Electronic properties of crystals: 10 key ideas

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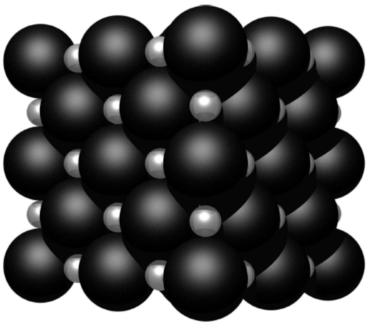
Aschroft & Mermin, chapters 1-11

1. Simplicity vs. complexity

- Crystals are complex quantum many-body systems.
- Yet rudimentary classical models such as the Drude model and

packing of hard spheres can describe some properties of elemental materials.



2. Where the action is

The Sommerfeld model shows that for elemental metals the Fermi temperature is much larger than room temperature.

Hence, many electronic and thermodynamic properties are dominated by the electrons which have energy (wavevector) close to the Fermi energy (surface).

3. Repetition leads to limited options

Crystal structure = Bravais lattice + atomic basis

There are 14 distinct Bravais lattices.

- Symmetry is powerful.
- Aside: None have 5-fold symmetry.

4. The reciprocal lattice

- Think about crystals in reciprocal space rather than real space. (i.e., do a Fourier transform).

- Each reciprocal lattice vector G corresponds to
- Family of planes in the real space lattice.
- A Miller index (klm)
- Specific x-ray diffraction peak
- Bragg scattering is described by k'=k+G.

5. Crystal structure determination

- Possible because an x-ray diffraction pattern allows one to determine the reciprocal lattice.
- The reciprocal lattice of the reciprocal lattice is the real space lattice.
- There are 230 possible crystal structures.

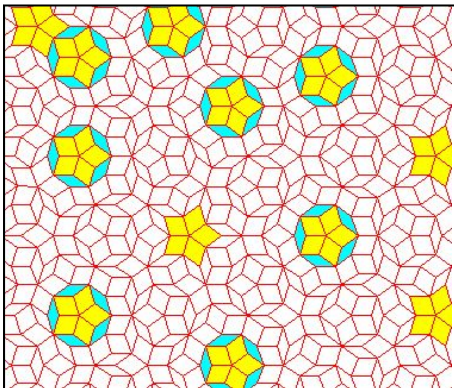
- The first x-ray diffraction experiment ``can be regarded as the most important ever undertaken in the study of condensed matter''

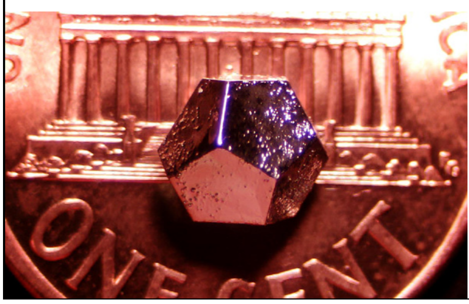
R. Cotterill,

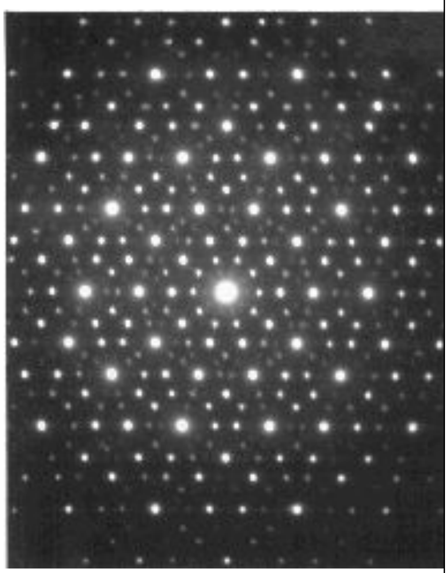
Cambridge Guide to the Materials World

6. Question conventional wisdom

- A implies B does not mean B implies A.
- Discovery of quasi-crystals showed that a periodic arrangement of atoms was a sufficient but NOT necessary condition for the presence of sharp diffraction peaks.
- Diffraction patterns with 5-fold symmetry are possible.

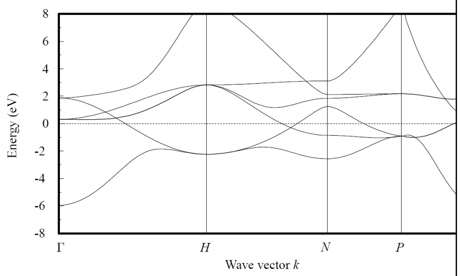






7. Bloch's theorem

- Gives us an important quantum number (the Bloch wavevector) for the electronic eigenstates in the periodic potential associated with the crystal.

