Primer on Semiconductors

Unit 1: Material Properties

Lecture 1.3: Miller indices

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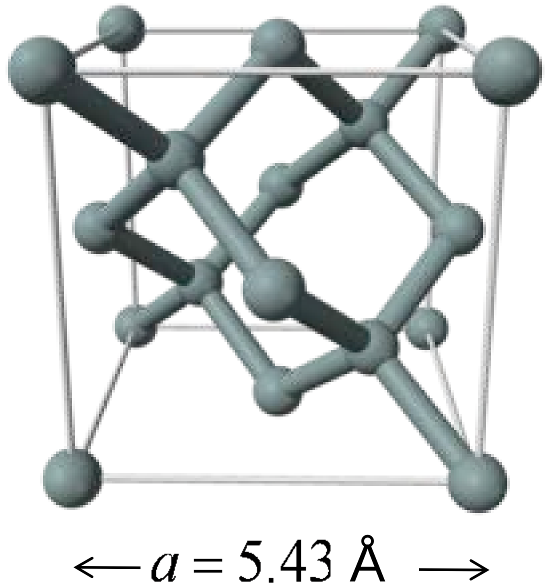
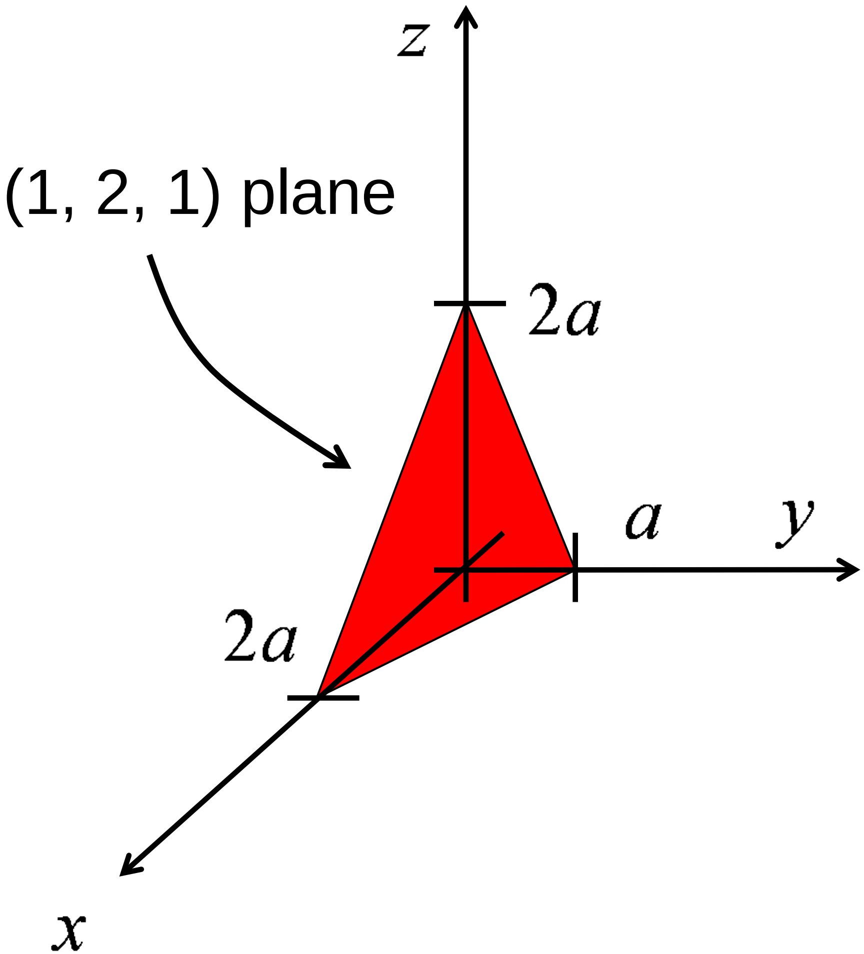
Si crystal structure (diamond lattice)



How do we specify planes and directions in a crystal?

For cubic crystals, there is a simple prescription.

