a shear strain of 0.3. What distance a dislocation could move, if dislocation density remains constant at 10^{14} /m^2? What will be the average dislocation velocity if strain rate is 10^{-2} /s? Estimate its shear strength.

21. Polycrystalline aluminum with average grain size of 10micron is subjected to shear stress of 50MPa. If a dislocation source located at the centre of a grain emits dislocations which pile up at the boundary what is the stress it would experience? (G=70GPa, b=0.3nm)

22. Estimate the distance between dislocations in a tilt boundary of alumunium if the misorientation angle is 5^o. Given lattice parameter of Al = 0.405nm. Crystal structure is fcc.

23. A more precise expression for low energy grain biundary is given by $E = \frac{Gb}{4\pi(1-\nu)}\theta(A - ln\theta)$ where A is an constant. This is valid over the range 0 < θ < 10^o. Find a reasonable estimate of A. Given lattice parameter of Ni (fcc) = 0.35nm, G = 76MPa Poisson ratio = 0.3 (Hint: assume dislocation core radius as 5b & the minimum distance between dislocation to be twice this. The doslocation core energy $= \frac{Gb^2}{10}$)

24. Estimate the dislocation spacing and energy of a low angle boundary in copper crystal (fcc b = 0.25nm) if tilt angle = 1^o. Given G = 48MPa & ν = 0.3

25. Use the expression given in problem 2 to find our the tilt angle (θ_{max})at which enegry of the low angle boundary is maximum. Hence show that $\frac{E}{E_{max}} = \frac{\theta}{\theta_{max}}\left(1 - ln\frac{\theta}{\theta_{max}}\right)$

26. Estimate the energy of the free surface of polycrystalline copper from its heat of sublimation. Does this vary from grain to grain? Given L_s = 338 kJ/mole; a = 0.36 nm

Answer:

1. FCC has the maximum packing density (74%). However the interstitial sites where the carbon atoms are located are larger than those in BCC structure. Packing density in BCC is relatively low (68%). However there is more number of interstitial sites for every Fe atom. The gaps are distributed amongst more number of sites. Therefore these are too small to accommodate carbon atoms. This is why solubility is low.

2. The fraction of vacant lattice sites in a crystal is given by $\frac{n_v}{n} = exp\left(-\frac{q_v}{kT}\right)$ where k is Boltzmann constant, q_v is the energy needed to create a vacancy and T is the temperature in degree Absolute. As the T increases $\frac{n_v}{n}$ too increases.

3. Ionic crystals must maintain charge neutrality. In this iron oxide fraction of vacant Fe^{2+} sites = 1-0.994 = 0.006. The reason that stoichiometry is not maintained indicates that for every O^{2-} vacancy there are 2 Fe^{3+} ions. Thus fraction of vacant O^{2-} sites = 0.003. Note that to maintain charge neutrality there could have been 0.006 vacant O^{2-} sites. In that event stoichiometry would have been FeO.

4.

Nature	Edge	Screw
Burgers vector	Perpendicular to dislocation	Parallel to dislocation
Slip plane	The plane containing both Burgers vector & the dislocation	Any plane containing the dislocation
Cross slip	Not possible	Possible
Climb	Can climb	Cannot climb
Atomic arrangements around dislocation	There is an extra plane of atoms above slip plane	Atoms along the dislocation are arranged in a helix like a screw

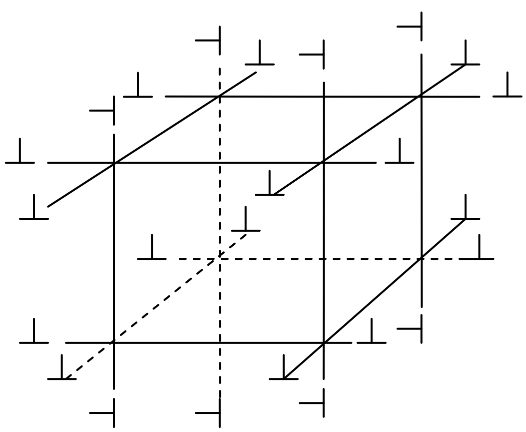
5. Dislocation: [t1 t2 t3] = $[\bar{1}01]$ & Burgers vector [b1 b2 b3] = $\frac{a}{2}[0\bar{1}1]$. Since b does not lie along t it is not a screw dislocation. The angle between the two is given by $cos\theta = \frac{t_1b_1+t_2b_2+t_3b_3}{\sqrt{t_1^2+t_2^2+t_3^2}\sqrt{b_1^2+b_2^2+b_3^2}} = \frac{0+0+1}{\sqrt{2}\sqrt{2}}$ = ½. Since θ = 60˚ it a mixed dislocation. It can move only in a plane containing both t & b. If the indices of the plane is (hkl) then: $t_1h + t_2k + t_3l = 0$ & $b_1h + b_2k + b_3l = 0$. Therefore –h+l = 0 & -k+l = 0; or h = k= l Therefore slip plane is (111)

