Spots on detector ("reflexes")

$h=2$ $h=1$ $h=0$ $h=1$ $h=2$

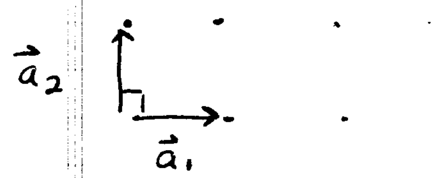
S_2 S_1 S_0 S_1 S_2

Spacings proportional to $\frac{1}{a} \equiv a^*$ and λ

small $a \rightarrow$ large a^* $\beta = h\lambda a^*$

large $a \rightarrow$ small a^*

Now consider a 2D surface lattice:

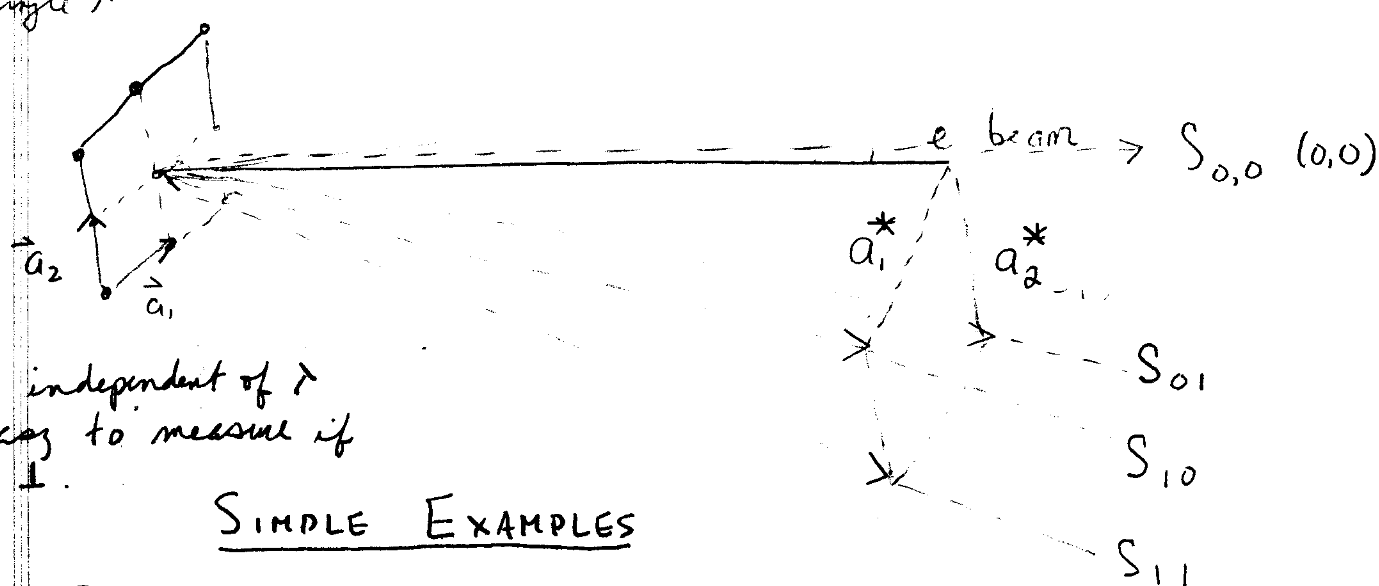


For each dimension of periodicity, there is a diffraction equation:

$$a_1 \cos\alpha_1 = a_1 \sin\beta_1 = h_1 \lambda$$
$$a_2 \cos\alpha_2 = a_2 \sin\beta_2 = h_2 \lambda$$

$$\beta_1 = \frac{h_1 \lambda}{a_1} \qquad \beta_2 = \frac{h_2\lambda}{a_2} \qquad \text{or} \quad \beta_1 = h_1 \lambda a_1^*$$
$$\beta_2 = h_2 \lambda a_2^*$$

can do with single λ

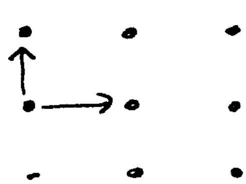


(0,0) independent of λ so easy to measure if not $\perp$.

