LN–6 IDLE MIND SOLUTIONS

1. The number of defects (vacancies) in a given atomic assembly N is proportional to $e^{-\Delta H_v/kT}$ where ΔH_v is the energy of defect formation and k is the Boltzmann constant.

$$n_v \propto Ne^{-\Delta H_v/kT}$$

$$n_v = ANe^{-\Delta H_v/kT} \text{(unless otherwise stated, we assume A = 1)}$$

$$\text{and} \quad \frac{n_v}{N} = e^{-\Delta H_v/kT} = e^{-\frac{1.12 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23} \times 1724}} = 5.36 \times 10^{-4}$$

For $n_v = 1$, we find:

$$N = \frac{1}{5.36 \times 10^{-4}} = \boxed{1.87 \times 10^3 \text{ filled sites/vac.}}$$

2. This problem is analog to problem 1.

Required:
$n_v = ANe^{-(H_v/kT)}$
Cr, $T_M = 2130K$
$H_v = 1.08$ eV

$$n_v = Ne^{-H_v/kT}$$

Here we want to find N for $n_v = 1$.

$$1 = Ne^{-H_v/kT}$$

$$N = \frac{1}{e^{-H_v/kT}} = e^{H_v/kT}$$

$$= 2.718^{\frac{1.08 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23} \times 2129}}$$

$$\boxed{N = 358 \text{ filled sites/vacancy}}$$

3. To solve this problem we must first convert n_V/cm^3 into n_V/N, which is simple since the molar volume for Al is 10 cm^3 ($N = N_A/\text{Mol.Vol.} = 6.02 \times 10^{22}$). Accordingly, we have:

$$\frac{n_v}{N} = \frac{2 \times 10^{17}}{6.02 \times 10^{22}} = 3.32 \times 10^{-6} = \exp(-\Delta H_v/kT)$$

$$\ln 3.32 \times 10^{-6} = -\Delta H_V/kT$$

$$\Delta H_V = -kT \times \ln 3.32 \times 10^{-6} = 1 \times 10^{-19}\ \text{J}$$

$$\Delta H_v = 1 \times 10^{-19}\ \text{J} \times \frac{1\ \text{eV}}{1.6 \times 10^{-19}\ \text{J}} = \boxed{0.63\ \text{eV/vac.}}$$

4. Required:

$$n_V = ANe^{-(H_v/kT)}$$
$$T^oK = T^oC + 273.16$$

Given is:

$$\frac{n_V(T_1)}{n_V(T_2)} = 2 \times 10^{-3} = \frac{ANe^{-H_v/kT_1}}{ANe^{-H_v/kT_2}}$$

$$= \frac{e^{-H_v/kT_1}}{e^{-H_v/kT_2}} = e^{-H_v/kT_1} \times e^{-H_v/kT_2}$$

$$2 \times 10^{-3} = e^{-\frac{H_v}{k}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)}$$

In logarithmic form:

$$\ln (2 \times 10^{-3}) = -\frac{H_v}{k}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

$$H_v = -\frac{k \times \ln(2 \times 10^{-3})}{\frac{1}{T_1} - \frac{1}{T_2}} = -\frac{1.38 \times 10^{-23} \times (-6.22)}{\frac{1}{773.16} - \frac{1}{1173.16}}$$

$$= \boxed{1.95 \times 10^{-19}\ \text{J} = (1.22\ \text{eV})}$$

5. We have: (1) $1/10^{10} = A\exp(-\Delta H_v/kT_1)$
(2) $1/(3\text{x}10^9) = A\exp(-\Delta H_v/kT_2)$

We see that by dividing we can get rid of the constant:

$$\frac{3 \text{ x } 10^9}{10^{10}} = 0.3 = \exp\left[-\frac{\Delta H_v}{k}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right]$$

and

$$\ln 0.3 = -\frac{\Delta H_v}{k}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

$$\Delta H_v = -\frac{k \text{ x } \ln 0.3}{\frac{1}{T_1} - \frac{1}{T_2}} = \boxed{2.09 \text{ x } 10^{-19} \text{ J/vacancy}}$$

6. $$\frac{n_v}{N} = A\exp\left(-\frac{\Delta H_v}{kT}\right) = \frac{1}{10^5} = 10^{-5}$$

Assuming A to be close to 1, we have: $\ln 10^{-5} = -(\Delta H_v)/(kT_x)$

$$T_x = -\frac{H_v}{k \text{ x } \ln 10^{-5}} = -\frac{1.05 \text{ x } 1.6 \text{ x } 10^{-19}}{1.38 \text{ x } 10^{-23} \text{ x } (-)11.5} = \boxed{1059\text{K} = 786^o\text{C}}$$

