Background: The Free Electron DOS

Basis:

Denstity of electronic states in momentum space (k-space) for a free particle with mass m in dimension n from periodic boundary conditions in cube (square, line) with length L:

$$H_n\left(\vec{k}\right) = 2 \cdot \left(\frac{L}{2\pi}\right)^n$$ constant in k-space; factor 2 from spin degeneracy

$$E\left(\vec{k}\right) = \frac{\hbar^2}{2m} k^2 \;\Leftrightarrow\; k(E) = \frac{\sqrt{2m}}{\hbar} E^{1/2}$$ dispersion relation, valid for all n

Number N of states with energy <E = sphere (circle, line) with radius k(E):

$$N_3(E) = H_3 \cdot \tfrac{4}{3}\pi \cdot k(E)^3 \qquad N_2(E) = H_2 \cdot \pi \cdot k(E)^2 \qquad N_1(E) = 2 \cdot H_1 \cdot k(E)$$

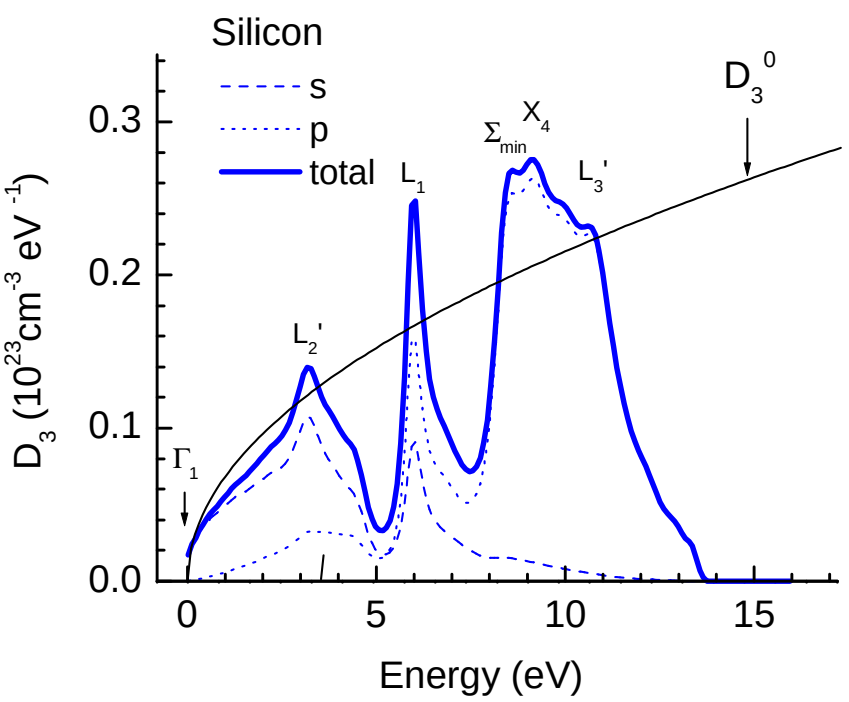
Density of States per volume (area, length) L^n and energy increment dE: $L^{-n}\frac{dN_n}{dE}$

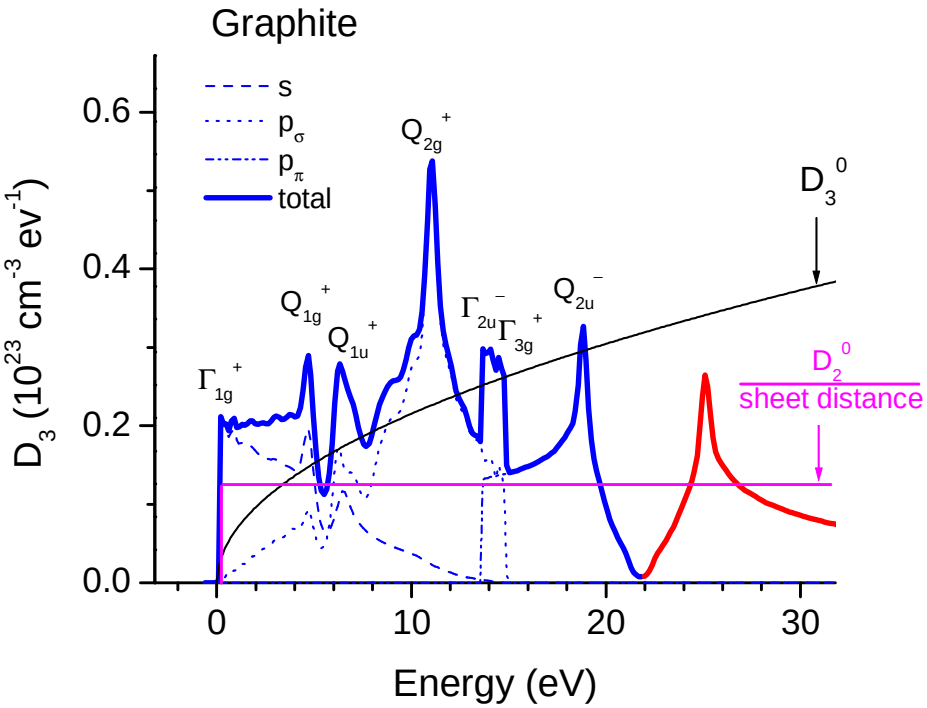
$$D_3^0(E) = 8\sqrt{2}\,\pi\left(m/h^2\right)^{3/2}\sqrt{E} \qquad D_2^0(E) = 4\pi\left(m/h^2\right) \qquad D_1^0(E) = 2\sqrt{2}\,\sqrt{m/h^2}\cdot\frac{1}{\sqrt{E}}$$

constant!

singularity at E=0 !

Examples





Note:

- Peaks (= so-called ‚critical points' of the DOS) are labelled with symmetry notations for the corresponding wave functions.
- Graphite is a sheet crystal with weakly bound ‚graphene layers' 3.35 Å apart!