Notes for ECE-606: Spring 2013

L2: Miller Indices

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prescription for describing planes

x, y, and z-axis intercepts:
2a, 1a, 2a
2, 1, 2

invert:
½, 1, ½

Rationalize:
1, 2, 1
where it comes from

Equation of a plane:

\[
\frac{x}{x_{int}} + \frac{y}{y_{int}} + \frac{z}{z_{int}} = 1
\]

describe with numbers:

\[
\frac{1}{x_{int}/a}, \frac{1}{y_{int}/a}, \frac{1}{z_{int}/a}
\]

equivalent to:

\[
\frac{1}{x_{int}/a}, \frac{1}{y_{int}/a}, \frac{1}{z_{int}/a}
\]

prescription for describing directions

equation of a vector:

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

describe with components:

\(2a, 2a, 3a\)

equivalent to:

\(2, 2, 3\)
direction normal to a plane

\[ (1, 2, 1) \text{ plane} \]

\[ \vec{v} = [1, 2, 1] \]

where it comes from

\[ \text{equation of a plane:} \]

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

\[ \text{normal to a plane:} \]

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

\[ \vec{N} = \frac{1}{x_{\text{int}}} \hat{x} + \frac{1}{y_{\text{int}}} \hat{y} + \frac{1}{z_{\text{int}}} \hat{z} \]
angle between planes

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

(1, 0, 0) plane

\( \theta \)

(1, 1, 1) plane

(KOH etching)

\[ \vec{N}_2 = [1, 1, 1] \]

\[ \vec{N}_1 \cdot \vec{N}_2 = N_1 N_2 \cos \theta \]

\[ \cos \theta = \frac{\vec{N}_1 \cdot \vec{N}_2}{N_1 N_2} \]

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

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

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

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

\[ \vec{N}_2 = [1, 1, 1] \]

\[ \cos \theta = \frac{1 + 0 + 0}{\sqrt{1^2 + 0^2 + 0^2} \sqrt{1^2 + 1^2 + 1^2}} \]

\[ \cos \theta = \frac{1}{\sqrt{3}} \]

\[ \theta = 54.7^\circ \]
distance between adjacent planes

$(h,k,l)$

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

distance $d = \frac{1}{|\tilde{N}|}$

$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

References:


The diamond lattice

FCC Bravais lattice

Basis of 2 atoms per site
(000) and \((\frac{1}{4} \frac{1}{4} \frac{1}{4})\)

https://nanohub.org/tools/crystal_viewer
The diamond lattice

Atoms per unit cell

8 times $\frac{1}{8}$ + 6 times $\frac{1}{2}$ + 4

8 atoms per unit cell

https://nanohub.org/tools/crystal_viewer

Silicon: density

Lattice constant: $a = 5.4307$ Ang

Density = total mass/vol. of unit cell.

Atomic mass of Si: 28.0855 amu

1 amu = $1.6605 \times 10^{-27}$ kg

$$\rho = \frac{8 \times 28.0855 \times 1.6605 \times 10^{-27}}{(5.4307 \times 10^{-10})^3} \text{ kg/m}^3$$

$$\rho = 2.3296 \text{ g/cm}^3$$

https://nanohub.org/tools/crystal_viewer
Silicon: NN spacing

Lattice constant: $a = 5.4307$ Ang

Body diagonal = $\sqrt{3}a$.

NN spacing = $\sqrt{3}a/4$

https://nanohub.org/tools/crystal_viewer

Silicon: packing density

Lattice constant: $a = 5.4307$ Ang

NN spacing = $\sqrt{3}a/4$

Radius of atom = $\frac{1}{2}$ NN spacing

= $\sqrt{3}a/8$

Vol of atom = $(4/3)\pi R^3$

$$PF = \frac{8 \times \frac{4}{3} \pi R^3}{(a)^3} = \frac{\sqrt{3}\pi}{16} = 34\%$$
Silicon: atoms / cm² on (100)

Lattice constant: 5.4307 Å
Atoms on face = 4 times \( \frac{1}{4} + 1 = 2 \)

\[ N_s = \frac{2}{a^2} \]

\[ N_s = 6.81 \times 10^{14} / \text{cm}^2 \]

https://nanohub.org/tools/crystal_viewer