Condensed Matter Physics – FK7060, Feb. 15, 2018.

Lecture 11 – Dielectric properties, defects in crystals

Reading

Ashcroft & Mermin, Ch. 25 (p. 501-503), Ch. 26 (p. 523-528), Ch. 27 (p. 554-557), Ch. 30

Content

- Umklapp process
- Temperature dependence of electrical resistivity
- Pyroelectricity, piezoelectricity, ferroelectricity
- Vacancies, interstitials
- Color centers
- Dislocations
- Surface defects
- Low-angle grain boundary

Central concepts

- **Umklapp process, Ch. 25 (p. 501-503)**

  At low temperatures, $T << \Theta_D$, only phonons with $\omega << \omega_D$ are present in significant numbers. The available phonon wave vectors are thus short. When phonons collide (due to anharmonic terms) the energy is conserved. For short initial wave vectors, the resulting wave vector must then also be short, i.e., there is no additional reciprocal lattice vector G in the crystal momentum conservation law. Such a process is a *normal process*.

  If, however (at higher temperatures) the initial and final states differ by a nonzero reciprocal lattice vector, the process is an *umklapp process*. Normal collisions alone cannot bring a system to full thermodynamic equilibrium. In fact, without umklapp processes, the thermal conductivity of an insulating crystal would be infinite.

- **Temperature dependence of electrical resistivity, Ch. 26 (p. 523-528)**

  The conductivity of Bloch electrons in a perfect periodic potential is infinite. The resistivity is thus from imperfections (point defects, dislocations, grain boundaries) and interactions with lattice vibrations. Simplified, the (always present) phonon contribution gives

  $$\rho \sim T \qquad , \qquad T >> \Theta_D$$

  and

  $$\rho \sim T^5 \qquad , \qquad T << \Theta_D$$

- **Pyroelectricity, piezoelectricity, ferroelectricity, Ch. 27 (p. 554-557)**

  Pyroelectric crystals have a nonvanishing dipole moment of their natural primitive cell.

  Piezoelectric crystals are nonpyroelectric but can obtain a nonvanishing dipole moment through suitable strain.

  Ferroelectric crystals are pyroelectric below a certain temperature, the *Curie temperature* and nonpyroelectric above. The transition is typically of second order (continuous transition without latent heat).

- **Vacancies, insterstitials**

  Vacancies, also known as *Schottky defects*, are point defects where an atom/ion is missing.

  Interstitials are point defects where an extra atom/ion is sqeezed in between the regular crystal structure.

  Point defects are important for the color and electrical conductivity of ionic crystals.

  The number of point defects follows a thermally activated behavior:

  $$n_v = N_0 e^{-U_0/k_B T}$$

  where U_0 is roughly the cohesive energy per atom, i.e. of the order of 1 eV.

  If an atom/ion is moved to create an interstitial, the resulting vacancy/interstitial pair is called a *Frenkel defect*.

- **Color centers**

  The charge of a negative ion vacancy can be balanced by a positive ion vacancy. But it can also be balanced by a bound electron, attracted by the positively charged center where the negative ion should have been. Such an electron-defect structure is called a *color center*, since it gives the color to otherwise transparent crystals.

- **Dislocations**

  A dislocation is a line defect. It comes as a *screw dislocation* or an *edge dislocation*.

  The *Burger vector* is a measure of the dislocation strength. It is obtained by going around the dislocation with a selected number of steps in each direction (equal number left and right etc), following the perfect crystal bonds. If start and stop are not the same, the loop contains one or several dislocations. The burger vector is perpendicular to an edge dislocation and parallel to a screw dislocation.

  Although it is extremely difficult to prepare a crystal without dislocations, their equilibrium concentration is zero. They are thus metastable, but frozen in. Cold-work /work hardening and deformations increase their number. The yield strength of a crystal is closely related to the presence of dislocations and their motion. Crystal growth is strongly enhanced around screw dislocations.

- **Surface defects**

  A surface defect where the crystal orientation suddenly is mirrored is known as a *twin boundary*. Another kind of surface defect is the *stacking fault*, where the order of close-packed planes suddenly change.

- **Low-angle grain boundary**

  A *grain boundary* is the boundary between two single crystals of different orientation. If the orientation is only slightly mismatched, the boundary is called a *low-angle grain boundary*. Such a boundary can be seen as a set of equally spaced dislocations, using edge dislocations for the *tilt* boundary and screw dislocations for the *twist* boundary.