SIMPLE EXAMPLES

(a) Primitive cubic: no reconstruction of 100

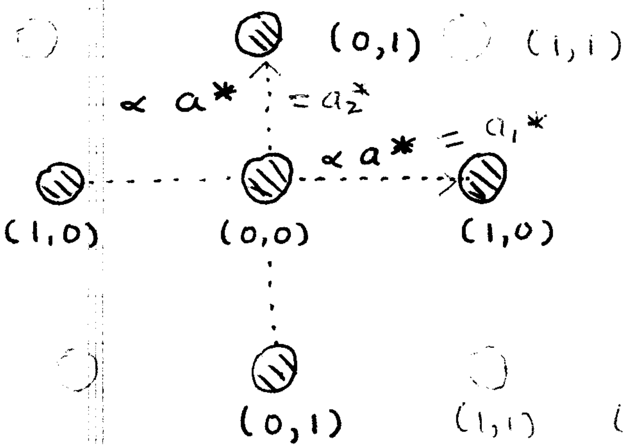
$|\vec{a}_1| = |\vec{a}_2| = a$



1st order LEED pattern:

$$a_1^* = \frac{1}{a_1} = \frac{1}{a} = a^*$$

$$a_2^* = \frac{1}{a_2} = \frac{1}{a} = a^*$$



Add higher orders

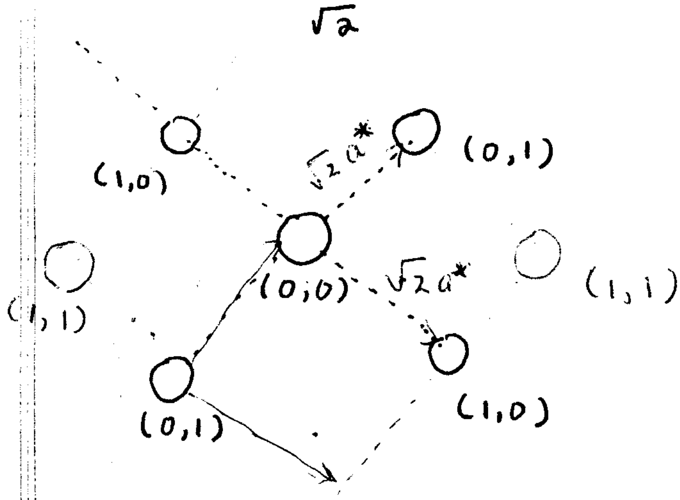
"inverse net"

Increase $\lambda \Rightarrow$ Increase Size of spacing

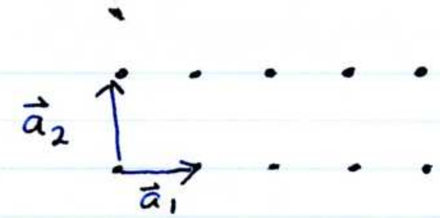
(b) fcc (100)

$$a_1 = \frac{\sqrt{2}}{2}\, a \qquad a_2 = \frac{\sqrt{2}}{2}\, a$$

$$a_1^* = \frac{2}{\sqrt{2}}\, a^* \qquad a_2^* = \frac{2}{\sqrt{2}}\, a^*$$

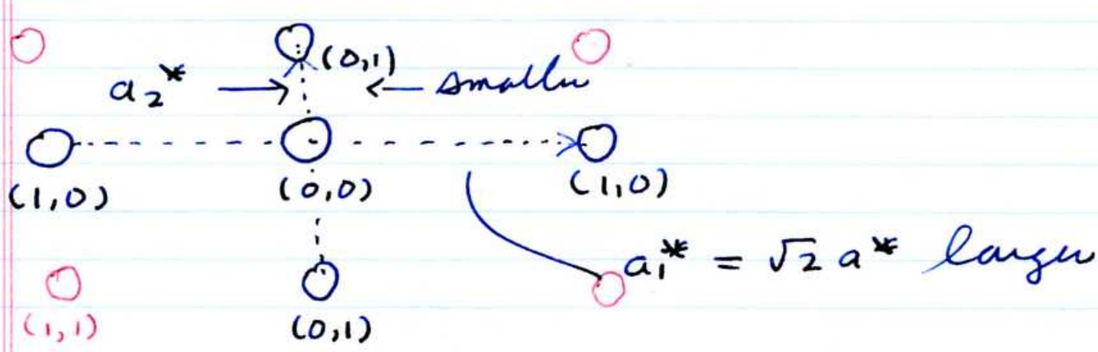


c) fcc (110)

