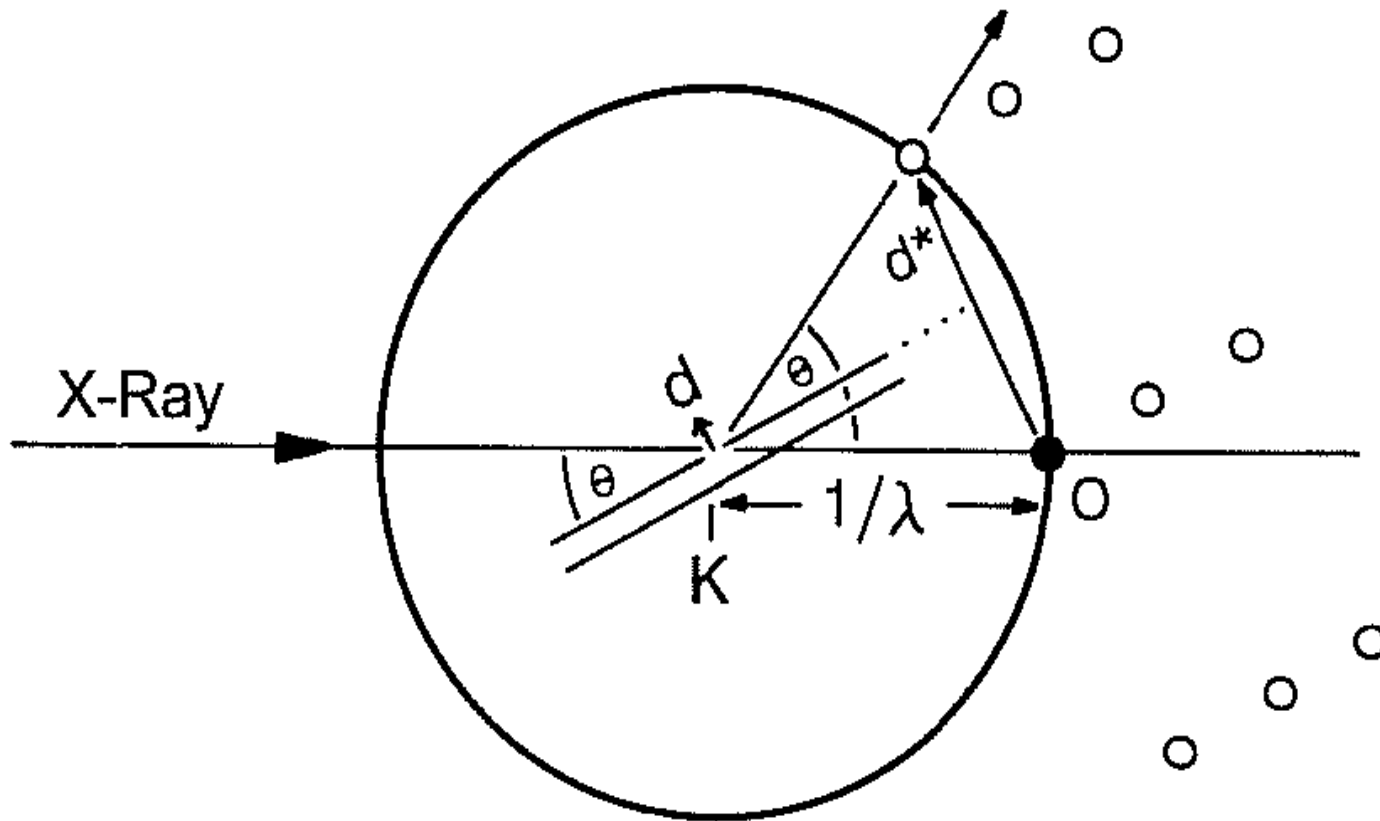


**Fig. 4.3.** Example of a reciprocal lattice, divided into layers along  $c^*$ .

Where are the real space vectors  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ ?  
 What does each of these points represent?



