Summary of Key Concepts in Solid State Physics

The structure of crystalline solids

- Solid state physics is the study of atoms assembled in periodic structures called **crystals**, and includes their electronic, optical and transport properties.
- The structures of crystalline solids are classified according to their **Bravais lattice**, in which every lattice site is specified in terms of **primitive lattice vectors** with integer coefficients. In a Bravais lattice, every lattice site is equivalent.

Electrons in crystalline solids

- The wave functions of electrons in crystals reflect the periodicity of the lattice by taking the form of **Bloch functions**, $\psi_{\boldsymbol{k}}(\boldsymbol{x}) = e^{i\boldsymbol{k}\cdot\boldsymbol{x}} u_{\boldsymbol{k}}(\boldsymbol{x})$, which is a periodic function u modulated by a plane wave.
- The periodicity of the lattice is also manifested in the energy bands. Whenever the Bragg condition is satisfied, an **energy gap** appears because propagation is suppressed; only stranding waves are allowed. Thus, the **band structure** of a solid consists of continuous bands of energy levels separated by energy gaps.
- The existence of gaps explains the difference between **metals** and **insulators** as solids which have partially filled bands (metals) and those which have completely filled bands (insulators). Most elements solids are derived from partially filled atomic energy levels and are, therefore, metals.
- By virtue of their partially filled energy bands, metals are good conductors of electricity and heat. Insulators, on the other hands, are poor conductors of electricity (but can conduct heat by lattice vibrations).

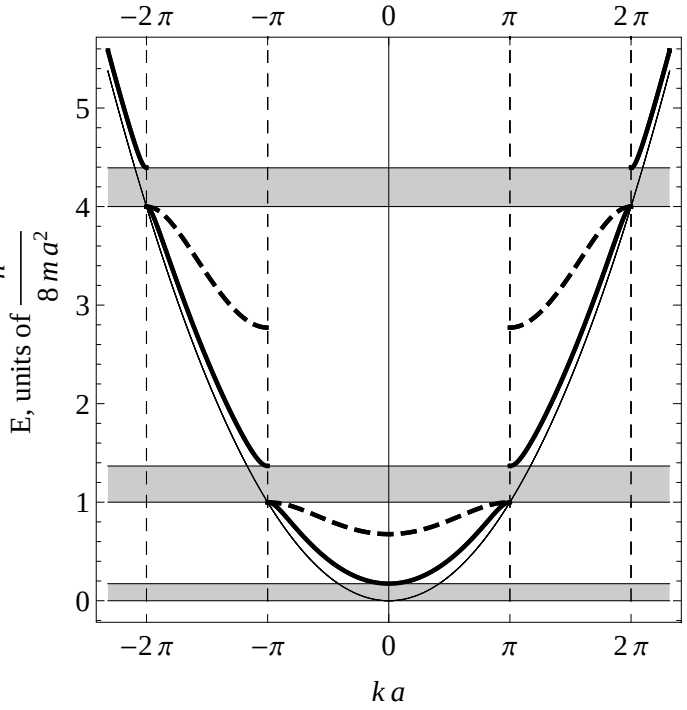
Electrons and holes in semiconductors

- A semiconductor is an insulator at $T = 0$ with electrical properties that can be controlled by doping with electrically active atoms. A pure semiconductor is called **intrinsic** and a semiconductor with dopants is called **extrinsic**. At $T = 0$, the completely filled bands are called **valence bands** and the empty bands are called **conduction bands**.
- Dopants are called either **donors** or **acceptors**, depending on whether they donate an electron into the conduction bands (donors) or holes into the valence band (acceptors). Semiconductors with donors are called n-type, and those with acceptors are called p-type, reflecting the dominant carrier type as being either electrons (n) or holes (p).
- Many electronic properties of semiconductors such as Si and Ge can be understood as the **rehybridization** of the atomic s^2p^2 electronic configuration to the sp^3 configuration in the tetrahedral environment of the crystalline solid.
- In a **direct band gap** semiconductor, the highest energy in the valence bands and the lowest energy in the conduction bands occurs at the same **k**-point, so excitations can occur by the absorption of a photon. For an **indirect band gap** semiconductor, however, the extrema of the valence and conduction bands are at different **k**-points, so the absorption of a photon, must be accompanied by the absorption of a phonon to provide the additional momentum to complete the transition.