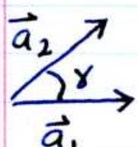


$[00\bar{1}]$ $\quad a_1 = a/\sqrt{2} < a_2 = a$

REFLEXES: $\quad a_1^* = \sqrt{2}\, a^* > a_2^* = a^*$



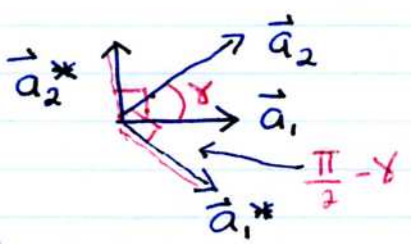
Non-Orthogonal Axes



A general relation to define the inverse mesh is: $\vec{a}_i \cdot \vec{a}_j^* = \delta_{ij}$ $\quad \vec{a}_1 \perp \vec{a}_2^*$

$\vec{a}_2 \perp \vec{a}_1^*$

preserve right-handedness



$\measuredangle(\vec{a}_1^*, \vec{a}_2^*) = \pi - \gamma \equiv \gamma^*$

Lengths *

$$\vec{a}_1 = a_1 \vec{i} \qquad \vec{a}_2 = a_2(\cos\gamma\, \vec{i} + \sin\gamma\, \vec{j})$$

$$\vec{a}_1^* = a_1^* \left(\cos(\pi/2 - \gamma)\, \vec{i} - \sin(\pi/2 - \gamma)\, \vec{j} \right)$$

$$\vec{a}_1 \cdot \vec{a}_1^* = \delta_{11} = 1 = a_1 a_1^* \cos(\pi/2 - \gamma) = a_1 a_1^* \sin\gamma$$

$$\therefore \; a_1^* = \frac{1}{a_1 \sin\gamma}$$

* don't really need $\vec{i}, \vec{j}$ analysis – see next page

Lengths w/o Vectors

$$\vec{a}_1 \cdot \vec{a}_1^{\,*} = 1 = a_1 a_1^* \cos(\pi/2 - \gamma) = a_1 a_1^* \sin\gamma$$

$$a_1^* = \frac{1}{a_1 \sin\gamma}$$

$$\vec{a}_2 \cdot \vec{a}_2^{\,*} = 1 = a_2 a_2^* \cos(\pi/2 - \gamma) = a_2 a_2^* \sin\gamma$$

$$a_2^* = \frac{1}{a_2 \sin\gamma}$$ spreads out inverse net

Similarly $\vec{a}_2 \cdot \vec{a}_2^* = 1 \Rightarrow a_2 a_2^* \sin\gamma = 1$

$$a_2^* = \frac{1}{a_2 \sin\gamma}$$ spreads out inverse net

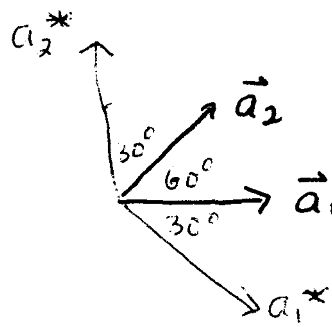
Example: fcc (111)

$\gamma = 60°$

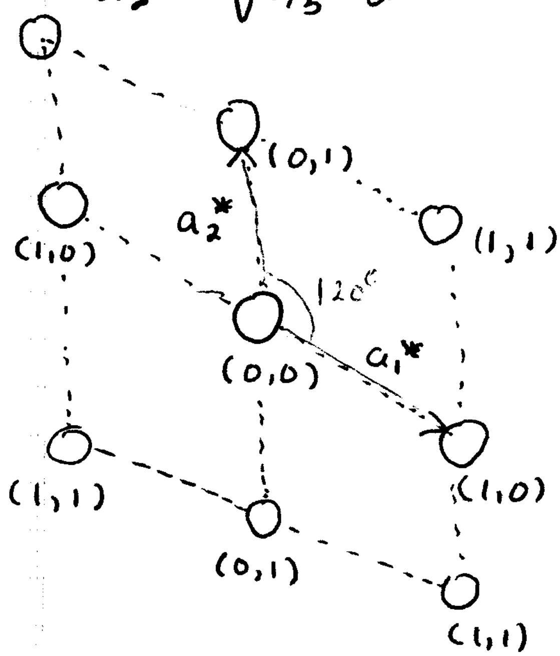
$a_1 = a/\sqrt{2} \quad a_2 = a/\sqrt{2} \qquad \sin 60° = \sqrt{3}/2$

$$a_1^* = \frac{1}{a_1 \sin\gamma} = \frac{\sqrt{2}}{a\sqrt{3}/2} = \frac{2\sqrt{2}}{a\sqrt{3}} = \sqrt{\frac{8}{3}}\ a^*$$

$a_2^* = \sqrt{8/3}\ a^*$



$\pi - \gamma = 120°$



(look on opposite side of paper: inverse mesh not really different from normal mesh)