### The Ewald Sphere

Monochromatic X-rays come in at left, wavelength  $\lambda$

Radius of the sphere is  $1/\lambda$

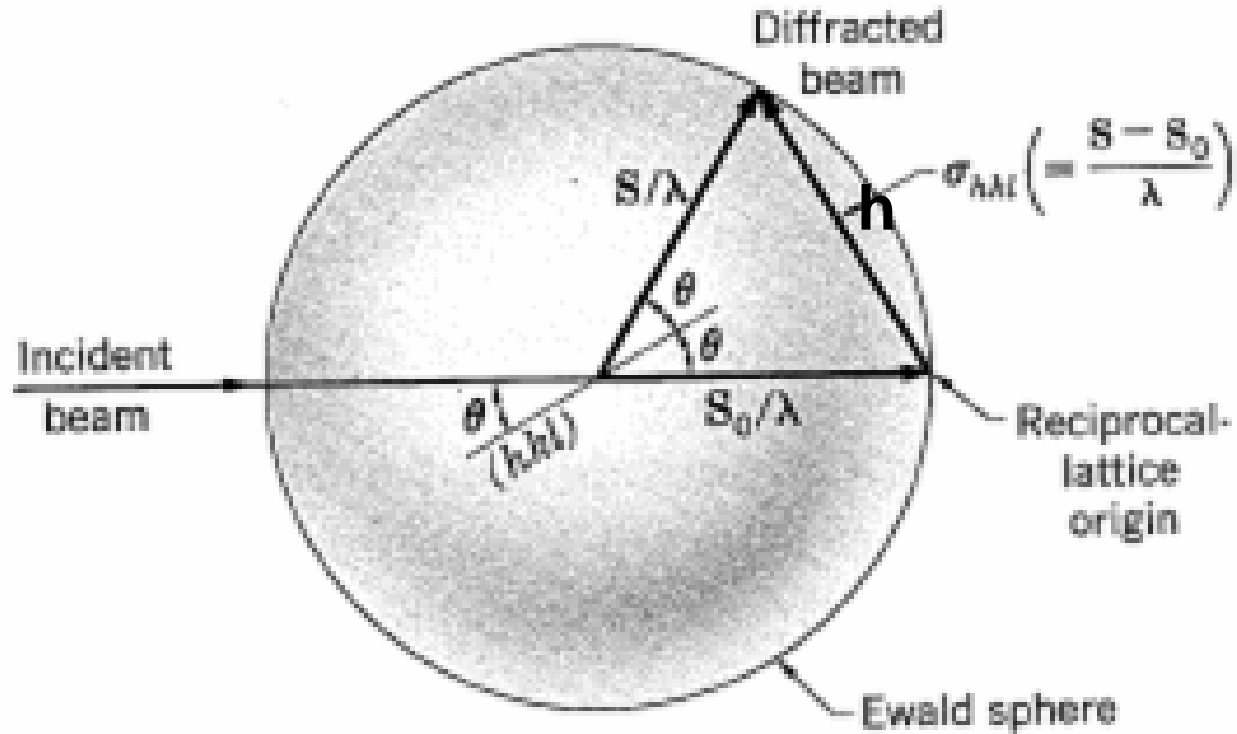
Crystal at center (K)

Origin of the reciprocal lattice is at O

When a reciprocal lattice point touches the sphere  
diffraction occurs, as shown

What happens as  $\lambda$  gets smaller?