Miller index prescription for describing planes



1) x, y, and z-axis intercepts:

2a, 1a, 2a
2, 1, 2

2) invert:

½ 1, ½

3) Rationalize:

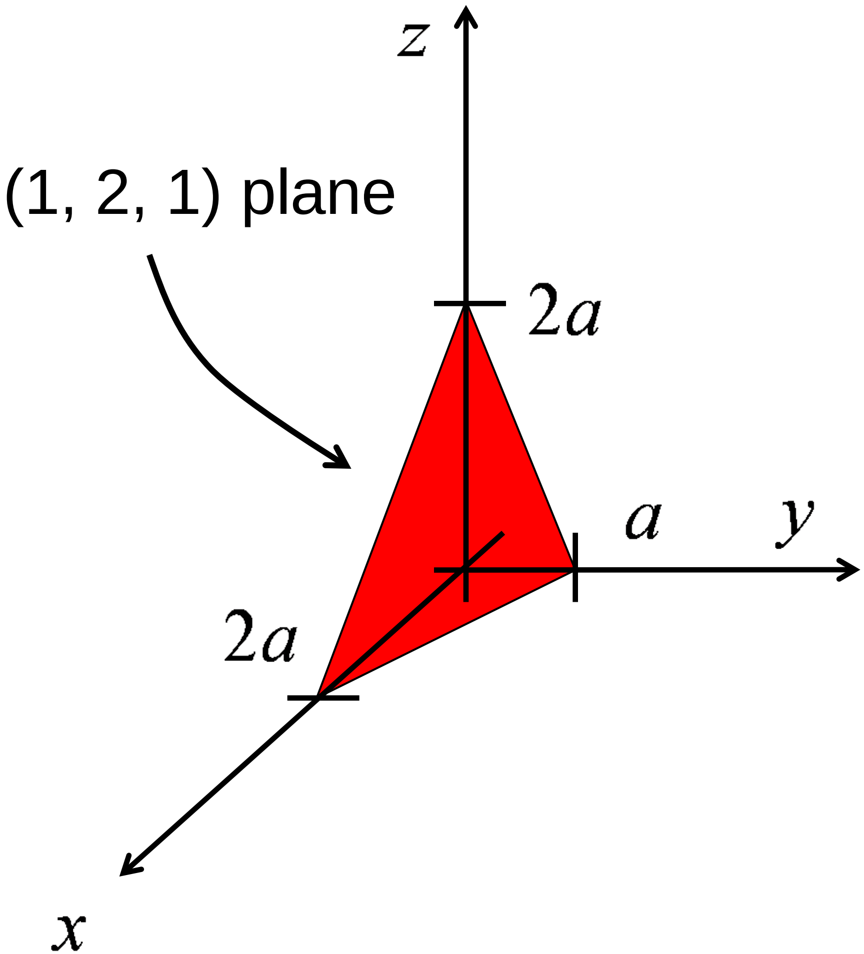
1, 2, 1

Question

Where does this prescription come from?

Answer: If we remember the equation for a plane, we can figure it out.

Where it comes from?



equation of a plane:

$$\frac{x}{x_{\text{int}}} + \frac{y}{y_{\text{int}}} + \frac{z}{z_{\text{int}}} = 1$$

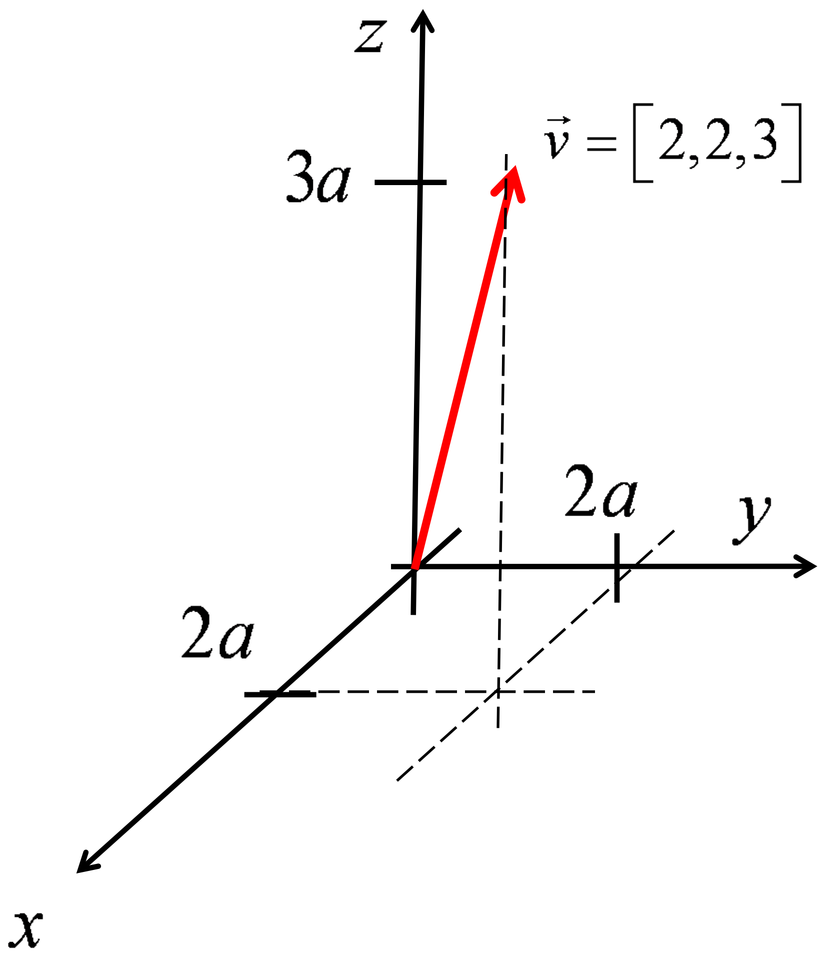
describe with the numbers:

