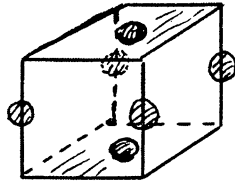(1.1)
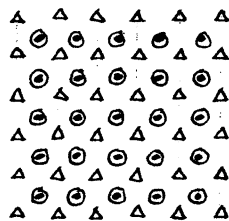
(a)

... $\frac{1}{2}$ atom inside cell on top and bottom faces
... $\frac{1}{4}$ atom along each vertical edge

TOTAL ATOMS $= 2 \times \frac{1}{2} + 4 \times \frac{1}{4} = \underline{\underline{2}}$

(b)

⇐ TOP VIEW
• ... plane # 1
△ ... plane # 2
○ ... plane # 3

(c)   bcc

(1.2)

(a) The diamond lattice is composed of two interpenetrating fcc lattices. Each fcc lattice unit cell contains 4 atoms. ($\frac{1}{2}$ atom at each of 6 faces and $\frac{1}{8}$ atom at each of 8 corners.) Thus the Si lattice contains [8 ATOMS] per unit cell. Inspecting Fig. 1.5a leads to the same conclusion -- there are 4 atoms totally inside the cube and an fcc arrangement on the faces of the cube.
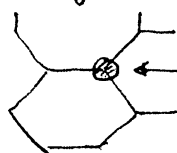
(b)

$$\frac{\text{Si ATOMS}}{\text{CM}^3} = \frac{\text{ATOMS/UNIT CELL}}{a^3} = \frac{8}{(5.431 \times 10^{-8})^3} = 4.994 \times 10^{22} \;✓$$

$\swarrow$ from Table 1.5

(c) Looking at Fig. 1.5a we note that the upper front corner atom and the atom along the body diagonal through the upper front corner are nearest neighbors. These are separated by $1/4 \times$ length of a body diagonal. Thus

$$d = \frac{1}{4}\sqrt{3}\,a = \frac{\sqrt{3}}{4}(5.431\times10^{-8}) = 2.352\times10^{-8}\ \text{cm}$$

(1.3) Looking at Fig. 1.6a we conclude (counting Cd ↔ N atoms in the figure)

each bottom/top face atom shared with 6 cells

$\therefore \frac{1}{6}\times6 = 1$ atom total inside cell on top and bottom faces AT corners

$\therefore \frac{1}{2}$ atom also at center of top + bottom faces

$\therefore$ Total of 3 atoms on top + bottom faces

ALSO, there are 3 atoms inside cell near middle

[6 atoms] of N per unit cell

As stated in the text, the hexagonal unit cell volume is $\frac{3\sqrt{3}}{2}a^2c$. Thus

$$\frac{N\ \text{atoms}}{\text{cm}^3} = \frac{6}{\frac{3\sqrt{3}}{2}a^2c} = \frac{4}{\sqrt{3}\,a^2c} = \frac{4}{\sqrt{3}(3.1115\times10^{-8})^2(4.9798\times10^{-8})}$$

$$= 4.790\times10^{22}$$

(1.4)

(a) (i) 6, 3, 2   ... normalized intercepts
         1/6, 1/3, 1/2 ... 1/[INTERCEPTS]
         1, 2, 3   .... MULTIPLY X 6 to get whole numbers
         (1 2 3)   .... MILLER INDICES OF PLANE

    (ii) [1 2 3]   ... direction normal to plane has same
                            indices as plane in cubic crystals

(b)   2, ∞, 3   ... normalized intercepts
      1/2, 0, 1/3   ... 1/INTERCEPTS
      3, 0, 2   ... multiply X 6
      (3 0 2)   ... MILLER INDICES

(c) $1, 1, -\frac{1}{2}, 1$ ... intercepts
      $1, 1, -2, 1$ .... 1/intercepts — already whole numbers
      $(1\,1\,\bar{2}\,1)$ ... MILLER INDICES

    NOTE: $h + k + l = 0$, thus the i index associated with
    the a_3 axis must be $\bar{2}$.   There is REALLY no need to
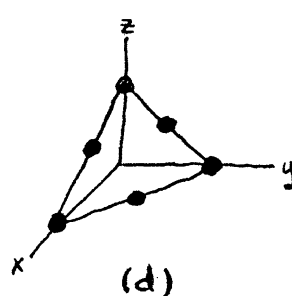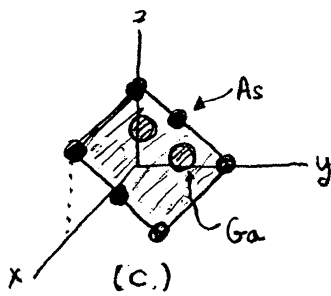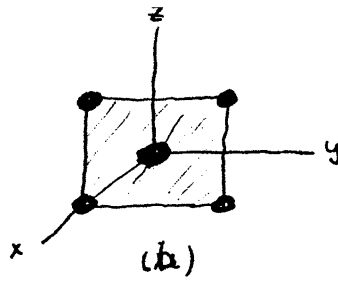   work out the intermediate steps for this index.

