

4. Kinematics and dynamics of electrons and holes in energy bands

Key ideas

A free electron in an energy band can be represented semiclassically by a *wave packet* of Bloch states that is *spatially localized*. The velocity of the center of the wave packet is the *group velocity* v_g .

The curvature of an energy band is proportional to the *inverse effective mass*. The *inverse effective mass tensor* is defined by

$$\left(\frac{1}{m^*}\right)_{\alpha\beta} = \frac{1}{\hbar^2} \frac{\partial^2 E_{nk}}{\partial k_\alpha \partial k_\beta}.$$

An *external force* F acting on a band electron produces a change of its wave vector k with time,

$$F = \hbar \frac{dk}{dt},$$

which is analogous to the classical relation of force to time rate of change of momentum p :

$$F = \frac{dp}{dt}.$$

Electrons and holes in energy bands

4.1 Group velocity

4.2 Inverse effective mass tensor

4.3 Force equation

One therefore defines the *crystal momentum* to be $\hbar k$.

4.4 Dynamics of electrons

An electric field \mathcal{E} produces an accelerated electron wave packet:

$$\frac{dv_g}{dt} = -e \left(\frac{1}{m^*}\right) \cdot \mathcal{E}.$$

4.5 Dynamics of holes

A *hole* is an *empty state* in an otherwise filled band. Both the *electric charge* of a hole and its *effective mass* are *positive*.

4.6 Cyclotron resonance

The effective mass of a charge carrier can be measured by *cyclotron resonance*.

4.7 Hall effect

The concentration and charge sign of a charge carrier can be measured by the *Hall effect*.

The valence electrons are responsible of the charge carrier generation, too, and in case of intrinsic semiconductors, in particular. Electrons are excited from the valence band to conduction band leaving the holes behind.

The charge carrier properties, however, follow from the band structure, as discussed below.

4.1. Group velocity

To consider electrons as spatially localized charge carriers moving in the crystal from one location to another we define the concept *wave packet* (aaltopaketti). The wave packet can be created as a superposition

$$f_{n\mathbf{k}_0}(\mathbf{r}, t) = \int a_{n\mathbf{k}} \psi_{n\mathbf{k}}(\mathbf{r}, t) d\mathbf{k}, \quad (4.1)$$

of the time-dependent Bloch functions

$$\psi_{n\mathbf{k}}(\mathbf{r}, t) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) e^{-i(E_{n\mathbf{k}}/\hbar)t}. \quad (4.2)$$

The $E_{n\mathbf{k}}$ is the eigenenergy of the Bloch state.

4.2. Inverse effective mass tensor

4.3. Force equation

4.4. Dynamics of electrons

Assume an external electric field \mathbf{E} with a force

$$\mathbf{F} = -e \mathbf{E} \quad (4.17)$$

on the electron. Thus, the crystal momentum or wave vector is changing in time

$$\frac{d\mathbf{p}}{dt} = m^* \frac{d\mathbf{v}_g}{dt} = \hbar \frac{d\mathbf{k}}{dt} = -e \mathbf{E}. \quad (4.18-4.19)$$

Deceleration due to scattering of the accelerating electrons leads to a dynamical balance of charge carrier flow or electrical current.

4.5. Dynamics of holes

For the holes in valence band we infer:

4.6. Experimental determination of effective masses: cyclotron resonance in semiconductors

4.7. Experimental determination of carrier charge and concentration: Hall effect

Consider DC current in a bar (in x-direction). Due to the Lorentz force

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \quad (4.55)$$

where $\mathbf{B} = B_z \hat{\mathbf{k}}$, there is a force component $F_y = q(E_y - v_x B_z)$ on the charge carriers. Therefore,

$$E_y = v_x B_z \quad (4.57)$$

and $V_H = E_y w$. Suppose the charge carriers are holes, in which case $J_x = qp_0 v_x$ and

$$E_y = J_x / qp_0 B_z = R_H J_x B_z, \text{ where } R_H = 1 / qp_0. \quad (4.58-59)$$

R_H is *Hall coefficient* (Hall-vakio). Thus, measurement of Hall coefficient gives both the charge carrier concentration and charge of the carriers (including sign) from

$$p_0 = 1 / qR_H = J_x B_z / qE_y.$$

Measurement of the resistivity $\rho = Rwt/L = 1/\sigma$, too, allows evaluation of the mobility

$$\mu_p = \sigma / qp_0$$

in case there is only one type of charge carriers.

