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# ELG6380 Theory of Semiconductor Devices

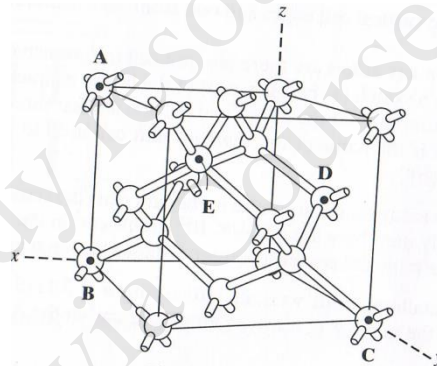
## Assignment 1

Due: 2 February 2017

From Pierret, 2<sup>nd</sup> ed., Advanced Semiconductor Fundamentals

**1.5** Referring to the unit cell of the SI lattice reproduced in Fig. P1.5, and noting that the origin of coordinates is located at the lower back corner of the unit cell:

- What are the Miller indices of the plane passing through the points ABC?
- What are the Miller indices of the plane passing through the points BCD?
- What are the Miller indices of the direction vector running from the origin of coordinates to the point D?
- What are the Miller indices of the direction vector running from the origin of coordinates to the point E?



...see next page

1.9 A SI wafer will tend to cleave (break apart) along  $\{111\}$  planes if sufficient stress is applied to the surface of the wafer. If the top surface of the wafer is a  $(100)$  plane as pictured in Fig. P1.9:

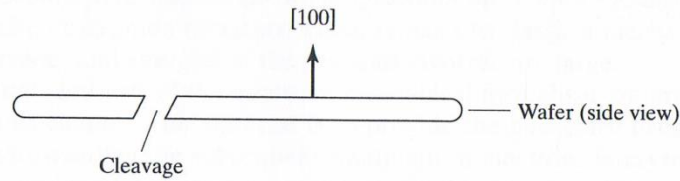
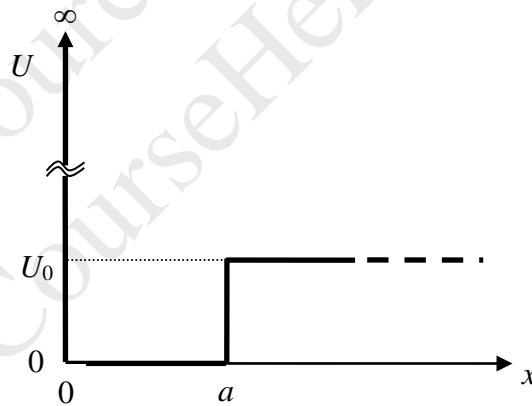


Figure P1.9

- What are the possible angles between the normal to the top surface and the cleavage planes?
- If pressure is applied to a point on the surface of the wafer and  $\{111\}$  plane cleavage occurs through the pressure point, into how many pieces at maximum will the wafer break? (A million pieces is not the correct answer.)
- Assuming cleavage occurs along a  $\{111\}$  plane, how will the broken edge of the wafer be oriented relative to the primary wafer flat?

2.6 A particle of mass  $m$  and fixed total energy  $E$ , where  $0 < E < U_0$ , is placed in the one-dimensional potential well shown on the right:



- Write down the simplified form of Schrödinger's equation appropriate for the various spatial regions.
- Indicate the general solutions to your part (a) equations.
- List the boundary conditions appropriate for the given problem.
- Establish the simultaneous equations that result by applying the part (c) boundary conditions.
- Obtain the equation that must be solved to determine the allowed particle energies.

1.5) (a) The plane passing through ABC :

intercepts :  $1, 1, \infty$

invert :  $1, 1, 0$

integer set :  $1, 1, 0$

Miller indices :  $(110)$

(b) The plane passing through BCD :

intercepts :  $1, 1, 1$  (D is a face centre)

invert :  $1, 1, 1$

integer set :  $1, 1, 1$

Miller indices :  $(111)$

(c) Direction vector, origin to D :

D lies on the  $yz$ -plane face centre

Projection :  $0, \frac{1}{2}, \frac{1}{2}$

integer set :  $0, 1, 1$

Direction :  $[011]$

(d) Direction vector, origin to E :

E lies along the main cube diagonal,  $\frac{3}{4}$  of the diagonal length from the origin.

