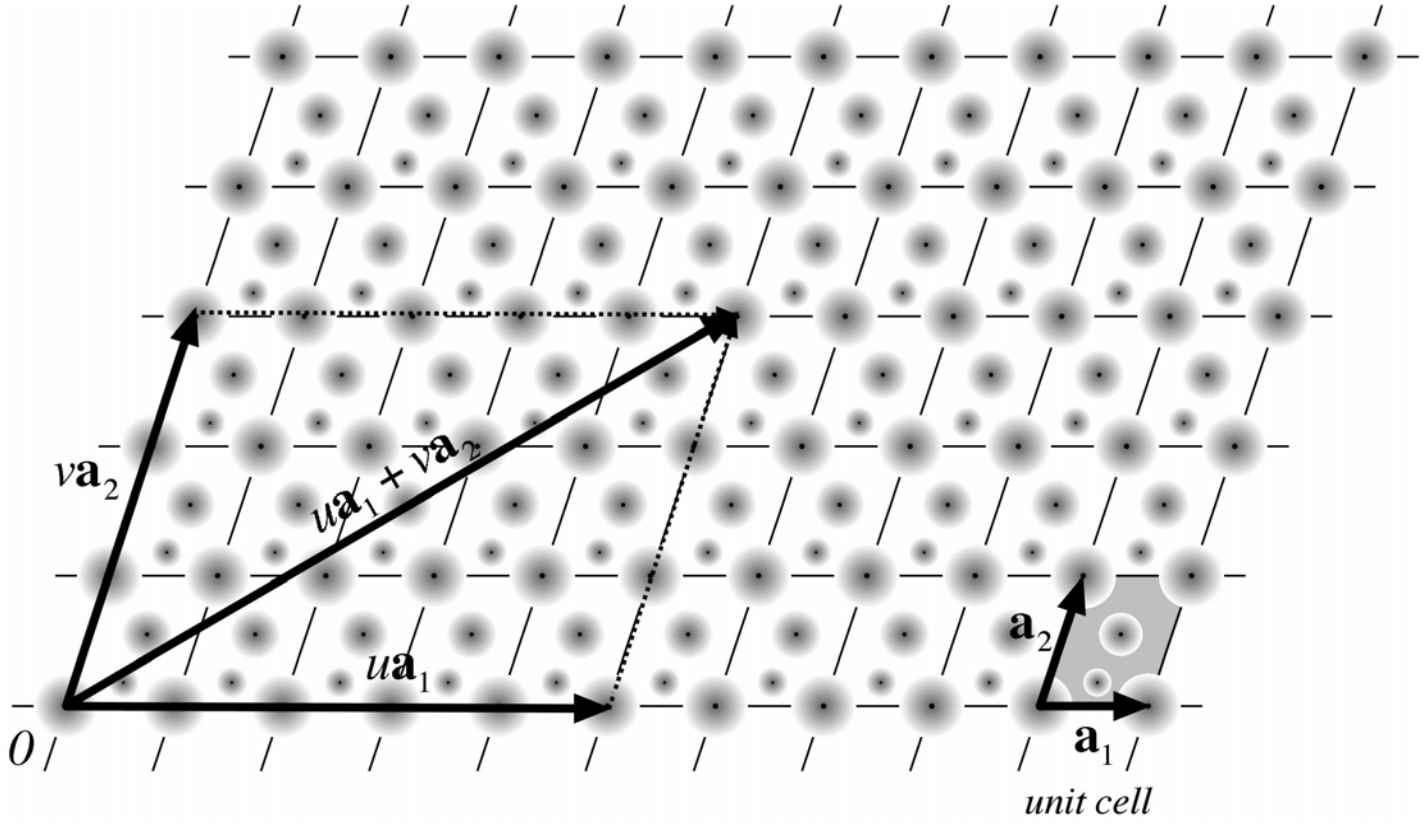
Direct lattice

A crystal is a periodic structure in real space



Infinite crystal, translational symmetry: All unit cells are equivalent

Lattice vectors

A real-space (direct) lattice vector can be represented as:

$$\mathbf{r}_{uvw} = u\mathbf{a}_1 + v\mathbf{a}_2 + w\mathbf{a}_3$$

where (u,v,w) are integers.

$\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ are the direct-lattice basis vectors

A reciprocal-space lattice vector can be represented as:

$$\mathbf{g}_{hk\ell} = h\mathbf{b}_1 + k\mathbf{b}_2 + \ell\mathbf{b}_3$$

where (h,k,ℓ) are integers.

$\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ are the reciprocal-lattice basis vectors

Scalar and vector products

Two ways of "multiplying" vectors:

$$\mathbf{r}_1 = x_1\hat{\mathbf{x}} + y_1\hat{\mathbf{y}} + z_1\hat{\mathbf{z}}$$
$$\mathbf{r}_2 = x_2\hat{\mathbf{x}} + y_2\hat{\mathbf{y}} + z_2\hat{\mathbf{z}}$$

$$\hat{\mathbf{x}}\cdot\hat{\mathbf{x}} = 1,\ \hat{\mathbf{x}}\cdot\hat{\mathbf{y}} = 0,\ \hat{\mathbf{x}}\cdot\hat{\mathbf{z}} = 0$$
$$\hat{\mathbf{y}}\cdot\hat{\mathbf{x}} = 0,\ \hat{\mathbf{y}}\cdot\hat{\mathbf{y}} = 1,\ \hat{\mathbf{y}}\cdot\hat{\mathbf{z}} = 0$$
$$\hat{\mathbf{z}}\cdot\hat{\mathbf{x}} = 0,\ \hat{\mathbf{z}}\cdot\hat{\mathbf{y}} = 0,\ \hat{\mathbf{z}}\cdot\hat{\mathbf{z}} = 1$$