$$\frac{1}{x_{\text{int}}}, \frac{1}{y_{\text{int}}}, \frac{1}{z_{\text{int}}}$$

equivalent to:

$$\frac{1}{x_{\text{int}}/a}, \frac{1}{y_{\text{int}}/a}, \frac{1}{z_{\text{int}}/a}$$

Prescription for describing directions



1) equation of a vector:

$$\vec{v} = 2a\hat{x} + 2a\hat{y} + 3a\hat{z}$$

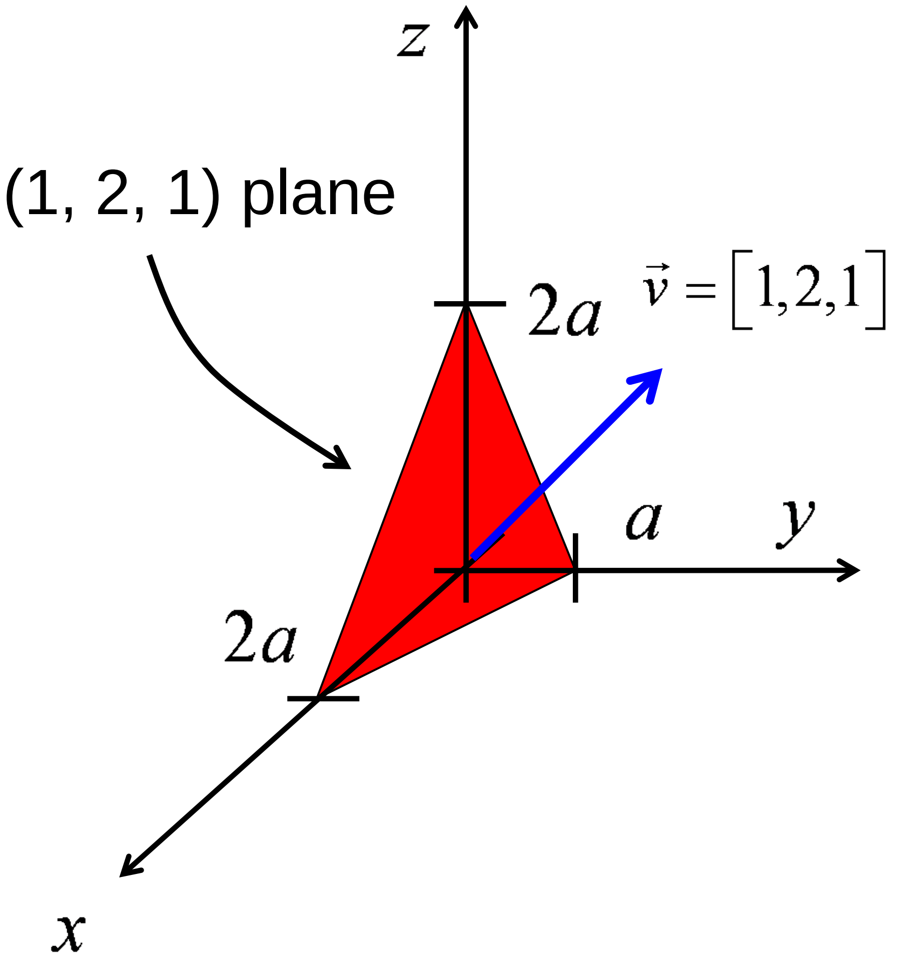
2) describe with components:

$$2a, 2a, 3a$$

3) equivalent to:

$$2,2,3$$

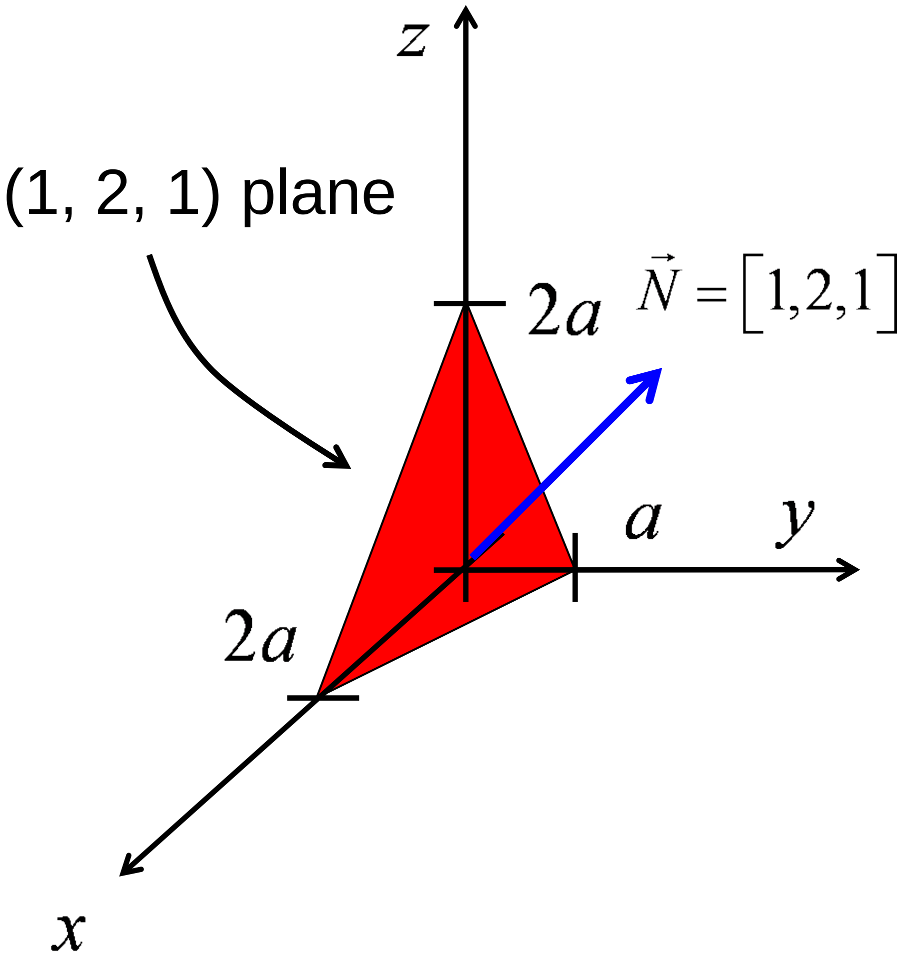
Direction normal to a plane



The vector [1, 2, 1] is normal to the plane (1, 2, 1).

Why?

Why is [h k l] normal to (h k l)?



equation of a plane:

$$f(x,y,z) = \frac{x}{x_{\text{int}}} + \frac{y}{y_{\text{int}}} + \frac{z}{z_{\text{int}}} = 1$$