The diagonal direction is  $[111]$

1.9) Si wafer with a (100) surface. The wafer cleaves along  $\{111\}$  planes.

(a) Since  $\cos \theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{[(h_1^2 + k_1^2 + l_1^2)(h_2^2 + k_2^2 + l_2^2)]^{1/2}}$

For  $[h_2 k_2 l_2] = [100]$ , and  $\sqrt{h_1^2 + k_1^2 + l_1^2} = \sqrt{3}$ , this reduces to

$$\cos \theta = \frac{h_1}{\sqrt{3}}$$

The 8 equivalent planes in the  $\{111\}$  set can be classified by  $h_1 = +1$  or  $h_1 = -1$ . For the former,  $(111)$ ,  $(1\bar{1}1)$ ,  $(11\bar{1})$ ,  $(1\bar{1}\bar{1})$  yield

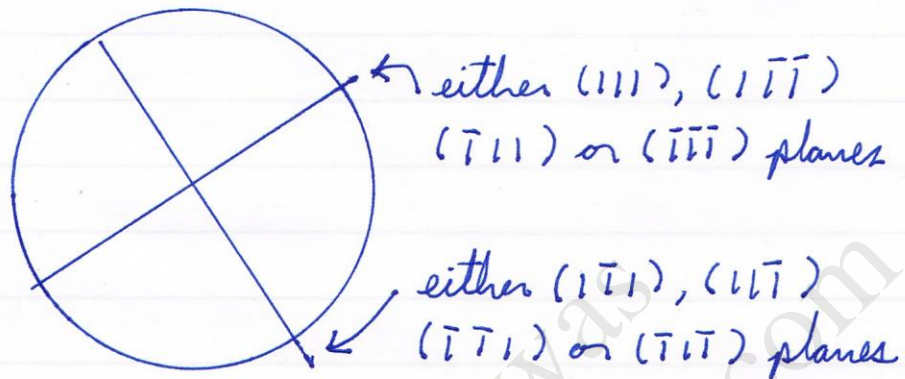
$$\cos \theta = \frac{1}{\sqrt{3}} \Rightarrow \theta = 54.74^\circ$$

For the latter,  $(\bar{1}11)$ ,  $(\bar{1}\bar{1}1)$ ,  $(\bar{1}1\bar{1})$ ,  $(\bar{1}\bar{1}\bar{1})$  yield

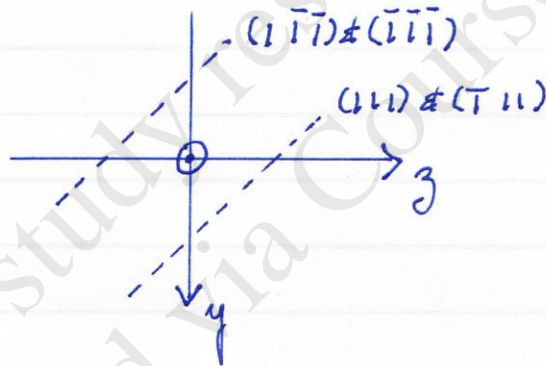
$$\cos \theta = \frac{-1}{\sqrt{3}} \Rightarrow \theta = 125.26^\circ$$

These angles are equivalent under inversion of the surface normal.