1) Scalar (Dot) Product:

$$\mathbf{r}_1\cdot\mathbf{r}_2 = x_1x_2 + y_1y_2 + z_1z_2$$

2) Vector (Cross) Product:

$$\mathbf{r}_1\times\mathbf{r}_2 = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \end{vmatrix} = \left(y_1z_2 - z_1y_2\right)\hat{\mathbf{x}} - \left(x_1z_2 - z_1x_2\right)\hat{\mathbf{y}} + \left(x_1y_2 - y_1x_2\right)\hat{\mathbf{z}}$$

Determining reciprocal lattice basis vectors

Unit-Cell Volume: $$V = \left|\mathbf{a}_1 \cdot \left(\mathbf{a}_2 \times \mathbf{a}_3\right)\right|$$

$$\mathbf{b}_1 = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V} \qquad \mathbf{b}_2 = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V} \qquad \mathbf{b}_3 = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V}$$

Additional Properties: $$\mathbf{b}_i \cdot \mathbf{a}_i = 1 \qquad \mathbf{b}_i \cdot \mathbf{a}_j = 0, \ \left(i \neq j\right)$$

Matrix representation

$$\mathbf{a}_1 = \begin{pmatrix} a_{1x} \\ a_{1y} \\ a_{1z} \end{pmatrix}, \mathbf{a}_2 = \begin{pmatrix} a_{2x} \\ a_{2y} \\ a_{2z} \end{pmatrix}, \mathbf{a}_3 = \begin{pmatrix} a_{3x} \\ a_{3y} \\ a_{3z} \end{pmatrix} \qquad \mathbf{A} = \begin{pmatrix} a_{1x} & a_{2x} & a_{3x} \\ a_{1y} & a_{2y} & a_{3y} \\ a_{1z} & a_{2z} & a_{3z} \end{pmatrix} \qquad \mathbf{r}_{uvw} = \mathbf{A} \cdot \begin{pmatrix} u \\ v \\ w \end{pmatrix}$$

$$\mathbf{b}_1 = \begin{pmatrix} b_{1x} \\ b_{1y} \\ b_{1z} \end{pmatrix}, \mathbf{b}_2 = \begin{pmatrix} b_{2x} \\ b_{2y} \\ b_{2z} \end{pmatrix}, \mathbf{b}_3 = \begin{pmatrix} b_{3x} \\ b_{3y} \\ b_{3z} \end{pmatrix} \qquad \mathbf{B} = \begin{pmatrix} b_{1x} & b_{2x} & b_{3x} \\ b_{1y} & b_{2y} & b_{3y} \\ b_{1z} & b_{2z} & b_{3z} \end{pmatrix} \qquad \mathbf{g}_{hkl} = \mathbf{B} \cdot \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

$$\mathbf{A}^T \cdot \mathbf{B} = \begin{pmatrix} \mathbf{a}_1 \cdot \mathbf{b}_1 & \mathbf{a}_1 \cdot \mathbf{b}_2 & \mathbf{a}_1 \cdot \mathbf{b}_3 \\ \mathbf{a}_2 \cdot \mathbf{b}_1 & \mathbf{a}_2 \cdot \mathbf{b}_2 & \mathbf{a}_2 \cdot \mathbf{b}_3 \\ \mathbf{a}_3 \cdot \mathbf{b}_1 & \mathbf{a}_3 \cdot \mathbf{b}_2 & \mathbf{a}_3 \cdot \mathbf{b}_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathbf{1}$$

$$V = \det \mathbf{A}, \qquad \frac{1}{V} = \det \mathbf{B}$$

$$\Rightarrow \ \mathbf{B} = \left(\mathbf{A}^T \right)^{-1} = \left(\mathbf{A}^{-1} \right)^T$$

Computational method to find RLVs

Another property of RLVs

Notice,

$$\mathbf{g}_{hk\ell} \cdot \mathbf{r}_{uvw} = hu + kv + \ell w = n, \text{ (where } n \text{ is an integer)}$$

So, $$e^{2\pi i \mathbf{g}_{hk\ell} \cdot \mathbf{r}_{uvw}} = 1$$

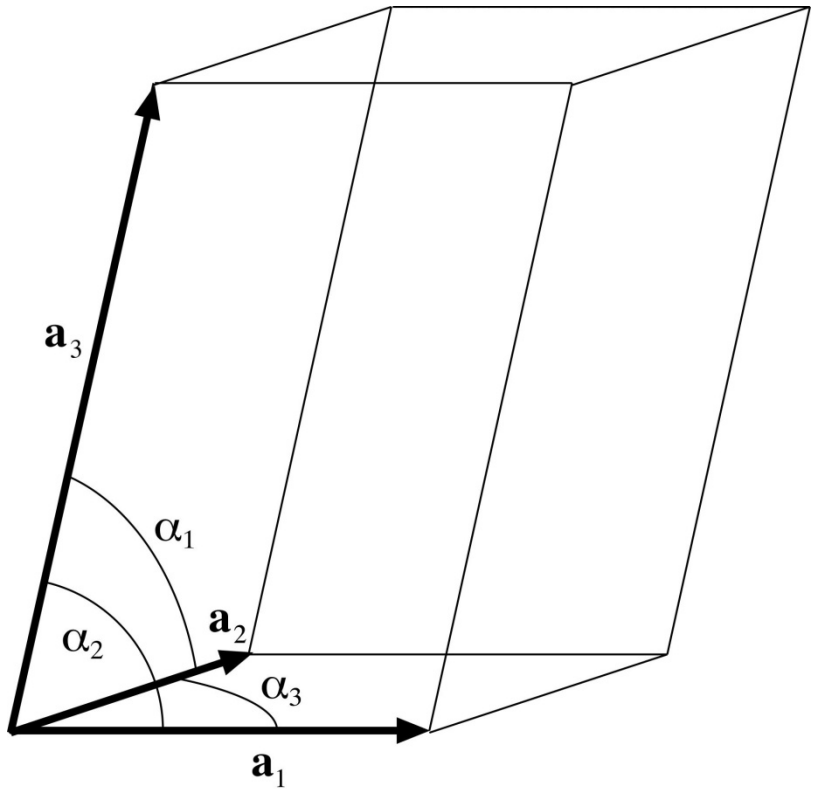
Lattice Sum:

$$\sum_{u,v,w} e^{2\pi i \mathbf{g}_{hk\ell} \cdot \mathbf{r}_{uvw}} = \sum_{n=1}^{N} e^{2\pi i \mathbf{g}_{hk\ell} \cdot \mathbf{r}_{n}} = \sum_{n=1}^{N} (1) = N$$

