Diffraction & Crystallography

Why do we get Bragg spots ?

When light interacts with electrons the elastic component of the *scattering amplitude* is given by:

$$A = \int_{\text{all space}} r(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}').\mathbf{r}} d\mathbf{r} = N \int_{cell} r(\mathbf{r}) e^{-i?\,\mathbf{k}.\mathbf{r}} d\mathbf{r}$$

$$?\,\mathbf{k} = \mathbf{k}' - \mathbf{k}$$

Fourier analyse the density…

The charge density is periodic

$$r(\mathbf{r}+\mathbf{R}) = r(\mathbf{r})$$

$$r(\mathbf{r}) = \sum_{\mathbf{G}} r_{\mathbf{G}}\, e^{i\mathbf{G}.\mathbf{r}}$$

$$A_{\mathbf{G}} = N \sum_{\mathbf{G}} \int_{cell} r_{\mathbf{G}}\, e^{i(\mathbf{G}-?\,\mathbf{k}).\mathbf{r}}\, d\mathbf{r}$$

If $G=\Delta k$ $A=\rho_G$ and 0 otherwise ….. the diffraction spots.

The intensity of the spots…

The density is built from atomic contributions (roughly speaking)

$$r(r) = \sum_{j}^{N} r_j(r - R_j)$$

$$A_G = \sum_{j}^{N} \int_{cell} r_j(r - R_j)\, e^{-iG.r}\, dV$$

$$s \equiv r - R_j$$

$$A_G = \sum_{j}^{N} e^{-iG.R_j} \int_{cell} r_j(s)\, e^{-iG.s}\, dV$$

$$= \sum_{}^{N} f_j e^{-iG.R_j}$$

The Atomic Form Factor

$$A_G = \sum_j^N \int_{cell} r_j(r - R_j) e^{-iG.r} dV$$

$$s \equiv r - R_j$$

$$A_G = \sum_j^N e^{-iG.R_j} \int_{cell} r_j(s) e^{-iG.s} dV = \sum_j^N f_j e^{-iG.R_j}$$

$$f_j = \int_{cell} r_j(s) e^{-iG.s} dV$$

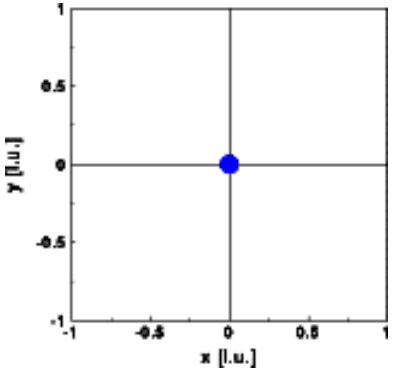
Summary – Diffraction..

$$A_G = \sum_j^N f_j e^{-iG.R_j}$$

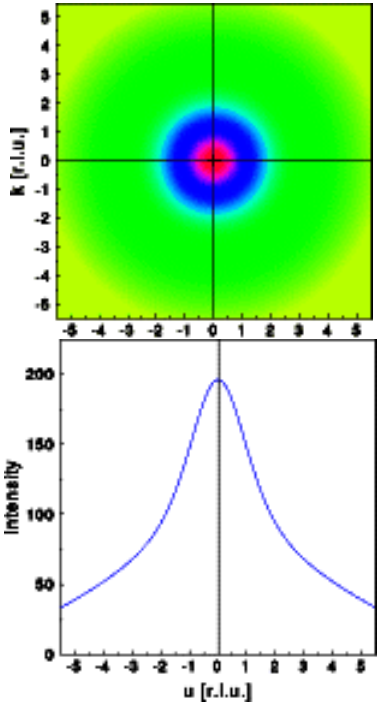
The form factor is the Fourier Transform of the atomic charge density, the total diffraction amplitude is a Fourier Series based on the lattice periodicity – the Fourier coefficients are the form factors these govern the intensity in each peak.

