Task 1: Band gap dependence on potential height V_0

1. Kronig-Penney Model Setup

We have a periodic potential with:

- Well width: $a = 1.5$ Å
- Barrier width: $b = 1.0$ Å
- Period: $L = a + b = 2.5$ Å
- Barrier height: V_0 variable (0–10 eV)

The Kronig-Penney equation for rectangular barriers:

$$\cos(kL) = \cos(\alpha a)\cosh(\beta b) + \frac{\beta^2 - \alpha^2}{2\alpha\beta}\sin(\alpha a)\sinh(\beta b)$$

where:

- $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$ (well region, E > 0)
- $\beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$ (barrier region, E < V_0)

2. Band Gap Calculation

The band gap occurs at the Brillouin zone boundary $k = \pi/L$. For small V_0, we can use perturbation theory.

The Fourier component of the potential for reciprocal vector $G = 2\pi/L$:

$$V_G = \frac{1}{L}\int_0^L V(x)e^{-iGx}dx$$

For our rectangular potential:

$$V(x) = \begin{cases} 0 & 0 < x < a \\ V_0 & a < x < L \end{cases}$$

$$V_G = \frac{1}{L}\int_a^L V_0 e^{-iGx}dx = \frac{V_0}{L}\left[\frac{e^{-iGx}}{-iG}\right]_a^L$$

$$V_G = \frac{V_0}{-iGL}(e^{-iGL} - e^{-iGa})$$

Since $GL = 2\pi$ and $Ga = 2\pi a/L = 2\pi \times 1.5/2.5 = 1.2\pi$:

$$V_G = \frac{V_0}{-iGL}(1 - e^{-i1.2\pi})$$

Magnitude:

$$|V_G| = \frac{V_0}{GL}|1 - e^{-i1.2\pi}| = \frac{V_0}{2\pi}|1 - \cos(1.2\pi) + i\sin(1.2\pi)|$$

$$|1 - e^{-i1.2\pi}| = \sqrt{(1 - \cos(1.2\pi))^2 + \sin^2(1.2\pi)} = \sqrt{2 - 2\cos(1.2\pi)}$$

$$= 2|\sin(0.6\pi)| \approx 2\sin(108°) \approx 2 \times 0.951 = 1.902$$

Thus:

$$| V_G | \approx \frac{V_0}{2\pi} \times 1.902 \approx 0.303 V_0$$

The band gap is approximately:

$$E_g \approx 2 | V_G | \approx 0.606 V_0$$

3. Dependence and Plot

For small V_0, the gap increases linearly with V_0. For larger V_0, the dependence becomes sublinear as higher-order terms matter.

Plot description:

- x-axis: V_0 (eV)
- y-axis: E_g (eV)
- Curve: Starts at (0,0), rises linearly with slope ~0.6 for small V_0, then curves toward saturation

$$E_g(V_0) \approx 0.606 V_0 \text{(for small } V_0\text{)}$$

Task 2: Band gap dependence on barrier width b

1. Modified Parameters

- $a = 1.5$ Å fixed
- $V_0 = 5$ eV fixed
- b variable, $L = a + b$

2. Fourier Component Analysis

$$V_G = \frac{1}{L}\int_0^b V_0 e^{-iGx} dx = \frac{V_0}{L} \cdot \frac{1 - e^{-iGb}}{iG}$$

Magnitude:

$$| V_G | = \frac{V_0}{GL} \cdot | 1 - e^{-iGb} | = \frac{V_0}{GL} \cdot 2 | \sin(Gb/2) |$$

Since $G = 2\pi/L$, $GL = 2\pi$, so:

$$| V_G | = \frac{V_0}{2\pi} \cdot 2 | \sin(\pi b/L) | = \frac{V_0}{\pi} | \sin(\pi b/L) |$$