N = # of unit cells

Unit-cell specification

Most tabulations provide lattice parameter(s) and angles between direct-lattice basis vectors.



$$a_1 = |\mathbf{a}_1|,\ a_2 = |\mathbf{a}_2|,\ a_3 = |\mathbf{a}_3|$$

$$\mathbf{a}_2 \cdot \mathbf{a}_3 = a_2 \cdot a_3 \cdot \cos\alpha_1$$

$$\mathbf{a}_3 \cdot \mathbf{a}_1 = a_3 \cdot a_1 \cdot \cos\alpha_2$$

$$\mathbf{a}_1 \cdot \mathbf{a}_2 = a_1 \cdot a_2 \cdot \cos\alpha_3$$

Example

Orthorhombic Lattice: $a_1 \neq a_2 \neq a_3,\ \alpha_1 = \alpha_2 = \alpha_3 = 90°$

Direct Lattice Vectors: $\mathbf{a}_1 = a\hat{\mathbf{x}},\ \mathbf{a}_2 = b\hat{\mathbf{y}},\ \mathbf{a}_3 = c\hat{\mathbf{z}}$

Unit-Cell Volume: $V = \left|\mathbf{a}_1 \cdot \left(\mathbf{a}_2 \times \mathbf{a}_3\right)\right| = abc$

Reciprocal-Lattice Basis Vectors:

$$\mathbf{b}_1 = \frac{\begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ 0 & b & 0 \\ 0 & 0 & c \end{vmatrix}}{abc} = \left(\frac{\cancel{b}\,\cancel{c}\,\hat{\mathbf{x}}}{a\cancel{b}\,\cancel{c}}\right) = \left(\frac{1}{a}\right)\hat{\mathbf{x}}$$

$$\mathbf{b}_2 = \frac{\begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ 0 & 0 & c \\ a & 0 & 0 \end{vmatrix}}{abc} = \left(\frac{1}{b}\right)\hat{\mathbf{y}}$$

$$\mathbf{b}_3 = \frac{\begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ a & 0 & 0 \\ 0 & b & 0 \end{vmatrix}}{abc} = \left(\frac{1}{c}\right)\hat{\mathbf{z}}$$

Reciprocal lattice is also orthorhombic.

Miller indices

Consider an arbitrary vector: $\mathbf{r} = x\mathbf{a}_1 + y\mathbf{a}_2 + z\mathbf{a}_3$

A plane normal to $\mathbf{g}_{hk\ell}$ is defined by: $\mathbf{g}_{hk\ell} \cdot \mathbf{r} = hx + ky + \ell z = A$

General equation for a plane: $\frac{x}{x_i} + \frac{y}{y_i} + \frac{z}{z_i} = 1$

The intercepts are: $\mathbf{a}_1 = a_1\hat{\mathbf{a}}_1 : \; y = z = 0 \rightarrow x_i = \frac{A}{h}$

$\mathbf{a}_2 = a_2\hat{\mathbf{a}}_2 : \; z = x = 0 \rightarrow y_i = \frac{A}{k}$

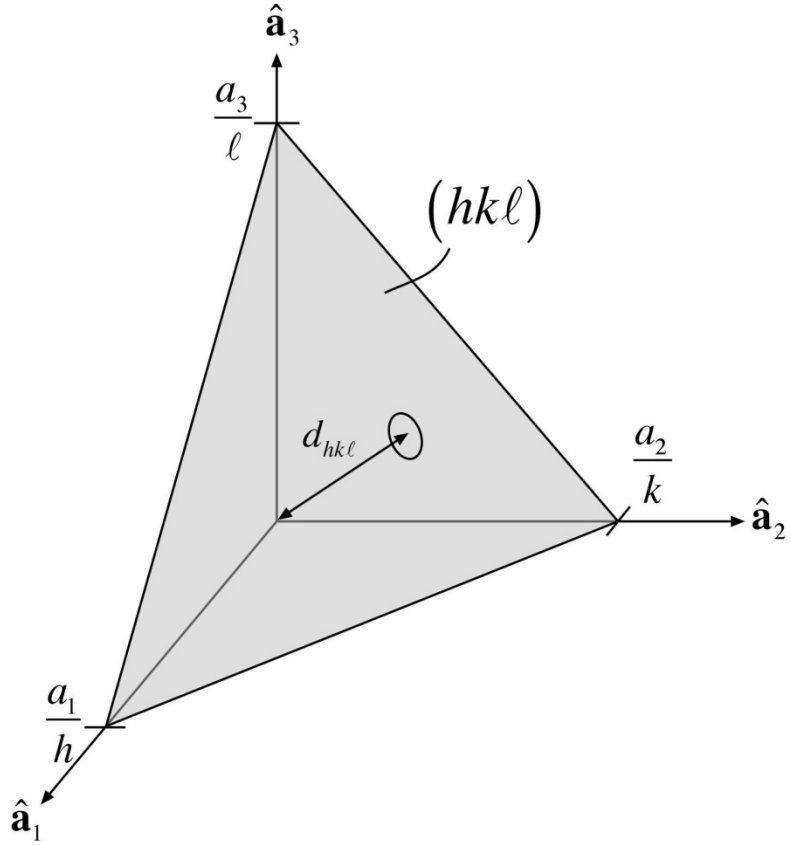
$\mathbf{a}_3 = a_3\hat{\mathbf{a}}_3 : \; x = y = 0 \rightarrow z_i = \frac{A}{\ell}$

If intercepts are lattice points: $\frac{x}{p} + \frac{y}{q} + \frac{z}{r} = 1$

where p, q, r are integers.