7. Slip along <111> directions suggests a “BCC” system, corresponding to {110}, <111> slip. Therefore:

$$a\sqrt{3} = 4r$$

$$a = \frac{4r}{\sqrt{3}} = 1.78 \text{ x } 10^{-10} \text{ m}$$

Densest planes are {110}

We find:

$$\frac{2 \text{ atoms}}{a^2\sqrt{2}} = \boxed{4.46 \text{ x } 10^{19} \text{ atoms x m}^{-2}}$$

8. According to LN6–15: $N = 2^{n-1}$ where N = number of grains/inch^2 if viewed at a magnification of 100X and n = grain size number. Taking n=7:

$$N = 2^6 \times 10^4 \text{ grains/inch}^2 = 6.4 \times 10^5 \text{ grains/inch}^2$$

Knowing N, we can compute an average grain diameter:

$$d_{grain} = N^{1/2} = 1.25 \times 10^{-3} \text{ inch} = 3.12 \times 10^{2} \text{ mm} = \mathbf{31.2\ \mu m}$$

In more expanded form: If we have 64 x 10^5 grains (cubic – exposing square areas under the microscope) per inch^2 (N grains), then in linear arrangement we have $\sqrt{N}$ = 800 grains/inch. The side of each grain is then:

$$1/800 \text{ inch} = 1.25 \times 10^{-3} \text{ inch} = 1.25 \times 10^{-3} \times 25 \text{ mm} = 3.12 \times 10^{-3} \text{ mm} = \mathbf{31.2\ \mu m}$$

We can now establish a convenient list for grain size numbers in the metric scale.

ASTM No. n	Grain/mm^2	Approximate Grain Diameter (μm)
–3	1	1000.0
–2	2	708.0
–1	4	500.0
0	8	354.0
1	16	250.0
2	32	177.0
3	64	125.0
4	128	88.4
5	256	62.5
6	512	44.2
7	1024	31.2

9. For example:
   - (1) dopant elements in semiconductors → affect electrical conductivity
   - (2) vacancies in close packed metals → explain solid state diffusivity
   - (3) edge dislocations → explain slip; visible as etch pits and in X–ray topography
   - (4) grain boundaries → visible in reflected light; evidence by X–ray diffraction
   - (5) micro–precipitates → visible in X–ray transmission, IR transmission

10. The information provided is:

$$\frac{n_d(T_1)}{n_d(T_2)} = 10^{-3} = \frac{ANe^{-\frac{E_d}{kT_1}}}{ANe^{-\frac{E_d}{kT_2}}} \qquad (T_1 = 773K, T_2 = 1073K)$$

$$10^{-3} = \frac{e^{-(E_d/kT_1)}}{e^{-(E_d/kT_2)}} = e^{-\frac{E_d}{kT_1}} \text{ x } e^{-\frac{E_d}{kT_2}} = e^{-\frac{E_d}{k}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)}$$

$$\ln 10^{-3} = -\frac{E_d}{k}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

$$E_d = -\frac{k \ln 10^{-3}}{\left(\frac{1}{T_1} - \frac{1}{T_2}\right)} = -\frac{1.38 \text{ x } 10^{-23} \text{ x } (-6.9)}{\frac{1}{773} - \frac{1}{1073}}$$

$$\boxed{E_d = 2.63 \text{ x } 10^{-19} \text{ J x } \frac{1 \text{ eV}}{1.6 \text{ x } 10^{-19} \text{ J}} = 1.64 \text{ eV}}$$

11. At the melting point: $\frac{N_d}{N} = e^{-(E_d/kT)} = e^{-\frac{1.2 \text{ x } 1.6 \text{ x } 10^{-19}}{1.38 \text{ x } 10^{-23} \text{ x } 1357}} = 3.56 \text{ x } 10^{-5}$

(1 of 28570 sites is “absorbed vacancy”.)

At room temperature: $\frac{N_d}{N} = e^{-(E_d/kT)} = e^{-\frac{1.2 \text{ x } 1.6 \text{ x } 10^{-19}}{1.38 \text{ x } 10^{-23} \text{ x } 300}} = 7.2 \text{ x } 10^{-21}$

(1 of 1.4 x 10^{20} sites is vacant.)