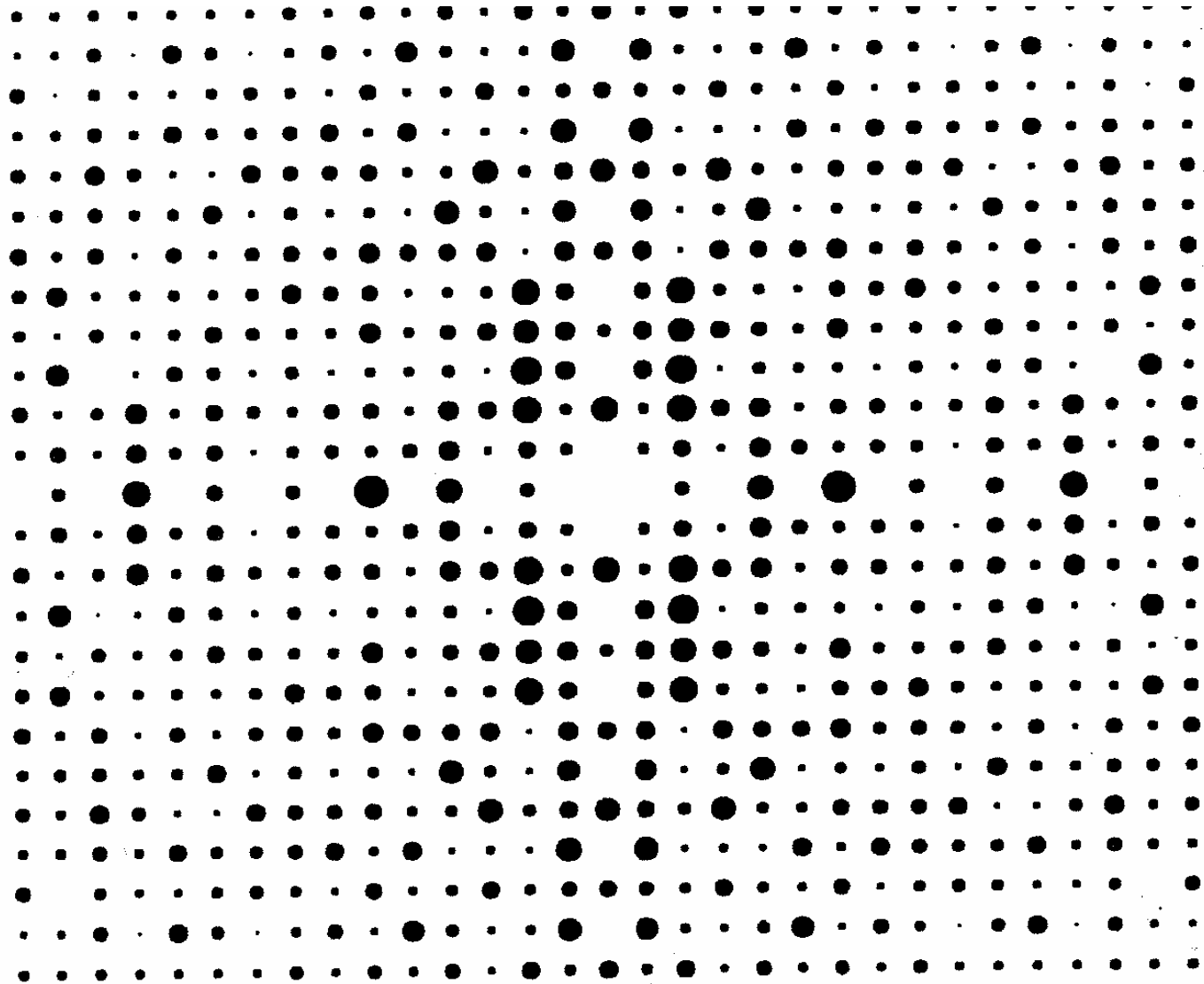
As the real lattice constants get bigger?



### Ewald Sphere..more

Notice that the incoming X-ray beam has both a direction and length (if we set the length to  $1/\lambda$  as done in the Ewald sphere). It is thus a vector. This is also true for the diffracted beam. These are shown here as, respectively,  $\mathbf{S}_0/\lambda$  and  $\mathbf{S}/\lambda$  (where bold face indicates a vector). The Bragg diffraction condition then becomes the vector equation

$\mathbf{h} = \mathbf{S}/\lambda - \mathbf{S}_0/\lambda$ , where  $\mathbf{h}$  is the reciprocal lattice position (and Miller index)  $h, k, l$



A computer generated model of a Precession camera photograph. This type of camera gives an undistorted view of the reciprocal lattice, one plane of which is shown in this view. What symmetry do you see? What systematic absences?

