Advanced Electromagnetics:
21st Century Electromagnetics

Lattice Vectors

Lecture Outline

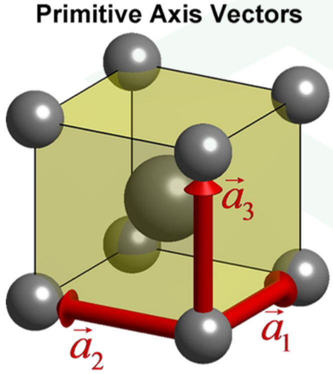
- Direct lattice vectors
- Reciprocal lattice vectors
- Converting between direct and reciprocal lattice vectors

Direct Lattice Vectors

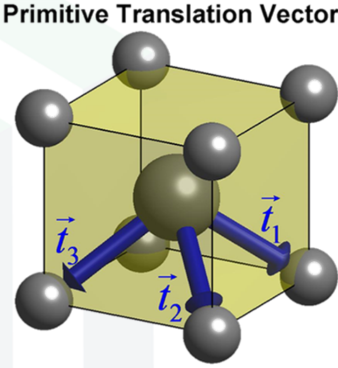
Slide 3

Direct Lattice Vectors

Primitive Axis Vectors



Primitive Translation 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.

Slide 4

Calculating Translation Vectors From Axis Vectors

Simple

$$\begin{bmatrix}\vec{t}_1\\\vec{t}_2\\\vec{t}_3\end{bmatrix}=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}\begin{bmatrix}\vec{a}_1\\\vec{a}_2\\\vec{a}_3\end{bmatrix}$$

Body-Centered

$$\begin{bmatrix}\vec{t}_1\\\vec{t}_2\\\vec{t}_3\end{bmatrix}=\begin{bmatrix}-1/2&1/2&1/2\\1/2&-1/2&1/2\\1/2&1/2&-1/2\end{bmatrix}\begin{bmatrix}\vec{a}_1\\\vec{a}_2\\\vec{a}_3\end{bmatrix}$$

Face-Centered

$$\begin{bmatrix}\vec{t}_1\\\vec{t}_2\\\vec{t}_3\end{bmatrix}=\begin{bmatrix}0&1/2&1/2\\1/2&0&1/2\\1/2&1/2&0\end{bmatrix}\begin{bmatrix}\vec{a}_1\\\vec{a}_2\\\vec{a}_3\end{bmatrix}$$

Base-Centered

$$\begin{bmatrix}\vec{t}_1\\\vec{t}_2\\\vec{t}_3\end{bmatrix}=\begin{bmatrix}-1/2&1/2&0\\1/2&1/2&0\\0&0&1/2\end{bmatrix}\begin{bmatrix}\vec{a}_1\\\vec{a}_2\\\vec{a}_3\end{bmatrix}$$

Trigonal

$$\begin{bmatrix}\vec{t}_1\\\vec{t}_2\\\vec{t}_3\end{bmatrix}=\begin{bmatrix}1&1/3&1/3\\-1/3&1/3&1/3\\-1/3&-1&1/3\end{bmatrix}\begin{bmatrix}\vec{a}_1\\\vec{a}_2\\\vec{a}_3\end{bmatrix}$$

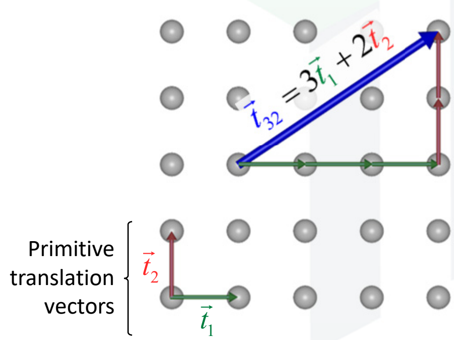
EMPossible

Slide 5

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*.



$$\vec{t}_{pqr}=p\vec{t}_1+q\vec{t}_2+r\vec{t}_3$$

$$p=\cdots,-2,-1,0,1,2,\cdots$$
$$q=\cdots,-2,-1,0,1,2,\cdots$$
$$r=\cdots,-2,-1,0,1,2,\cdots$$