Multiply: $(qr)x + (pr)y + (pq)z = pqr$

$A = pqr = \text{an integer}$



The planes with *A*=any integer are identified by the Miller indices (*hkl*).

Interplanar spacing

The distance from the origin to an plane ($hk\ell$) is:

$$\frac{\mathbf{g}_{hk\ell}}{\left|\mathbf{g}_{hk\ell}\right|}\cdot\mathbf{r}=\frac{hx+ky+\ell z}{\left|\mathbf{g}_{hk\ell}\right|}=\frac{A}{\left|\mathbf{g}_{hk\ell}\right|}$$

The distance from A=0 to A=1 is:

$$d_{hk\ell}=\frac{1}{\left|\mathbf{g}_{hk\ell}\right|}$$

So $\mathbf{g}_{hk\ell}$:

1) is normal to the plane ($hk\ell$), and

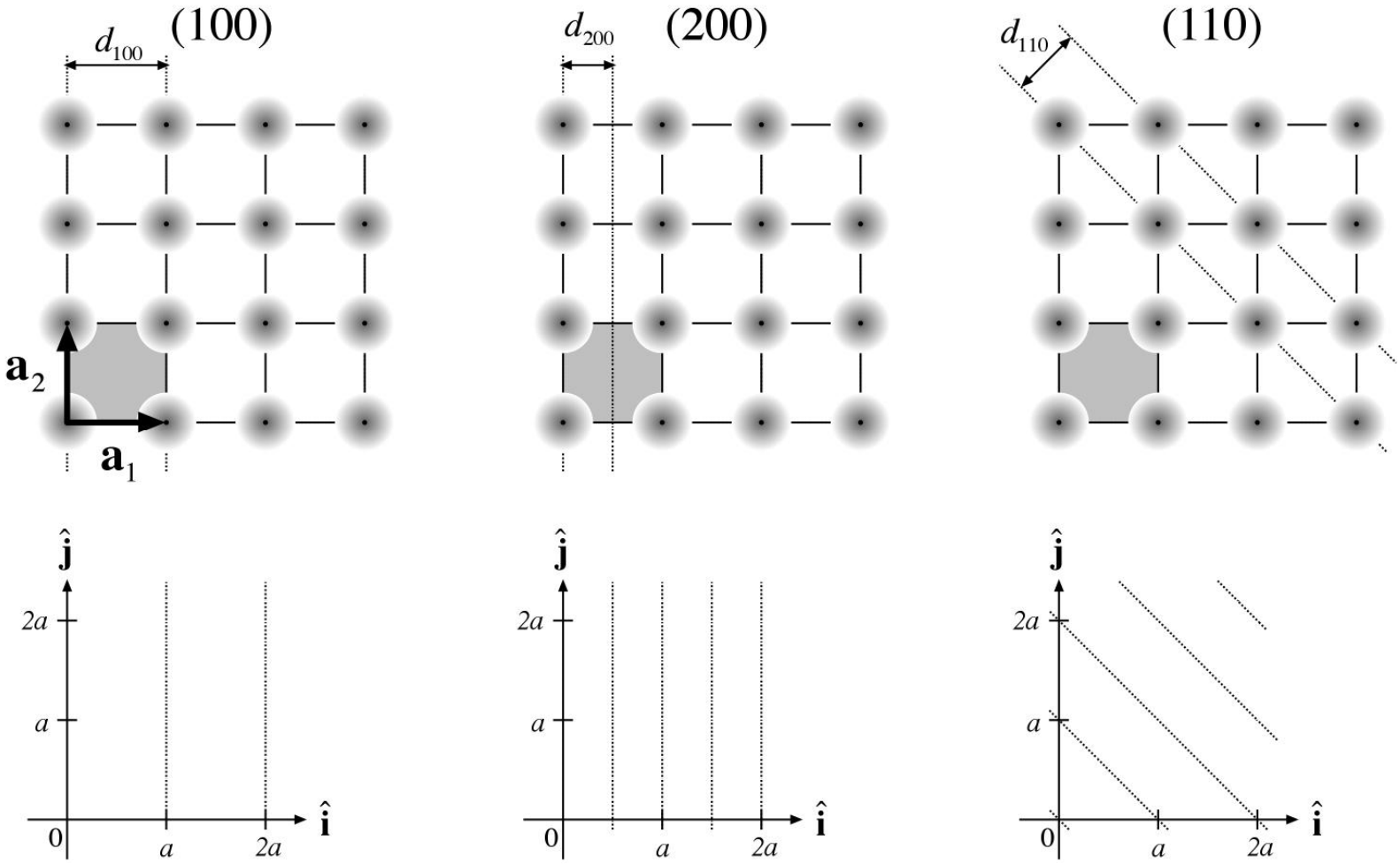
2) has length $1/d_{hk\ell}$

Note: The direction of $\mathbf{g}_{hk\ell}$ is also written ($hk\ell$)

Notation for planes, directions, & reflections

Direct Lattice	Reciprocal Lattice	Notation
vector, direction, or point	plane	[*uvw*]
family of vectors or directions	family of planes	<*uvw*>
plane	vector, direction or point	(*hkℓ*)
family of planes	family of vectors or directions	{*hkℓ*}
diffracting plane	reflection	*hkℓ*