Single Atom

Charge density - ρ(r)



Fourier Transform - ρ(k)

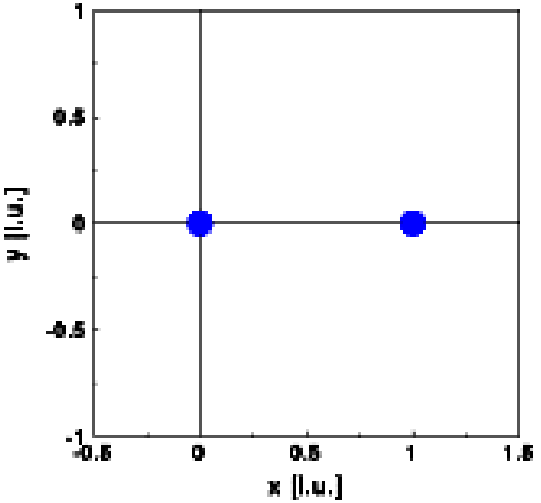


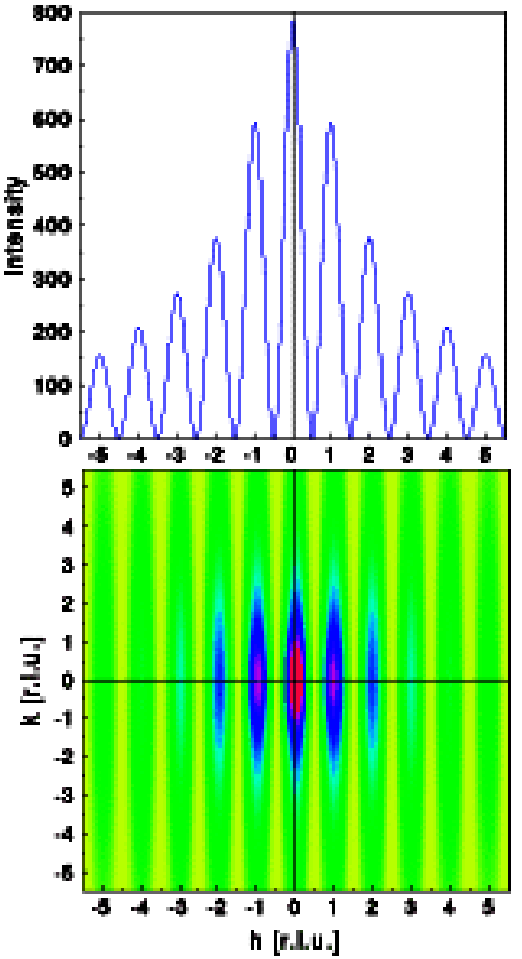
2D

1D

ρ(k) - spherically symmetric, decays as k increases

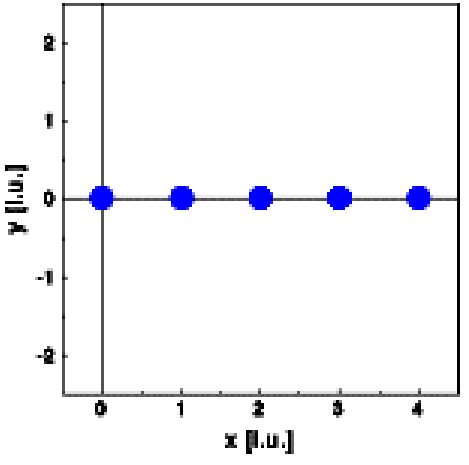
2 Atoms

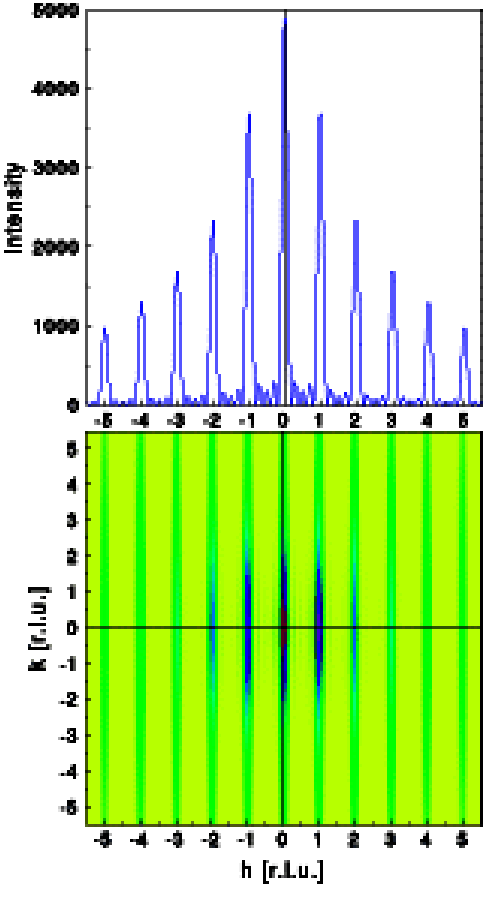




Scattered intensity falls off for large k but is modulated in the direction linking the atoms due to interference the scattered waves

