Electron-matter interactions: Elastic scattering (I)

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Contents

Introduction to e⁻ scattering

- Electron wave: wavelength and speed
- Plane wave for free electron: solving the Schrödinger eq.
- Plane wave in uniform potential
- Scattering by atomic potential
- Mott formula

The electron wave

- De Broglie relations: $\lambda = \dfrac{h}{p}$ $\qquad E_{\mathrm{el}} = \hbar\omega$ (1.1)

- Momentum given by: $p = mv$ where $m = \dfrac{m_0}{\left(1 - v^2/c^2\right)^{\frac{1}{2}}}$ (1.2)

- Relativistic total energy of electron: $W = mc^2 = E_{\mathrm{kin}} + m_0 c^2$ (1.3)

The electron wave: λ

- Electron accelerated by potential difference (high tension) E_0:

- Find relativistic wavelength:

$$\lambda = \frac{h}{\left[2m_0 eE_0\left(1+\frac{eE_0}{2m_0c^2}\right)\right]^{1/2}} \qquad (1.4)$$

The free electron: v

- Find speed of electron:

$$v = c\sqrt{1 - \frac{1}{\left(1 + \frac{eE_0}{m_0c^2}\right)^2}} \qquad (1.5)$$

Plane wave: wave function

- Wave function of type: $$\psi(\vec{r},t) = \psi_0 \exp\left(2\pi i \vec{k}.\vec{r} - i\omega t\right) \tag{1.6}$$

where: $$\left|\vec{k}\right| = \frac{1}{\lambda} \tag{1.7}$$

Plane wave: Schrödinger equation

- Schrödinger equation: $$\hat{H}\psi\left(\vec{\boldsymbol{r}},t\right)=i\hbar\frac{\partial\psi\left(\vec{\boldsymbol{r}},t\right)}{\partial t} \qquad (1.8)$$

- Energy of electron eigenstate E_{eig}:

Plane wave: Schrödinger eq. for free e⁻

- Hamiltonian: $$\hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{\boldsymbol{r}},t) \qquad (1.9)$$

- Momentum operator: $$\hat{p} = -i\hbar\nabla \qquad (1.10)$$

- Solve considering $V(\vec{\boldsymbol{r}},t) = 0$:

Plane wave: Schrödinger eq. for free e⁻

- Energy of electron: $E_{\text{eig}} = \hbar\omega$ $\qquad E_{\text{eig}} = \dfrac{h^2 k^2}{2m}$ (1.11)

- From now on use a *time independent* wave function for the electron plane wave:

- Schrödinger equation simplifies to:

$$\nabla^2 \psi(\vec{\boldsymbol{r}}) + 4\pi^2 k^2 \psi(\vec{\boldsymbol{r}}) = 0 \tag{1.12}$$

- Solutions: $\psi = \exp(2\pi i \vec{\boldsymbol{k}}.\vec{\boldsymbol{r}})$ and $\psi = \exp(-2\pi i \vec{\boldsymbol{k}}.\vec{\boldsymbol{r}})$ (1.13)

e^- in uniform potential field

- Suppose electron travels in uniform potential field:
- Schrödinger equation becomes:

e⁻ in uniform potential field

- Schrödinger eq.: $$-\frac{h^2}{8\pi^2 m}\nabla^2\psi(\vec{\boldsymbol{r}})+V\psi(\vec{\boldsymbol{r}})=E_{\mathrm{eig}}\psi(\vec{\boldsymbol{r}}) \qquad (1.14)$$

- For uniform potential ϕ_0:

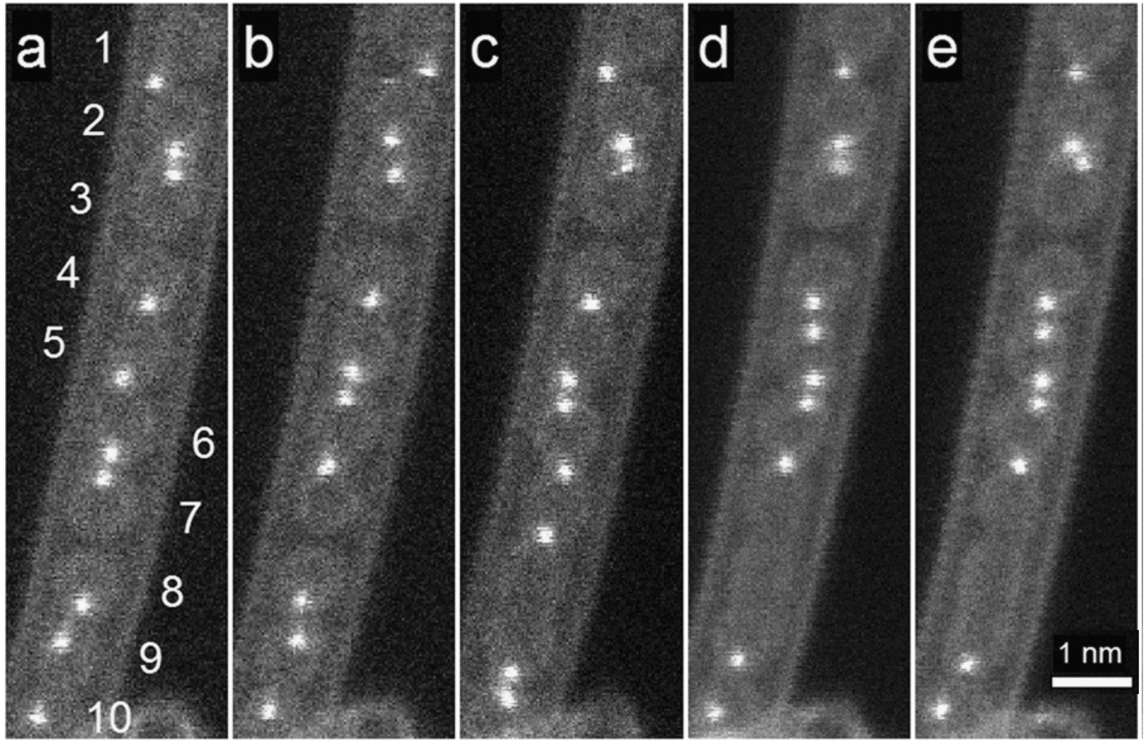
e⁻ in uniform potential field

- For uniform potential ϕ_0 derive refractive index n:

$$n = \sqrt{\left(1 + \frac{\phi_0}{E_0}\right)} \tag{1.15}$$

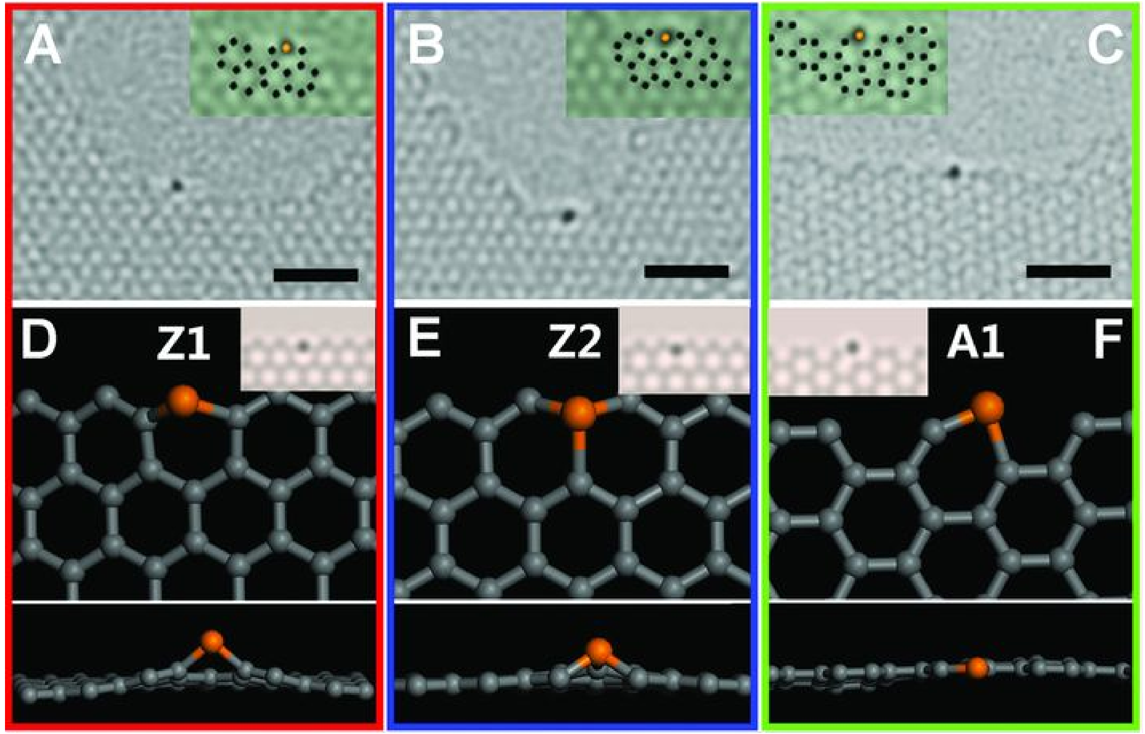
- Typical $\phi_0 \approx$ 10–20 V:

TEM imaging of individual atoms



Cs-corrected canning TEM (STEM) time sequence of Er atoms in carbon nanotube "pea pods"

O.L. Krivanek et al. Ultramicroscopy **110** (2010) 935–945



Cs-corrected high resolution TEM of single Fe atoms at edge of graphene monolayer

J. Zhao et al. Science **343** (2014) 1228–1232

Schrödinger eq. for atomic potential $\phi(\vec{\boldsymbol{r}})$

- Aim: study scattering of plane wave by single atomic potential described by function $\phi(\vec{\boldsymbol{r}})$:

- Rewrite equation 1.14: $$-\frac{h^2}{8\pi^2 m}\nabla^2\psi(\vec{\boldsymbol{r}})+V\psi(\vec{\boldsymbol{r}})=E_{\mathrm{eig}}\psi(\vec{\boldsymbol{r}})$$

$$\nabla^2\psi(\vec{\boldsymbol{r}})+\frac{8\pi^2 me}{h^2}\left[E_0+\phi(\vec{\boldsymbol{r}})\right]\psi(\vec{\boldsymbol{r}})=0 \qquad (1.16)$$

- Substitute in: $$k^2=\frac{1}{\lambda^2}=\frac{2meE_0}{h^2} \qquad U(\vec{\boldsymbol{r}})=\frac{2me}{h^2}\phi(\vec{\boldsymbol{r}}) \qquad (1.17)$$

Schrödinger eq. for atomic potential $\phi(\vec{\boldsymbol{r}})$

- Equation:

$$\nabla^2\psi(\vec{\boldsymbol{r}})+4\pi^2\left[k^2+U(\vec{\boldsymbol{r}})\right]\psi(\vec{\boldsymbol{r}})=0 \qquad (1.18)$$

has integral form (see Mott and Massey):

$$\psi(\vec{\boldsymbol{r}})=\psi_0(\vec{\boldsymbol{r}})+\pi\int\frac{\exp\{2\pi ik|\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'|\}}{|\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'|}U(\vec{\boldsymbol{r}}')\psi(\vec{\boldsymbol{r}}')\mathrm{d}\vec{\boldsymbol{r}}' \qquad (1.19)$$

- Scattering geometry:

Schrödinger eq. for atomic potential $\phi(\vec{\boldsymbol{r}})$

- For: $$\psi(\vec{\boldsymbol{r}}) = \psi_0(\vec{\boldsymbol{r}}) + \pi \int \frac{\exp\{2\pi ik|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}'|\}}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}'|} U(\vec{\boldsymbol{r}}')\psi(\vec{\boldsymbol{r}}')\mathrm{d}\vec{\boldsymbol{r}}'$$

- Solution given by **Born series**: $\psi(\vec{\boldsymbol{r}}) = \sum_{n=0}^{\infty} \psi_n(\vec{\boldsymbol{r}})$

- First Born approximation: assume that $\psi(\vec{\boldsymbol{r}})$ in integral can be replaced by $\psi_0(\vec{\boldsymbol{r}})$

- For plane incident wave $\psi_0(\vec{\boldsymbol{r}}) = \exp\{2\pi i\vec{\boldsymbol{k}}_0 \cdot \vec{\boldsymbol{r}}\}$ this gives:

$$\psi_0(\vec{\boldsymbol{r}}) + \psi_1(\vec{\boldsymbol{r}}) = \exp\{2\pi i\vec{\boldsymbol{k}}_0 \cdot \vec{\boldsymbol{r}}\} + \pi \int \frac{\exp\{2\pi \mathrm{i}k|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}'|\}}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}'|} U(\vec{\boldsymbol{r}}')\exp\{2\pi \mathrm{i}\vec{\boldsymbol{k}}_0 \cdot \vec{\boldsymbol{r}}'\}\mathrm{d}\vec{\boldsymbol{r}}' \tag{1.20}$$

Scattering from atomic potential $\phi(\vec{\boldsymbol{r}})$

$$\int \frac{\exp\left\{2\pi \mathrm{i} k\left|\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'\right|\right\}}{\left|\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'\right|} U\left(\vec{\boldsymbol{r}}'\right)\exp\left\{2\pi \mathrm{i}\vec{\boldsymbol{k}}_0\cdot\vec{\boldsymbol{r}}'\right\}\mathrm{d}\vec{\boldsymbol{r}}'$$