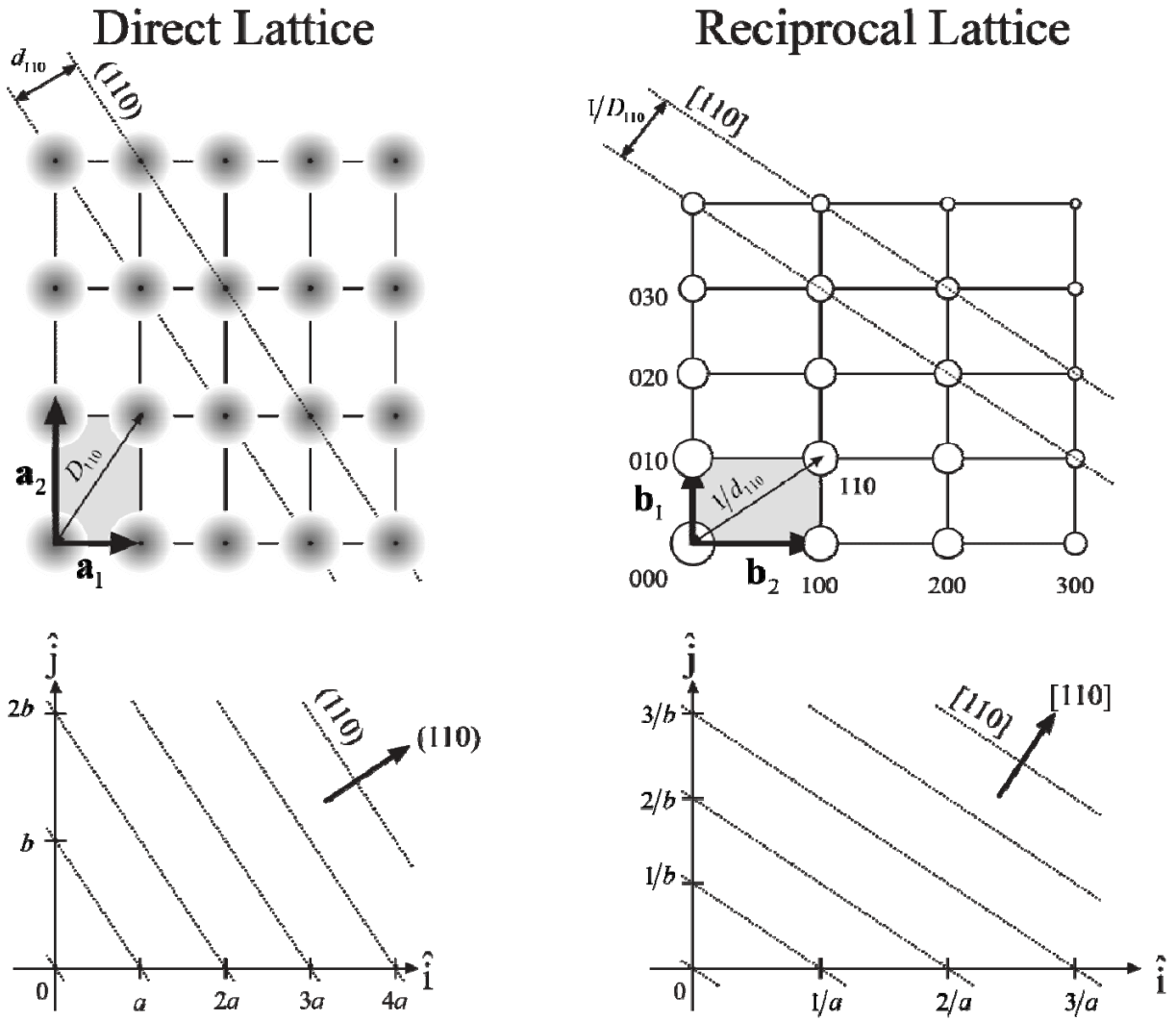
Visualizing direct-lattice planes: Cubic



Arbitrary Origin

Direct and reciprocal lattices: Non-cubic

$(hkl) \not\parallel [uvw]$

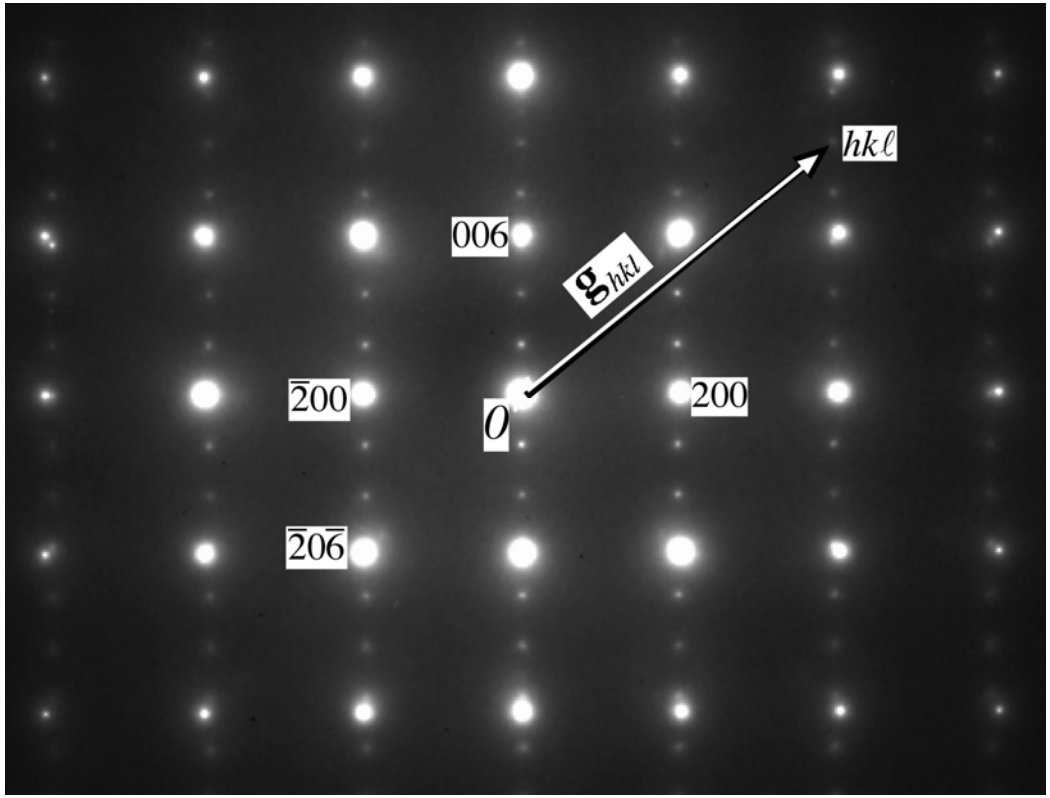


(*hkl*): direct plane/reciprocal vector

[*uvw*]: reciprocal plane/direct vector

Reciprocal lattice vectors and diffraction

Every diffraction spot $hk\ell$ (usually) has an associated $\mathbf{g}_{hk\ell}$