(inverse same)

Adsorbate / Substrate Problems (- inverse)

$\vec{a}_1, \vec{a}_2$ substrate $\quad \vec{b}_1, \vec{b}_2$ adsorbate

can be done without matrices

$$\vec{b}_1 = G_{11}\vec{a}_1 + G_{12}\vec{a}_2$$
$$\vec{b}_2 = G_{21}\vec{a}_1 + G_{22}\vec{a}_2$$

matrix approach requires primitive lattices MUST BE COMMENSURATE

$$\begin{pmatrix} \vec{b}_1 \\ \vec{b}_2 \end{pmatrix} = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} \begin{pmatrix} \vec{a}_1 \\ \vec{a}_2 \end{pmatrix}$$

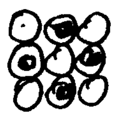
Also: $\begin{pmatrix} \vec{b}_1{}^* \\ \vec{b}_2{}^* \end{pmatrix} = \begin{pmatrix} G_{11}^* & G_{12}^* \\ G_{21}^* & G_{22}^* \end{pmatrix} \begin{pmatrix} \vec{a}_1{}^* \\ \vec{a}_2{}^* \end{pmatrix}$

$$G = \left([G^*]^{-1} \right)^{\dagger} = \frac{1}{|G^*|} \begin{pmatrix} G_{22}^* & -G_{21}^* \\ -G_{12}^* & G_{11}^* \end{pmatrix}$$

$$|G^*| = G_{11}^* G_{22}^* - G_{12}^* G_{21}^*$$

Real Space

$\vec{a}_1, \vec{a}_2$
$\vec{b}_1, \vec{b}_2$
G



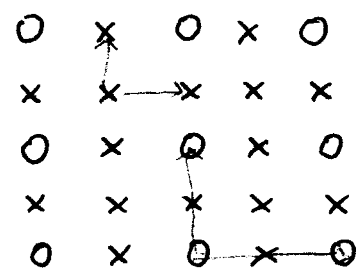
$\longleftrightarrow$

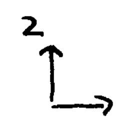
Inverse Space (LEED)

$\vec{a}_1{}^* \quad \vec{a}_2{}^*$ o o o
$\vec{b}_1{}^* \quad \vec{b}_2{}^*$ x x x
G^* (additional)

Example I: Inverse Problem

LEED Pattern
$\Theta = 0.25$ of O
on Cu (100) fcc





no reconstruction

$$\vec{b}_1{}^* = \tfrac{1}{2}\vec{a}_1{}^* \qquad \vec{b}_2{}^* = \tfrac{1}{2}\vec{a}_2{}^*$$

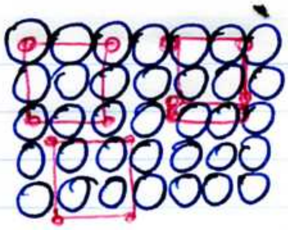
$$G^* = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \qquad |G^*| = 1/4$$

$$G = \frac{1}{1/4} \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

$$G \Rightarrow \vec{b}_1 = 2\vec{a}_1 \qquad \vec{b}_2 = 2\vec{a}_2$$

While such a procedure allows an exact definition of the 2-D periodicity of the overlayer relative to the substrate, it says <u>nothing</u> about the actual adsorption sites:

$$\Theta = \frac{a_1 \times a_2}{b_1 \times b_2} \quad ?$$



CN = 1, 2, or 4

$$Cu(100) - \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} - O - (0.25\,ML)$$

Note: to use matrix approach to determine LEED pattern;

$$G = \left([G^*]^{-1}\right)^{+}$$

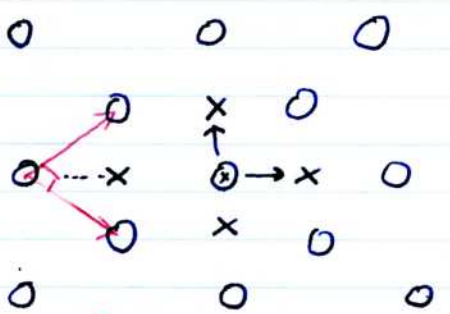
$$G^{+} = (G^*)^{-1}$$

$$(G^{+})^{-1} = G^* = \begin{pmatrix} G_{11} & G_{21} \\ G_{12} & G_{22} \end{pmatrix}^{-1}$$

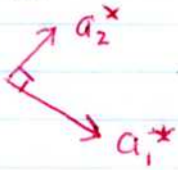
$$G^* = \frac{1}{|G|} \begin{pmatrix} G_{22} & -G_{21} \\ -G_{12} & G_{11} \end{pmatrix}$$