5. Electronic effects of impurities

<p>Key ideas</p> <p><i>Donor impurities</i> in <i>n-type semiconductors</i> provide free electrons to the conduction band and positively charged <i>donor ions</i>. <i>Acceptor impurities</i> in <i>p-type semiconductors</i> provide free holes to the valence band and negatively charged <i>acceptor ions</i>.</p> <p><i>Shallow impurities</i> have ionization energies that are small compared to the fundamental gap. Their energy levels and eigenfunctions are well described by <i>effective mass theory</i>.</p> <p>The <i>anisotropic effective mass</i> of the conduction band in Si and Ge causes a splitting of energy levels associated with <i>p-like</i> hydrogenic states. A set of donor levels is associated with each conduction band minimum: six minima for Si and four for Ge.</p> <p>The wave vector dependence of the dielectric constant leads to coupling between impurity states associated with different extrema of an energy band and a splitting of degeneracies.</p> <p>In materials such as InSb, the small effective mass and large dielectric constant lead to a large <i>effective Bohr radius</i> of <i>donor levels</i>.</p> <p><i>Degeneracy</i> and <i>warping</i> of the valence bands lead to complicated structure of <i>acceptor levels</i>.</p>	<p>Impurities in semiconductors</p> <p>5.1 Qualitative aspects of impurities</p> <p>5.2 Effective mass theory</p> <p>5.3 Donor impurities in Si and Ge</p> <p>5.4 Donor impurities in III–V semiconductors</p> <p>5.5 Acceptor impurities</p>
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<p><i>Deep level centers</i> have energy levels near the midpoint of the fundamental gap. The ground state ionization energy depends significantly on the nature of the impurity or defect. <i>Central cell corrections</i> are required in the impurity potential.</p> <p>At sufficiently high impurity concentrations, the wave functions of neighboring impurities overlap sufficiently to produce an <i>impurity band</i>.</p>	<p>5.6 Central cell corrections and deep levels</p> <p>5.7 Impurity bands</p>
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By doping with impurities the electronic properties of semiconductors can be controlled or tuned as desired. Impurities are one type of defects, whose electronic states we consider next. In general, defects can be either useful or harmful.

5.1. Qualitative aspects of impurities

The most general defects are *point defects* (pistevika), *line defects* (viivavika) and *complexes* (kertymä).

Classification of point defects:

- vacancy (vakanssi)	V_A	A	B	A	B	B	A	B	A
- interstitial (välikköatomi)	I_A				A				
- substitutional (korvaus-)	C_A	B	A	B	A	B	A	B	A
- antisite	B_A								
- Frenkel defect pair	V_A-I_A	A	B	B	B	C	B	A	B
		B	A	B	A	B	A	B	A

Impurities like C_A involving foreign atoms are *extrinsic* defects, whereas the others are *native* or *intrinsic*.

Donors

acceptors

double donors

double acceptors

isovalent substitutional

5.2. Effective mass theory

Impurities whose electrons can be treated by s.c. "*effective mass approximation*" are called *shallow* (matala) and the others are called *deep* (syvä). The effective mass approximation or theory is based on simplifying assumptions:

1. The impurity potential is weak, because the impurity is strongly screened by the high dielectric constant of a typical semiconductor crystal.
2. The impurity potential is slowly varying over the crystal lattice constant.
3. The impurity state is very spread out and only wave vectors near the band extremum (Γ -point) are essential to consider.

Thus, consider a donor with a weakly bound electron, e.g. $P_{Si}@Si$. Describe the electronic state with a hydrogen like orbital in the potential

$$V_i(\mathbf{r}) = -Ze^2 / (4\pi\epsilon_0 \epsilon r), \quad (5.6)$$

where the dielectric constant ϵ takes into account the screening of the medium and Z is the charge of the impurity.

Thus, for the donor state $\psi_i(\mathbf{r})$ we solve the Schrödinger equation

$$(H_0 + V_i(\mathbf{r})) \psi_i(\mathbf{r}) = E_i \psi_i(\mathbf{r}), \quad (5.1)$$

where H_0 is the one-electron hamiltonian of the perfect crystal.

Let us expand the solution in terms of Luttinger–Kohn functions (see the text book) or localized Wannier functions

$$\psi_i(\mathbf{r}) = N^{-1/2} \sum_n F_n(\mathbf{R}_i) w_n(\mathbf{r} - \mathbf{R}_i), \quad (5.3)$$

where the coefficients $F_n(\mathbf{R}_i)$ can be regarded as amplitudes of the contributing Wannier functions, or the *envelope wave function*.

By substituting (5.3) into (5.1) and assuming isotropic, nondegenerate and parabolic lowest conduction band

$$E_c(\mathbf{k}) = E_c(\mathbf{0}) + \hbar^2 \mathbf{k}^2 / 2m^* \quad (5.7)$$

we are left with an equation for the envelope function

$$\left[-\frac{\hbar^2}{2m^*} \nabla^2 + V_i(\mathbf{R}) \right] F(\mathbf{R}) = (E - E_c(0)) F(\mathbf{R}), \quad (5.8)$$

which is similar to the Schrödinger equation of a particle with mass m^* in a potential $V_i(\mathbf{R})$, whose reference (zero) energy is $E_c(\mathbf{0})$. This is the *effective mass approximation* for the donor state (envelope wave function) or the *charge carrier with effective mass m^* in medium described by the dielectric function ϵ* .

The variable \mathbf{R} in (5.8) assumes the discrete values of lattice vectors, only. However, in the range of tens or hundreds of Ångströms we can consider \mathbf{R} continuous or quasi-continuous. As the potential $V_i(\mathbf{R})$ is essentially that of the point charge with effective ϵ , the solution $F(\mathbf{R})$ is the hydrogen atom wave function for a particle with effective mass m^* . There are both discrete bound eigenstates and continuum states with a continuous energy spectrum available for the charge carrier.

By denoting the states with principal quantum number N , angular momentum quantum number L (and M_L and M_S) we obtain the *bound Rydberg states* or levels

$$E_N = E_c(\mathbf{0}) - R / N^2, \quad (5.11)$$

where $N = 1, 2, 3, \dots$; and R is the *donor Rydberg constant*.