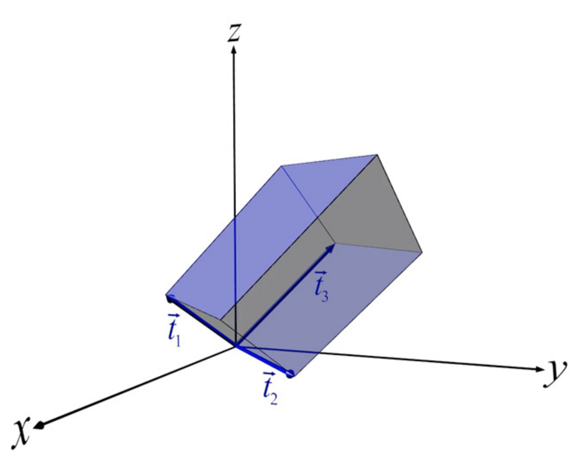
EMPossible

Slide 6

Reciprocal Lattice Vectors

Slide 7

The Reciprocal Lattice (1 of 8)

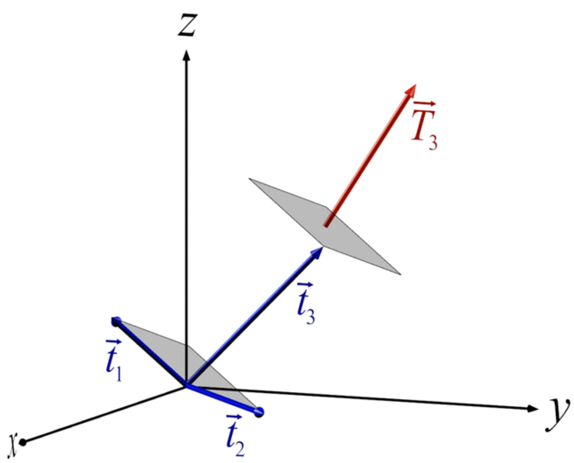


Direct lattice vectors $\vec{t}_1$, $\vec{t}_2$ and $\vec{t}_3$ define the *direct* lattice.

EMPossible

Slide 8

The Reciprocal Lattice (2 of 8)



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

This plane repeats itself through the lattice with a spacing of Λ_3.

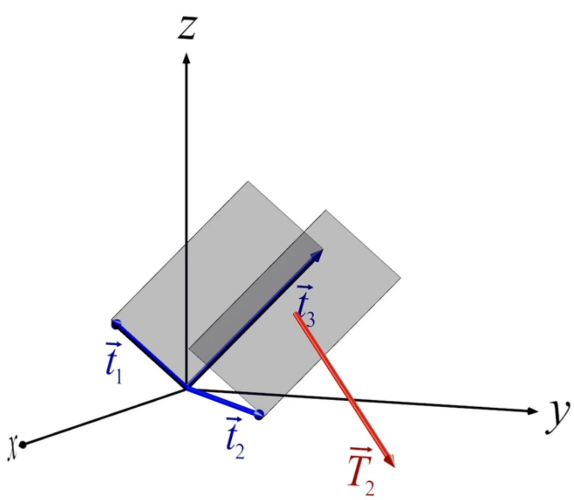
Reciprocal lattice vector $\vec{T}_3$ is defined to be perpendicular to these planes with magnitude Λ_3.

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

EMPossible

Slide 9

The Reciprocal Lattice (3 of 8)



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

This plane repeats itself through the lattice with a spacing of Λ_2.