$$f = \frac{E_a}{E_e} \quad dq = \rho dV$$

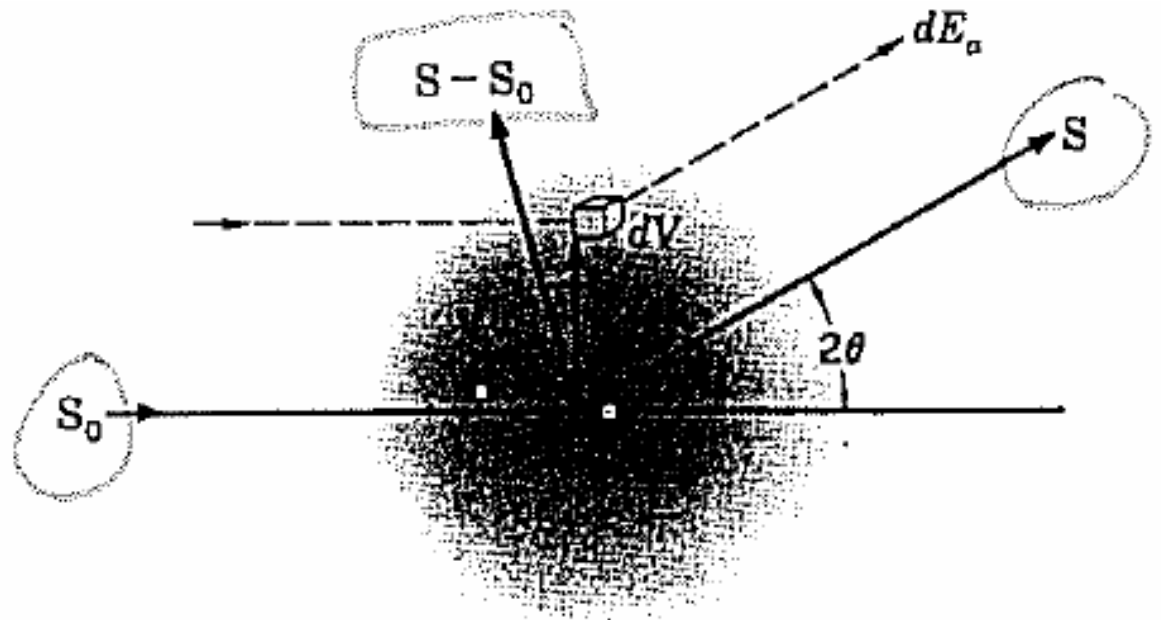
$$\frac{dE_a}{E_e} = \frac{dq}{e} = \frac{\rho dV}{e}$$

$$df = \frac{\rho(r)}{e} e^{(2\pi i/\lambda)(S-S_0)\cdot r} dV$$

$$dV = 2\pi r^2 \sin \varphi d\varphi dr$$

$$f = \frac{1}{e} \int_{r=0}^{\infty} \int_{\varphi=0}^{\pi} \rho(r) e^{ikr \cos \varphi} 2\pi r^2 \sin \varphi d\varphi dr$$

$$f = \frac{4\pi}{e} \int_0^{\infty} r^2 \rho(r) \frac{\sin kr}{kr} dr \quad \text{where} \quad k = \frac{4\pi \sin \theta}{\lambda}$$