The *donor Rydberg constant* is

$$R = \frac{m^*}{m_0} \frac{1}{\epsilon^2} R_H = \frac{m^*}{m_0} \frac{1}{\epsilon^2} \frac{e^4 m_0}{(4\pi\epsilon_0)^2 2\hbar^2}.$$

The donor Bohr radius is

$$a^* = \epsilon \frac{m_0}{m^*} a_0 = \epsilon \frac{m_0}{m^*} \frac{(4\pi\epsilon_0) \hbar^2}{e^2 m_0} \quad (5.9)$$

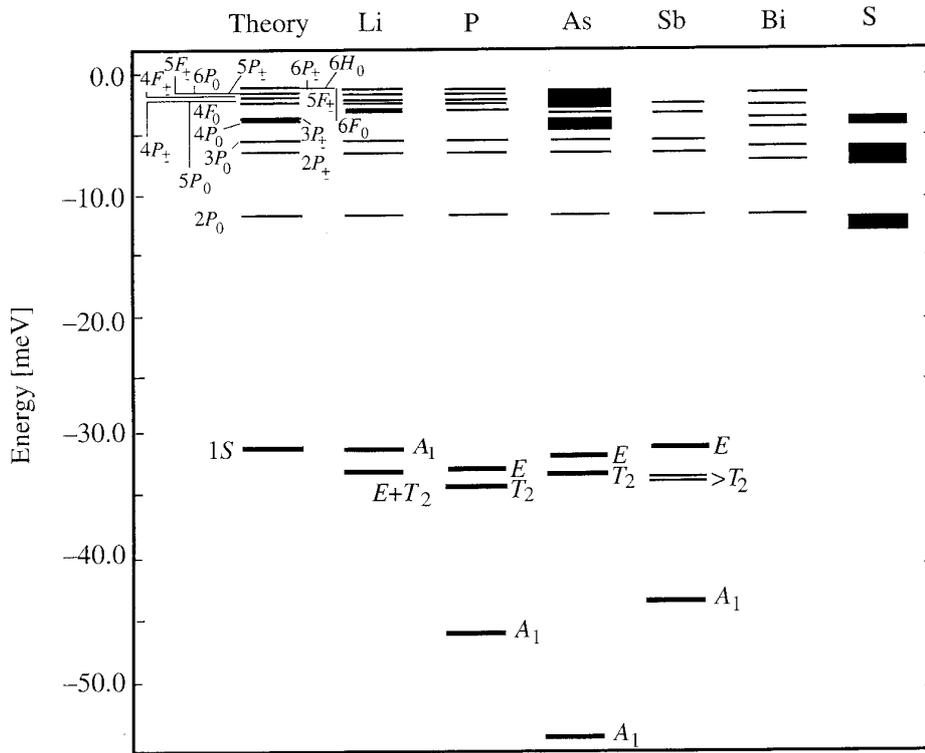
and the lowest energy wave function (1S)

$$C_{1S}(\mathbf{R}) = \frac{1}{\sqrt{\pi a^{*3}}} \exp\left(\frac{-R}{a^*}\right).$$

Thus, a simplified description of the shallow donor wave function is

$$\psi_i(\mathbf{r}) = u_0(\mathbf{r}) F(\mathbf{r}).$$

5.3. Donor impurities in Si and Ge



5.4. Donor impurities in III-V semiconductors

5.5. Acceptor impurities

5.6. Deep centers (syvät tilat)

The shallow impurity states extend over many primitive cells and need only a few Bloch functions to form the descriptive Wannier function. The deep center levels are characterized by much stronger localization and need of several Bloch functions (\mathbf{k}) from several bands (n) for the description.

The deep levels often relate to the lattice distortion (or relaxation), which takes energy E_D . A shallow level conversion to a deep level of energy E_0 is favorable and minimizes the total energy, if $|E_0| > E_D$.

Si_{Ga} in GaAs is a shallow hydrogenic donor, but in GaAlAs with more than 25% of Al it converts to a deep center with $E_0 \approx 0.4$ eV. Such deep donor is called a *DX center*.

5.7. Impurity bands

At high impurity concentrations, $n_I \geq 10^{18} \text{ cm}^{-3}$, the neighboring impurities are close enough to interact and form impurity bands. This may lead to high enough charge carrier concentration to screen the donor Coulomb potential to the form

$$V(r) = -e^2 / (4\pi\epsilon_0 r) e^{-q_s r}, \quad (5.16)$$

where q_s is the inverse screening length specified by $q_s = 4(3n_I / \pi)^{1/3} / a^*$. This binds the electron only if $q_s < 1.19 / a^*$ or

$$n_I^{1/3} a^* < 0.36. \quad (5.17)$$

6. Semiconductor statistics

Key ideas

In an *intrinsic semiconductor* free charge carriers arise from the excitation of electrons from the valence band to the conduction band creating equal concentrations of free electrons in the conduction band and free holes in the valence band.

At thermal equilibrium the *Fermi–Dirac distribution function* specifies the *occupation number* of a state.

The *density-of-states* in an energy band is the number of states per unit volume per unit energy interval.

The *intrinsic carrier concentration* enters the *law of mass action* that relates the concentration of electrons and holes.

In *extrinsic semiconductors* the charge carriers arise primarily from impurities.