- Assume point of observation for $\vec{\boldsymbol{r}}$ which is very large compared to scattering field

- Scattering vector: $\vec{\boldsymbol{q}}=\vec{\boldsymbol{k}}'-\vec{\boldsymbol{k}}_0$ (1.21)

- Then:

$$\psi_0\left(\vec{\boldsymbol{r}}\right)+\psi_1\left(\vec{\boldsymbol{r}}\right)=\exp\left\{2\pi i\vec{\boldsymbol{k}}_0\cdot\vec{\boldsymbol{r}}\right\}+\pi\frac{\exp\left\{2\pi \mathrm{i}kr\right\}}{r}\int U\left(\vec{\boldsymbol{r}}'\right)\exp\left\{-2\pi \mathrm{i}\vec{\boldsymbol{q}}\cdot\vec{\boldsymbol{r}}'\right\}\mathrm{d}\vec{\boldsymbol{r}}' \quad (1.22)$$

Scattering from atomic potential $\phi(\vec{\boldsymbol{r}})$

- Scattered wave: $$\psi_1(\vec{\boldsymbol{r}}) = \frac{2\pi me}{h^2}\frac{\exp\{2\pi ikr\}}{r}\int \phi(\vec{\boldsymbol{r}}')\exp\{-2\pi \mathrm{i}\vec{\boldsymbol{q}}\cdot\vec{\boldsymbol{r}}'\}\mathrm{d}\vec{\boldsymbol{r}}' \qquad (1.23)$$

- Define scattering amplitude $f(\vec{\boldsymbol{q}})$ such that: $$\psi_1(\vec{\boldsymbol{r}}) = \frac{\exp\{2\pi ikr\}}{r}f(\vec{\boldsymbol{q}}) \qquad (1.24)$$

- Therefore: $$f(\vec{\boldsymbol{q}}) = \frac{2\pi me}{h^2}\int_{-\infty}^{\infty}\phi(\vec{\boldsymbol{r}})\exp\{-2\pi \mathrm{i}\vec{\boldsymbol{q}}\cdot\vec{\boldsymbol{r}}\}\mathrm{d}\vec{\boldsymbol{r}} \qquad (1.25)$$

Mott formula derivation

- Introduce Poisson's equation: $$\nabla^2\phi(\vec{\boldsymbol{r}}) = -4\pi e\left[\rho_{\mathrm{n}}(\vec{\boldsymbol{r}}) - \rho_{\mathrm{e}}(\vec{\boldsymbol{r}})\right] \quad (1.26)$$

- First rewrite $f(\vec{\boldsymbol{q}})$:

$$f(\vec{\boldsymbol{q}}) = -\frac{me}{2\pi h^2 q^2}\int_{-\infty}^{\infty}\phi(\vec{\boldsymbol{r}})\nabla^2 \exp\{-2\pi \mathrm{i}\vec{\boldsymbol{q}}\cdot\vec{\boldsymbol{r}}\}\mathrm{d}\vec{\boldsymbol{r}} \quad (1.27)$$

- Integrating by parts gives: $$f(\vec{\boldsymbol{q}}) = -\frac{me}{2\pi h^2 q^2}\int_{-\infty}^{\infty}\nabla^2\phi(\vec{\boldsymbol{r}})\exp\{-2\pi \mathrm{i}\vec{\boldsymbol{q}}\cdot\vec{\boldsymbol{r}}\}\mathrm{d}\vec{\boldsymbol{r}} \quad (1.28)$$

- Substitute in $\nabla^2\phi(\vec{\boldsymbol{r}})$:

Mott formula

- Scattering amplitude: $$f(\vec{\boldsymbol{q}}) = \frac{2me^2}{h^2q^2}\int_{-\infty}^{\infty}\left[\rho_{\mathrm{n}}(\vec{\boldsymbol{r}}) - \rho_{\mathrm{e}}(\vec{\boldsymbol{r}})\right]\exp\{-2\pi\mathrm{i}\vec{\boldsymbol{q}}\cdot\vec{\boldsymbol{r}}\}\mathrm{d}\vec{\boldsymbol{r}} \qquad (1.29)$$

- Charge density of nucleus: $$\rho_{\mathrm{n}}(\vec{\boldsymbol{r}}) = Z\delta(\vec{\boldsymbol{r}}) \qquad (1.30)$$

- Find: $$f(\vec{\boldsymbol{q}}) = \frac{2me^2}{h^2q^2}\left[Z - f_{\mathrm{x}}(\vec{\boldsymbol{q}})\right] \qquad (1.31)$$