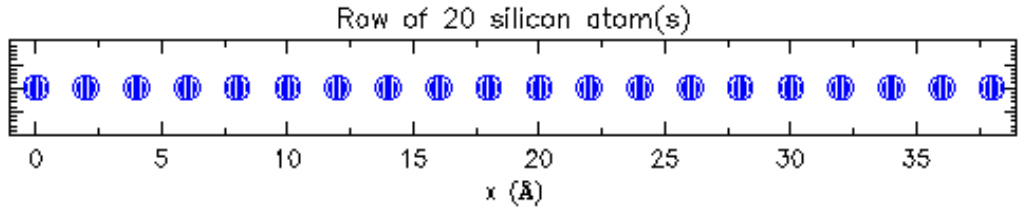
5 atoms

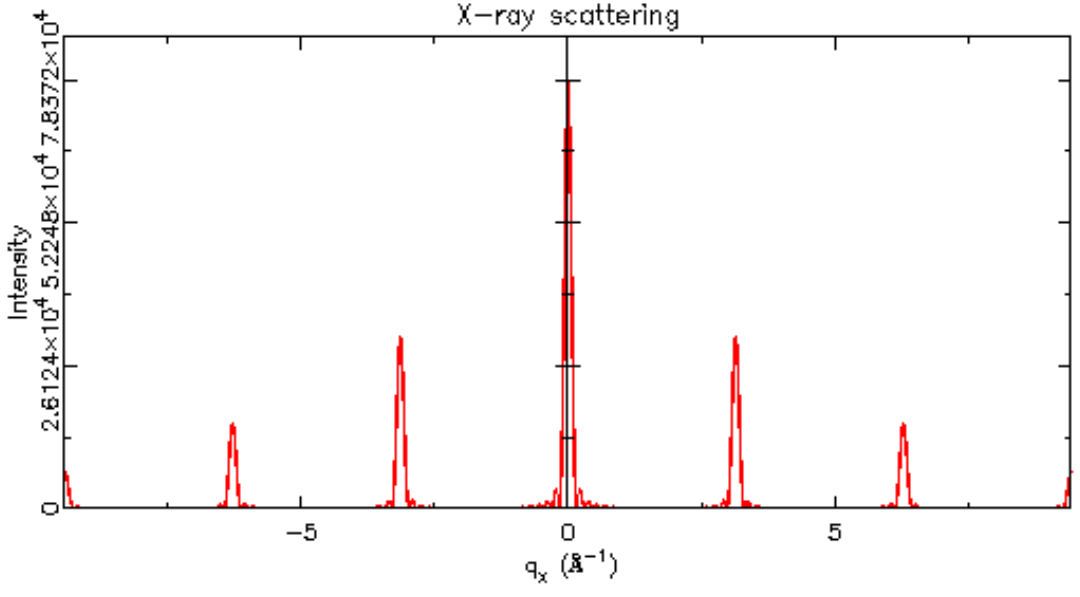




Sharper “Bragg” reflections – small maxima in between

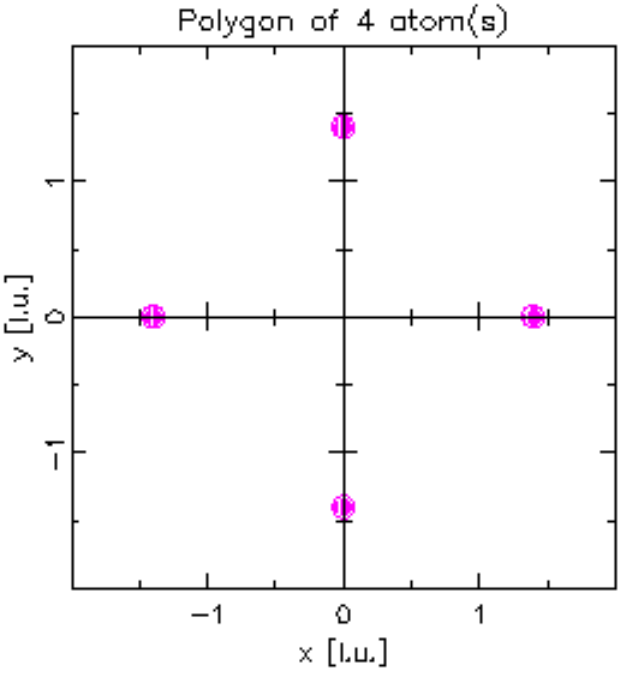
20 Atoms – 2Å spacing

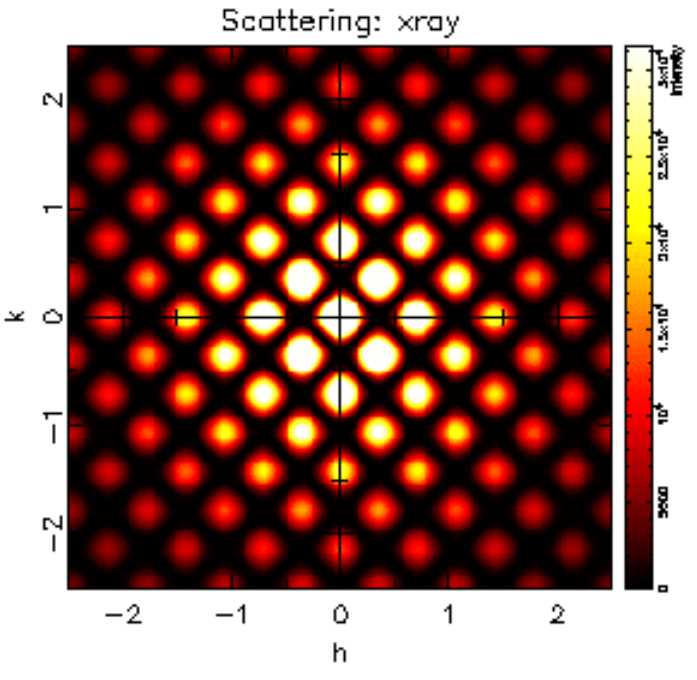




Peaks at $2\pi/2 = \pi$ Å^{-1}