$(3\ \ -2\ 4) = (3\bar{2}4)$: "three bar two four"

Bragg condition

$$\vec{\mathbf{k}}' = \vec{\mathbf{k}} + \vec{\mathbf{g}}$$

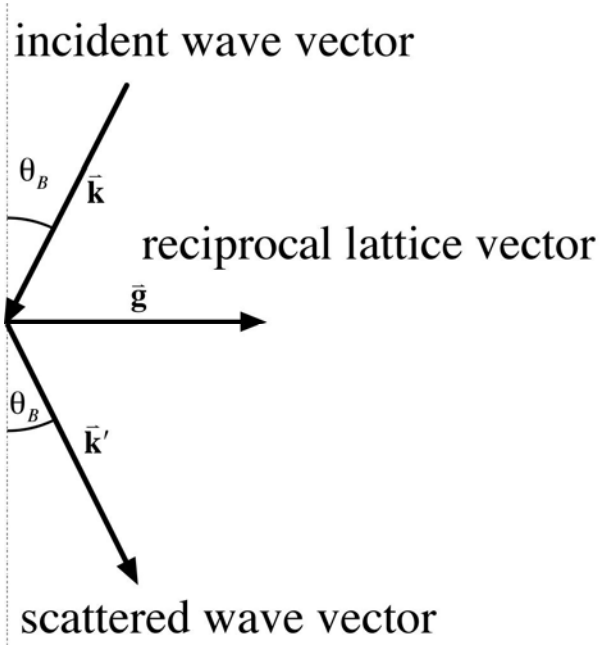
$$k = \left|\vec{\mathbf{k}}\right| = \left|\vec{\mathbf{k}}'\right| = \frac{1}{\lambda}$$

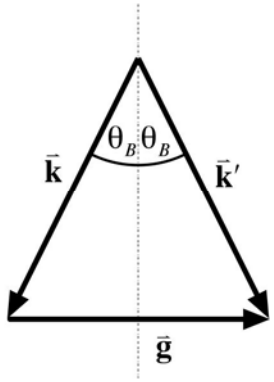
$$g = \left|\vec{\mathbf{g}}\right| = \frac{1}{d}$$

$$k^2 = \left(\vec{\mathbf{k}} + \vec{\mathbf{g}}\right)^2 = k^2 + g^2 + 2\vec{\mathbf{k}} \cdot \vec{\mathbf{g}}$$

$$\vec{\mathbf{k}} \cdot \vec{\mathbf{g}} = -k \cdot g \cdot \sin\theta_B$$

$$g = 2 \cdot k \cdot \sin\theta_B$$



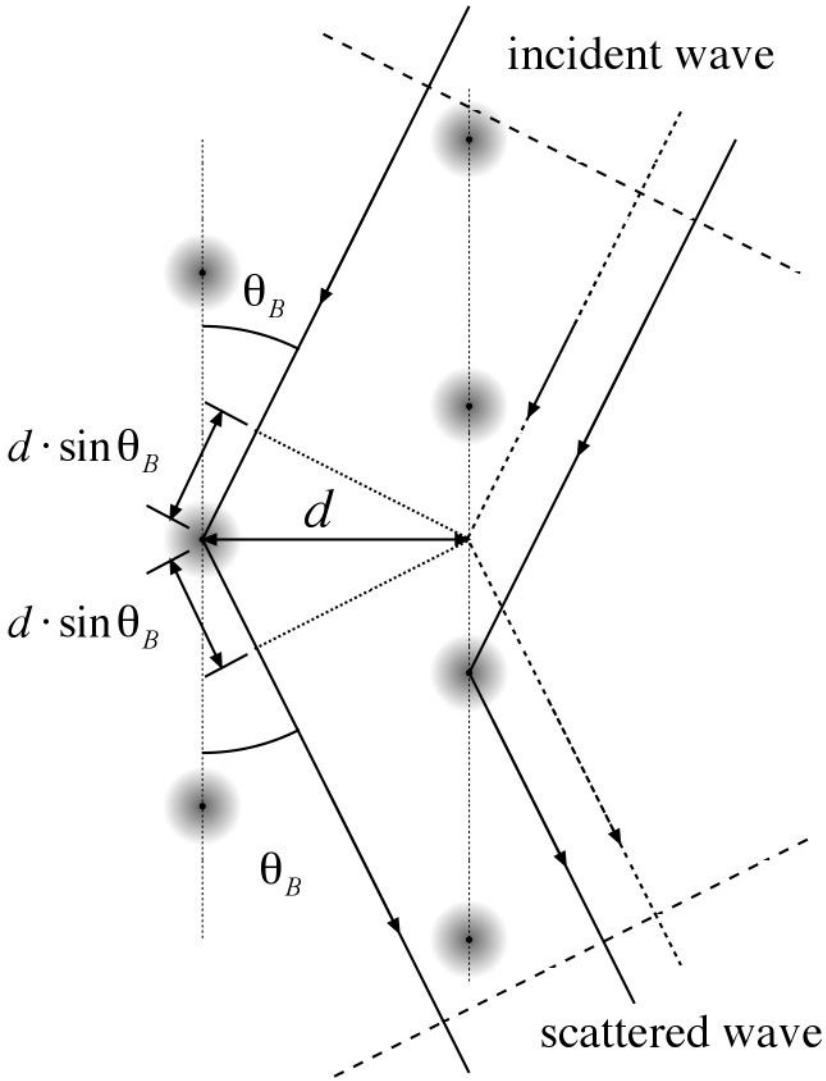


$$\Rightarrow 2 \cdot d \cdot \sin\theta_B = \lambda$$ Bragg's Law

$$\Delta\vec{\mathbf{p}} = h\left(\vec{\mathbf{k}}' - \vec{\mathbf{k}}\right) = h\vec{\mathbf{g}}$$