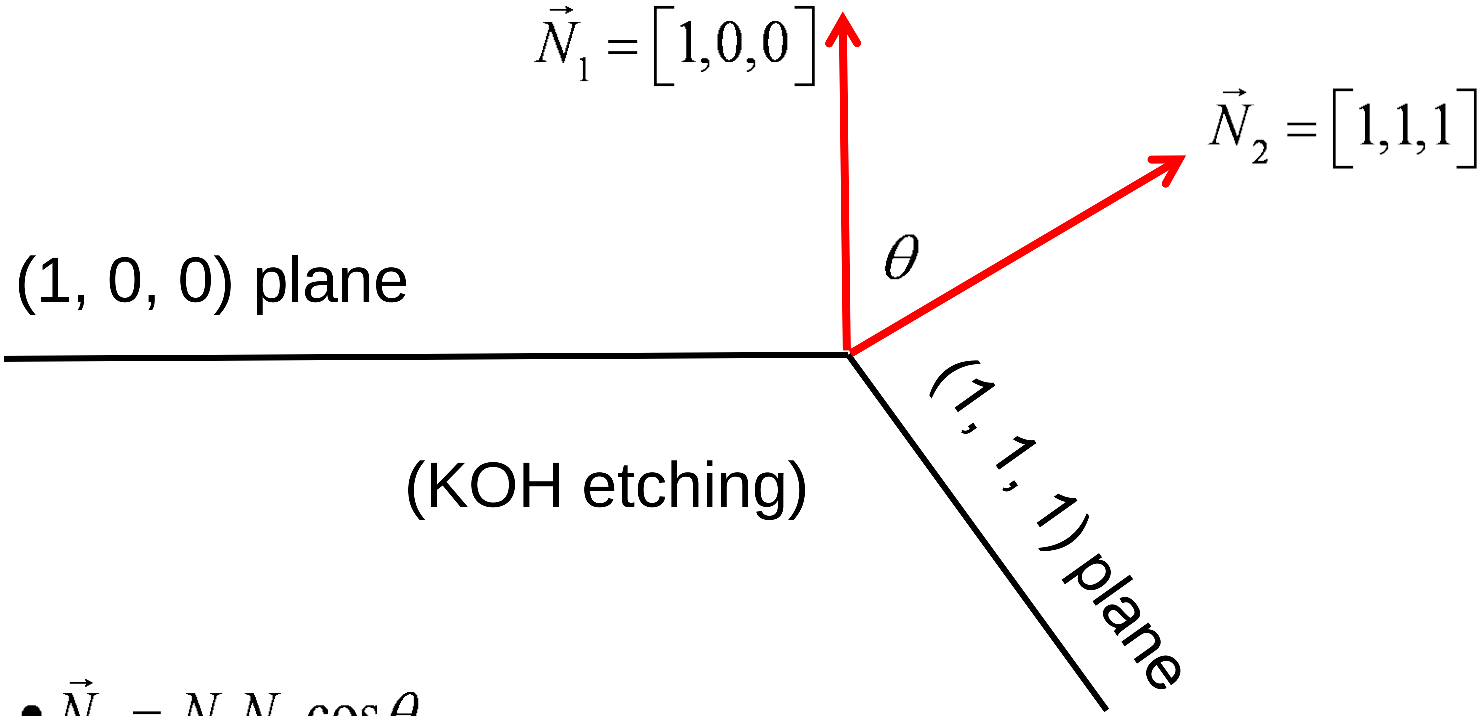
normal to a plane:

$$\vec{N} = \nabla f(x,y,z) = \frac{\partial f}{\partial x}\hat{x} + \frac{\partial f}{\partial y}\hat{y} + \frac{\partial f}{\partial z}\hat{z}$$

(gradient)

$$\vec{N} = \frac{1}{x_{\text{int}}}\hat{x} + \frac{1}{y_{\text{int}}}\hat{y} + \frac{1}{z_{\text{int}}}\hat{z}$$

Angle between planes



$$\vec{N}_1 \bullet \vec{N}_2 = N_1 N_2 \cos\theta$$

$$\cos\theta = \frac{\vec{N}_1 \bullet \vec{N}_2}{N_1 N_2}$$

Angle between planes

$$\cos\theta = \frac{\vec{N}_1 \bullet \vec{N}_2}{N_1 N_2}$$

$$\vec{N}_1 = \left[h_1, k_1, l_1\right]$$

$$\vec{N}_2 = \left[h_2, k_2, l_2\right]$$

$$\boxed{\cos\theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}}}$$

$$\vec{N}_1 = \left[1,0,0\right]$$

$$\vec{N}_2 = \left[1,1,1\right]$$

$$\cos\theta = \frac{1+0+0}{\sqrt{1^2 + 0^2 + 0^2}\sqrt{1_2^2 + 1_2^2 + 1_2^2}}$$

$$\cos\theta = \frac{1}{\sqrt{3}}$$

$$\theta = 54.7^\circ$$

Notation for planes and directions

$\left(h\ k\ l \right)$ A specific plane.