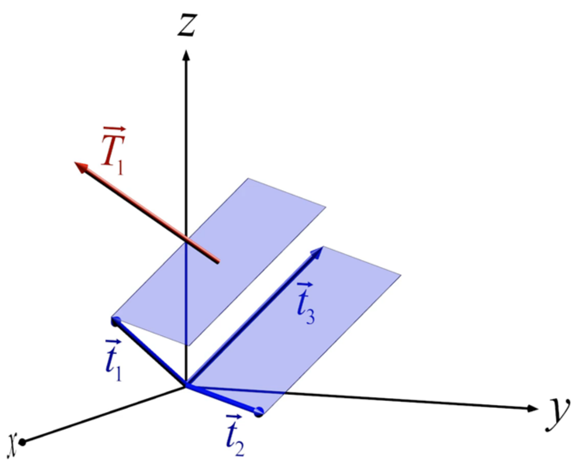
Reciprocal lattice vector $\vec{T}_2$ is defined to be perpendicular to these planes with magnitude Λ_2.

$$\left|\vec{T}_2\right| = \frac{2\pi}{\Lambda_2}$$

EMPossible

Slide 10

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 Λ_1.

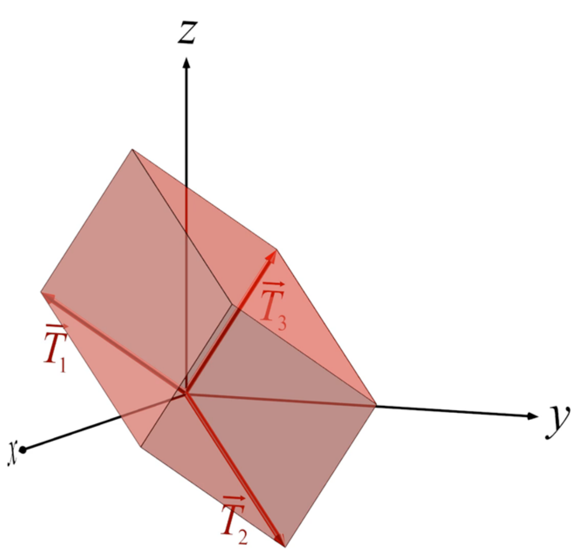
Reciprocal lattice vector $\vec{T}_1$ is defined to be perpendicular to these planes with magnitude Λ_1.

$$\left|\vec{T}_1\right| = \frac{2\pi}{\Lambda_1}$$

EMPossible

Slide 11

The Reciprocal Lattice (5 of 8)

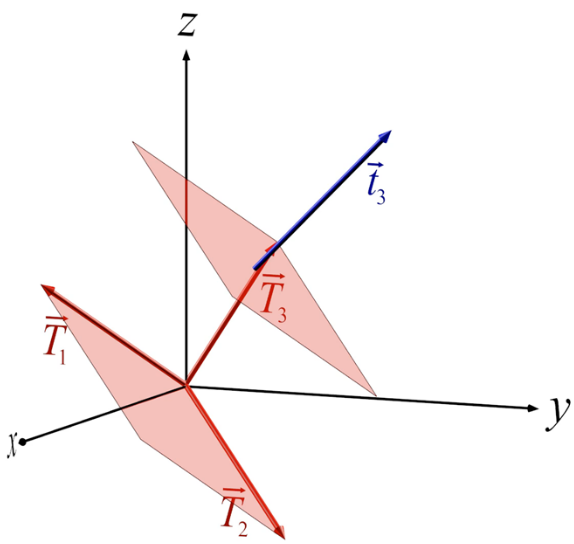


Reciprocal lattice vectors $\vec{T}_1$, $\vec{T}_2$ and $\vec{T}_3$ define the *reciprocal* lattice.

EMPossible

Slide 12

The Reciprocal Lattice (6 of 8)



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

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

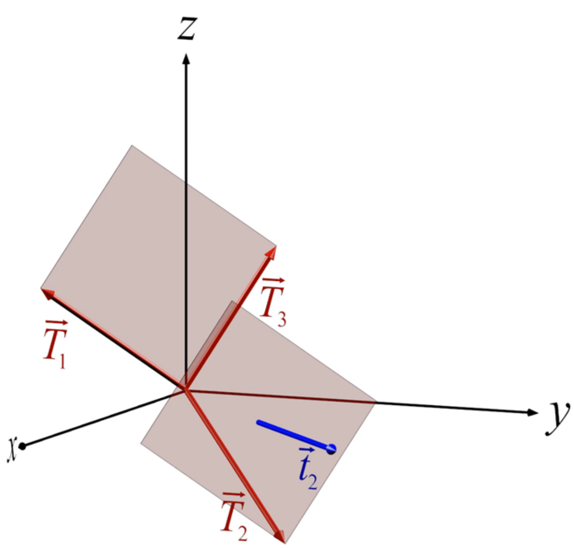
Direct lattice vector $\vec{t}_3$ is defined to be perpendicular to these planes with magnitude a_3.

