Condensed Matter Physics

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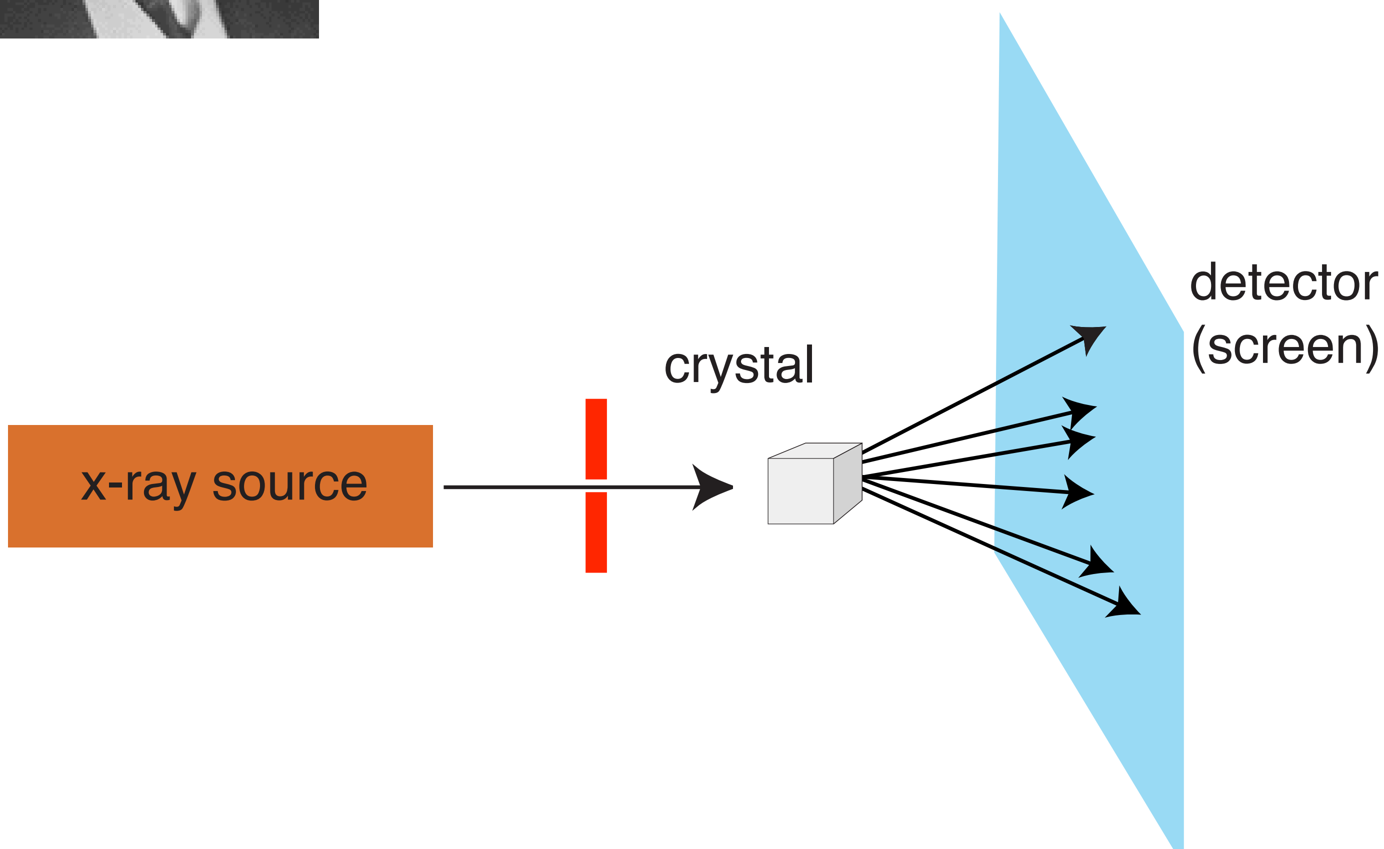
Crystal structure determination