The volume change (as specified) is due to the vacancies generated at the melting point – no significant vacancies exist at room temperature!! Therefore, the volume change is:

3.5 x 10^{-5} **ΔV = 0.0035%**

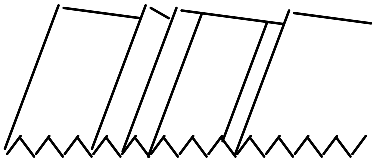
12. Silicon = 2.33 g/cm^3 (density)
Al: 10^{21}/m^3 = 10^{15}/cm^3

$$\text{Al (g/cm}^3\text{)} = \frac{10^{15} \times 26.98}{6.02 \times 10^{23}} = 4.48 \times 10^{-8}\ \text{g}$$

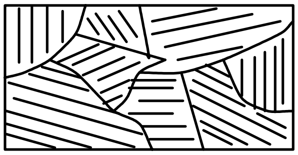
$$\text{Wt.\% Al in Si} = \frac{100 \times 4.48 \times 10^{-8}}{2.33} = \boxed{1.9 \times 10^{-6}\ \%}$$

13. The tensile strength is largely controlled by slip, which in FCC systems (Al) involves the twelve {111} <110> slip systems. The mobility of dislocations, which controls slip, is high in single crystals because of the high degree of crystal perfection and slip proceeds from one external surface to another. In polycrystalline Al the mobility of dislocations is slowed down because of mutual interference (high density of dislocations) and, because of precipitates frequently encountered, slip is retarded. Slip, moreover, is arrested at grain boundaries and proceeds from there into different directions; the strength of polycrystalline material is higher than that of single crystals.

slip systems in
single crystals



slip systems in poly–
crystalline materials



14. $$1/2000 = 5 \times 10^{-4} = \frac{N_d}{N} = e^{-\frac{E_d}{RT_M}} \qquad T_M = 3680\text{K}$$

$$\ln 5 \times 10^{-4} = -\frac{E_d}{8.314 \times 3680}$$

$$E_d = 7.6 \times 8.314 \times 3680$$

$$\boxed{E_d = 2.3 \times 10^5\ \text{J/mole} = 230\ \text{kJ/mole}}$$

15. (a) (1) impurities
        (2) dislocations
        (3) grain boundaries
        (4) “surfaces”

    (b) (2) and (3)

    (c) (2)

    (d) vacancies

16. As a first approximation we have $n_V/N = \exp-(\Delta H_V)/(kT)$. (In metals the pre–exponential is generally found to be close enough to unity to be neglected.)

$$n_v = N \exp - \frac{\Delta H_v}{kT}$$

Presently N = no. of lattice sites per cm^3 of Cu:

$$N = \frac{6.02 \text{ x } 10^{23}}{7.1} = \boxed{8.5 \text{ x } 10^{22} \text{ sites/cm}^3}$$

$$n_v = 8.5 \text{ x } 10^{22} \text{ x } \exp - \frac{4 \text{ x } 1.6 \text{ x } 10^{-19}}{1.38 \text{ x } 10^{-23} \text{ x } 1350} = \boxed{1 \text{ x } 10^8/\text{cm}^3}$$

17. (a) The change in density due to the formation of Schottky defects upon heating of Cu is a density change caused by an increase in the number of vacancies; the atoms originally at the vacated sites move to the surface and thus increase the atomic volume:

$$\Delta n_v = n_{T_2} - n_{T_1} = N\left[\exp\left(-\frac{\Delta H_v}{kT_2}\right) - \exp\left(-\frac{\Delta H_v}{kT_1}\right)\right]$$

$$= N\,(1.84 \text{ x } 10^{-4} - 1.2 \text{ x } 10^{-15})$$

Taking molar quantities: $N = 6.02 \text{ x } 10^{23}$
$\Delta n_V = 1.1 \text{ x } 10^{20}$ vacancies

The volume change, ΔV, associated with the “arrival” of 1.1 x 10^{20} atoms at the surface (coming from the interior) is:

(continued)

17. (a) Continued.

$$\Delta V = \frac{7.1 \text{ x } 1.1 \text{ x } 10^{20}}{6.02 \text{ x } 10^{23}} = \boxed{1.3 \text{ x } 10^{-3} \text{ cm}^3}$$

$$\%\Delta V = \frac{100 \text{ x } 1.3 \text{ x } 10^{-3}}{7.1} = 2 \text{ x } 10^{-2}\ \%$$

This volume change corresponds to a 2 x 10^{-2} % increase, relating to a density change from 8.96 g/cm^3 (= 8.96g/1.0002 cm^3) which is meaningless since it is beyond the precision of the density given in the P/T.

