

45.1 Bragg diffraction and electron-gas heat capacity

Name: _____ Class: _____ Date: _____ **Total: 11 marks**

KEY WORDS Bragg condition • Fermi energy

Objective

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. Original public practice; not an ETS paper.

1 Key knowledge and worked examples

Bragg: $2d \sin\theta = n\lambda$ with θ from the plane; require $\lambda/(2d) \leq 1$. Cubic planes: $d = a/\sqrt{h^2 + k^2 + l^2}$.

Free electrons fill states to $k_F = (3\pi^2 n)^{1/3}$; $E_F = \hbar^2 k_F^2 / 2m$ and $T_F = E_F / k_B$, typically 10^4 – 10^5 K.

Only about T/T_F of electrons are thermally excited, so the electronic heat capacity is linear in T .

Low- T metal heat capacity: $C = \gamma T + \beta T^3$; a C/T versus T^2 plot separates the electronic intercept from the lattice slope.

■ Worked method

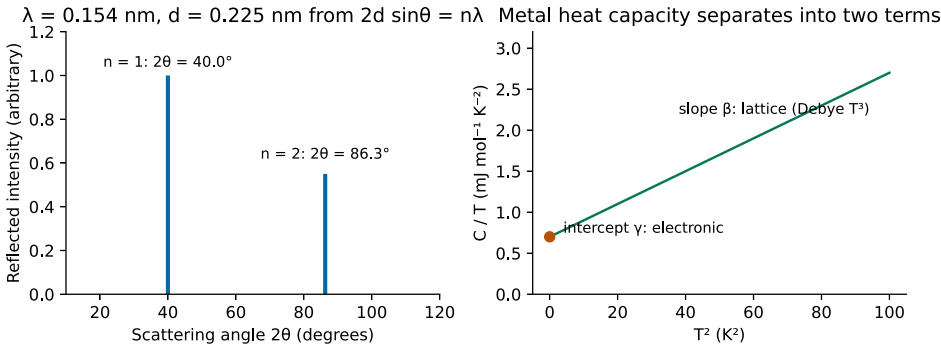
Bragg diffraction uses angle θ from the crystal plane, not from its normal.

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

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.



2 Practice

2.1 Choose one answer. X-rays of wavelength 0.154 nm show a first-order Bragg peak at $\theta = 20^\circ$. The plane spacing is about: [1]

- **A** 0.075 nm
- **B** 0.113 nm
- **C** 0.225 nm
- **D** 0.308 nm
- **E** 0.450 nm

2.2 Choose one answer. In the low-temperature metal heat capacity $C = \gamma T + \beta T^3$, the linear term γT comes from: [1]

- **A** lattice phonons
- **B** conduction electrons
- **C** magnetic ordering
- **D** surface atoms
- **E** thermal expansion

2.3 For $\lambda = 0.10 \text{ nm}$ and plane spacing $d = 0.25 \text{ nm}$, the first-order Bragg condition gives $\sin\theta = \underline{\hspace{2cm}}$. Show your relation and units. [2]

[2]

[5]

Solutions

2.1 C $d = \lambda / (2 \sin \theta) = 0.154 / (2 \times 0.342) \approx 0.225 \text{ nm}$.

Compare the rejected options: 0.075 nm; 0.113 nm; 0.308 nm; 0.450 nm. Use the stated model and conditions.

2.2 B Only a T/T_F fraction of conduction electrons are excited, giving a linear-T electronic term; βT^3 is the Debye lattice term.

Compare the rejected options: lattice phonons; magnetic ordering; surface atoms; thermal expansion. Use the stated model and conditions.

2.3 0.2. $\sin \theta = \lambda / (2d) = 0.10 / 0.50 = 0.2$.

2.4 False. The sine doubles, not the angle; and no order exists once $\lambda / (2d)$ exceeds 1.

3.1 $\beta = (5.2 - 2.8) / (16 - 4) = 0.20 \text{ mJ} / (\text{mol K}^4)$. $\gamma = 2.8 - 0.20(4) = 2.0 \text{ mJ} / (\text{mol K}^2)$. Equality requires $\gamma T = \beta T^3$ for T positive, hence $T = \sqrt{\gamma / \beta} = \sqrt{10} \text{ K} = 3.16 \text{ K}$. Award transformed axes, slope, intercept, condition and temperature/units. Two constructed points cannot independently establish the model or experimental uncertainty.