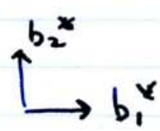
Example 2: slight variation 100 fcc again

LEED pattern



x - extra (adsorbate)





$$\vec{a}_1^* = \vec{b}_1^* - \vec{b}_2^*$$

$$\vec{a}_2^* = \vec{b}_1^* + \vec{b}_2^*$$

$$\vec{b}_1^* = \frac{1}{2}\left(\vec{a}_1^* + \vec{a}_2^*\right)$$

$$\vec{b}_2^* = \frac{1}{2}\left(-\vec{a}_1^* + \vec{a}_2^*\right)$$

$$a_1^* = \frac{2}{\sqrt{2}} a^*$$

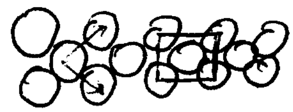
$$a_2^* = \frac{2}{\sqrt{2}} a^*$$

$$G^* = \begin{pmatrix} 1/2 & 1/2 \\ -1/2 & 1/2 \end{pmatrix}$$

$$G = \frac{1}{|G^*|} \begin{pmatrix} 1/2 & 1/2 \\ -1/2 & 1/2 \end{pmatrix} = \frac{1}{1/2} \begin{pmatrix} 1/2 & 1/2 \\ -1/2 & 1/2 \end{pmatrix}$$

$$G = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

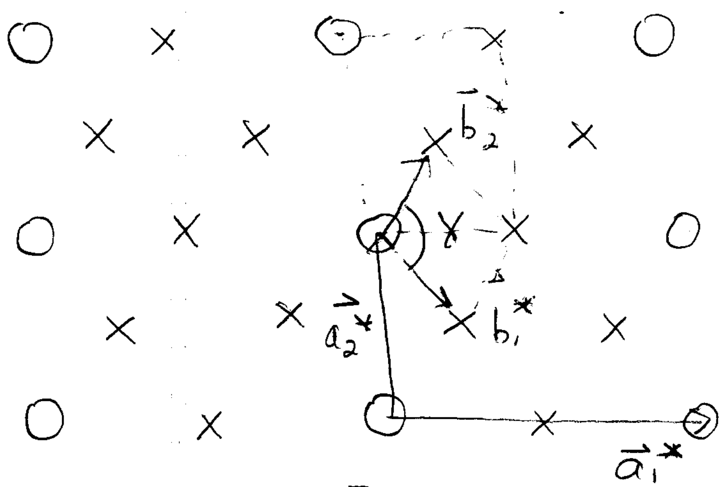
$\vec{b}_1 = \vec{a}_1 + \vec{a}_2 \qquad \vec{b}_2 = -\vec{a}_1 + \vec{a}_2$



$100 - \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$ Ask $\theta =$

Inverse + Non-orthogonal

LEED



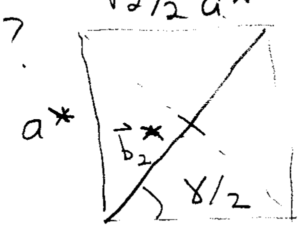
$|\vec{a}_1^*| = \sqrt{2}\,|\vec{a}_2^*|$

measured

$|\vec{a}_1^*| = \sqrt{2}\, a^*$

$|\vec{a}_2^*| = a^*$

$G^* = ?$



$\tan \gamma/2 = \dfrac{1}{\sqrt{2}/2}$

$\gamma/2 = \tan^{-1}\sqrt{2} = 54.74^\circ$

$\gamma = 109.47^\circ$

$\vec{b}_1^* = +\dfrac{\sqrt{2}}{4}\, a^* \vec{i} - \dfrac{1}{2}\, a^* \vec{j}$

$\vec{b}_1^* = \dfrac{1}{4}\,\vec{a}_1^* - \dfrac{1}{2}\,\vec{a}_2^*$

$\vec{b}_2^* = \dfrac{1}{4}\,\vec{a}_1^* + \dfrac{1}{2}\,\vec{a}_2^*$

$G^* = \begin{pmatrix} 1/4 & -1/2 \\ 1/4 & 1/2 \end{pmatrix}$

$G = \dfrac{1}{|G^*|} \begin{pmatrix} 1/2 & -1/4 \\ 1/2 & 1/4 \end{pmatrix} \qquad |G^*| = \dfrac{1}{8} - \left(-\dfrac{1}{8}\right) = \dfrac{1}{4}$