(b) The experimentally observed density change (–6.4%) can be attributed to lattice expansion associated with increased thermal vibrations of the atoms. The effective atomic radius increases with temperature.

18. The energy required to form one mole of vacancies in Cu (ΔH_v) = 20,000 cal x 4.18 J/cal. The formation of one vacancy requires:

$$\Delta H_v = \frac{83,600}{6.02 \text{ x } 10^{23}} = 1.39 \text{ x } 10^{-19} \text{ J/vac.}$$

$$\frac{n_v}{N} = \exp - \frac{1.39 \text{ x } 10^{-19}}{1.38 \text{ x } 10^{-23} \text{ x } 1350} = 5.6 \text{ x } 10^{-4} = \frac{1}{1740}$$

We find one vacancy per 1740 sites.

The number of sites per cm^3 is given by:

$$\frac{N_A}{\text{Mol.Vol.}} = \frac{6.02 \text{ x } 10^{23}}{7.1} = 8.5 \text{ x } 10^{22} \text{ sites/cm}^3$$

We now find:

$$n_v = \frac{8.5 \text{ x } 10^{22}}{1740} = \boxed{4.9 \text{ x } 10^{19}/\text{cm}^3}$$

19. According to LN6–15, $N = 2^{n-1}$ where N = number grains/inch^2 when viewed at a magntification of X100 (under a microscope) and n is the grain size number. Grains, 3–dimensional, when viewed under the microscope expose an area which can be approximated as <u>a square</u> with a particular side length. Any grain size analysis can thus be made along one dimension.

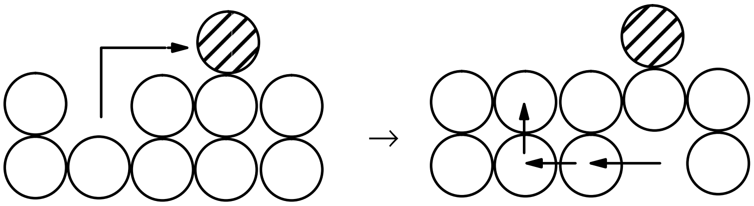
$$\text{no. averaged diameters (grains)/linear inch} = \frac{2.54 \text{ x } 10^{-2}}{100 \text{ x } 10^{-6} \text{ x } 100} = 2.54$$

Given:

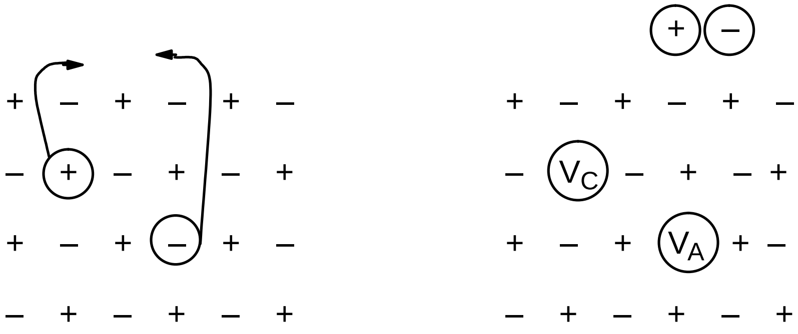
$$\begin{aligned} N &= 2^{n-1} \\ 6.45 &= 2^{(n-1)} \\ \ln 6.45 &= (n-1) \ln 2 \\ (n-1) &= (\ln 6.45)/(\ln 2) = 2.68 \end{aligned}$$

$$\boxed{n = 3.68 \sim 4}$$

20. (1)



(2)



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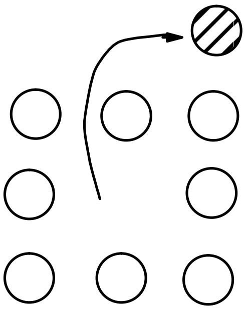

21. The fundamental relationship is $n_v/N = Ae^{-\Delta H_v/kT}$.

It can be applied at the two given temperatures, which allows us to eliminate the unknown constant A; solving, we obtain ΔH_V and with it the value of the constant A. needed to solve for the unknown temperature, T_X.