Momentum transfer (impulse) to electron

Bragg's law: Observations



$$2d \sin\theta_B = n\lambda$$

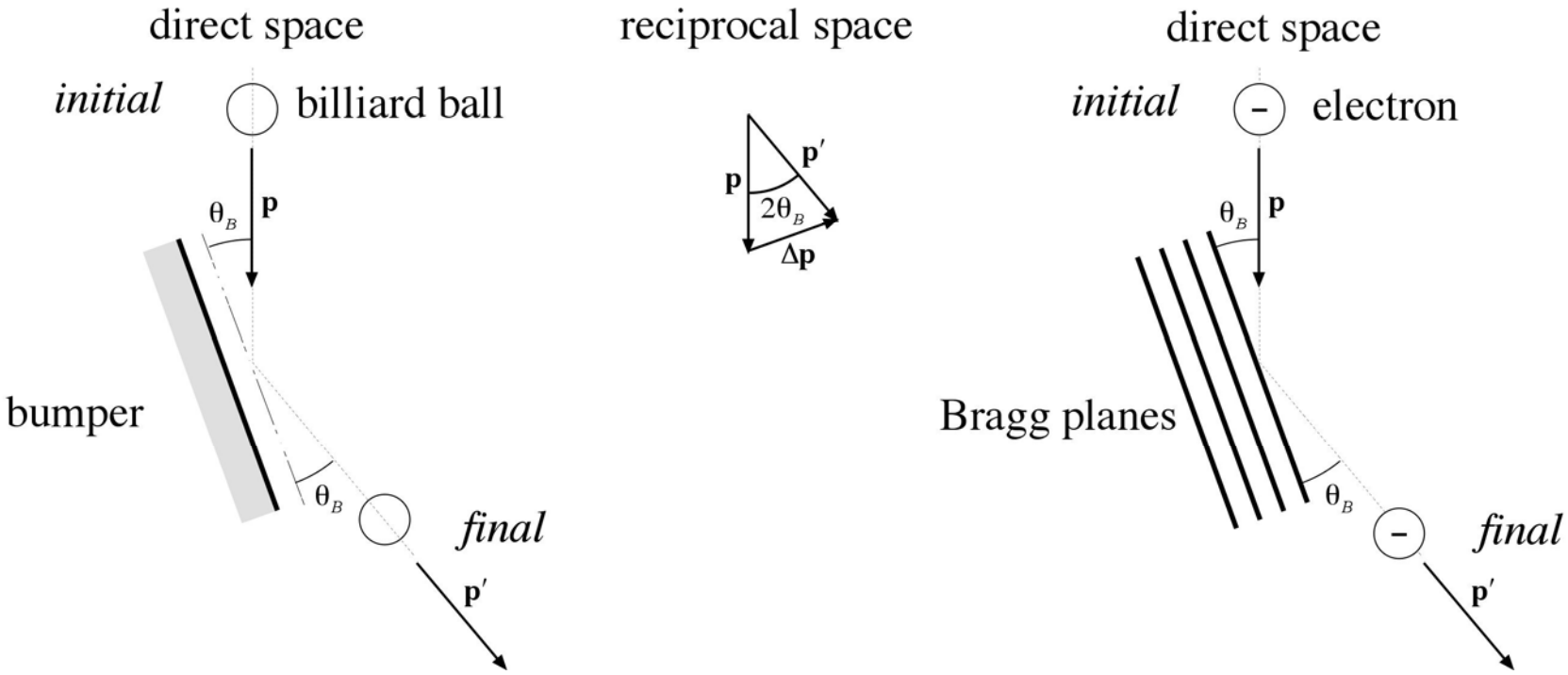
n = integer

1) Bragg's Law is insensitive to lateral shifting of planes; it only depends on the interplanar spacing.

2) We can interpret the n as arising from higher-order planes with spacing d/n.