Donor impurities produce an *n-type semiconductor*. In the *freeze-out range* the free carrier concentration increases exponentially with temperature, but in the *saturation range* it is nearly constant.

Acceptor impurities produce a *p-type semiconductor*.

In a *compensated semiconductor* both donor and acceptor impurities are present.

In an n-type semiconductor electrons are the *majority carriers* and holes are the *minority carriers*. In a p-type semiconductor the roles of electrons and holes are reversed.

Statistics

6.1 Intrinsic semiconductors

6.2 Extrinsic semiconductors

6.1. Intrinsic semiconductors

6.2. Extrinsic semiconductors

7. Lattice vibrations in semiconductors

Key ideas

In the *harmonic approximation* the equations of motion are linear in the displacement components of the atoms.

The *normal mode frequencies* of a monatomic linear chain are confined to a band between zero and a maximum frequency.

The normal mode frequencies of a diatomic linear chain lie in the *acoustic branch* or the *optical branch* with a *gap* between the branches.

Elastic continuum theory provides a simple treatment of long-wavelength modes of vibration.

Phonon dispersion curves are determined by *inelastic neutron scattering*. Short range interactions are insufficient to account for the experimental data. The deformability of the electron charge distribution is taken into account by the *shell model* and the *bond charge model*. The partial ionic character of the electron-pair bonds and the effective charge of the atom is taken into account by the *deformation dipole model*. The *linear response method* provides full phonon dispersion curves without fitting parameters to experimental curves.

In a *normal mode of vibration* all atoms vibrate with the same frequency.

The vibrational specific heat obeys the *Debye T^3 -law* at low temperatures and the *Dulong–Petit law* at higher temperatures.

Phonons

7.1 Equations of motion

7.2 Monatomic linear chain

7.3 Diatomic linear chain

7.4 Three-dimensional crystals

7.5 Lattice dynamical models

7.6 Normal coordinate transformation

7.7 Vibrational specific heat

Anharmonic effects are responsible for *thermal expansion* and *diffusive thermal conductivity*.

Impurities and other defects can give rise to *localized modes*.

Piezoelectricity can increase the elastic moduli and the speed of sound.

Applied *stress* can cause shifts and splittings of electronic and vibrational energy levels.

7.8 Anharmonic effects

7.9 Impurity effects on lattice vibrations

7.10 Piezoelectric effects

7.11 Effects of stress-induced atomic displacements

The atoms in any crystal vibrate around their equilibrium positions, that leads to several important phenomena. Vibration breaks the ideal and exact lattice symmetry leading to coupling with electrons and **electrical resistivity**. Vibration is also the main mechanism behind the **thermal phenomena**: heat capacity and thermal conductance. **Acoustics** in solids are described with one type of vibrations and one class of optical properties with another type.

The **quantized lattice vibrations** are called *phonons*.

7.1. Equations of motion

The most direct approach to vibration dynamics is based on the **Born–Oppenheimer approximation for evaluation of the potential energy hypersurface** (PES), where the *adiabatic ion core quantum dynamics* is solved. Such PES can be obtained from theoretical total energy calculations or by fitting observed phonon frequencies to suitably parameterized model of functional form. The simplest approximation is the collective or coupled *harmonic oscillator model* or *harmonic approximation* (not capable of explaining the thermal expansion).

It should be emphasized that the adiabatic Born–Oppenheimer dynamics does not include the *electron–phonon interaction* or scattering, which is an essential feature in transport phenomena.

With the position vector of an atom

$$\mathbf{u} = \mathbf{R} - \mathbf{R}^{(0)} \quad (7.2)$$

The classical equation of motion of the atom k with mass M_k is

$$M_k \ddot{\mathbf{u}}_k = -\nabla\Phi$$

or

$$M_k \ddot{u}_{k\alpha} = -\partial\Phi/\partial u_{k\alpha}, \quad (7.5)$$

where Φ is the PES, defined above.

In the quantum mechanical approach we consider the hamiltonian in a unit cell l .

Again, if \mathbf{u}_{kl} is the displacement of the atom from its equilibrium, in the harmonic approximation we write

$$H(\mathbf{u}_{kl}) = 1/2 M_k \dot{\mathbf{u}}_{kl}^2 + 1/2 \sum_{k'l'} \mathbf{u}_{kl} \cdot \Phi(\mathbf{k}l, \mathbf{k}'l') \cdot \mathbf{u}_{k'l'},$$

where Φ is the harmonic force constants (matrix).

7.2. Monatomic linear chain

By setting the force constant of the harmonic force field to be $\Phi = 2\sigma$, the equation of motion becomes now in form

$$M_k \ddot{\mathbf{u}}_k = \quad (7.22)$$

whose solution is

7.3. Diatomic linear chain

Consider two different atoms in the unit cell, where the reduced mass of internal dynamics M relates to the two atomic masses M_1 and M_2 as

$$M^{-1} = M_1^{-1} + M_2^{-1}. \quad (7.32)$$

The simplest procedure to find the main features of the phonon band is doubling the unit cell of the previous monatomic chain leading to halving the 1. Brillouin zone:

7.4. Three-dimensional crystals

As an extension to the 1-dimensional case, now, the dynamics of atoms is coupled to collective normal modes, which assume the form of Bloch waves

$$\mathbf{u}_{\mathbf{k}l}(\mathbf{q}, \omega) = \mathbf{u}_{\mathbf{k}0} \exp[i(\mathbf{q} \cdot \mathbf{R}_l - \omega t)], \quad (7.13)$$

where \mathbf{q} is the wave vector, ω is the frequency and \mathbf{R}_l are lattice vectors.