$$(1)\quad \frac{1}{10^{11}} = Ae^{-\Delta H_v/kT_1} \qquad T_1 = (750 + 273)K$$

$$(2)\quad \frac{1}{10^{10}} = Ae^{-\Delta H_v/kT_2} \qquad T_2 = (850 + 273)K$$

Dividing (1) by (2), we obtain:

$$10^{-1} = e^{-\frac{\Delta H_V}{k}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)}$$

$$-\ln 10 = -\frac{\Delta H_V}{k}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

$$\Delta H_v = \frac{k \text{ x } \ln 10}{\frac{1}{1023} - \frac{1}{1123}} = 3.65 \text{ x } 10^{-19} \text{ J/vac}$$

$$A = \frac{1}{10^{11}} e^{\frac{\Delta H_V}{kT_1}} = 1.69$$

$$\frac{1}{10^8} = Ae^{-\Delta H/kT_x}$$

$$T_x = \frac{\Delta H}{k \ln(A \text{ x } 10^8)} = 1396K = \boxed{1123^oC}$$

22. We know that the ratio of vacancies to sites is given as $\frac{n}{N} = Ae^{-\frac{\Delta H_V}{kT}}$ (A, not specified is assumed to be one), with ΔH_V, k and T given we still need to know N, the number of lattice sites/cm^3 for aluminum. We can get that from the atomic volume (10 cm^3/mole) which makes N = 6.02 x 10^{22}/cm^3.

$$\frac{n}{N} = Ae^{-\frac{\Delta H_V}{kT}} \quad ; \quad n = Ne^{-\frac{\Delta H_V}{kT}} = 6.02 \cdot 10^{22} e^{-\frac{1.05 \cdot 1.6 \cdot 10^{-19}}{1.38 \cdot 10^{-23} \cdot 883}}$$

$$n = 6.02 \text{ x } 10^{22} \text{ x } 1.03 \text{ x } 10^{-6}$$

$$= \boxed{6.2 \text{ x } 10^{16} \text{ vac/cm}^3}$$

23. The problem is simple in principle, but there are wrinkles: We deal with a simple cubic lattice – in the center of the unit cell we accomodate an atom; the maximum diameter will be $\left[a\sqrt{3} - 2r(O^{2})\right]$; the wrinkle – what is the atomic volume? The P/T gives an estimated density and an atomic volume not directly related to the density – atomic radii cannot be used when considering a solid.
I would answer this question by stating the given information and indicating how to solve the problem in principle (as above). I would also question the meaning of the data given.

24. Identify 3 types of crystal defects in solids and suggest for each of these one materials property which is adversely affected by its presence and one which is improved.

Defect	type	Improved Materials Properties	Adversely affected Materials Properties
Point Defect	Vacancy f(T)	– Diffusivity – Color Centers – Ionic Conductivity	– Electron mobility – Carrier Lifetime
	Substitutional	– Conductivity (dopant) – Strength (hardness) – Characteristic T (like T_M)	– Conductivity (impurities) – Ductility – Characteristic T
	Interstitial	– Strength – Characteristic T – Electrical Properties	– Ductility – Characteristic T – Electrical Properties
Line Defect	Dislocation	– Ductility (Malleability) – Strength (at high density)	– Strength – Yield Stress – Optical Properties – Lasing Action
Planar Defect	Grain Boundaries	– Strength – Electrical Properties – Magnetic Properties	– Creep – Electrical Properties – Magnetic Properties

25. (a) deBroglie wavelength

$$\lambda p = \frac{h}{mv}$$

where:

λ_p: particle wavelength
h: Planck’s constant
m: mass of particle
v: velocity of particle

(b) Bohr postulate

$$mvr = n\frac{h}{2\sqrt{\pi}}$$

where:

m: mass of electron
v: velocity of electron in orbit
h: Planck’s constant
n: quantum number of orbit
r: radius of electron orbit

(c) Schottky defect: A Schottky defect is a single vacancy (uncharged) or a pair of oppositely charged ion vacancies.

(d) Heisenberg uncertainty principle

$$\Delta E \cdot \Delta t \geq h \quad ; \quad \Delta p \cdot \Delta x \geq h$$

where:

h: Planck’s constant
ΔE: uncertainty in energy
Δt: uncertainty in time
Δp: uncertainty in linear momentum
Δn: uncertainty in position

(e) Schrödinger wave equation: The Schrödinger equation is a differential equation whose solutions yield the possible wave functions that can be associated with a particle such as an electron in a given physical situation; the equation tells us how the wave function changes as a result of the forces acting on the particle.

(f) Moseley relationship

$$\bar{\nu}_{K\alpha} = R(Z-1)^2 \cdot \frac{3}{4}$$

where:

R: Rydberg’s constant
Z: Atomic number of element
$\bar{\nu}_{K\alpha}$: wave number of K_α x–ray

(g) Bragg’s law

$$n\lambda = 2d_{(hkl)} \sin\theta$$