(1.5) (a) Intercepts ... 1, 1, ∞   (b) Intercepts ... 1, 1, 1
          1/Intercepts ... 1, 1, 0   1/Intercepts ... 1, 1, 1
          whole # set ... 1, 1, 0   whole # set ... 1, 1, 1
          Miller indices ... (110)   Miller indices ... (111)

      (c) Projections ... $0, \frac{1}{2}, \frac{1}{2}$ (d) Point E lies along the
          whole # set ... 0, 1, 1   cube diagonal.
          Direction ... [011]   DIRECTION ... [111]

1–3

(1.6)

(a)

(b)

(c)

(d)

(1.7)

(a) To lie in the (100) surface plane a direction must be perpendicular to the [100] direction. Using Eq.(1.3) we must have

$$\cos\theta = \frac{h_2}{(h_2^2 + k_2^2 + l_2^2)^{1/2}} = 0 \qquad \dots h_1 = 1, k_1 = 0, l_1 = 0$$

or $h_2 = 0$

Thus all directions [0kl] lie in the (100) surface plane.

$$[011], [0\bar{1}1], [01\bar{1}], [0\bar{1}\bar{1}] \dots \langle 110 \rangle \text{ directions lying in the (100) surface plane}$$

(b) For a direction to be perpendicular to the [111] direction we must have (using Eq.(1.3))

$$\cos\theta = \frac{h_2 + k_2 + l_2}{\sqrt{3}\,(h_2^2 + k_2^2 + l_2^2)^{1/2}} = 0 \qquad \dots h_1 = 1, k_1 = 1, l_1 = 1$$

$\left[\text{Any direction } [hkl] \text{ where } h+k+l = 0\right]$ will be perpendicular to the [111] direction. Possible answers are
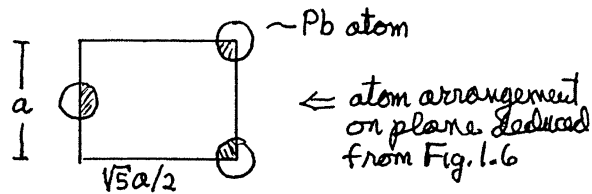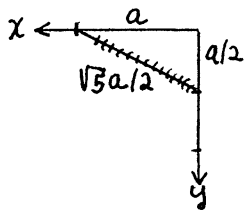
$$[11\bar{2}], [3\bar{1}\bar{2}] \text{ etc.}$$

1–4

(1.8)

(a) Cubic

(b) Examining Fig. 1.6, we conclude that there are 4 atoms within the unit cell. (There are 1/4 of 12 atoms along the cube edges and 1 interior atom. Alternatively, one might note that the Pb and S atoms lie on interpenetrating fcc lattices. The fcc lattice has 4 atoms per unit cell.)

$$\text{Pb atoms/cm}^3 = \frac{4}{a^3} = \frac{4}{(5.9362 \times 10^{-8})^3} = 1.9122 \times 10^{22}/\text{cm}^3$$

(c) A (120) plane has intercepts of $1, \frac{1}{2},$ and ∞ on the x, y and z axes, respectively.

← atom arrangement on plane deduced from Fig. 1.6

~Pb atom

$$\text{Pb atoms/cm}^2 \text{ on (120) plane} = \frac{1 \text{ atom}}{a \cdot \sqrt{5}a/2} = \frac{2}{\sqrt{5}(5.9362 \times 10^{-8})^2} = 2.5382 \times 10^{14}/\text{cm}^2$$

(1.9)

(a) If the cleavage plane is a (111), (1̄11), (11̄1) or (1̄1̄1) plane

$$\cos\theta = \frac{1}{\sqrt{3}} \Rightarrow \boxed{\theta = 54.74°}$$

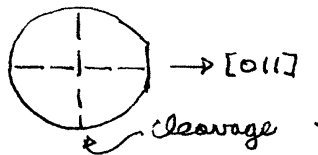If the cleavage plane is a (1̄11), (1̄1̄1), (1̄11̄) or (1̄1̄1̄) plane

$$\cos\theta = -\frac{1}{\sqrt{3}} \Rightarrow \boxed{\theta = 125.26°}$$

Actually, as inferred from Fig. P1.9, both of the above angles will be observed after a single break — one piece has a normal pointing upward, one has a normal pointing downward.