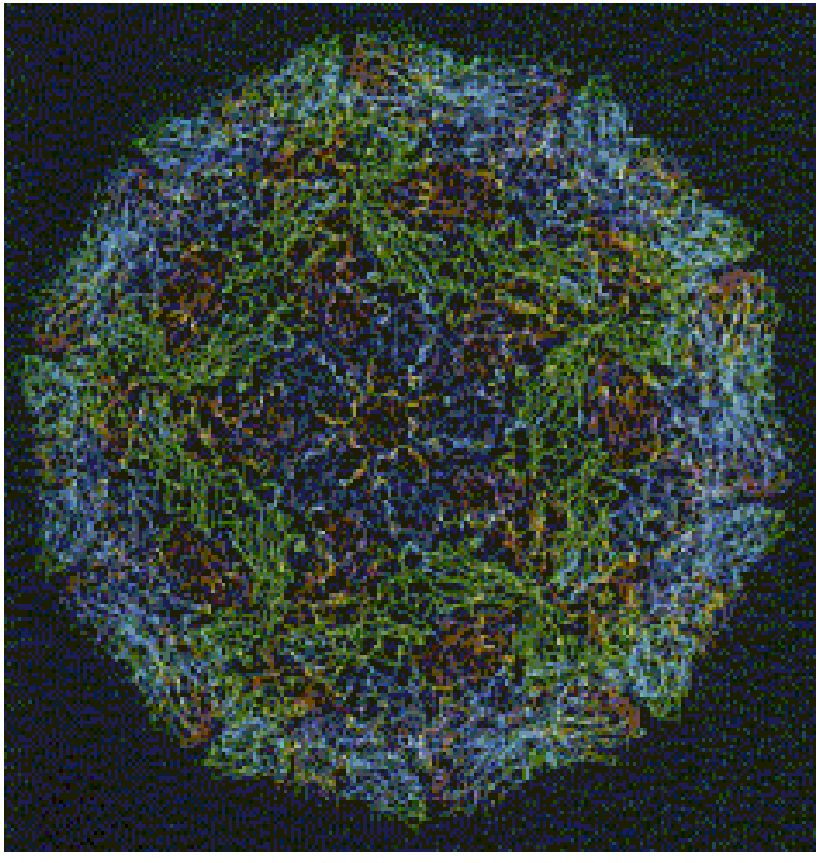
Lattices of Atoms – 2D





Crystallography

- Measure the positions and intensities of the Bragg peaks
- Figure out the structure.



Structure of the foot and mouth virus.

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