6. Energy of an edge dislocation of unit length: $E^e = \frac{Gb^2}{4\pi(1-\nu)} ln\left(\frac{r}{r_0}\right)$ & that of a screw dislocation: $E^s = \frac{Gb^2}{4\pi} ln\left(\frac{r}{r_0}\right)$ Therefore $\frac{E^e}{E^s} = \frac{1}{1-\nu}$ Most metal ν = 1/3. Therefore energy of an edge dislocation is 3/2 time that of a screw dislocation.

7. Hydrostatic stress: $\bar{\sigma} = \frac{\sigma_{11}+\sigma_{22}+\sigma_{33}}{3}$ Each of three terms is zero for a screw dislocation. $\bar{\sigma} = 0$

8. Hydrostatic stress: $\bar{\sigma} = \frac{\sigma_{11}+\sigma_{22}+\sigma_{33}}{3}$ Since $\sigma_{33} = \nu(\sigma_{11}+\sigma_{22})$, $\bar{\sigma} = \frac{1+\nu}{3}(\sigma_{11}+\sigma_{22})$ for an edge dislocation: $\sigma_{11} = -\frac{Gb}{2\pi(1-\nu)}\frac{x_2(3x_1^2+x_2^2)}{(x_1^2+x_2^2)^2}$ & $\sigma_{22} = \frac{Gb}{2\pi(1-\nu)}\frac{x_2(x_1^2-x_2^2)}{(x_1^2+x_2^2)^2}$ Thus: $\bar{\sigma} = -\frac{Gb(1+\nu)}{3\pi(1-\nu)}\frac{x_2}{(x_1^2+x_2^2)}$ The nature of stress is compressive above the slip plane. This is why the atoms are more closely placed above the slip plane.

9. Let L represents edge of a cube and each of these represent a dislocation line of length L. Repeated array of such a cube would represent a net work of dislocation. This is schematically shown as follows:



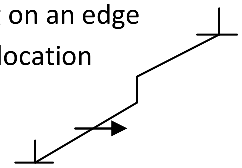
Volume of cube = L^3 Since each edge denotes dislocation of length L the total length of dislocation within the cube = 12 L / 4. This is because each edge belongs to 4 adjacent cubes. Therefore dislocation density ρ = total length of dislocation / volume of cube =3L/L^3. Or; $L = \sqrt{\frac{3}{\rho}}$. Therefore the distance between two dislocation is inversely proportional to the square root of dislocation density.

10. Previous problem shows that the average distance between two dislocation = L. The stress field of a dislocation can be assumed to extend over a distance = L/2. Or;$R = \frac{L}{2} = \sqrt{\frac{3}{4\rho}} = 0.86\rho^{-0.5}$ which is approximately: $\approx \frac{1}{\sqrt{\rho}}$ Energy of a dislocation consists of two parts. U = U_{core} + U_{strain} & $U_{core} = \frac{Gb^2}{10}$ The strain energy = $\frac{Gb^2(1-\nu\cos^2\alpha)}{4\pi(1-\nu)} ln\frac{R}{r_0}$ where α represents angle between dislocation and Burgers vector. For edge dislocation α = π/2 whereas for screw α=0. To estimate energy of a dislocation let us assume b=0.25nm and r_0 = 5b and R = $\rho^{-0.05}$ = 10^{-6} Therefore $U = \frac{Gb^2}{10} + \frac{Gb^2}{4\pi} ln\frac{10^{-6}}{5\times0.25\times10^{-9}} = Gb^2\left(\frac{1}{10}+\frac{1}{4\pi}ln800\right) = 0.63Gb^2 \approx 0.5Gb^2$. Assume G=50GPa Energy / unit length of dislocation = $0.5 \times 50 \times 10^9 \times 0.0625 \times 10^{-18}$ J/m^2 = 1.56 x 10^{-9} J/m Therefore elastic stored energy / unit volume = Uρ = 1.56 x 10^{-9} x 10^{12} = 1.56 kJ/m^3