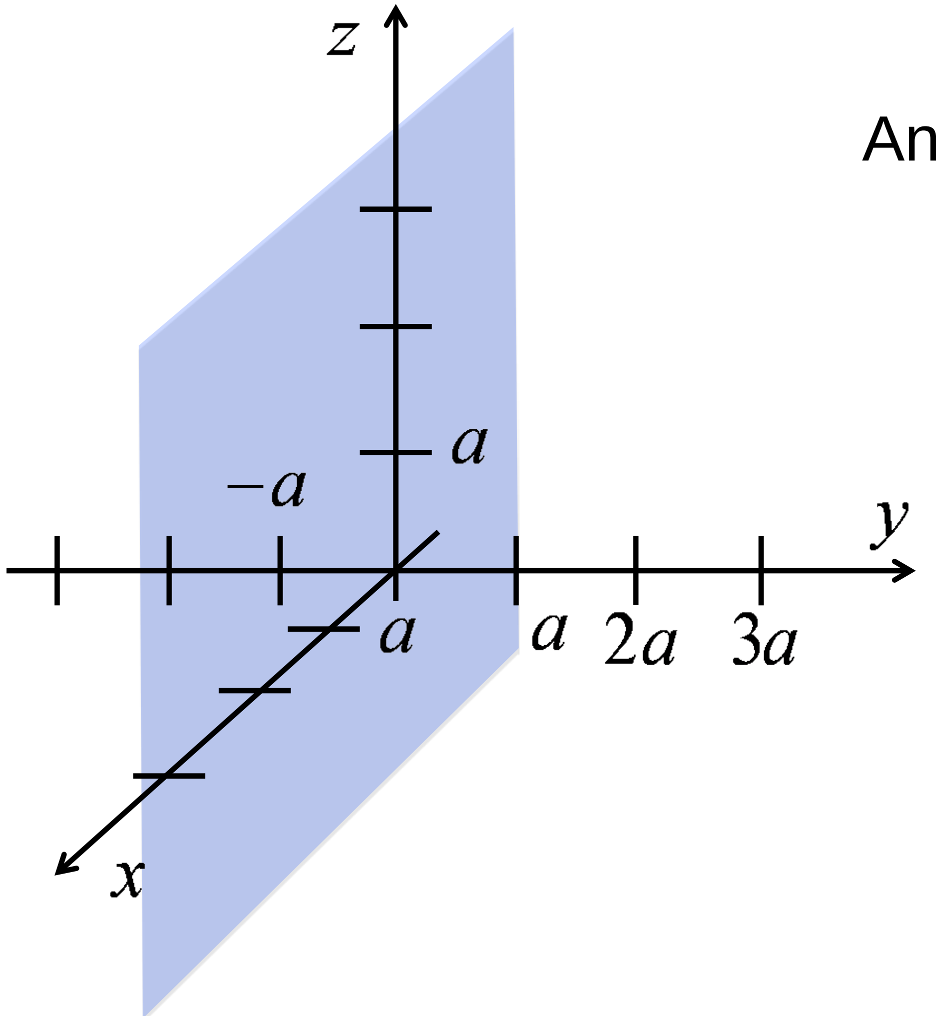
$\left[h\ k\ l \right]$ A direction normal to the plane above.

$$\vec{N} = ha\hat{x} + ka\hat{y} + la\hat{z}$$

$\left\{ h\ k\ l \right\}$ A set of equivalent planes.

$\left\langle h\ k\ l \right\rangle$ A set of equivalent directions.