(b) <u>Four</u> pieces (ideally).

← either $(1\bar{1}1)$, $(1\bar{1}\bar{1})$, $(\bar{1}11)$ or $(\bar{1}1\bar{1})$ cleavage plane

← either $(1\bar{1}1)$, $(11\bar{1})$, $(\bar{1}\bar{1}1)$ or $(\bar{1}1\bar{1})$ cleavage plane

(c) As discussed in the text, for a (100) plane, the primary flat along the edge of the wafer is a (011) plane. The intercept of a {111} plane and the (100) plane is always a <110> direction. Thus

→ [011]

↳ cleavage

(1.10) To determine the positioning of the ingot for sawing, we must determine the angles between the [001] ↔ [112] and [110] ↔ [112] directions.

For [001] ↔ [112]

$$\cos\Theta = \frac{2}{\sqrt{6}} \qquad \Rightarrow \quad \Theta = 35.26°$$

For [110] ↔ [112]

$$\cos\Theta = \frac{2}{\sqrt{12}} \qquad \Rightarrow \quad \Theta = 54.74°$$

If ⬦ are conceptually drawn about the ingot and flat normals we see that the normal to the saw plane lies in the plane of the aforementioned normals

[001]
[112]
[110]

SAW PLANE

FLAT

PROBLEM SOLUTIONS
CHAPTER 2

(2.1) We concluded from the Bohr atom analysis that

$$E_N = \frac{m_0 q^4}{2(4\pi \epsilon_0 N \hbar)^2} = -\frac{13.6}{N^2} \text{ eV} \qquad [Eq.(2.7)]$$

Thus for an exciton in the $n = 1$ state

$$E_{ex} = \frac{(m_0/2) q^4}{2(4\pi k_s \epsilon_0 \hbar)^2} = -\frac{1}{2 k_s^2} (13.6) \text{ eV}$$

$$= -0.0488 \text{ eV}$$

(2.2) We know

$$E = \tfrac{1}{2} m_0 v^2$$

$$p = m_0 v$$

$$\lambda = h/p = 2d\sin\theta \qquad \text{or} \qquad p = \frac{h}{2d\sin\theta}$$

Thus

$$E = \tfrac{1}{2} m_0 v^2 = \frac{p^2}{2m_0} = \frac{h^2}{2m_0 (2d\sin\theta)^2}$$

$$= \left(\frac{6.63 \times 10^{-34}}{10^{-9} \sin 1^\circ}\right)^2 \frac{1}{2(9.11 \times 10^{-31})} \cdot \frac{1}{1.6 \times 10^{-19}}$$

$$\qquad\qquad\qquad\qquad\qquad\qquad \text{converts to eV}$$

$$E = 4.95 \text{ KeV}$$

(2.3)(a) Using Eq. (2.18) and Table 2.1 we conclude

$$\langle p_x \rangle = \int_0^a \psi_N^* \; \frac{\hbar}{i} \; \frac{\partial \psi_N}{\partial x} \, dx$$

$$\psi_N^* = \psi_N = A_N \sin \frac{m\pi x}{a}$$

$$\frac{\partial \psi_N}{\partial x} = \frac{m\pi}{a} A_N \cos \frac{m\pi x}{a}$$

Thus

$$\langle p_x \rangle = A_N^2 \; \frac{m\pi}{a} \; \frac{\hbar}{i} \int_0^a \sin \frac{m\pi x}{a} \cos \frac{m\pi x}{a} \, dx$$

