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:
   - $\frac{1}{2}$, $1$, $\frac{1}{2}$

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:

\[
\frac{1}{x_{\text{int}}} \cdot \frac{1}{y_{\text{int}}} \cdot \frac{1}{z_{\text{int}}}
\]

equivalent to:

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

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

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

(1, 0, 0) plane

(KOH etching)

(1, 1, 1) plane

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

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

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Angle between planes

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

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

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

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

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

\[
\vec{N}_2 = \begin{bmatrix} 1, 1, 1 \end{bmatrix}
\]

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

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

\[
\theta = 54.7^\circ
\]
Notation for planes and directions

\[
\left( \begin{array}{c} h \\ k \\ l \end{array} \right) \quad \text{A specific plane.}
\]

\[
\begin{bmatrix} h & k & l \end{bmatrix} \quad \text{A direction normal to the plane above.}
\]

\[
\{ h k l \} \quad \text{A set of equivalent planes.}
\]

\[
\left< h k l \right> \quad \text{A set of equivalent directions.}
\]

\[
\vec{N} = h\hat{x} + k\hat{y} + l\hat{z}
\]
What plane is this?

Answer: (0 1 0)

(0 2 0)?
What plane is this?

Answer: $(0 \ 1 \ 0)$

\begin{align*}
\{1 \ 0 \ 0 \} \text{ set of equivalent planes} \\
(100) \ (010) \ (001) \\
(\overline{1}00) \ (\overline{0}10) \ (00\overline{1})
\end{align*}
What plane is this?

Answer: \((1 \ 1 \ 0)\)

What direction is this?
Silicon: atoms / cm² on a \{100\} plane

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

Lundstrom: 2018
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

\( (h \ k \ l) \) A specific plane.

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

\( \{h \ k \ l\} \) A set of equivalent planes.

\( \langle h \ k \ l \rangle \) A set of equivalent directions.