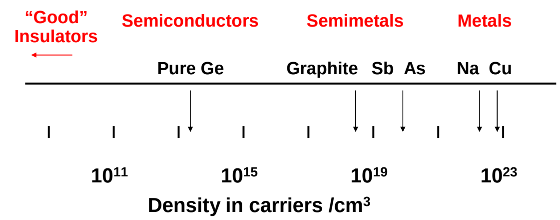
Metals vs Insulators

- An energy band holds two electrons
- Therefore an crystal with an odd number of electrons per cell MUST be a metal!
  - Partially filled bands
  - Conductivity because states can change and scatter when electric field is applied
- A crystal with an even number of electrons per cell MAY be an insulator!
  - Electrons “frozen” in filled bands
  - Gap in energy for any excitations of electrons

What is a semiconductor?

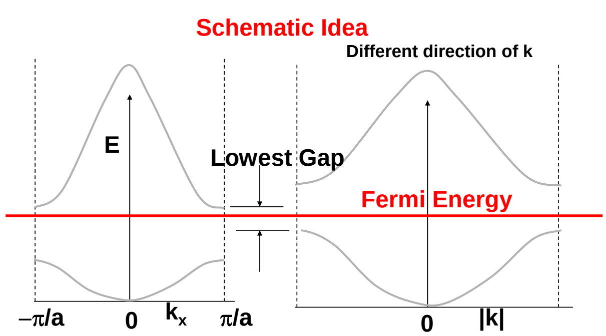
- **Density of electrical carriers in different crystals at room temperature**



- **Semiconductors:**
  - **carrier concentration varies dramatically with purity, can be changed or controlled**
  - **carriers can have different signs!**

Semiconductors

- **A material is a semiconductor if there is a small gap**
- **Roughly 0.1 eV - 2.0 eV**



Real Semiconductors - Si, Ge, GaAs, ...

- **All the common semiconductors (**Si, Ge, GaAs**) have diamond structure: FCC with two atoms per primitive cell**
- **8 valence electrons per cell**
- **Can be understood (roughly!) as nearly free electron-like**

Face Centered Cubic

All the common semiconductors (Si, Ge, GaAs) **have diamond structure: FCC with two atoms per primitive cell**

8 valence electrons per cell

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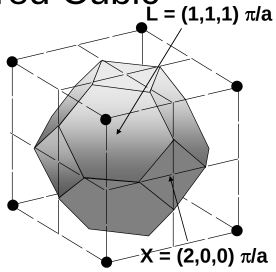
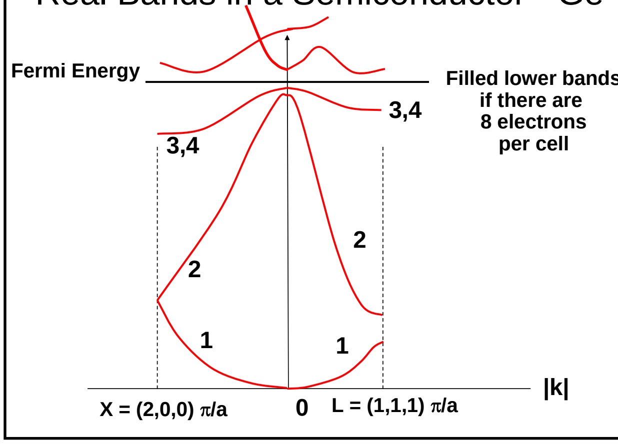


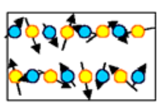
Brillouin Zone of FCC lattice

Real Bands in a Semiconductor - Ge



Magnetism and Ising model

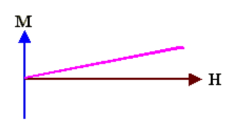
- Consider a collection of atoms, each having a permanent magnetic moment (spin)
- No interaction between the atoms/moments.
- The orientation of the moments fluctuates in time



- The system is characterized by its magnetization, or magnetic moment per unit volume.
- There is no permanent magnetism for non-interacting systems - paramagnet
- If external magnetic field applied
  The moments align with the field, so the magnetization increases

Magnetic susceptibility of paramagnets

The magnetization of paramagnets is proportional to the intensity of the external magnetic field



define the magnetic susceptibility = the ratio of the magnetization and the intensity of the magnetic field.

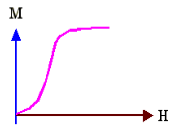
Curie law: $\chi = 1/T$

For a non-interacting system the magnetic susceptibility is inversely proportional to the temperature.

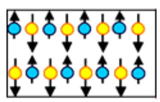
At room temperature, achievable magnetic fields produce only a weak alignment of the spins.

Interacting systems

- Non-interacting systems have achieve only a weak alignment of the spins
- If there are interactions between the spins which favor their parallel alignment then at high temperatures the susceptibility of the system is enhanced.



- The interactions lead to a spontaneous alignment of the spins at low temperatures, a phenomenon called ferromagnetism.

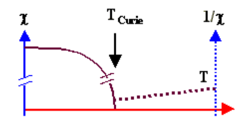


Temperature dependence of susceptibility

- The Curie-Weiss law gives

$$\chi = 1/(T-\theta),$$

- The Curie temperature is predicted by the mean-field theory of ferromagnetism to be $\theta = 4J$



Above the Curie temperature the magnetization behavior is qualitatively similar to paramagnetism.

Below the Curie temperature the susceptibility diverges (approaches infinity) - ferromagnetic behavior

2D Ising model

- A system of N atoms distributed on a square lattice, with spin variables which can take on only the values +1 and -1, corresponding to "up" and "down" orientations.
- The spins are assumed to interact with their nearest neighbors with an exchange energy –*J* if the neighbor is parallel, and +*J* if the neighbor is anti-parallel.
- Each spin also interacts with the applied magnetic field.
- The energy of the full system is

$$E = -\frac{1}{2}\sum_{ij} J_{ij} S_i S_j - \sum_i S_i H,$$

where $J_{ij} = J$ if *i* and *j* are neighbors and zero otherwise.

$$E = -\sum_i S_i \left(J \sum_n S^p - J \sum_n S^a + H \right)$$

- Assume that the magnetic field points in the positive direction
- "ising" selects a spin at random and determines an effective field at the selected spin, equal to the sum of the applied field and an exchange field from the neighbors.

When the spin also points in the positive direction

$$H^{eff} = (n_+ - n_-)J + H$$

where *n*+ and *n*- are the numbers of up and down-oriented neighbors.

- After selection the spin will point up with the probability

$$p(S_i = 1) = \frac{\exp(H_i^{eff}/T)}{\exp(-H_i^{eff}/T) + \exp(H_i^{eff}/T)}$$

T and *H* are measured in units of *J*.

and point down with the probability 1-p .

- This process is repeated for a number of sweeps, during which each spin is selected in once, on average.

This type of simulation is called a Monte Carlo simulation.