As above, since \mathbf{R}_l are lattice vectors, two phonons whose wave vectors differ by a reciprocal lattice vector are equivalent. In other words, the unit cell or interatomic distance sets limits to the shortest wavelength. Thus, the phonon dispersion $\omega(\mathbf{q})$ is the same in all Brillouin zones.

As diamond and zinc-blende structures have two atoms in the primitive cell, there are six phonon bands: 3 acoustic and 3 optical. In high symmetry directions these can be classified to 4 transverse and 2 longitudinal

7.5. Lattice dynamical models for semiconductors

The quantized normal modes are phonons. The phonon dispersion curves can be measured by inelastic neutron scattering and inelastic x-ray scattering experiments.

Phonon creation is called Stokes process and annihilation correspondingly anti-Stokes process. Thus, the energy and momentum conservation laws can be written

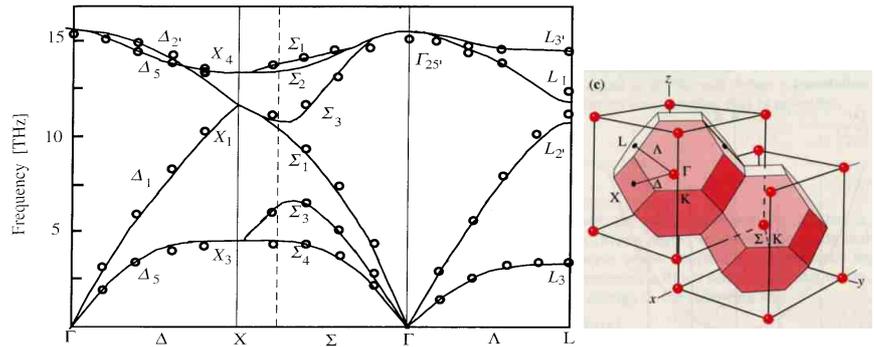


Fig. 3.1. Phonon dispersion curves in Si along high-symmetry axes. The circles are data points from [3.4]. The continuous curves are calculated with the adiabatic bond charge model of Weber [3.5]

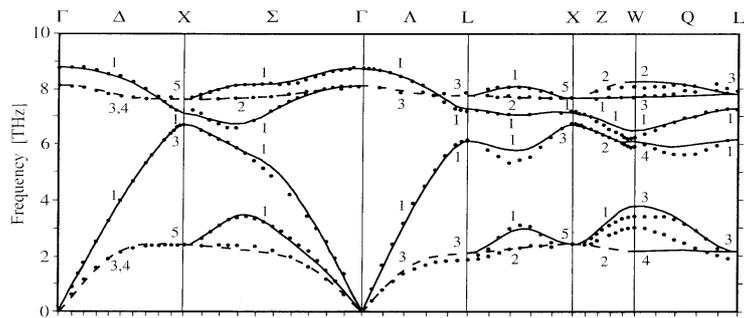


Fig. 3.2. Phonon dispersion curves in GaAs along high-symmetry axes [3.6]. The experimental data points were measured at 12 K. The continuous lines were calculated with an 11-parameter rigid-ion model. The numbers next to the phonon branches label the corresponding irreducible representations

7.6. Normal coordinate transformation

7.7. Vibrational specific heat

7.8. Anharmonic effects

8. Charge carrier scattering and transport properties

Key ideas	Transport properties
Charge carriers in semiconductors are characterized by their <i>mean free path</i> , <i>relaxation time</i> , and <i>mobility</i> .	8.1 Elementary transport theory
The <i>Boltzmann equation</i> governs the behavior of the carrier <i>distribution function</i> .	8.2 Boltzmann equation
The <i>mobility</i> of a carrier is proportional to the <i>average relaxation time</i> .	8.3 Electrical conductivity and mobility
In general, the <i>relaxation time</i> of a carrier depends on its <i>energy</i> and on the nature of the <i>scatterers</i> .	8.4 Energy dependence of the relaxation time
<i>Scattering mechanisms</i> such as those due to <i>ionized impurities</i> and <i>phonons</i> contribute to the relaxation time.	8.5 Relaxation times for specific scattering mechanisms
The <i>electrical conductivity</i> is modified by an <i>external magnetic field</i> .	8.6 Magnetotransport properties
The <i>Hall effect</i> enables one to measure the <i>carrier concentration</i> .	8.7 Thermoelectric phenomena
The presence of a <i>temperature gradient</i> gives rise to the <i>Seebeck effect</i> .	8.8 Thermal conductivity
An <i>electric current</i> can produce a <i>heat flux</i> through the <i>Peltier effect</i> .	8.9 Semi-insulating semiconductors
<i>Free carriers</i> contribute to the <i>thermal conductivity</i> of a semiconductor.	8.10 Hot carrier phenomena
Using <i>deep impurities</i> , <i>semi-insulating semiconductors</i> can be produced.	8.11 Variable-range hopping conductivity
In <i>high electric fields</i> , free carriers have a <i>higher effective temperature</i> and a <i>lower mobility</i> . <i>Negative differential conductivity</i> can arise that produces <i>Gunn oscillations</i> . High-energy carriers can generate additional carriers by <i>impact ionization</i> .	
In <i>disordered semiconductors</i> at low temperature, the electrical conductivity can have an $\exp(-BT^{-4})$ dependence due to <i>variable-range hopping</i> of carriers.	