$$\left|\vec{t}_3\right| = \frac{2\pi}{a_3}$$

EMPossible

Slide 13

The Reciprocal Lattice (7 of 8)



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

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

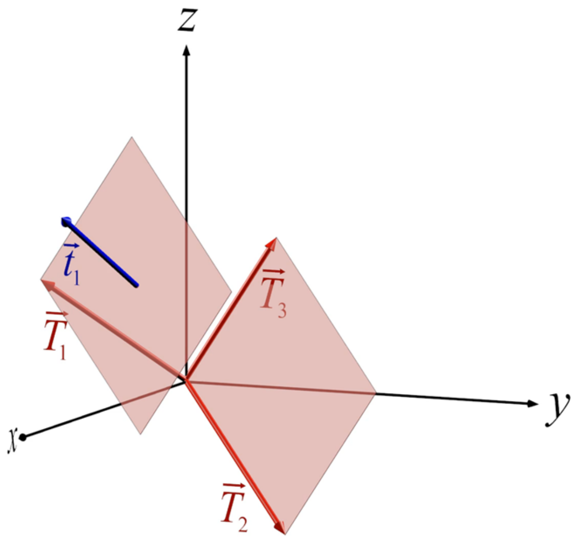
Direct lattice vector $\vec{t}_2$ is defined to be perpendicular to these planes with magnitude a_2.

$$\left|\vec{t}_2\right| = \frac{2\pi}{a_2}$$

EMPossible

Slide 14

The Reciprocal Lattice (8 of 8)



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

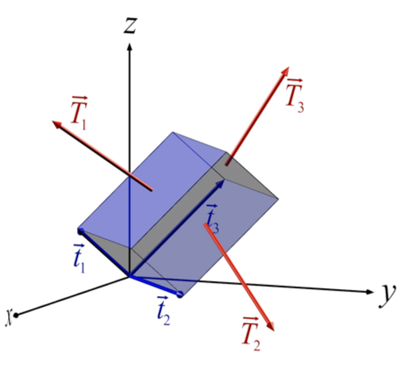
This plane repeats itself through the lattice with a spacing of a_1.

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

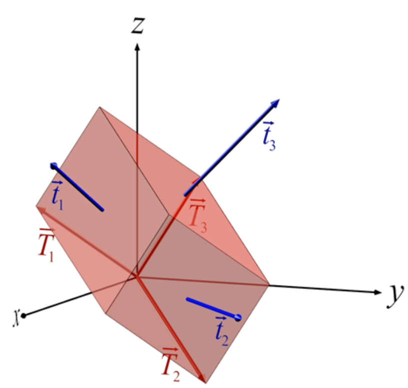
$$\left|\vec{t}_1\right| = \frac{2\pi}{a_1}$$

Direct & Reciprocal Lattices

Direct Lattice

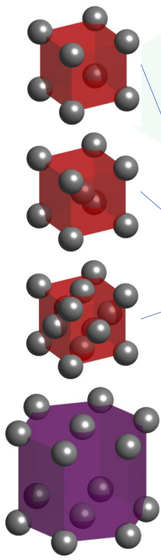


Reciprocal Lattice

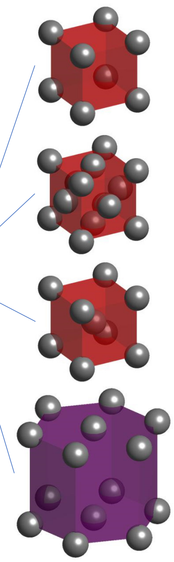


Each direct lattice has a unique reciprocal lattice so knowledge of one implies knowledge of the other.