The *p*-*n* junction

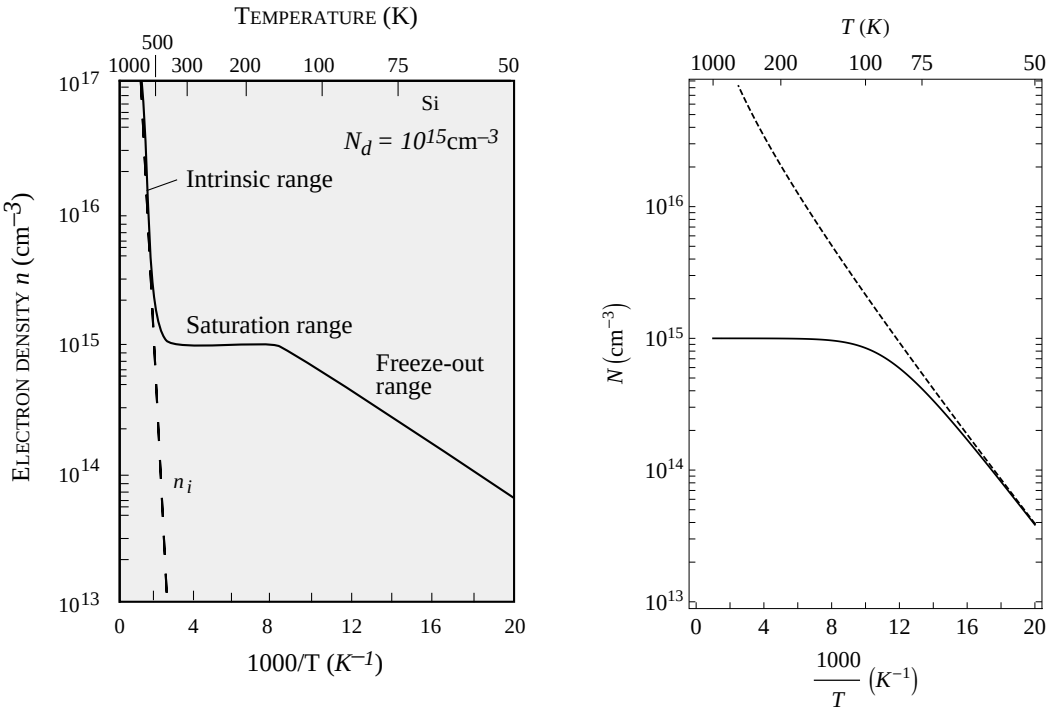
- A ***p*-*n* junction**, formed at the interface of an n-type and a p-type semiconductor, is the fundamental component of many semiconductor electronic devices, including diodes, transistors, solar cells, light-emitting diodes, and integrated circuits.
- There are two main types of current in a p-n junction: **diffusion**, where carriers flow from high to low concentrations, and **drift**, where carriers flow in response to an electric field.
- Without an external applied voltage, an equilibrium condition is reached in which a potential difference, called the **built-in potential**, is formed across the junction. This is the main feature of a p-n junction because the existence of this potential allows current to pass in one direction with far greater ease than in the other.
- When two p-n junctions are placed back-to-back, the resulting device, a **bipolar junction transistor**, allows current to be regulated. An n-p-n transistor, for example, allows the current of electrons through an n-type semiconductor to be controlled. Electrons flow through the device from one side, called the **emitter**, to the other side, called the **collector**, with the voltage at the **base** regulating the current between the emitter and collector.

Three diagrams



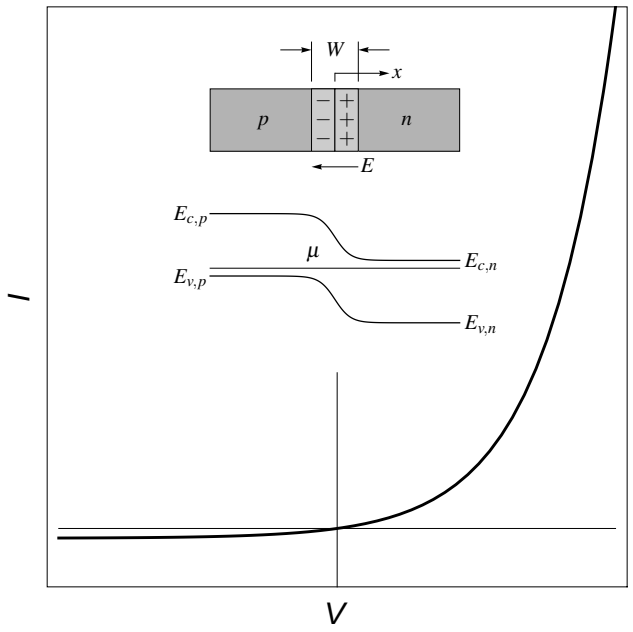
The energy bands of a one-dimensional 'crystal' composed of an infinite periodic array of δ-functions (the Kronig–Penney model) compared with the free-electron dispersion (light solid line). The main features of the Kronig–Penney solution that are found for real bands are:

- The Kronig–Penney model corresponds to a crystal whose 'atoms' are infinite potential wells. When these wells are brought together, and the well height reduced to a finite value, the electrons can hop between wells, which leads to the broadening of the discrete levels into energy bands..
- Continuous bands alternate with gaps, which are indicated by shading. Note that gaps do not occur for the free electron dispersion.
- The continuous bands correspond to propagating solutions within the one-dimensional crystal.
- The gaps correspond to regions of energy where propagating solutions are forbidden.
- The energy gaps occur whenever $ka = n\pi$, where n is any integer. This corresponds to the fulfilment of the Bragg condition, with the one-dimensional crystal acting as a diffraction grating for the electrons. Thus, at these points, only standing waves are possible. The vanishing of the group velocity of the electrons at these Bragg points is evident from the fact that the energy bands approach these points with zero slope.
- The energy gap arises because the complex propagating solutions are split into two real standing waves. The solution with maximum amplitude between the δ-functions have the lower energy, and those whose maximum amplitude is at the δ-functions have the higher energy.
- The widths of the bands and the magnitudes of the gaps are determined by the strength of the potentials, with weak potentials yielding wide bands that resemble those of free electrons, and strong potentials producing comparatively narrow bands.
- The form of the energy dispersion curves near the Bragg points can be regarded as free-electron-like, but with an effective mass that embodies the effect of the potential.



The measured carrier density of a Si crystal with a concentration 10^{15} cm^{-3} of donors (left) and the corresponding calculation at all but the highest temperatures (right).

- The measured carrier density shows three discernible temperature regions: the freeze-out range, the saturation range, and the intrinsic range.
- In the freeze-out range, the donors are beginning to be ionized and both plots show a gradual increase of the carrier density.
- The donors continue to be ionized until the temperature reaches the saturation range, when all donors are ionized and the carrier density remains constant at the dopant concentration. This is the operational range of devices, and the constant (and controllable) carrier density is the reason extrinsic semiconductor are used in devices.
- The dotted line in the right panel represents the simplest calculation of the carrier density and includes the Boltzmann approximation for both the donors and the conduction bands, While the Boltzmann approximation for the donor levels is valid at lower temperatures, the discrepancy between this calculation and measured densities increases with increasing temperature.
- A correct description of the saturation necessitates that the Fermi–Dirac distribution be used for the donor levels. The result is the solid curve in the right panel, which reproduces the behavior of the measured carrier density.
- In the intrinsic range, the temperature is high enough to excite electrons from the valence band to the conduction band. The calculations described above neglected this source of carriers. Including this effect (but still using the Boltzmann approximation for the conduction band) requires a numerical solution of the resulting equations.



Current-voltage diagram showing the rectification properties of a *p*-*n* junction, with a dramatic increase of current for forward bias ($V > 0$), but only a small current for reverse bias ($V < 0$). The inset shows a *p*-*n* junction, along with the profiles of the valence and conduction band edges, and the important parameters that characterize the junction.

- A *p*-*n* junction is formed at the interface of *p*-type material (that is, a semiconductor doped with acceptors) and *n*-type material (that is, a semiconductor doped with donors).
- The balance of diffusion current (in response to the concentration steps of holes and electrons at the interface) and drift current (in response to the field created by diffusing carriers leaving behind ionized dopants) leads to the formation of an equilibrium state in which the chemical potential is constant throughout the material.
- There are two main effects of the equilibrium state: (i) the bending of the bands to accommodate the constant chemical potential throughout the system, and (ii) the formation of an electrostatic potential due to the ionized dopants. Both effects are confined to a small region around the interface called the transition region.
- In the case of forward bias, the applied field acts in opposition to the in-built field, which reduces the potential barrier across the junction. The effect of reverse bias is to reinforce the in-built field, leading to a much greater barrier at the junction.
- The current in the forward bias direction is dominated by diffusion current of *extrinsic* carriers, but the the current in the reverse bias direction is due mainly to *intrinsic* carriers generated by excitation across the energy gap of the semiconductor.