- In SI units:

- Or for Bohr radius a_0: $$f(\vec{\boldsymbol{q}}) = \frac{1}{2\pi^2a_0q^2}\left[Z - f_{\mathrm{x}}(\vec{\boldsymbol{q}})\right] \qquad (1.32)$$

Scattering geometry

- Assume scattering by an angle 2θ

- Therefore atomic scattering amplitude:

$$f(\theta)=\frac{me^2}{2h^2}\left(\frac{\lambda}{\sin\theta}\right)^2\left[Z-f_x(\theta)\right] \tag{1.33}$$

Scattered intensity

- Scattered intensity at unit distance: $$I(\theta) = |f(\theta)|^2 \quad (1.34)$$

- For large scattering angles: $f_x(\vec{\boldsymbol{q}}) \to 0$ hence $$I(\theta)_{\theta \to \pi/2} = |f(\theta)|^2_{\theta \to \pi/2} = \frac{4m^2e^4}{h^4q^4}Z^2 \quad (1.35)$$

Relative scattering strength

- Applying "bandwidth" nature of Fourier transform:

$$\Delta q \Delta r \simeq 1$$

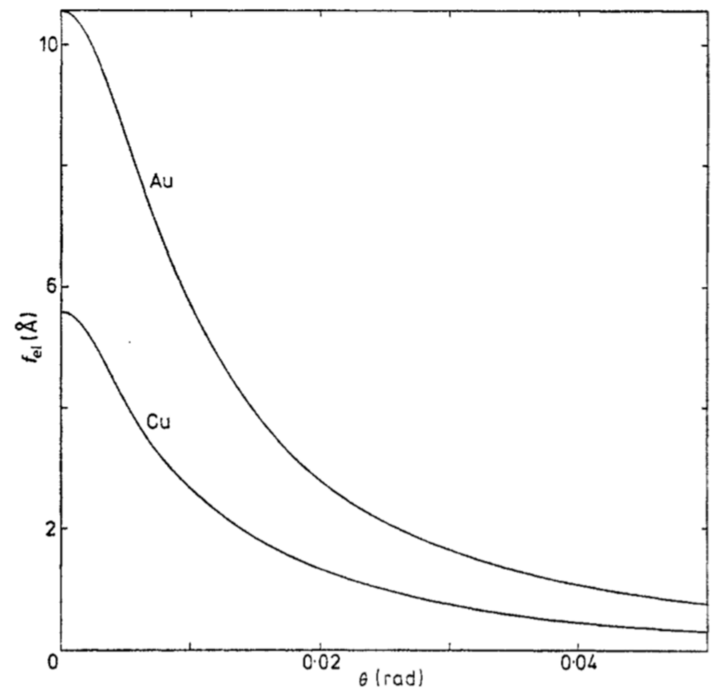


Figure 4. The first Born approximation scattering amplitude, $f^{B}(\boldsymbol{K}')$, as a function of θ for 100 keV electrons incident upon single atoms of gold and copper. The plots have been made using the relativistic Hartree–Fock scattering amplitudes of Doyle and Turner (1968).

Summary

Introduction to e⁻ scattering

- Free e⁻

$$\nabla^2\psi(\vec{\boldsymbol{r}})+4\pi^2k^2\psi(\vec{\boldsymbol{r}})=0$$

$$\psi=\exp\left(2\pi i\vec{\boldsymbol{k}}.\vec{\boldsymbol{r}}\right)$$

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

- Uniform potential

$$n=\sqrt{\left(1+\frac{\phi_0}{E_0}\right)}$$

- Scattering by atomic potential

$$f(\vec{\boldsymbol{q}})=\frac{2me^2}{h^2q^2}\left[Z-f_{\mathrm{x}}(\vec{\boldsymbol{q}})\right]$$

Bibliography

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- Electron Diffraction Techniques Vol. 1, ed. John M. Cowley, Oxford University Press 1992: Chapters 1 (Cowley) and 2 (Humphreys and Bithell)
- Elastic and Inelastic Scattering in Electron Diffraction and Imaging, by Z.L. Wang, Plenum Press, New York 1995: Chapters 1 and 2
- Peter Rez: “Scattering Cross Sections in Electron Microscopy and Analysis” Microsc. Microanal. **7** (2001) 356–362. Note: $\vec{\boldsymbol{q}}_{\mathrm{Rez}} = 2\pi\vec{\boldsymbol{q}}$
- The Theory of Atomic Collisions Vol. 1, Third Edition, by N.F. Mott and H.S.W. Massey, Oxford Science Publications 4965