Advanced Electromagnetics:
21st Century Electromagnetics

Lattice Vectors

Lecture Outline

• Direct lattice vectors
• Reciprocal lattice vectors
• Converting between direct and reciprocal lattice vectors
Direct Lattice Vectors

Axis vectors most intuitively define the shape and orientation of the unit cell. They cannot uniquely describe all 14 Bravais lattices, but they do uniquely identify the 7 crystal systems.

Translation vectors connect adjacent points in the lattice and can uniquely describe all 14 Bravais lattices. They are less intuitive to interpret.

Primitive lattice vectors are the smallest possible vectors that still describe the unit cell.
Calculating Translation Vectors From Axis Vectors

Simple
\[
\begin{bmatrix}
\ell_1 \\
\ell_2 \\
\ell_3 \\
\end{bmatrix} =
\begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
\end{bmatrix}
\begin{bmatrix}
\vec{a}_1 \\
\vec{a}_2 \\
\vec{a}_3 \\
\end{bmatrix}
\]

Body-Centered
\[
\begin{bmatrix}
\ell_1 \\
\ell_2 \\
\ell_3 \\
\end{bmatrix} =
\begin{bmatrix}
-1/2 & 1/2 & 1/2 \\
1/2 & -1/2 & 1/2 \\
1/2 & 1/2 & -1/2 \\
\end{bmatrix}
\begin{bmatrix}
\vec{a}_1 \\
\vec{a}_2 \\
\vec{a}_3 \\
\end{bmatrix}
\]

Face-Centered
\[
\begin{bmatrix}
\ell_1 \\
\ell_2 \\
\ell_3 \\
\end{bmatrix} =
\begin{bmatrix}
0 & 1/2 & 1/2 \\
1/2 & 0 & 1/2 \\
1/2 & 1/2 & 0 \\
\end{bmatrix}
\begin{bmatrix}
\vec{a}_1 \\
\vec{a}_2 \\
\vec{a}_3 \\
\end{bmatrix}
\]

Base-Centered
\[
\begin{bmatrix}
\ell_1 \\
\ell_2 \\
\ell_3 \\
\end{bmatrix} =
\begin{bmatrix}
-1/2 & 1/2 & 0 \\
1/2 & -1/2 & 0 \\
1/2 & 1/2 & 0 \\
\end{bmatrix}
\begin{bmatrix}
\vec{a}_1 \\
\vec{a}_2 \\
\vec{a}_3 \\
\end{bmatrix}
\]

Trigonal
\[
\begin{bmatrix}
\ell_1 \\
\ell_2 \\
\ell_3 \\
\end{bmatrix} =
\begin{bmatrix}
1 & 1/3 & 1/3 \\
-1/3 & 1/3 & 1/3 \\
-1/3 & -1/3 & 1/3 \\
\end{bmatrix}
\begin{bmatrix}
\vec{a}_1 \\
\vec{a}_2 \\
\vec{a}_3 \\
\end{bmatrix}
\]

Non-Primitive Lattice Vectors

Almost always, the label “lattice vector” refers to the translation vectors, not the axis vectors.

A translation vector is any vector that connects two points in a lattice. They must be an integer combination of the primitive translation vectors.

\[
\vec{t}_{pqr} = pt_1 + qt_2 + rt_3
\]

\[
p = \ldots, -2, -1, 0, 1, 2, \ldots
\]
\[
q = \ldots, -2, -1, 0, 1, 2, \ldots
\]
\[
r = \ldots, -2, -1, 0, 1, 2, \ldots
\]
Reciprocal Lattice Vectors

The Reciprocal Lattice (1 of 8)

Direct lattice vectors $\mathbf{i}_1$, $\mathbf{i}_2$, and $\mathbf{i}_3$ define the direct lattice.
The Reciprocal Lattice (2 of 8)

Direct lattice vectors $\vec{r}_1$ and $\vec{r}_2$ define a plane.