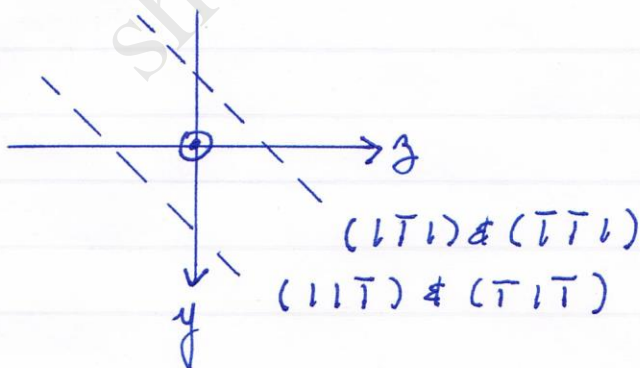
(b) The maximum number of pieces into which the wafer will break along  $\{111\}$  cleavage planes is 4, as noted below:



The top set of plane possibilities can be seen from planes intersecting the  $yz$ -plane as follows



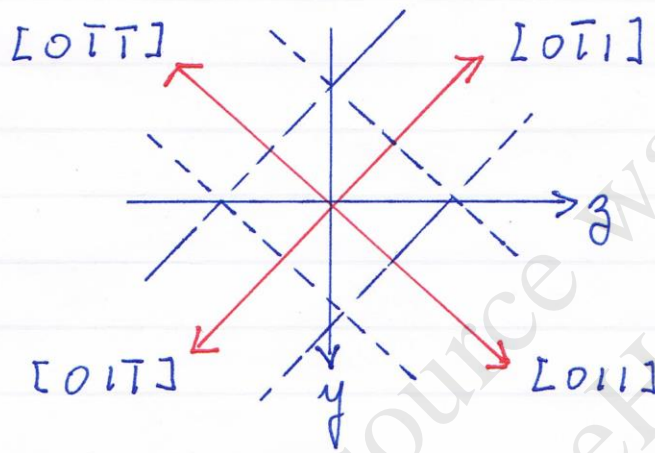
The bottom set is due to the other orientation



NB. The  $[100]$  direction is out of the page.

(c) For an Si wafer with a (100) surface, the primary flat is in the  $[011]$  direction.

as is noted below, the  $\{111\}$  planes intersect the (100) surface as follows:



These intercepts are  $\langle 011 \rangle$  directions. Thus, the broken edge will either be oriented along the flat, or at right angles to it.

(2.6) (a) Because the potential is infinite for  $x \leq 0$ , we only need to deal with the two regions  $0 < x < a$  and  $x > a$

$$\frac{d^2 \psi_0}{dx^2} + k^2 \psi_0 = 0, \quad 0 < x < a$$

$$\text{where } k^2 = 2mE/\hbar^2$$

$$\frac{d^2 \psi_+}{dx^2} - \alpha^2 \psi_+ = 0, \quad x > a$$

$$\text{where } \alpha^2 = 2m(V_0 - E)/\hbar^2$$

(b) The general solutions to the equations above are found from equations (2.39b) & (2.39c) in the notes as

$$\psi_0(x) = A_0 \sin(kx) + B_0 \cos(kx), \quad 0 < x < a$$

$$\psi_+(x) = A_+ e^{\alpha x} + B_+ e^{-\alpha x}, \quad x > a$$

(c) The appropriate boundary conditions are

$$\psi_0(0) = 0$$

$$\psi_+(+\infty) = 0$$

$$\psi_0(a) = \psi_+(a)$$

$$\left. \frac{d\psi_0}{dx} \right|_a = \left. \frac{d\psi_+}{dx} \right|_a$$

(d) Applying the boundary conditions yields

$$B_0 = 0, \quad A_+ = 0$$

$$A_0 \sin(ka) = B_+ e^{-\alpha a} \quad (*)$$

$$kA_0 \cos(ka) = -\alpha B_+ e^{-\alpha a} \quad (**)$$

(e) Dividing (\*) by (\*\*) yields

$$\frac{1}{k} \tan(ka) = -\frac{1}{\alpha}$$

$$\Rightarrow \tan(ka) = -\frac{k}{\alpha}$$

$$= -\sqrt{\frac{E}{U_0 - E}}$$