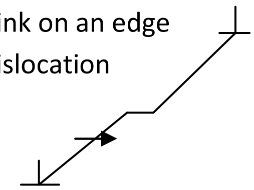
11. No. Because dislocations do not occur in isolation. If the average distance between dislocations is L average value of r = 0.5L. Therefore energy of dislocations is always finite. Approximately this is equal to 0.5 Gb^2.

12. Both kink & jog represent a step on the dislocation. The kink can glide on the slip plane of the parent dislocation. However its direction of motion is different. Glide plane of a jog is different from that of the parent dislocation.

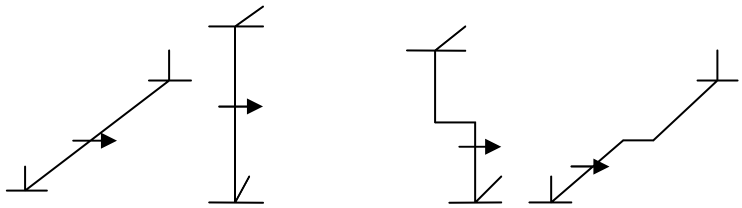
Jog on an edge dislocation



Kink on an edge dislocation



Note the jog is also an edge dislocation. Its slip plane is perpendicular to the glide plane of parent dislocation. The kink is a screw dislocation. Its direction of motion is along the length of the dislocation.



Here kinks are created on both. These have screw character.

13. The Burgers vectors of dislocations on these planes are given in the following table:

$(11\bar{1})$	$(1\bar{1}\bar{1})$
$\frac{a}{2}[101]$	$\frac{a}{2}[101]$
$\frac{a}{2}[\bar{1}10]$	$\frac{a}{2}[110]$
$\frac{a}{2}[011]$	$\frac{a}{2}[01\bar{1}]$

Note: if Burgers vector $b = \frac{a}{n}[hkl]$ $then$ $|b|^2 = \frac{a^2}{n^2}(h^2 + k^2 + l^2)$

Lomer lock: The two planes intersect along [101]
Favorable reactions producing edge dislocation are Lomer locks. It is immobile because the plane on which it lies is not a close packed plane on

No.	Reactions	Energy	Remark
1	$\frac{a}{2}[101] + \frac{a}{2}[101] = a[101]$	$\frac{a^2}{2} + \frac{a^2}{2} < 2a^2$	Unfavorable
2	$\frac{a}{2}[101] + \frac{a}{2}[110] = \frac{a}{2}[211]$	$\frac{a^2}{2} + \frac{a^2}{2} < \frac{3}{2}a^2$	Unfavorable
3	$\frac{a}{2}[101] + \frac{a}{2}[\bar{1}\bar{1}0] = \frac{a}{2}[0\bar{1}1]$	$\frac{a^2}{2} + \frac{a^2}{2} > \frac{a^2}{2}$	Favorable
4	$\frac{a}{2}[101] + \frac{a}{2}[01\bar{1}] = \frac{a}{2}[110]$	$\frac{a^2}{2} + \frac{a^2}{2} > \frac{a^2}{2}$	Favorable
5	$\frac{a}{2}[101] + \frac{a}{2}[0\bar{1}1] = \frac{a}{2}[1\bar{1}2]$	$\frac{a^2}{2} + \frac{a^2}{2} < \frac{3}{2}a^2$	Unfavorable
6	$\frac{a}{2}[\bar{1}10] + \frac{a}{2}[101] = \frac{a}{2}[011]$	$\frac{a^2}{2} + \frac{a^2}{2} > \frac{a^2}{2}$	Favorable
7	$\frac{a}{2}[\bar{1}10] + \frac{a}{2}[\bar{1}0\bar{1}] = \frac{a}{2}[\bar{2}1\bar{1}]$	$\frac{a^2}{2} + \frac{a^2}{2} < \frac{3}{2}a^2$	Unfavorable
8	$\frac{a}{2}[\bar{1}10] + \frac{a}{2}[110] = a[010]$	$\frac{a^2}{2} + \frac{a^2}{2} = a^2$	Unfavorable
9	$\frac{a}{2}[\bar{1}10] + \frac{a}{2}[\bar{1}\bar{1}0] = a[\bar{1}00]$	$\frac{a^2}{2} + \frac{a^2}{2} = a^2$	Unfavorable
10	$\frac{a}{2}[\bar{1}10] + \frac{a}{2}[01\bar{1}] = \frac{a}{2}[\bar{1}2\bar{1}]$	$\frac{a^2}{2} + \frac{a^2}{2} < \frac{3}{2}a^2$	Unfavorable
11	$\frac{a}{2}[\bar{1}10] + \frac{a}{2}[0\bar{1}1] = \frac{a}{2}[\bar{1}01]$	$\frac{a^2}{2} + \frac{a^2}{2} > \frac{a^2}{2}$	Favorable; Lomer Lock