This plane repeats itself through the lattice with a spacing of $\Lambda_3$.

Reciprocal lattice vector $\vec{T}_3$ is defined to be perpendicular to these planes with magnitude $\Lambda_3$.

$$|\vec{T}_3| = \frac{2\pi}{\Lambda_3}$$

The Reciprocal Lattice (3 of 8)

Direct lattice vectors $\vec{r}_1$ and $\vec{r}_3$ define a plane.

This plane repeats itself through the lattice with a spacing of $\Lambda_2$.

Reciprocal lattice vector $\vec{T}_2$ is defined to be perpendicular to these planes with magnitude $\Lambda_2$.

$$|\vec{T}_2| = \frac{2\pi}{\Lambda_2}$$
The Reciprocal Lattice (4 of 8)

Direct lattice vectors \( \vec{t}_2 \) and \( \vec{t}_3 \) define a plane.

This plane repeats itself through the lattice with a spacing of \( \Lambda_1 \).

Reciprocal lattice vector \( \vec{T}_1 \) is defined to be perpendicular to these planes with magnitude \( \Lambda_1 \).

\[
|\vec{T}_1| = \frac{2\pi}{\Lambda_1}
\]

The Reciprocal Lattice (5 of 8)

Reciprocal lattice vectors \( \vec{T}_1, \vec{T}_2 \) and \( \vec{T}_3 \) define the reciprocal lattice.
The Reciprocal Lattice (6 of 8)

Reciprocal lattice vectors $\mathbf{T}_1$ and $\mathbf{T}_2$ define a plane.

This plane repeats itself through the lattice with a spacing of $a_3$.

Direct lattice vector $\mathbf{t}_3$ is defined to be perpendicular to these planes with magnitude $a_3$.

$$|\mathbf{t}_3| = \frac{2\pi}{a_3}$$

The Reciprocal Lattice (7 of 8)

Reciprocal lattice vectors $\mathbf{T}_1$ and $\mathbf{T}_3$ define a plane.

This plane repeats itself through the lattice with a spacing of $a_2$.

Direct lattice vector $\mathbf{t}_2$ is defined to be perpendicular to these planes with magnitude $a_2$.

$$|\mathbf{t}_2| = \frac{2\pi}{a_2}$$
The Reciprocal Lattice (8 of 8)

Reciprocal lattice vectors $\mathbf{T}_2$ and $\mathbf{T}_3$ define a plane.

This plane repeats itself through the lattice with a spacing of $a_1$.

Direct lattice vector $\mathbf{t}_1$ is defined to be perpendicular to these planes with magnitude $a_1$.

$$|\mathbf{t}_1| = \frac{2\pi}{a_1}$$

Direct & Reciprocal Lattices

Each direct lattice has a unique reciprocal lattice so knowledge of one implies knowledge of the other.
Direct & Reciprocal Lattice Pairs

<table>
<thead>
<tr>
<th>Direct Lattice</th>
<th>Reciprocal Lattice</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple Cubic</td>
<td>Simple Cubic</td>
</tr>
<tr>
<td>Body-Centered Cubic</td>
<td>Face-Centered Cubic</td>
</tr>
<tr>
<td>Face-Centered Cubic</td>
<td>Body-Centered Cubic</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>Hexagonal</td>
</tr>
</tbody>
</table>

Converting Between Direct & Reciprocal Lattice Vectors
Calculating the Reciprocal Lattice Vectors (1 of 4)

The area of this parallelogram is calculated from the magnitude of the cross product...

\[ A = |\vec{t}_2 \times \vec{t}_3| \]

Calculating the Reciprocal Lattice Vectors (2 of 4)

The volume of this parallelepiped is calculated using the scalar triple product.

\[ V = \vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3) \]
Calculating the Reciprocal Lattice Vectors (3 of 4)