Thus:

$$E_g \approx 2 | V_G | = \frac{2V_0}{\pi} | \sin(\pi b/(a+b)) |$$

3. Behavior Analysis

- When $b = 0$: $\sin(0) = 0 \rightarrow E_g = 0$
- When $b/(a+b) = 0.5$: $\sin(\pi/2) = 1 \rightarrow$ maximum gap
- When $b \rightarrow \infty$: $b/(a+b) \rightarrow 1$, $\sin(\pi) = 0 \rightarrow$ gap $\rightarrow 0$

Maximum occurs when:

$$\frac{b}{a+b} = 0.5 \Rightarrow b = a = 1.5\ \text{Å}$$

Maximum gap value:

$$E_g^{max} = \frac{2 \times 5}{\pi} \approx 3.18\ \text{eV}$$

4. Plot Description

- x-axis: b (Å)
- y-axis: E_g (eV)
- Curve: Starts at 0, rises to peak at $b = 1.5$ Å, then decreases to 0 as $b \to \infty$

Task 3: Amorphous solids and band gaps

1. Short-Range Order in Amorphous Materials

Amorphous solids lack long-range periodicity but retain short-range order:

- Characteristic bond lengths
- Characteristic coordination numbers
- Similar local atomic environments as crystals

2. Relevance of Tasks 1 & 2

From Task 1: Band gap depends on **potential strength** (atomic potential depth)

- In amorphous SiO_2: Strong Si-O ionic potential → large gap (~9 eV)

From Task 2: Band gap depends on **spatial dimensions** (well/barrier widths)

- In amorphous materials: Average nearest-neighbor distance determines effective "well width"

3. Key Short-Range Properties

1. **Atomic potential strength** (determined by atomic number, ionization)
2. **Bond length** (determines effective well width a)
3. **Coordination number** (affects local potential shape)
4. **Bond angle distribution** (affects potential periodicity)

4. Explanation

Even without long-range order, the **local potential landscape** resembles the crystalline case. Electronic states feel similar scattering potential at wavevectors corresponding to inverse interatomic spacing. This creates a **pseudogap** rather than a true band gap, but for strong scatterers (like SiO_2), it becomes a full band gap.

Task 4: Bragg law and electron behavior

1. Bragg Law Derivation

Bragg condition: $2d\sin\,\theta = n\lambda$

For electrons: $\lambda = 2\pi/k$, so:

$$2d\sin\,\theta = n\frac{2\pi}{k} \Rightarrow k\sin\,\theta = \frac{n\pi}{d}$$

For normal incidence on atomic planes ($\theta = 90°$):

$$k = \frac{n\pi}{d}$$

2. Brillouin Zone Boundary

First Brillouin zone boundary occurs at:

$$k = \frac{\pi}{d}$$

which matches Bragg condition with $n = 1$.

3. Electron Behavior at BZ Boundary

At $k = \pi/d$, electrons satisfy Bragg condition → strong backscattering → standing waves form:

$$\psi_+ \propto e^{i\pi x/d} + e^{-i\pi x/d} = 2\cos(\pi x/d)$$
$$\psi_- \propto e^{i\pi x/d} - e^{-i\pi x/d} = 2i\sin(\pi x/d)$$

These have different electrostatic energies → band gap opens.

4. Electron Behavior at Other k-values

- **k ≪ π/d**: Nearly free electrons, weak scattering
- **k ≈ π/2d**: Intermediate scattering, band curvature changes (effective mass)
- **k far from BZ boundary**: Free-electron-like with modified effective mass due to periodic potential perturbation

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Task 5: Empty lattice model in 1D

1. Model Setup

Periodic potential V(x) = 0, but impose Bloch theorem with period a.

Free electron dispersion:

$$E(k) = \frac{\hbar^2 k^2}{2m}$$

Reduced zone scheme: Map all k to first Brillouin zone $(-\pi/a, \pi/a]$.