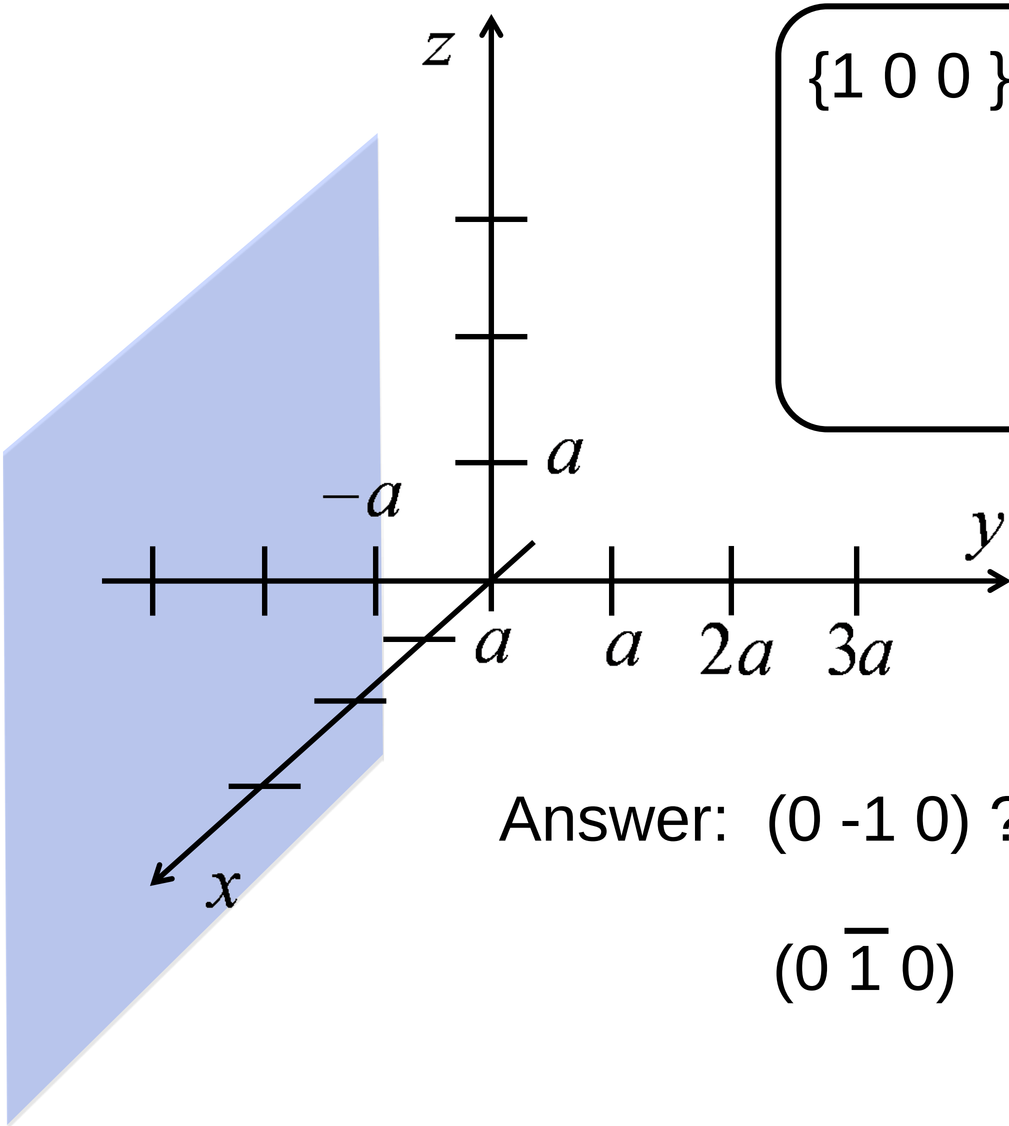
What plane is this?



Answer: (0 1 0)

(0 2 0) ?

What plane is this?



$\{1\ 0\ 0\}$ set of equivalent planes

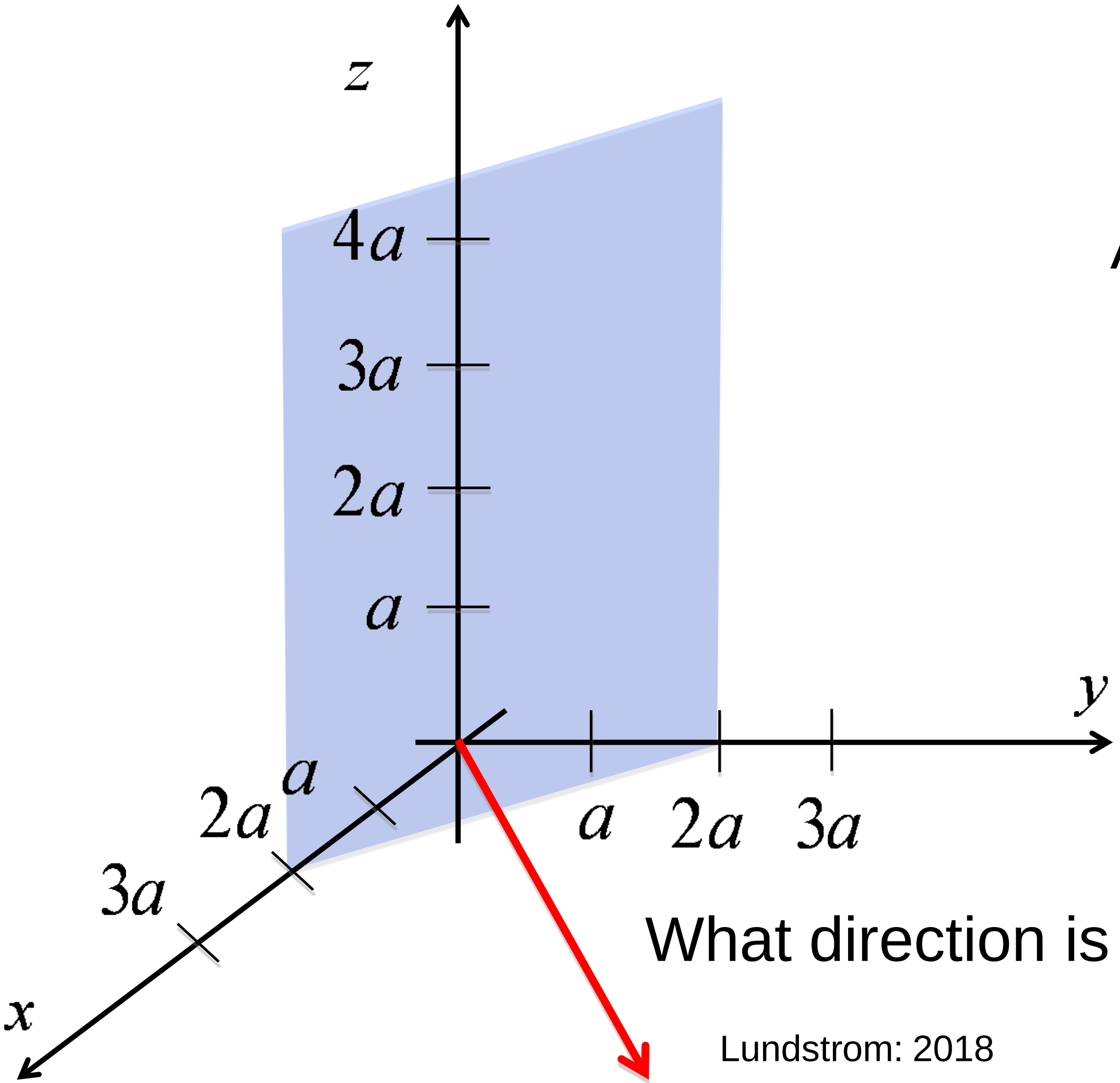
(100) (010) (001)