Consider next *free charge carriers*, electrons and holes, under the influence of an external field. In a *weak electric field* the behavior can be described by *Ohm's law*, but in *high fields* the behavior is different and the carriers are called *hot electrons*.

8.1. Simple phenomenological introduction to transport in semiconductors

We start with a simple phenomenological discussion for the externally driven *drift current* and concentration gradient driven *diffusion current*.

8.1.1. Electric conduction current

In the absence of external field the "low-density-noninteracting" charge carrier distribution could be viewed even with the classical statistics. Then, the *equipartition principle* would give for the mean thermal square speed s_{th}^2 a relation

$$1/2 m^* s_{th}^2 = 3/2 k_B T$$

or

$$(8.1)$$

The average time between collisions of charge carriers (*scattering or relaxation time* τ) is in the range $10^{-13} - 10^{-12}$ s leading to the *mean free path*

$$\Lambda = s_{th} \tau, \quad (8.2)$$

which thus is usually about 100 – 1000 Å.

For the drift current we assume that all electrons (holes) experience the same weak external field $\mathbf{E} = -\nabla\Phi(\mathbf{r})$ of the slowly and linearly varying external potential $\Phi(\mathbf{r})$.

By modeling "friction" due to the scattering of electrons by impurities and phonons with the above defined relaxation time τ , the classical equation of motion of electrons becomes as

$$m^* \ddot{\mathbf{r}} + (m^*/\tau) \dot{\mathbf{r}} = -e \mathbf{E}, \quad (8.3)$$

where the dot indicates time derivative.

From the steady-state condition $\ddot{\mathbf{r}} = 0$ (and denoting more generally $q = -e$) we derive the drift velocity of carriers

Define the *carrier mobility* μ by

$$\mathbf{v}_d = \mu \mathbf{E} \quad (8.10)$$

in the isotropic case leading to

$$\mu = q\tau / m^*. \quad (8.11)$$

By adding the contributions of both electrons and holes we obtain for the conductivity

$$\sigma = q (n_e \mu_e + n_h \mu_h). \quad (8.14)$$

8.1.2. Conductivity effective mass

8.1.3. Diffusion current

8.1.4. Displacement current

8.2. Boltzmann equation and its solution

Next we consider a more general case, where the carriers are distributed according to a temperature dependent *distribution function* and the scattering time is charge carrier energy dependent. This is also called the relaxation time approximation.

The distribution function $f_{\mathbf{k}}(T, \mathbf{r})$ gives the probability for the occupation of the band state $E_{\mathbf{k}}$ (at \mathbf{r}) at temperature T . In the absence of the external field and thermal equilibrium this is the *Fermi–Dirac distribution*

$$f_{\mathbf{k}}^0 = \frac{1}{\exp\left[\frac{(E_{\mathbf{k}} - \mu_F)}{k_B T}\right] + 1} \quad (8.72)$$

for fermions, like electrons, where μ_F is the *chemical potential* and k_B is the Boltzmann constant.

In the presence of external perturbation the distribution function obeys the *Boltzmann equation*

$$\frac{df_{\mathbf{k}}}{dt} = \left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{field}} + \left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{diff}} + \left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{scatt}}. \quad (8.45)$$

The three terms on the right hand side include the effects from the external field, diffusion of charge carriers and scattering of carriers by phonons and impurities.

Let us assume that diffusion is negligible and the applied field is weak enough that we can expand the distribution function

$$f_{\mathbf{k}} = f_{\mathbf{k}}^0 + g_{\mathbf{k}}(\mathbf{E}),$$

where $g_{\mathbf{k}}(\mathbf{E})$ is the change induced by the external field \mathbf{E} . Thus,

(8.46)

For the third term we write within the *relaxation time approximation*

$$\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{scatt}} = -\frac{g_{\mathbf{k}}}{\tau_{\mathbf{k}}}, \quad (8.55)$$

which assumes the relaxation time to be \mathbf{k} -dependent. Relaxation is due to scattering processes, which we consider later.

Note, that a transient perturbation $g_{\mathbf{k}}$ decays away exponentially.

Now, in the steady state (e.g. in external field), from the Boltzmann equation

9. Surface properties of semiconductors

Key ideas

The *wave function amplitude* of *electronic surface states* decreases strongly from the surface to the interior of the crystal.

The *wave function* of a *surface state* in the *nearly free electron approximation* is constructed from Bloch functions with *complex wave vectors*. The *energy eigenvalue* lies in the *gap* between the energy bands of the bulk crystal.

In the *tight binding method* the surface state wave function is a *linear combination of atomic orbitals* with coefficients that *decay exponentially* toward the interior of the crystal.

Surface elastic waves have displacement amplitudes that *decay exponentially* from the surface to the interior. Their *velocity* is *less* than that of *bulk waves*.

In diatomic semiconductors *surface modes of vibration* can occur with frequencies in the gap between acoustic and optical branches.

The *shell model*, the *bond charge model* and *ab initio methods* can be used to calculate the properties of surface modes in real semiconductors.