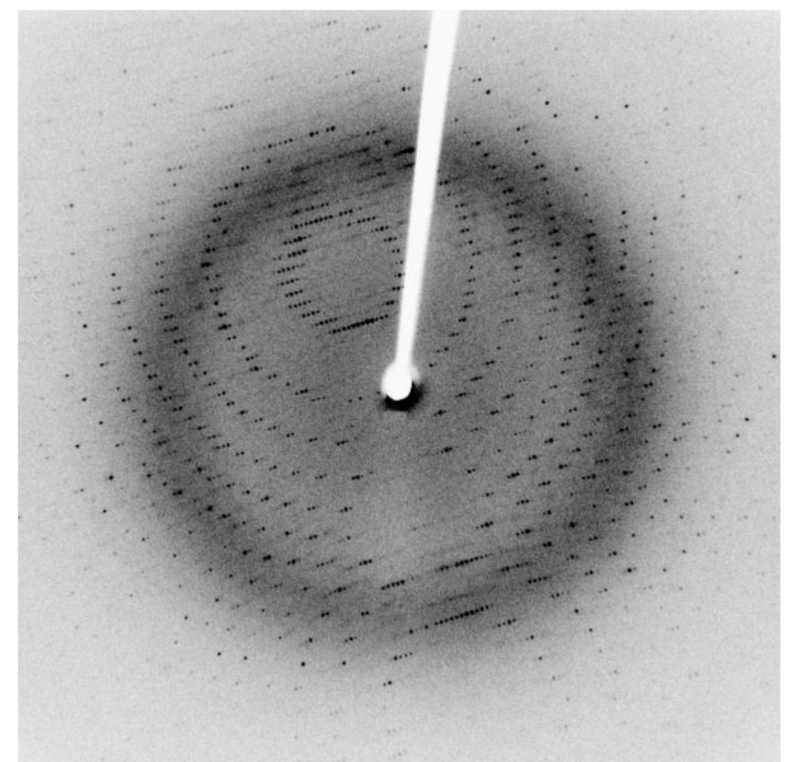
X-ray diffraction

- The atomic structure of crystals cannot be determined by optical microscopy because the wavelength of the photons is much too long (400 nm or so).
- So one might want to build an x-ray microscope but this does not work for very small wavelength because there are no suitable x-ray optical lenses.
- The idea is to use the diffraction of x-rays by a perfect crystal.
- Here: monochromatic x-rays, elastic scattering, kinematic approximation

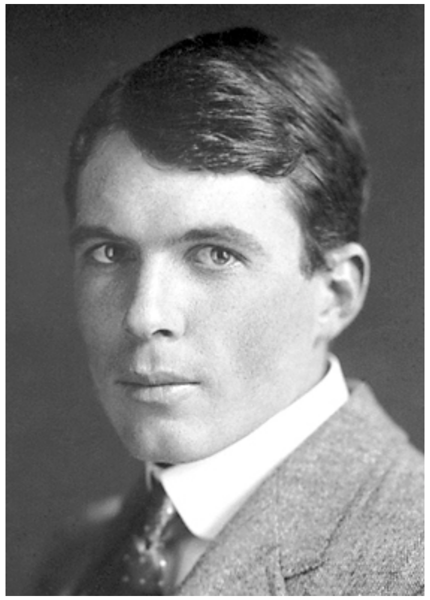
X-ray diffraction

- The crystals can be used to diffract X-rays (von Laue, 1912).





The Bragg description (1912): specular reflection



- Fig 2.8 Solid State Physics: An Introduction, by Philip Hofmann Wiley-VCH Berlin.

$$2AB = n\lambda$$

$$d \sin \Theta \quad d \sin \Theta$$

$$\sin \Theta = \frac{AB}{d}$$

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

and this only works for $\lambda < 2d$

- The Bragg condition for constructive interference holds for any number of layers, not only two (why?)

X-ray diffraction: the Bragg description

- The X-rays penetrate deeply and many layers contribute to the reflected intensity
- The diffracted peak intensities are therefore very sharp (in angle)
- The physics of the lattice planes is totally obscure!

A little reminder about waves and diffraction

$$\mathbf{A}(\mathbf{r},t) = \mathbf{A}_0 e^{i\mathbf{k}\cdot\mathbf{r} - i\omega t}$$

$$|\mathbf{k}| = \frac{2\pi}{\lambda}$$

$$\mathbf{A}_0 \cdot \mathbf{k} = 0$$

λ = 1 Å
hν = 12 keV

complex notations

$$\mathbf{A}(\mathbf{r},t) = \mathbf{A}_0 \cos(\mathbf{k}\cdot\mathbf{r} - \omega t) = \Re\left[\mathbf{A}_0 e^{i\mathbf{k}\cdot\mathbf{r} - i\omega t}\right]$$

(for real $\mathbf{A_0}$)

$$e^{i\phi} = \cos\phi + i\sin\phi$$

X-ray diffraction, von Laue description

- Fig 2.10 Solid State Physics: An Introduction, by Philip Hofmann Wiley-VCH Berlin.

X-ray diffraction, von Laue description

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incoming wave at **r**

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0 e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})-i\omega t}$$

absolute E_0 of no interest

$$\mathbf{E}(\mathbf{r},t) \propto e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})} e^{-i\omega t}$$

outgoing wave in detector

$$\mathbf{E}(\mathbf{R}',t) \propto \mathbf{E}(\mathbf{r},t)\rho(\mathbf{r}) e^{i\mathbf{k}'\cdot(\mathbf{R}'-\mathbf{r})}$$

$$\mathbf{E}(\mathbf{R}',t) \propto e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})}\rho(\mathbf{r}) e^{i\mathbf{k}'\cdot(\mathbf{R}'-\mathbf{r})} e^{-i\omega t}$$

$$= e^{i(\mathbf{k}'\cdot\mathbf{R}'-\mathbf{k}\cdot\mathbf{R})}\rho(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} e^{-i\omega t}$$

X-ray diffraction, von Laue description

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field at detector for one point

$$\mathbf{E}(\mathbf{R}', t) \propto e^{i(\mathbf{k}'\cdot\mathbf{R}' - \mathbf{k}\cdot\mathbf{R})}\rho(\mathbf{r})e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}e^{-i\omega t}$$

$$\mathbf{E}(\mathbf{R}', t) \propto \rho(\mathbf{r})e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}e^{-i\omega t}$$

and for the whole crystal

$$\mathbf{E}(\mathbf{R}', t) \propto e^{-i\omega t}\int_V \rho(\mathbf{r})e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}dV$$

X-ray diffraction, von Laue description

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$$\mathbf{E}(\mathbf{R}', t) \propto e^{-i\omega t} \int_V \rho(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} dV$$

so the measured intensity is

$$I(\mathbf{K}) \propto |\int_V \rho(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} dV|^2 = |\int_V \rho(\mathbf{r}) e^{-i\mathbf{K}\cdot\mathbf{r}} dV|^2$$

with

$$\mathbf{K} = \mathbf{k}' - \mathbf{k}$$