Direct & Reciprocal Lattice Pairs



Direct Lattice	Reciprocal Lattice
Simple Cubic	Simple Cubic
Body-Centered Cubic	Face-Centered Cubic
Face-Centered Cubic	Body-Centered Cubic
Hexagonal	Hexagonal



EMPossible

Slide 17

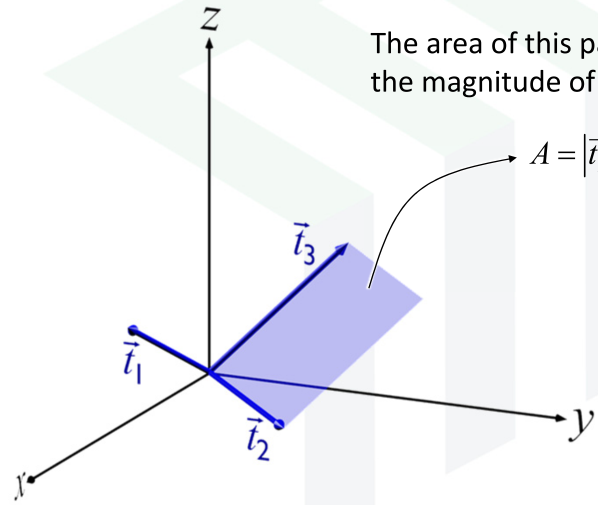
Converting Between Direct & Reciprocal Lattice Vectors

Slide 18

Calculating the Reciprocal Lattice Vectors (1 of 4)

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

$$A = \left|\vec{t}_2 \times \vec{t}_3\right|$$



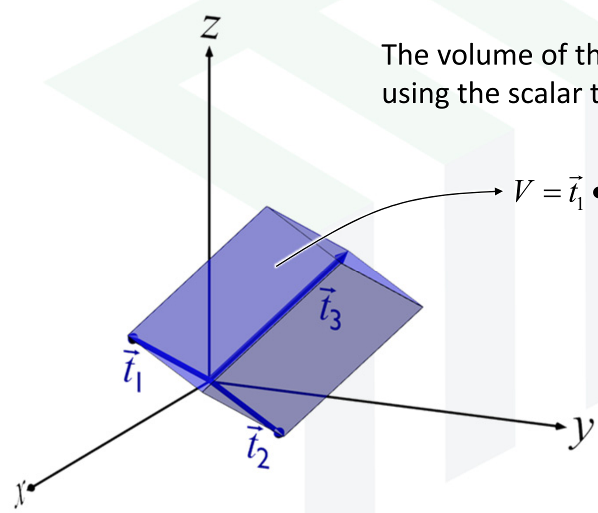
EMPossible

Slide 19

Calculating the Reciprocal Lattice Vectors (2 of 4)

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

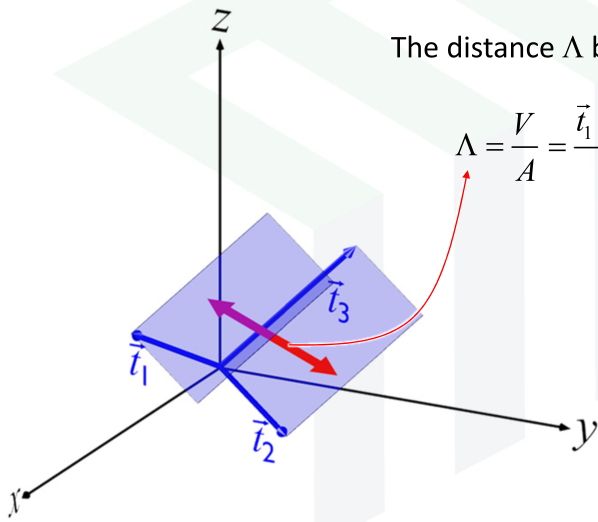
$$V = \vec{t}_1 \bullet \left(\vec{t}_2 \times \vec{t}_3\right)$$