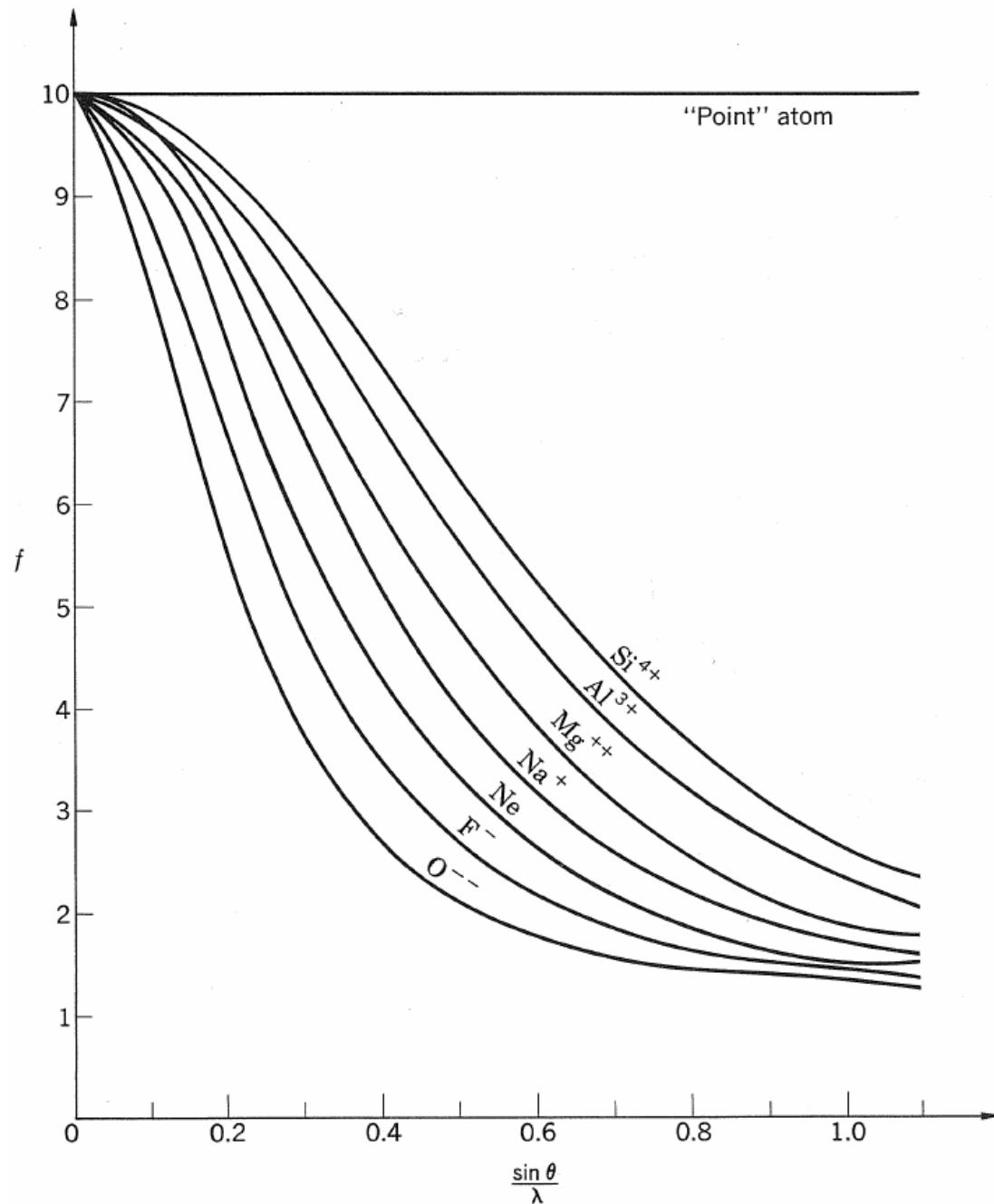
## The atomic scattering factor (compared to scattering by a free electron)

The distribution of electron density around atoms is approximately spherical. At the nucleus it is a maximum and goes to zero at large distance from the nucleus. Consider a volume element  $V$  at position  $r$  from the nucleus, where we can work in Cartesian coordinates and so  $r$  is just the positional coordinates  $x, y, z$  in Angstroms (or polar,  $r, \theta, \varphi$ ). Compared to the scattering from a volume element at the origin (along the same path as shown here for the diffraction vector) there is a phase shift, since the distance traversed by the two beams is different.