The distance $\Lambda$ between the planes is

$$\Lambda = \frac{V}{A} = \frac{\vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3)}{|\vec{t}_2 \times \vec{t}_3|}$$

Calculating the Reciprocal Lattice Vectors (4 of 4)

The reciprocal lattice vector has a magnitude of

$$|\vec{T}_1| = \frac{2\pi}{\Lambda}$$

and direction of

$$\frac{\vec{T}_1}{|\vec{T}_1|} = \frac{\vec{t}_2 \times \vec{t}_3}{|\vec{t}_2 \times \vec{t}_3|}$$

$$\vec{T}_1 = |\vec{T}_1| \frac{\vec{t}_2 \times \vec{t}_3}{|\vec{t}_2 \times \vec{t}_3|} = \frac{2\pi}{\Lambda} \frac{\vec{t}_2 \times \vec{t}_3}{|\vec{t}_2 \times \vec{t}_3|} = \frac{2\pi}{\vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3)} \frac{\vec{t}_2 \times \vec{t}_3}{|\vec{t}_2 \times \vec{t}_3|} = 2\pi \frac{\vec{t}_2 \times \vec{t}_3}{\vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3)}$$
Summary of Reciprocal Equations for 3D Lattices

The reciprocal lattice vectors can be calculated from the direct lattice vectors (and the other way around) as follows:

\[
\vec{T}_1 = 2\pi \frac{\vec{t}_2 \times \vec{t}_3}{\vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3)} \quad \vec{T}_2 = 2\pi \frac{\vec{t}_3 \times \vec{t}_1}{\vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3)} \quad \vec{T}_3 = 2\pi \frac{\vec{t}_1 \times \vec{t}_2}{\vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3)}
\]

\[
\vec{t}_1 = 2\pi \frac{\vec{T}_2 \times \vec{T}_3}{\vec{T}_1 \cdot (\vec{T}_2 \times \vec{T}_3)} \quad \vec{t}_2 = 2\pi \frac{\vec{T}_3 \times \vec{T}_1}{\vec{T}_1 \cdot (\vec{T}_2 \times \vec{T}_3)} \quad \vec{t}_3 = 2\pi \frac{\vec{T}_1 \times \vec{T}_2}{\vec{T}_1 \cdot (\vec{T}_2 \times \vec{T}_3)}
\]

Summary of Reciprocal Equations for 3D Lattices

The reciprocal lattice vectors can be calculated from the direct lattice vectors (and the other way around) as follows:

\[
\vec{T}_1 = \frac{2\pi}{t_{1,x}t_{2,y} - t_{2,x}t_{1,y}} \begin{bmatrix} t_{2,y} \\ -t_{2,x} \end{bmatrix} \quad \vec{T}_2 = \frac{2\pi}{t_{1,x}t_{2,y} - t_{2,x}t_{1,y}} \begin{bmatrix} -t_{1,y} \\ t_{1,x} \end{bmatrix}
\]

\[
\vec{t}_1 = \frac{2\pi}{T_{1,x}T_{2,y} - T_{2,x}T_{1,y}} \begin{bmatrix} T_{2,y} \\ -T_{2,x} \end{bmatrix} \quad \vec{t}_2 = \frac{2\pi}{T_{1,x}T_{2,y} - T_{2,x}T_{1,y}} \begin{bmatrix} -T_{1,y} \\ T_{1,x} \end{bmatrix}
\]
There also exists *primitive reciprocal lattice vectors*. All *reciprocal lattice vectors* must be an integer combination of the *primitive reciprocal lattice vectors*.

\[
\vec{T}_{PQR} = P\vec{T}_1 + Q\vec{T}_2 + R\vec{T}_3
\]

\[
P = \ldots, -2, -1, 0, 1, 2, \ldots
\]

\[
Q = \ldots, -2, -1, 0, 1, 2, \ldots
\]

\[
R = \ldots, -2, -1, 0, 1, 2, \ldots
\]