EMPossible

Slide 20

Calculating the Reciprocal Lattice Vectors (3 of 4)



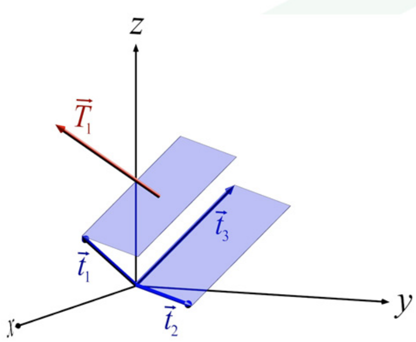
The distance Λ between the planes is

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

EMPossible

Slide 21

Calculating the Reciprocal Lattice Vectors (4 of 4)



The reciprocal lattice vector has a magnitude of

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

and direction of

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

$$\vec{T}_1 = \left|\vec{T}_1\right| \frac{\vec{t}_2 \times \vec{t}_3}{\left|\vec{t}_2 \times \vec{t}_3\right|} = \frac{2\pi}{\Lambda} \frac{\vec{t}_2 \times \vec{t}_3}{\left|\vec{t}_2 \times \vec{t}_3\right|} = \frac{2\pi}{\frac{\vec{t}_1 \bullet \left(\vec{t}_2 \times \vec{t}_3\right)}{\left|\vec{t}_2 \times \vec{t}_3\right|}} \frac{\vec{t}_2 \times \vec{t}_3}{\left|\vec{t}_2 \times \vec{t}_3\right|} = 2\pi \frac{\vec{t}_2 \times \vec{t}_3}{\vec{t}_1 \bullet \left(\vec{t}_2 \times \vec{t}_3\right)}$$

EMPossible

Slide 22

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:

$$\vec{T}_1 = 2\pi \frac{\vec{t}_2 \times \vec{t}_3}{\vec{t}_1 \bullet \left(\vec{t}_2 \times \vec{t}_3\right)} \qquad \vec{T}_2 = 2\pi \frac{\vec{t}_3 \times \vec{t}_1}{\vec{t}_1 \bullet \left(\vec{t}_2 \times \vec{t}_3\right)} \qquad \vec{T}_3 = 2\pi \frac{\vec{t}_1 \times \vec{t}_2}{\vec{t}_1 \bullet \left(\vec{t}_2 \times \vec{t}_3\right)}$$

$$\vec{t}_1 = 2\pi \frac{\vec{T}_2 \times \vec{T}_3}{\vec{T}_1 \bullet \left(\vec{T}_2 \times \vec{T}_3\right)} \qquad \vec{t}_2 = 2\pi \frac{\vec{T}_3 \times \vec{T}_1}{\vec{T}_1 \bullet \left(\vec{T}_2 \times \vec{T}_3\right)} \qquad \vec{t}_3 = 2\pi \frac{\vec{T}_1 \times \vec{T}_2}{\vec{T}_1 \bullet \left(\vec{T}_2 \times \vec{T}_3\right)}$$

EMPossible

Slide 23

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:

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

$$\vec{t}_1 = \frac{2\pi}{T_{1,x}T_{2,y} - T_{2,x}T_{1,y}} \begin{bmatrix} T_{2,y} \\ -T_{2,x} \end{bmatrix} \qquad \vec{t}_2 = \frac{2\pi}{T_{1,x}T_{2,y} - T_{2,x}T_{1,y}} \begin{bmatrix} -T_{1,y} \\ T_{1,x} \end{bmatrix}$$

EMPossible

Slide 24

Primitive Reciprocal Lattice Vectors

There also exists *primitive reciprocal lattice vectors*. All *reciprocal lattice vectors* must be an integer combination of the *primitive reciprocal lattice vectors*.

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

$$P = \cdots,-2,-1,0,1,2,\cdots$$
$$Q = \cdots,-2,-1,0,1,2,\cdots$$
$$R = \cdots,-2,-1,0,1,2,\cdots$$

EMPossible

Slide 25