WEISS INDICES (CELL PARAMETERS), MILLER INDICES, MILLER PLANES

WEISS INDICES

- Once a unit cell is defined. and the lengths of the cell axes (a, b, and c) determined, these can be placed and mapped against a three-dimensional Cartesian-like plot, where the axes are defined by x, y, and z.
- Lets consider an orthorhombic P-type cell in which all angles are equivalent to 90°, and all unit cell lengths are nol equal. where a = 2, b = l, and c = 3,

Figure 2.1 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

- These planes. known as Miller planes, can be identified by a set of three integer values (zero, positive or negative values), h, k, l, known as Miller indices. Miller indices generally refer to sets of parallel planes. The use of Miller indices is also helpful in explaining and further understanding diffraction patterns that result from an X-ray diffraction experiment.

- Miller indices are written in brackets (/1, k, 1)

Table 2.1 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

DETERMINING MILLER INDICES AND IDENTIFYING MILLER PLANES

- Miller indices are determined from the intercepts of the planes along the crystallographic axes. This is done by:

(a) First, *determining the intercepts* of the face along the crystallographic axes (if a plane is parallel to an axis, its value is infinite, ∞);

(b) Then, taking the reciprocals;

(c) Clearing the fractions; and

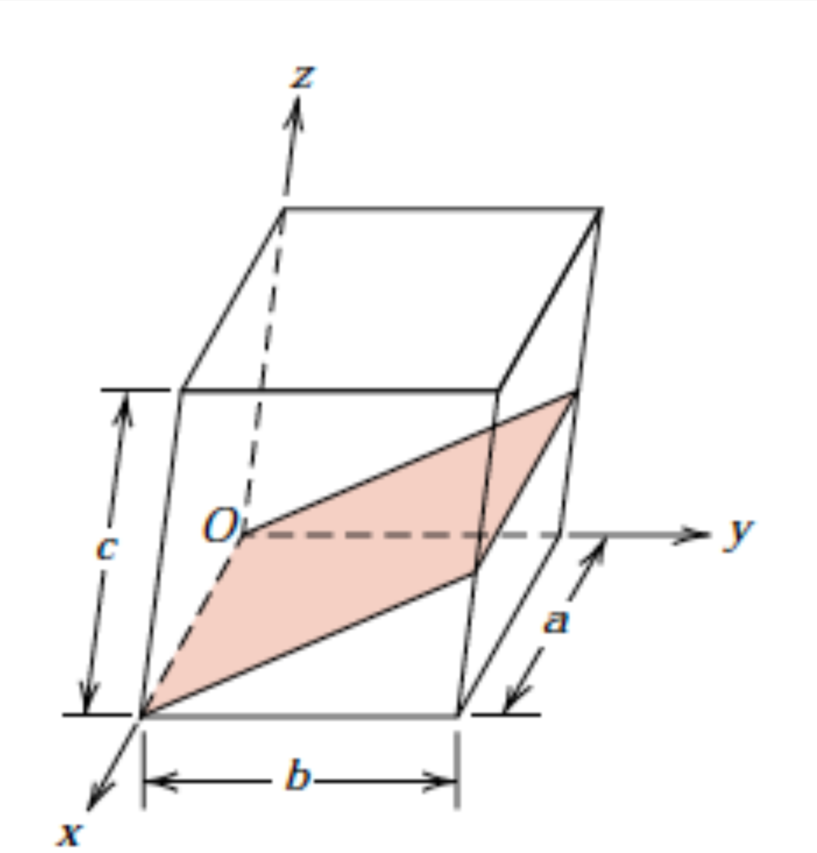
(d) Finally, reducing the indices to lowest terms.

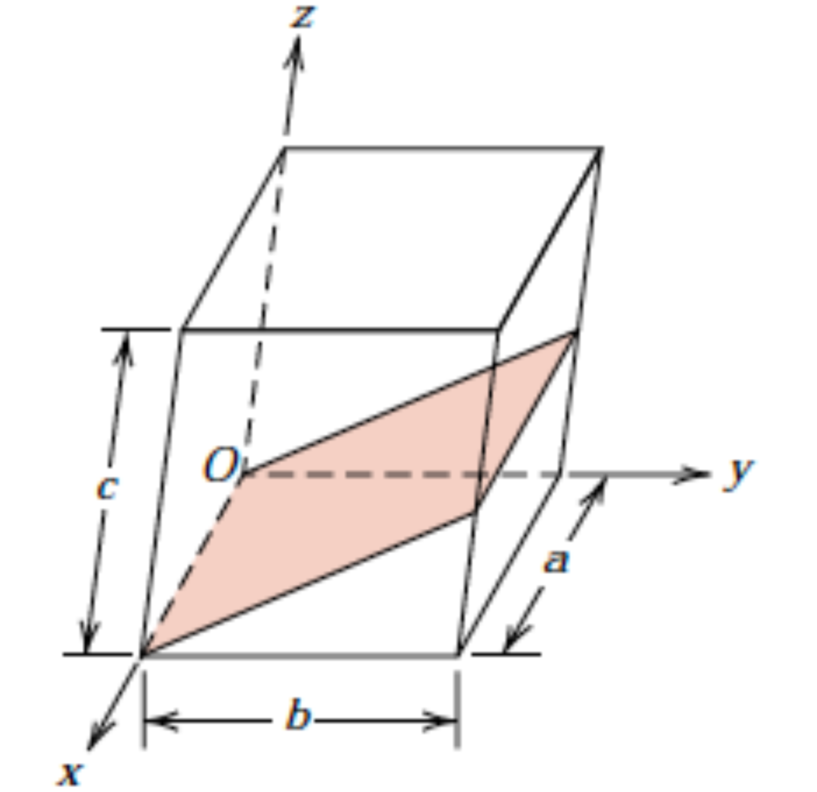
Figure 2.2a Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