## Atomic scattering factor, $f$

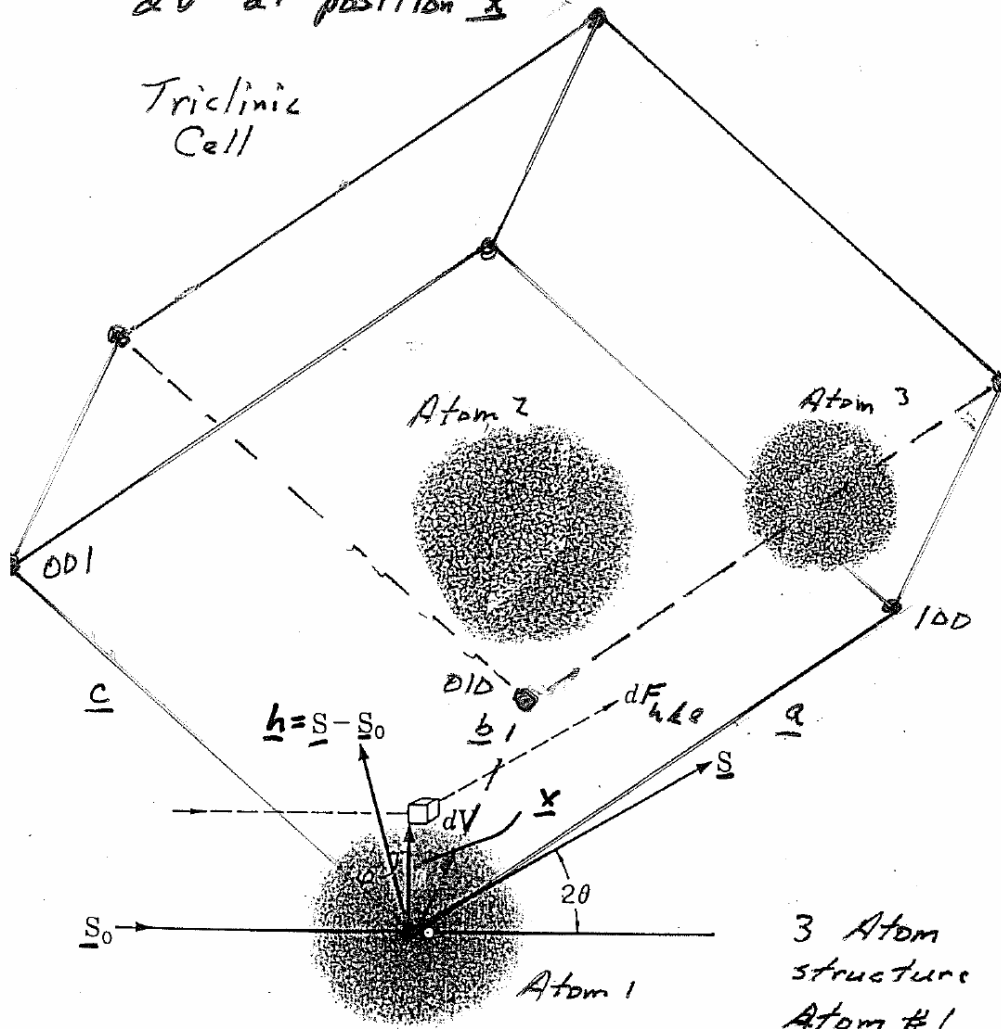
Units of  $f$  are electrons.

- Why 10 at the origin?
- Why does  $O^{2-}$  drop off faster than  $Si^{4+}$ ?
- Why rapid drop at the beginning and less rapid later?
- Why is axis in  $(\sin \theta)/\lambda$ ?



Phase shift for  $e^-$  density in volume  $dV$  at position  $\underline{x}$

Triclinic Cell



$$\underline{h} = h\underline{a}^* + k\underline{b}^* + l\underline{c}^*$$

$$\underline{x} = x\underline{a} + y\underline{b} + z\underline{c}$$

3 Atom structure  
Atom #1  
at cell  
origin

Note different  
units.

The crystal structure factor:  
 $F(h,k,l)$

Now we consider the scattering by the entire unit cell contents of the crystal. [We know that all the other unit cells scatter in phase.] As an illustration consider this three atom structure in a triclinic unit cell (Picasso could not do better).

Now we need to keep track of coordinates. The unit cell contents are in triclinic fractional coordinates. The Miller indices  $h, k, l$  are in reciprocal lattice units. We have seen that the phase shift in cycles is the dot product of the reciprocal lattice vector  $\underline{h}$  with the positional coordinate, here called  $\underline{x}$