Let $\quad \xi = \frac{m\pi}{a} x; \quad d\xi = \frac{m\pi}{a} dx; \quad \xi \Big|_0^{m\pi} \leftrightarrow x \Big|_0^a$

$$\langle p_x \rangle = A_N^2 \; \frac{\hbar}{i} \int_0^{m\pi} \sin\xi \cos\xi \, d\xi = A_N^2 \; \frac{\hbar}{i} \; \frac{\sin^2 \xi}{2} \Big|_0^{m\pi}$$

or

$$\langle p_x \rangle = \underline{\underline{0}}$$

(b) Given $\quad \psi_N = A_N \sin \frac{m\pi x}{a}$

we require $\quad \int_0^a \psi_N^* \psi_N \, dx = A_N^* A_N \int_0^a \sin^2 \left(\frac{m\pi x}{a}\right) dx = 1$

Letting $\quad \xi = \frac{m\pi}{a} x \quad$ as in part (a) yields

$$\frac{A_N^* A_N}{m\pi/a} \int_0^{m\pi} \sin^2 \xi \, d\xi = \frac{A_N^* A_N}{m\pi/a} \left(\frac{1}{2}\xi - \frac{1}{4}\sin 2\xi\right)\Big|_0^{m\pi} = \frac{|A_N|^2}{m\pi/a} \; \frac{m\pi}{2} = \frac{a}{2}|A_N|^2$$

Thus

$$|A_N|^2 = \frac{2}{a}$$

and taking A_N to be real

$$A_N = \sqrt{\frac{2}{a}}$$

(c) Referring to Eq. (2.18) and Table 2.1, we conclude

$$\langle x \rangle = \int_0^a \psi_N^* \, x \, \psi_N \, dx = \int_0^a A_N^* A_N \, x \sin^2\!\left(\frac{N\pi x}{a}\right) dx = \frac{2}{a} \int_0^a x \sin^2\!\left(\frac{N\pi x}{a}\right) dx$$

Let $y = \frac{N\pi x}{a} \Rightarrow dy = \frac{N\pi}{a} dx \qquad y\Big|_0^{N\pi}$

$$\langle x \rangle = \frac{2a}{(N\pi)^2} \int_0^{N\pi} y \sin^2 y \, dy = \frac{2a}{(N\pi)^2}\left[\frac{y^2}{4} - \frac{y \sin 2y}{4} - \frac{\cos 2y}{8}\right]\Bigg|_0^{N\pi} = \frac{a}{2}$$

(2.4) There are a number of ways to approach this problem. For example, we note first of all that, with $\xi = E/U_0 \lesssim 0.01$,

$$f(\xi) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1} \simeq -2\sqrt{\xi} \lesssim -0.2$$

all solutions therefore lie on the lower (negative) segment of the Fig. 2.7 $f(\xi)$ plot very close to $\xi = 0$, $f(\xi) = 0$. Also, with $\alpha_0 a \sqrt{\xi_{MAX}} \gg \pi$, the $\tan \alpha_0 a \sqrt{\xi}$ exhibits a large number of zeros between $\xi = 0$ and $\xi = 0.01$. Thus the tan function is almost vertical as it crosses the ξ-axis of the Fig. 2.7 plot. We therefore conclude that there will be little difference between the zeros of the tan function, corresponding to the infinite well solutions, and the intercepts on the $f(\xi)$ curve, corresponding to the finite well solutions. Clearly, for the specified situation, the energy states of the finite potential well will be very closely approximated by those of the infinitely deep potential well.

(2.5)

(a) Equations to be solved

$$\frac{d^2\psi_0}{dx^2} + k^2\psi_0 = 0 \qquad k = \sqrt{2mE/\hbar^2} \quad \ldots -a/2 < x < a/2$$

$$\frac{d^2\psi_\pm}{dx^2} - \alpha^2\psi_\pm = 0 \qquad \alpha = \sqrt{2m(U_0-E)/\hbar^2} \quad \ldots x < -\frac{a}{2}; \; x > \frac{a}{2}$$

The general solutions are

$$\psi_-(x) = A_- e^{\alpha x} + B_- e^{-\alpha x} \qquad\qquad \ldots x < -\frac{a}{2}$$

$$\psi_0(x) = A_0 \sin kx + B_0 \cos kx \qquad\qquad \ldots -\frac{a}{2} < x < \frac{a}{2}$$

$$\psi_+(x) = A_+ e^{\alpha x} + B_+ e^{-\alpha x} \qquad\qquad \ldots x > \frac{a}{2}$$