Surface vibrational modes can be studied experimentally using *Brillouin scattering*, *Raman scattering*, *electron scattering*, *helium atom scattering*, and *infrared spectroscopy*.

The *recombination* of electrons and holes can be *enhanced* at a surface or interface of a semiconductor.

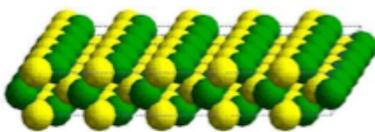
Surface Properties

9.1 Surface effects on electronic states

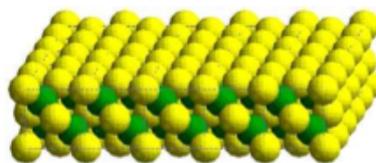
9.2 Surface effects on lattice vibrations

9.3 Surface recombination

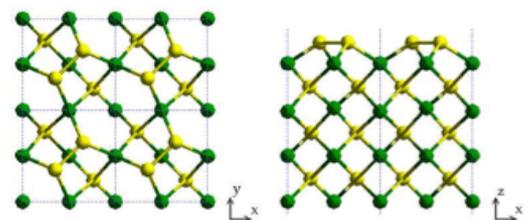
Surface atomic structure



Kuva 4.5: Galliumarsenidin (110)-katkaisupinta.



Kuva 4.7: Galliumarsenidin (100)-katkaisupinta.



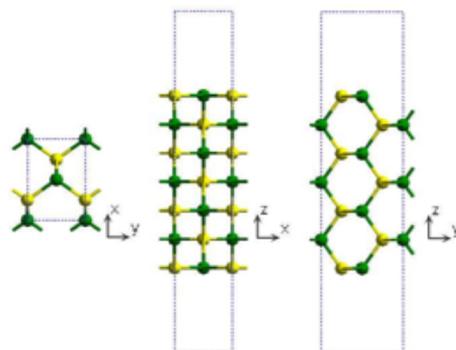
Kuva 5.11: (100)-pinnan arseeniterminoitu (1x1)-rekonstruktio.

with the slab model:

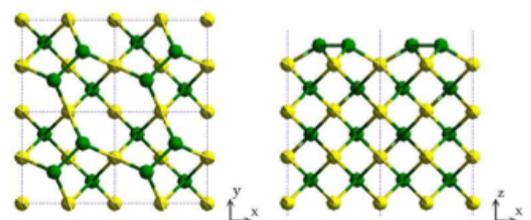
Pictures from

Ville Arpiainen:

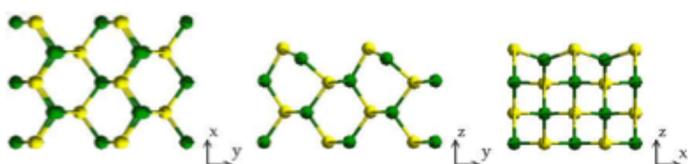
Electronic structure and simulated STM images of GaAs cleavage surface (Master of Science Thesis, TUT 2004).



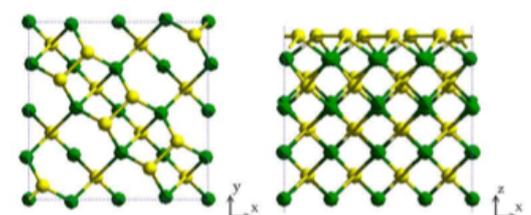
Kuva 5.7: (110)-pinnan seitsemän atomitasoa sisältävä slab-malli.



Kuva 5.12: (100)-pinnan galliumterminoitu (1x1)-rekonstruktio.

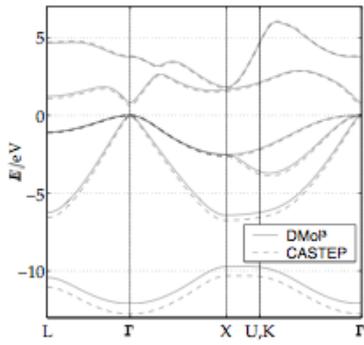


Kuva 5.8: (110)-pinnan relaksaatio.

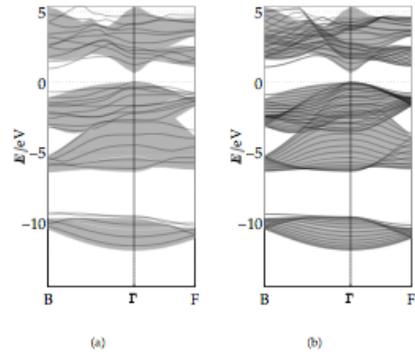
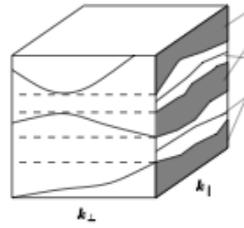


Kuva 5.13: (100)-pinnan arseeniterminoitu (2x2)-rekonstruktio.