12	$\frac{a}{2}[011]+\frac{a}{2}[101]=\frac{a}{2}[112]$	$\frac{a^2}{2}+\frac{a^2}{2}<\frac{3}{2}a^2$	Unfavorable
13	$\frac{a}{2}[011]+\frac{a}{2}[\bar{1}0\bar{1}]=\frac{a}{2}[\bar{1}10]$	$\frac{a^2}{2}+\frac{a^2}{2}>\frac{a^2}{2}$	Favorable: it can glide on $(11\bar{1})$
14	$\frac{a}{2}[011]+\frac{a}{2}[110]=\frac{a}{2}[121]$	$\frac{a^2}{2}+\frac{a^2}{2}<\frac{3}{2}a^2$	Unfavorable
15	$\frac{a}{2}[011]+\frac{a}{2}[\bar{1}\bar{1}0]=\frac{a}{2}[\bar{1}01]$	$\frac{a^2}{2}+\frac{a^2}{2}>\frac{a^2}{2}$	Favorable; Lomer Lock
16	$\frac{a}{2}[011]+\frac{a}{2}[01\bar{1}]=a[010]$	$\frac{a^2}{2}+\frac{a^2}{2}=a^2$	Unfavorable
17	$\frac{a}{2}[011]+\frac{a}{2}[0\bar{1}1]=a[001]$	$\frac{a^2}{2}+\frac{a^2}{2}=a^2$	Unfavorable

14. Let the slip plane be one of the 12 {110} planes. Dislocation & the Burgers vector must lie on slip plane. The Possible glide planes are $(1\bar{1}0),(10\bar{1}),(01\bar{1})$. The best way to check if dot product of Burgers vector & plane normal is equal to zero (b.n = 0). If the slip plane were of type {112} the slip plane for this case would be $(\bar{2}11),(1\bar{2}1)$ & $(11\bar{2})$. Try to find out the possible slip plane of type {123}.

    If it were an edge dislocation one must specify its direction. It could glide only if it lies on one of the slip planes. For example an edge dislocation $\frac{a}{2}[111]$lying along $[\bar{2}11]$could glide on $(01\bar{1})$. Find other possibilities.

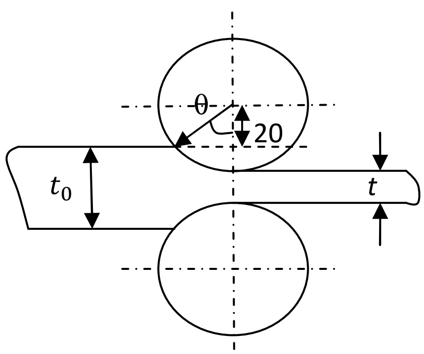
15. Look at the standard project & identify the the slip plane & direction having highest resolved shear stress. In this case it is $(\bar{1}11)[101]$. Therefore resolved shear stress:$\tau=\sigma\, cos\varphi\, cos\lambda$. $cos\varphi=\frac{-1\times1+1\times2+1\times3}{\sqrt{3}\sqrt{14}}=\frac{4}{\sqrt{42}}$ & $cos\lambda=\frac{1\times1+0\times2+1\times3}{\sqrt{2}\sqrt{14}}=\frac{4}{2\sqrt{7}}$ The force on dislocation which is mobile is given by $F=\tau b=\sigma b cos\varphi cos\lambda=100\times\frac{0.36}{\sqrt{2}}\times10^{-9}\times\frac{16}{14\sqrt{6}}$=0.012 N/m