$$2\left(\frac{d}{n}\right)\sin\theta_B = \lambda$$

Direct vs. reciprocal space

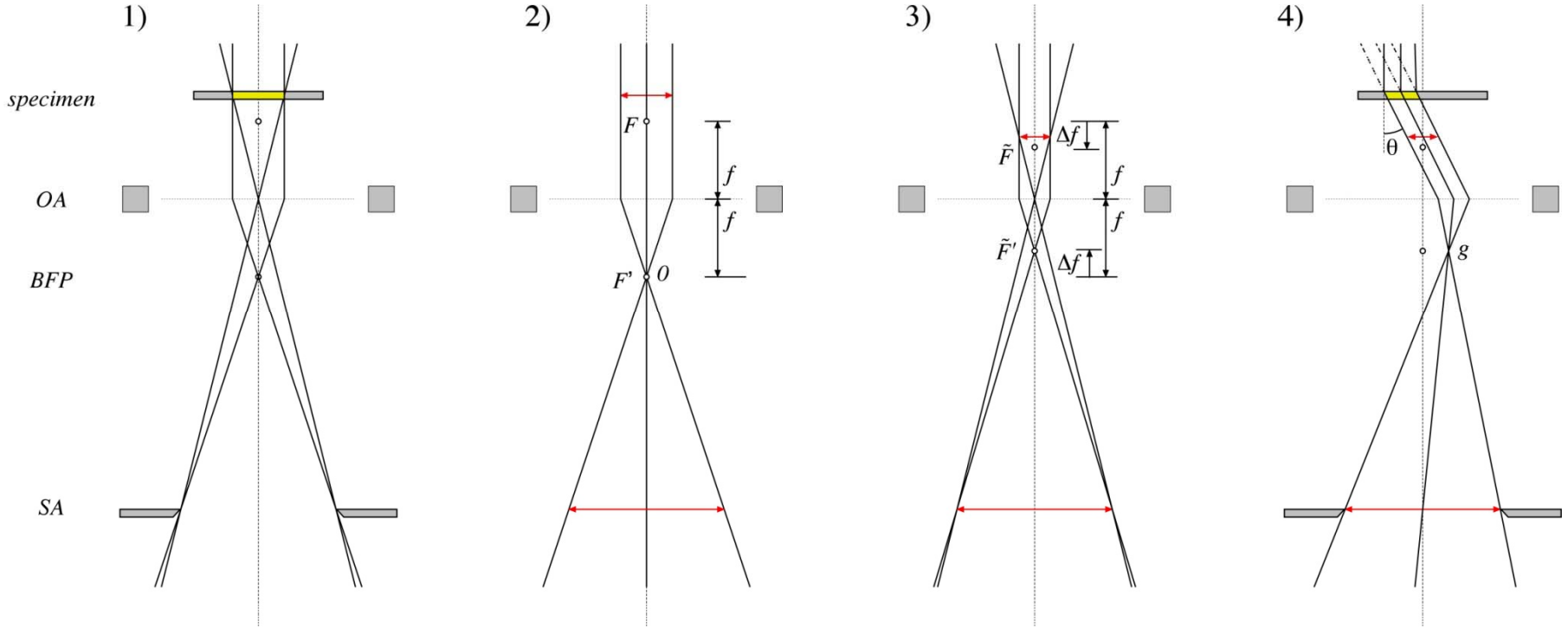


A diagram in direct space shows trajectories or rays.
A diagram in reciprocal space shows momentum or wave vectors.

Selected-area diffraction error

Spherical aberration causes selected region to differ for each reflection

1) Nominal selected area: SA in first image plane
2) Paraxial beams cross in BFP
3) Focal length shorter for tilted beams: find corresponding object
4) Find area selected for *g*, tilted by θ from axis



Influence of C_s on selected area

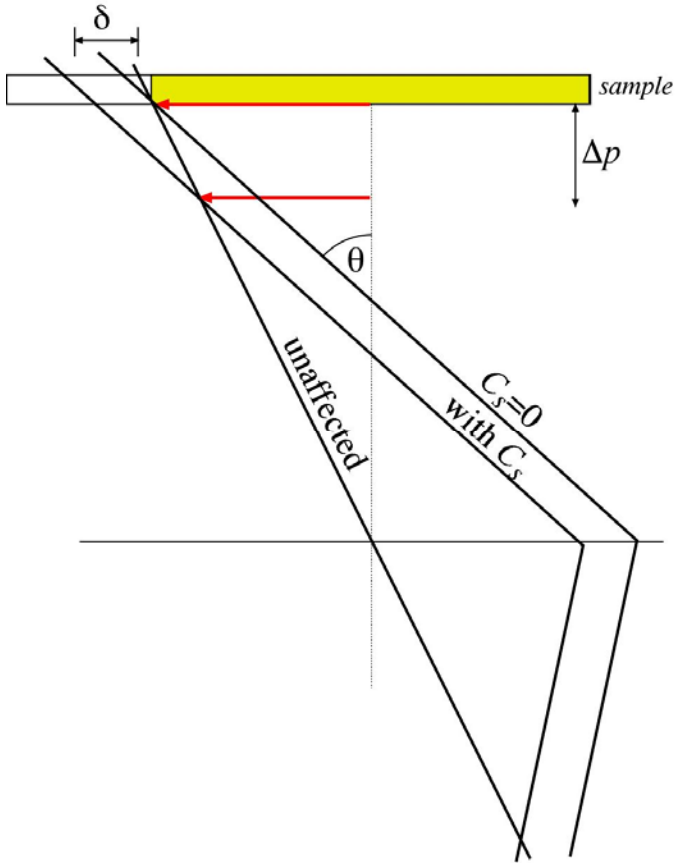
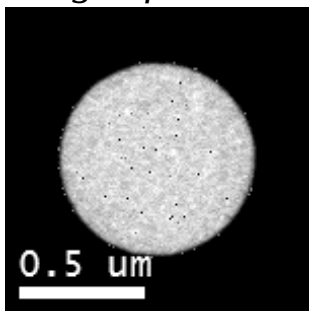


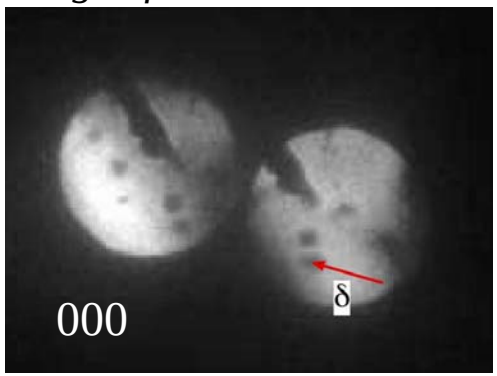
image of SA



SA4

Actual size ~ 50 μm

image of DP



$$\Delta p \approx \Delta f = C_s \theta^2$$

$$\delta \approx \Delta p \cdot \theta = C_s \cdot \theta^3$$

$$\theta = 2\theta_{B,004} = \frac{\lambda}{d_{004}} = 22 \text{ mrad} \qquad \delta = 0.21 \text{ μm}$$

Estimate C_s? $\quad C_s = \dfrac{\delta}{\theta^3} = 19 \text{ mm}$

Too big! (Other contributions to δ.)