

Bragg diffraction and electron-gas heat capacity

GRE · GRE Subject Test · GRE Physics

Bragg diffraction and electron-gas heat capacity

Rotating a crystal in an X-ray beam maps its atomic planes, because constructive reflection happens only at discrete angles.

Prerequisites: 8, 36.

- Apply the Bragg condition to find plane spacings or diffraction angles
- Estimate free-electron Fermi energy and Fermi temperature
- Distinguish electronic and lattice heat-capacity contributions

Apply the Bragg condition

Bragg reflection from parallel planes spaced d interferes constructively when $2d \sin\theta = n\lambda$, with θ measured from the plane surface (the glancing angle), not from the normal. First order $n=1$ gives the smallest angle. For $\lambda=0.154$ nm and a peak at $\theta=20^\circ$, $d=0.154/(2 \sin 20^\circ) \approx 0.225$ nm. If $2d < \lambda$ no order exists; the sine must stay at or below 1.

Read the lattice constant

In a cubic crystal the (hkl) plane spacing is $d=a/\sqrt{h^2+k^2+l^2}$ with lattice constant a ; the (110) planes give $a/\sqrt{2}$. A measured Bragg angle therefore measures the lattice constant. Systematic absences from the basis (for example body-centred lattices missing $h+k+l$ odd) carry structure information beyond the spacing formula.

Fill the electron sea

The free-electron model packs N conduction electrons into states up to the Fermi wavevector $k_F = (3\pi^2 n)^{1/3}$ for number density n , giving $E_F = \hbar^2 k_F^2 / (2m)$. For $n = 8.5 \times 10^{28} \text{ /m}^3$, $k_F \approx 1.36 \times 10^{10} \text{ /m}$, $E_F \approx 7.05 \text{ eV}$ and $T_F = E_F / k_B \approx 8.2 \times 10^4 \text{ K}$. Since T_F far exceeds room temperature, only a fraction of order T/T_F of the electrons are thermally excited.

Separate the heat capacities

Metals therefore have two low-temperature heat-capacity terms: an electronic term γT linear in T and a lattice (Debye) term βT^3 . Plotting C/T against T^2 gives intercept γ and slope β . At room temperature the lattice part approaches the classical Dulong–Petit value and dominates; the electronic term matters at low T , where the T^3 lattice

term collapses faster.

Worked method

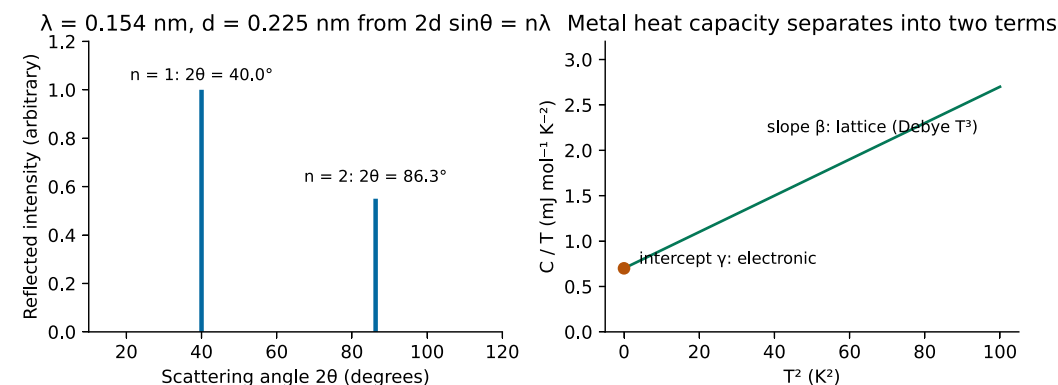
Bragg diffraction uses angle θ from the crystal plane, not from its normal.

$$2d \sin \theta = n\lambda, \quad d = \lambda / (2 \sin \theta) = (0.154 \text{ nm}) / [2 \sin(20^\circ)] = 0.225 \text{ nm}.$$

Low-temperature metal heat capacity has separate electronic and lattice terms:

$$C = \gamma T + \beta T^3, \quad C/T = \gamma + \beta T^2.$$

A plot of C/T against T squared has intercept γ and slope β . A straight line identifies this model's regime.



Bragg diffraction and electron-gas heat capacity: original GRE teaching diagram.

Check conditions and vocabulary

Measuring θ from the plane normal instead of the plane, or assigning the whole low- T heat capacity to electrons. The sine condition and the two-term decomposition are where these calculations fail.

Bragg condition: Constructive reflection from lattice planes when $2d \sin\theta = n\lambda$, with θ measured from the plane.

Fermi energy: The highest occupied electron energy at zero temperature in the free-electron model.