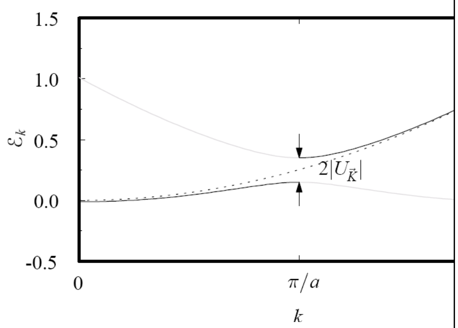


- Leads to energy bands
- N allowed k values in FBZ for a crystal containing N primitive cells.

8. Maximum impact

The periodic potential has the largest effect on electrons whose Bloch wavevector is close to the boundary of the first Brillouin zone (FBZ).

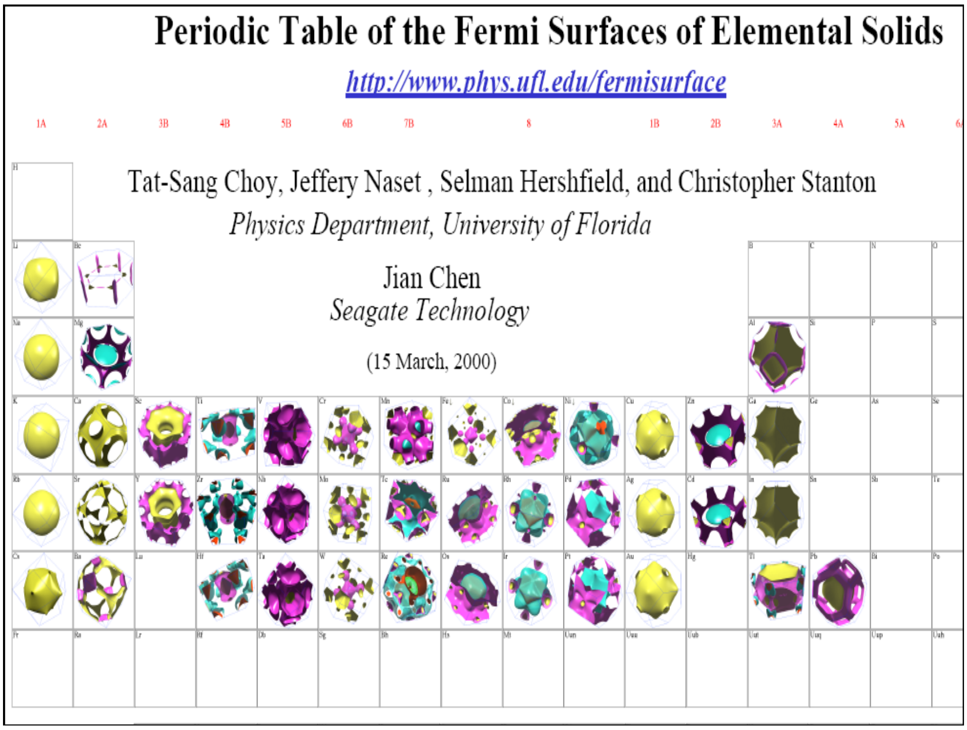
This Bragg scattering of electrons produces band gaps at the zone boundary.



9. Bloch rocks!

Key successes of Bloch model (failures of Sommerfeld)

- explains difference between metals, insulators, and semiconductors
- explains anomalous sign of the Hall co-efficient and thermopower in terms of holes
- hole = absence of an electron = positively charged quasi-particle
- electrons and holes have an effective mass which can be as much as an order of magnitude different to the mass of a free electron
- Fermi surface can have complex geometry and topology

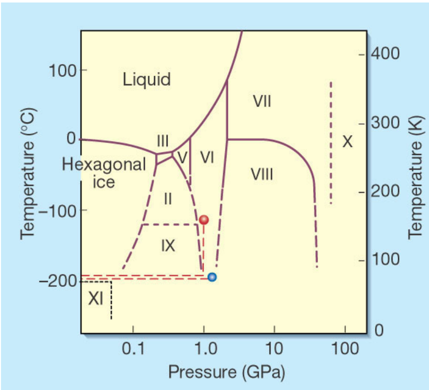


Tight-binding model

- Energy bands arise from the overlap of orbitals on neighbouring atoms in crystal.
- Band width increases
  - as the atoms move closer and
  - as spatial extent of orbitals increase.
- Hence, d-orbitals in transition metals are associated with narrow bands and large density of states.

10. A subtle fight

- Even is simple materials there is a subtle competition between different states (e.g., crystal structures) for the most stable.
- Example: there are more than ten different crystal structures for ice



Looking forward

- How do we experimentallly determine the Fermi surface of a metal?
  dHvA and SdH effect
- Why does the Bloch model work so well?
  Fermi liquid theory
- Failures of the Bloch model: magnetic states and superconductivity.
- Technological applications: how can semiconductors be used to make diodes, and transistors?

Things you should also know about

- Emergence
- Pseudo-potentials
- Hybridisation of atomic orbitals
- Covalent bonding
- Harrison’s solid state table of elements
- Boltzmann-Bloch theory of transport