16. The force on a dislocation is given by $F_i=\epsilon_{ijk}\,\sigma_{jl}\,b_l\,t_k$ The subscripts can have values 1, 2 or 3. Since only non zero compoments of **σ**, **b** & **t** are σ_{22}, b_2 & t_1. $F_i=\epsilon_{i21}\,\sigma_{22}\,b_2t_1$ Therefore subscript i has to be 3 ($\epsilon_{ijk}=1\, for\; i\neq j\neq k\; else\; \epsilon_{ijk}=0$ & $\epsilon_{321}=-1$) Thus $F_3=-\sigma_{22}b$ This being an edge dislocation can climb noly due to a force acting along its Burgers vector. Since the force is along x3 it can help it climb down.

17. Assume both dislocations lie on (001) plane. Let this be the glide plane. Since x2 = 0 only non zero force acting on the dislocation is given by $F_1=\frac{Gb^2}{2\pi(1-\nu)x_1}$ Since both dislocations have positive b they would repel each other. Here it is balanced by a force acting on the second dislocation which is τb. Therefore the distance between the two is given by $x_1=\frac{Gb}{2\pi(1-\nu)\tau}=\frac{210\times10^3\times0.25\times10^{-9}}{2\times\pi\times(1-0.3)\times140}=59.7nm$

18. Shear stress τ is given by $\tau = \frac{Gb}{l} = \frac{100\times10^3\times0.25}{1\times10^3} = 25MPa$ This represents shear strength. YS is usually = 2 x shear stregth = 50MPa.

19. Look at the following schematic diagram given below relating different parameters during rolling. Assume that plate width is 1 & initial length is l_0. Since the volume during rolling does not change it can be shown that strain is given by $\varepsilon = ln\left(\frac{l}{l_0}\right) = ln\frac{t_0}{t} = ln2$ The time to achieve this strain is estimated as follows:



If R is the roll radius ω is the angular velocity, time it takes to give this deformation =θ/ω. Since R=25, $\theta = cos^{-1}\left(\frac{R-\frac{t_0-t}{2}}{R}\right) = cos^{-1}\left(\frac{20}{25}\right) = cos^{-1}0.8$ & $\omega = \frac{2\pi rpm}{60} = \frac{2\pi\times200}{60} = \frac{20\pi}{3}s^{-1}$Thus time = $\frac{3cos^{-1}0.8}{20\pi} = 0.031$& strain rate =$\dot{\varepsilon} = \frac{ln2}{0.031} = 22.56s^{-1}$. Stored energy due to increased dislocation density =$0.5Gb^2\rho$ = 0.5 x 200 x 10^9 x $(0.25)^2$ x 10^{-18} x 10^{11} x 10^4 = 6.25 MJ/m^3

Energy spent =flow stress x strain = 300 ln(2) = 208 MJ/m^3. This shows only a very small amount of the total enegy is stored within the metal. Bulk of it is dissipated as heat. Assuming the process of rolling is adiabatic temperature increase $\Delta T = \frac{E}{\rho s} = \frac{(208-6.25)\times10^6}{8907\times0.49\times10^3} \approx 46°C$

20. Total strain (ε) is given by $\varepsilon = \rho b\bar{x}$ where ρ is dislocation density, b is Burgers vector & $\bar{x}$ is the average glide distance of dislocation. Burgers vector b = a/√3 =0.248nm. Therefore $\bar{x} = \frac{\varepsilon}{\rho b} = \frac{0.3}{0.248\times10^{-9}\times10^{14}} = 1.21\times10^{-5}m$. This is equal to 1.21micron which is less than its grain size. The average velocity = 1.21×10^{-3} m/s.