The boundary conditions are

$$\psi_-(-\infty) = 0 \; ; \qquad\qquad \psi_+(+\infty) = 0$$

$$\psi_-(-\tfrac{a}{2}) = \psi_0(-\tfrac{a}{2}) \; ; \qquad \psi_0(\tfrac{a}{2}) = \psi_+(\tfrac{a}{2})$$

$$\left.\frac{d\psi_-}{dx}\right|_{-\frac{a}{2}} = \left.\frac{d\psi_0}{dx}\right|_{-\frac{a}{2}} \; ; \qquad \left.\frac{d\psi_0}{dx}\right|_{\frac{a}{2}} = \left.\frac{d\psi_+}{dx}\right|_{\frac{a}{2}}$$

(b) $\psi_-(-\infty) = 0$ requires $B_- = 0$
$\psi_+(+\infty) = 0$ requires $A_+ = 0$
Invoking $\psi(-x) = \pm\psi(x)$ in the $-a/2 < x < a/2$ region yields

$$A_0 \sin(-kx) + B_0 \cos(-kx) = \pm A_0 \sin kx \pm B_0 \cos kx$$

or $\quad -A_0 \sin kx + B_0 \cos kx = \pm A_0 \sin kx \pm B_0 \cos kx$
and $\qquad -2A_0 \sin kx = 0 \Rightarrow A_0 = 0$ if even parity
$\qquad\qquad 2B_0 \cos kx = 0 \Rightarrow B_0 = 0$ if odd parity

The general solutions thus simplify to

$$\psi_-(x) = A_- e^{\alpha x}$$

$$\psi_0(x) = \begin{cases} B_0 \cos kx & \ldots \text{EVEN PARITY} \\ A_0 \sin kx & \ldots \text{ODD PARITY} \end{cases}$$

$$\psi_+(x) = B_+ e^{-\alpha x}$$

(c) Applying the continuity boundary conditions yields

EVEN PARITY

$$A_- e^{-\alpha a/2} = B_0 \cos \frac{ka}{2}$$

$$\alpha A_- e^{-\alpha a/2} = +k B_0 \sin \frac{ka}{2}$$

$$B_0 \cos \frac{ka}{2} = B_+ e^{-\alpha a/2}$$

$$-k B_0 \sin \frac{ka}{2} = -\alpha B_+ e^{-\alpha a/2}$$

ODD PARITY

$$A_- e^{-\frac{\alpha a}{2}} = -A_0 \sin \frac{ka}{2} \qquad ①$$

$$\alpha A_- e^{-\alpha a/2} = +k A_0 \cos \frac{ka}{2} \qquad ②$$

$$A_0 \sin \frac{ka}{2} = B_+ e^{-\alpha a/2} \qquad ③$$

$$k A_0 \cos \frac{ka}{2} = -\alpha B_+ e^{-\alpha a/2} \qquad ④$$

Combining either equations ① and ② or ③ and ④, we conclude

$$\alpha = \begin{cases} k \tan \frac{ka}{2} & \text{... even parity} \\ -k \cot \frac{ka}{2} & \text{... odd parity} \end{cases}$$

(d) Eq. (2.43b) reads $\tan ka = \frac{2\alpha k}{k^2 - \alpha^2}$, or taking the HINT

$$\tan ka = \frac{2 \tan(ka/2)}{1 - \tan^2(ka/2)} = \frac{2\alpha k}{k^2 - \alpha^2} = \frac{2\alpha/k}{1 - (\alpha/k)^2} \equiv 1/\gamma$$

or

$$2 \tan(ka/2) = [1 - \tan^2(ka/2)]/\gamma$$

$$\tan^2(ka/2) + 2\gamma \tan(ka/2) - 1 = 0 \quad \Leftarrow \text{Quadratic Equation}$$

$$\therefore \quad \tan(ka/2) = -\gamma \pm [\gamma^2 + 1]^{1/2}$$

but $\gamma^2 + 1 = \left[\frac{1 - (\alpha/k)^2}{2\alpha/k}\right]^2 + 1 = \frac{1 - 2(\alpha/k)^2 + (\alpha/k)^4 + 4(\alpha/k)^2}{4(\alpha/k)^2} = \left[\frac{1 + (\alpha/k)^2}{2\alpha/k}\right]^2$

thus

$$\tan \frac{ka}{2} = -\left[\frac{1 - (\alpha/k)^2}{2\alpha/k}\right] \pm \left[\frac{1 + (\alpha/k)^2}{2\alpha/k}\right] = \begin{cases} \alpha/k & \text{... (+) root} \\ -k/\alpha & \text{... (-) root} \end{cases}$$

$\qquad\qquad\qquad\qquad\qquad\qquad \Leftarrow$ same as part (c) result