$(\bar{1}00)$ $(0\bar{1}0)$ $(00\bar{1})$

Answer: (0 -1 0) ?

$(0\ \bar{1}\ 0)$

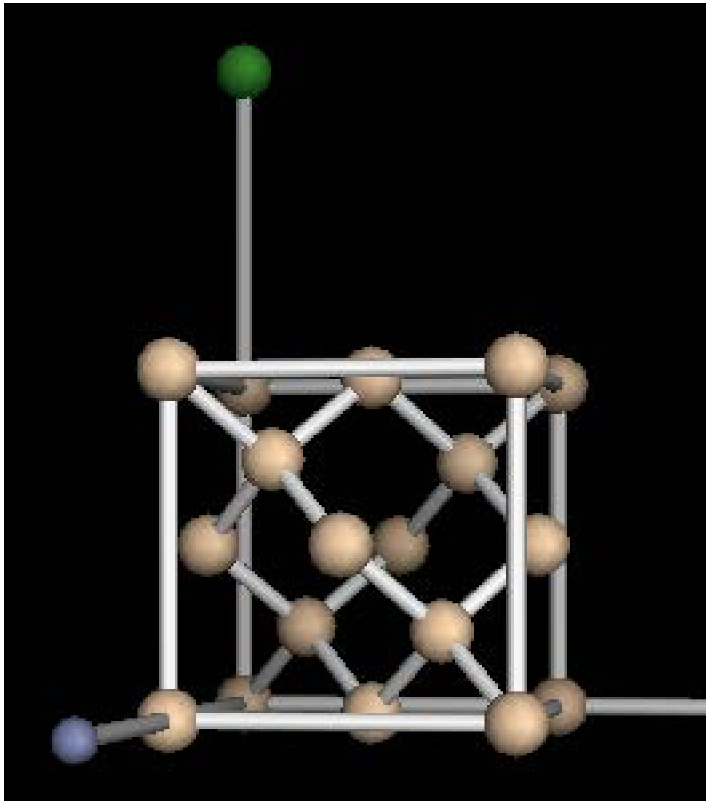
What plane is this?



Answer: (1 1 0)

What direction is this?

Silicon: atoms / cm^2 on a {100} plane



Lattice constant: 5.4307 Å

Atoms on face = (4 times ¼) +1 = 2

$N_S = 2/a^2$

$N_S = 6.81\text{x } 10^{14} /cm^2$

https://nanohub.org/tools/crystal_viewer

Summary

Miller indices provide a simple way to describe planes and directions in crystals.

For cubic systems, the prescription is simple.

Summary of Miller index notation

$\left(h\,k\,l\right)$ A specific plane.

$\left[h\,k\,l\right]$ A direction normal to the plane above.

$\left\{h\,k\,l\right\}$ A set of equivalent planes.

$\left\langle h\,k\,l\right\rangle$ A set of equivalent directions.