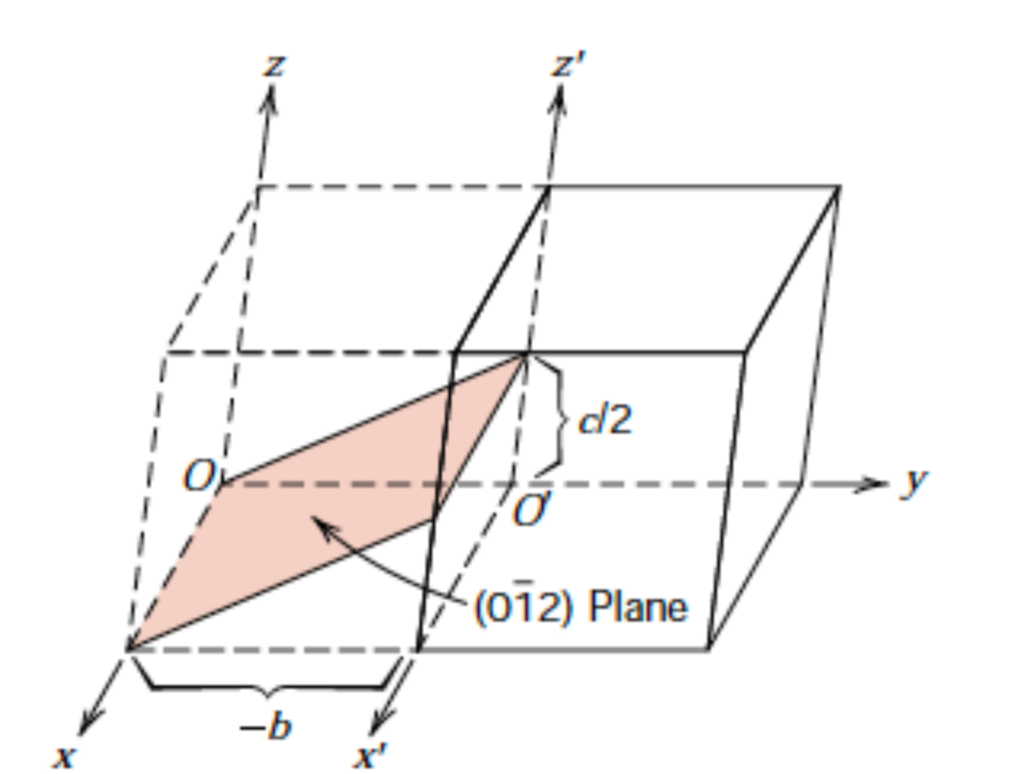
Figure 2.2b Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

QUESTION

Determine the Miller indices for the plane shown in the accompanying sketch (a).







Since the plane passes through the selected origin O, a new origin must be chosen at the corner of an adjacent unit cell, taken as O and shown in sketch (b). This plane is parallel to the x axis, and the intercept may be taken as a. The y and z axes intersections, referenced to the new origin O', are -b and c/2, respectively. Thus, in terms of the lattice parameters a, b, and c, these intersections are ∞, 1, and 1/2. The reciprocals of these numbers are 0, -1, and 2; and since all are integers, no further reduction is necessary. Finally, enclosure in parentheses yields (012).

	x	y	z
Intercepts	∞a	$-b$	$c/2$
Intercepts (in terms of lattice parameters)	∞	-1	$\frac{1}{2}$
Reciprocals	0	-1	2
Reductions (unnecessary)			
Enclosure		$(0\bar{1}2)$	

QUESTION

1. Determine the Miller Indices of the shaded areas in the diagrams below.

Figure 2.3 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

HOWEWORK

- llustrate (100), (110), (111), and (112) planes in cubic lattice and direction indices of [010], [111], [$\bar{1}$00], and [120].

X-RAY DIFFRACTION

- **Diffraction by crystals:** During an X-ray diffraction experiment, a crystal is irradiated with X-rays. The interaction between the oscillating electrons within each atom and the incoming X-ray beam causes the X-rays to diffract in all directions. The diffracted X-ray beams from all the Miller sets gives rise to 'diffraction spots'. The diffraction spots represent the diffraction pattern of the crystal being examined.

Figure 2.5 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

BRAGG'S LAW

- Bragg's law is able to provide a Simplified explanation as to how diffraction spots and patterns are produced from the incident X-ray beam.

Figure 2.6 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

When the incident X-rays collide with the crystal lattice at specific points, the X-rays are reflected or diffracted out from these points giving rise to diffraction spots.

Figure 2.6 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

The path taken by the incident and reflected beam can be calculated as the sum of AY and YB and this is equal to the wavelength of the incident X-ray beam, nλ. If the angle at which the incident beam collides with the crystal is θ, then we can calculate the path difference in terms of d, θ, and λ.

$$AY + YB = n\lambda,$$

and we know that

$$\sin\theta = AY/d,$$

rearranging the equation

$$AY = d\sin\theta \quad (AY = YB),$$

therefore, the path difference is

$$2d\sin\theta = n\lambda.$$