21. The force experienced by a dislocation due to another at a distance x on the slip plane is given by $F = \frac{Gb^2}{2\pi(1-\nu)x}$. Since the dislocation source is at the centre of the grain, it is at a distance = d/2 from the disloaction at grain boundary. Therefore x=d/2. Thus $F = \frac{Gb^2}{2\pi(1-\nu)\frac{d}{2}}$ This may be assumed to be the resisting force acting on the source. The net force acting on the source = *τb-F* which is $= \tau b - \frac{Gb^2}{\pi(1-\nu)} = 50\times10^6\times0.3\times10^{-9} - \frac{70\times10^9\times0.09\times10^{-18}}{\pi\times0.7\times5\times10^{-6}} = 0.015 - 0.00057 \approx 0.014N/m$

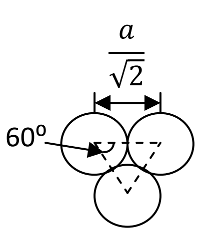
22. Burgers vector of a dislocation in a tilt boundary = $\frac{a}{2}[110] = \frac{a}{\sqrt{2}} = \frac{0.405}{\sqrt{2}} = 0.29nm$ The spacing between two dislocations is given by $h = \frac{b}{\theta} = \frac{0.29}{5\pi}\times180 = 3.32nm$

23. Burgers vector $= \frac{a}{\sqrt{2}} = \frac{0.35}{\sqrt{2}} = 0.25nm$ When the dislocations are 10b apart energy of the low angle boundary $= \frac{Gb^2}{10h}$ (since boundary consists of one dislocation of unit length at every distance of h). h = 2r$_0$ =10b. Thus $\frac{Gb^2}{100b} = \frac{Gb}{4\pi(1-\nu)}\theta(A - ln\theta)$ where q = b/10b = 0.1rad & A$= \frac{4\pi(1-\nu)}{100\times\theta} + ln\theta$ =-1.42

24. Since poisson ration is same as in the previous problem $E = \frac{Gb}{4\pi(1-\nu)}\theta(-1.42 - ln\theta) = \frac{48\times10^9\times0.25\times10^{-9}}{4\times\pi\times(1-0.3)}\frac{\pi}{180}\left(-1.42 - ln\frac{\pi}{180}\right) = 0.13$ J/m^2

25. Differentiating the expression for E: $\frac{dE}{d\theta} = \frac{Gb}{4\pi(1-\nu)}\left(A - \theta\frac{1}{\theta} - ln\theta\right) = 0$ Thus $ln\theta_{max} = A - 1$ On substituting the magtitude of A from the previous problem $\theta_{max} = 5.1^0$ & $E_{max} = \frac{Gb}{4\pi(1-\nu)}\theta_{max}$ *(note A = 1+ln θ_{max})* $\frac{E}{E_{max}} = \frac{\theta}{\theta_{max}}(A - ln\theta) = \frac{\theta}{\theta_{max}}(1 + ln\theta_{max} - ln\theta) = \frac{\theta}{\theta_{max}}\left(1 - ln\frac{\theta}{\theta_{max}}\right)$

26. Energy of the free surface depends on the way atoms are arranged. This varies from grain to grain depending on their orientations. If Z is the cordination number, the number of bonds of type AA in one mole of pure metal $= \frac{1}{2}ZN_0$ where N_0 is Avogrado number. If ε is the energy of one bond, $L_s = \frac{1}{2}ZN_0\varepsilon$ where L_s is heat of sublimation. The free surface has a set of broken bonds. Energy of a broken bond is approximately $\varepsilon/2$. The number depends on the indices of the top surface. If it were (111) there will be 3 broken bonds / atom (There are 6 bonds on the plane 3 beneath & 3 above it). Energy of free surface is therefore = 3ε/2 J/atom. If n_a is number of atom / unit area surcae free energy $\gamma_s = \frac{3}{2}\frac{L_s n_a}{ZN_0}$ The arrangements of atom in (111) plane is shown below. On substituion in expression for $\gamma_s = \frac{3}{2}\frac{L_s}{ZN_0}\frac{4}{\sqrt{3}a^2} = \frac{2\sqrt{3}}{ZN_0}\frac{L_s}{a^2} = 2.5J/m^2$



$$n_a = \frac{0.5}{0.5\left(\frac{a}{\sqrt{2}}\right)^2 sin60} = \frac{4}{\sqrt{3}a^2}$$