Condensed Matter Physics

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Applications of the reciprocal lattice

1D chain of atoms

- Fig 2.11, Solid State Physics: An Introduction, by Philip Hofmann, Wiley-VCH Berlin.

example of charge density 1

example of charge density 2

- Greatly simplifies the description of lattice-periodic functions (charge density, one-electron potential...).

Applications of the reciprocal lattice

example: charge density in the chain

$$\rho(x) = \rho(x+a)$$

Fourier series

$$\rho(x) = \rho_0 + \sum_{n=1}^{\infty} \left\{ C_n cos(x2\pi n/a) + S_n sin(x2\pi n/a) \right\}$$

alternatively

$$\rho(x) = \sum_{n=-\infty}^{\infty} \rho_n e^{ixn2\pi/a} \qquad \rho^*_{-n} = \rho_n$$

Applications of the reciprocal lattice

$$\rho(x) = \sum_{n=-\infty}^{\infty} \rho_n e^{ixn2\pi/a}$$

1D reciprocal lattice

$$g = n\frac{2\pi}{a}$$

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Applications of the reciprocal lattice

1D

$$\rho(x) = \sum_{n=-\infty}^{\infty} \rho_n e^{ixn2\pi/a} = \sum_{n=-\infty}^{\infty} \rho_n e^{igx}$$

$$g = n\frac{2\pi}{a}$$

$$\rho^*_{-n} = \rho_n$$

3D

$$\rho(\mathbf{r}) = \sum_{\mathbf{G}} \rho_{\mathbf{G}} e^{i\mathbf{G}\mathbf{r}}$$

$$\rho^*_{-\mathbf{G}} = \rho_{\mathbf{G}}$$

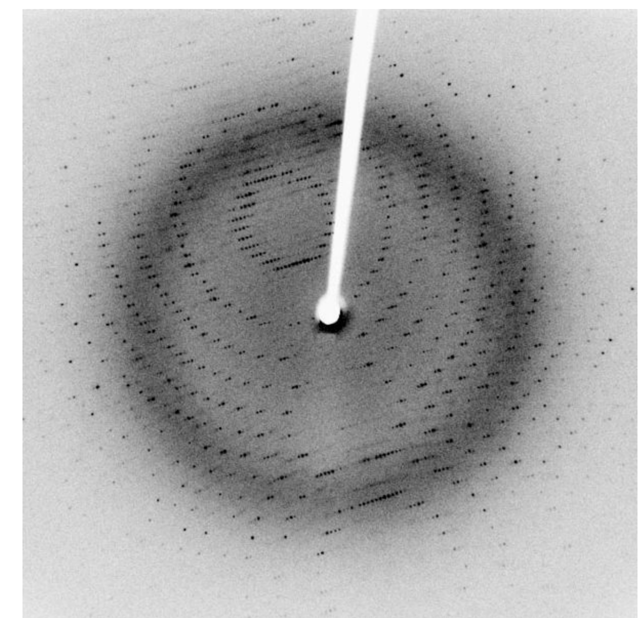
X-ray diffraction, von Laue description

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

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



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$$I(\mathbf{K}) \propto |\sum_{\mathbf{G}} \rho_{\mathbf{G}} \int_V e^{i(\mathbf{G}-\mathbf{K})\cdot\mathbf{r}} dV|^2$$

structive interference when $\mathbf{K} = \mathbf{k}' - \mathbf{k} = \mathbf{G}$ Laue condition

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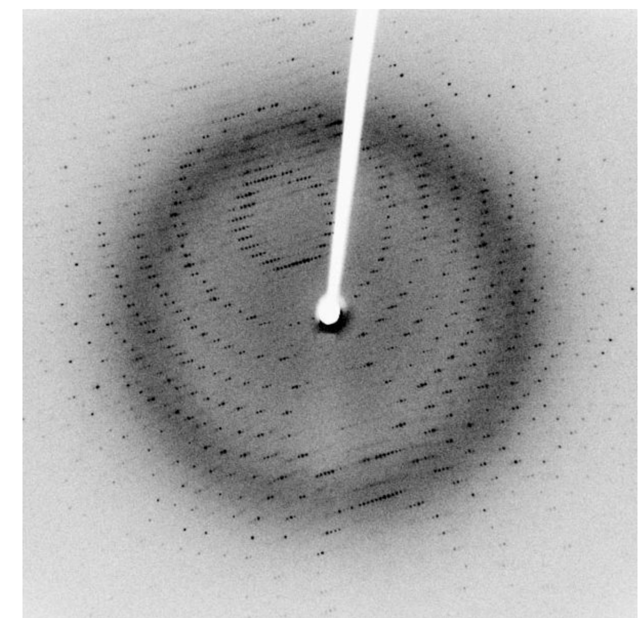

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for a specific spot

$$I(\mathbf{K} = \mathbf{G}) \propto |\rho_{\mathbf{G}}|^2$$

X-ray diffraction, von Laue description

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Volume
V

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