2. Band Construction

For each band index n:

$$E_n(k) = \frac{\hbar^2}{2m}(k + \frac{2\pi n}{a})^2, k \in \text{1st BZ}$$

First three bands:

Band 1 (n = 0):

$$E_0(k) = \frac{\hbar^2 k^2}{2m}$$

Band 2 (n = -1):

$$E_{-1}(k) = \frac{\hbar^2}{2m}(k - \frac{2\pi}{a})^2$$

Band 3 (n = 1):

$$E_1(k) = \frac{\hbar^2}{2m}(k + \frac{2\pi}{a})^2$$

3. Specific Values

Let $E_0 = \frac{\hbar^2}{2m}(\frac{\pi}{a})^2$ be the unit.

At $k = 0$:

- $E_0 = 0$
- $E_{-1} = E_1 = \frac{\hbar^2}{2m}(\frac{2\pi}{a})^2 = 4E_0$

At $k = \pi/a$:

- $E_0 = E_0$
- $E_{-1} = \frac{\hbar^2}{2m}(-\frac{\pi}{a})^2 = E_0$
- $E_1 = \frac{\hbar^2}{2m}(\frac{3\pi}{a})^2 = 9E_0$

4. Wavefunctions

Bloch form: $\psi_{nk}(x) = e^{ikx}u_{nk}(x)$

For empty lattice: $u_{nk}(x) =$ constant $\cdot\, e^{iG_n x}$, where $G_n = \frac{2\pi n}{a}$

Thus:

$$\psi_{nk}(x) \propto e^{i(k+G_n)x}$$

Simple plane waves.

Task 6: 2D square lattice, X to M direction

1. Reciprocal Space Setup

Square lattice constant a. Reciprocal lattice vectors:

$$\mathbf{G}_{mn} = \frac{2\pi}{a}(m, n), m, n \in \mathbb{Z}$$

High-symmetry points:

- X: $(\pi/a, 0)$
- M: $(\pi/a, \pi/a)$

Path: X → M: $\mathbf{k} = (\pi/a, k_y)$, with k_y from 0 to π/a

2. Empty Lattice Bands

$$E(\mathbf{k}) = \frac{\hbar^2}{2m} | \mathbf{k} + \mathbf{G}_{mn} |^2$$

Let $K = \pi/a$, then $\mathbf{k} = (K, k_y)$

$$E_{mn}(k_y) = \frac{\hbar^2}{2m}[(K + m\frac{2\pi}{a})^2 + (k_y + n\frac{2\pi}{a})^2]$$

3. Specific Bands Calculation

Use units where $\frac{\hbar^2}{2m}(\frac{\pi}{a})^2 = 1$, so $K = 1$ in these units.

Then $\frac{2\pi}{a} = 2$ in these units.

Band 1: G = (0,0)

$$E = (1)^2 + k_y^2 = 1 + k_y^2$$

Band 2: G = (-1,0)

$$\mathbf{k} + \mathbf{G} = (1 - 2, k_y) = (-1, k_y) \Rightarrow E = 1 + k_y^2$$(degenerate with Band 1)

Band 3: G = (0,-1)

$$\mathbf{k} + \mathbf{G} = (1, k_y - 2) \Rightarrow E = 1 + (k_y - 2)^2$$

Band 4: G = (-1,-1)

$$\mathbf{k} + \mathbf{G} = (-1, k_y - 2) \Rightarrow E = 1 + (k_y - 2)^2$$(degenerate with Band 3)

Band 5: G = (1,0)

$$\mathbf{k} + \mathbf{G} = (3, k_y) \Rightarrow E = 9 + k_y^2$$

4. Band Values at Key Points

At X point ($k_y = 0$):

- Bands 1,2: E = 1
- Bands 3,4: E = 1 + 4 = 5
- Band 5: E = 9

At M point ($k_y = 1$):

- Bands 1,2: E = 1 + 1 = 2
- Bands 3,4: E = 1 + 1 = 2
- Band 5: E = 9 + 1 = 10

5. Plot Description

Plot E vs k_y from 0 to 1 (units of π/a):

- Two degenerate bands starting at E=1, rising parabolically
- Two degenerate bands starting at E=5, decreasing to E=2
- One high band starting at E=9, rising slowly

All bands cross freely (no gaps in empty lattice).