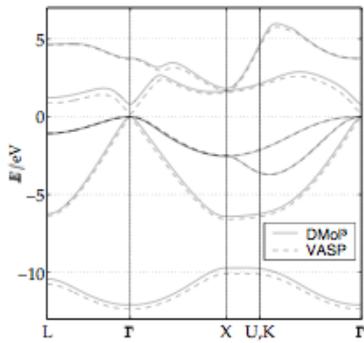
9.1. Surface effects on electronic states



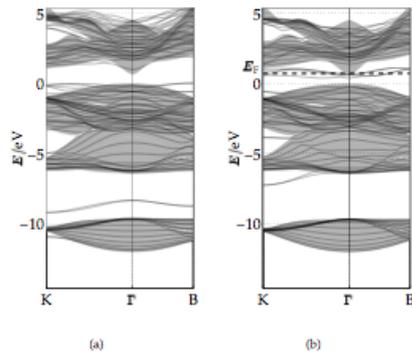
Kuva 5.3: CASTEP- ja DMol³-energiavyöt [Mäk03].



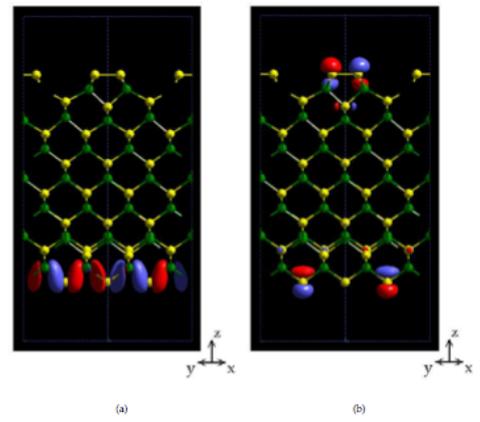
Kuva 5.10: (110)-pinnan energiavyöt ja bulk-tilojen projektioit. Slab-mallin paksuus (a) viisi atomitasa (b) 15 atomitasa.



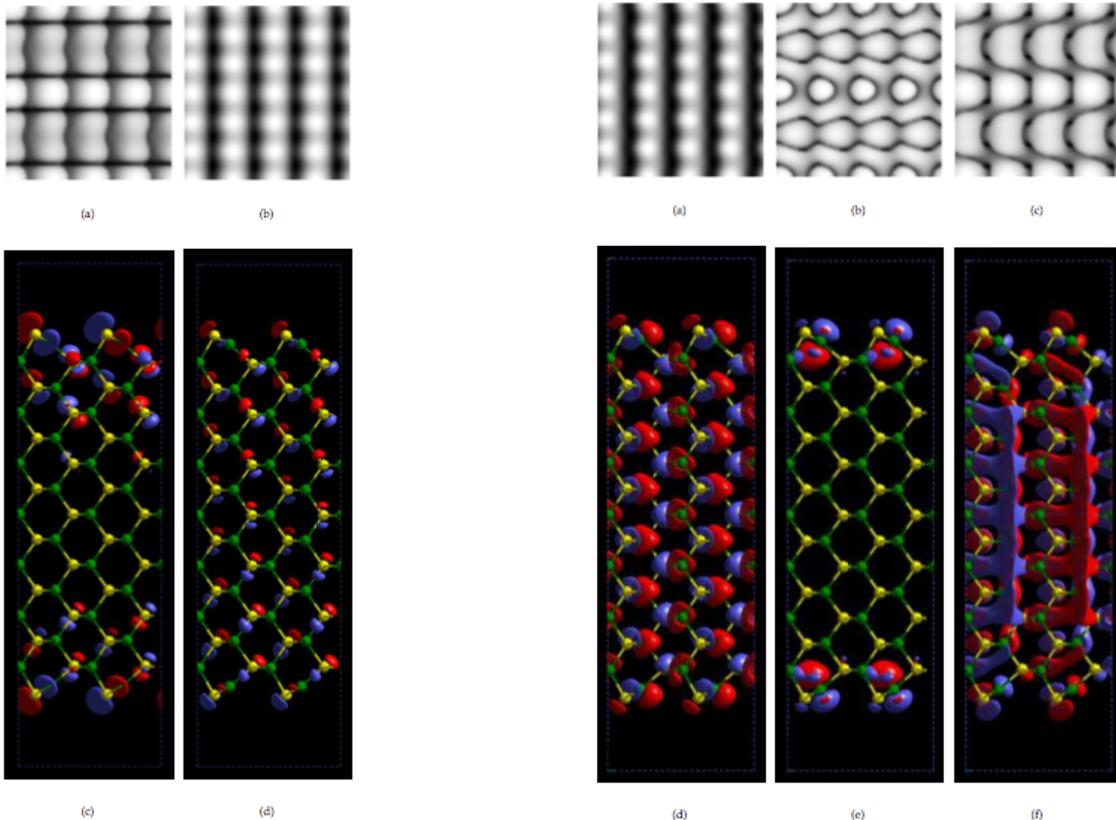
Kuva 5.4: VASP- ja DMol³-energiavyöt [Kom03].



Kuva 5.14: (100)-pinnan vyökaaviot. (a) Arseeniterminoitu (1x1)-rele tu (1x1)-rekonstruktio (c) Arseeniterminoidun (2x2)-rekonstruktio



Kuva 5.15: (100)-pinnan orbitaalit. (a) Ylin miehittetty. (b) Alin miehittämätön.



Kuva 6.3: (110)-pinnan miehittetyt tilat joilla on merkittävä kontribuutio STM-kuviin (a),(c) Dangling-bond -tila, energia -0,57 eV. (b),(d) Pintaresonanssitala, energia -0,15 eV.

Kuva 6.5: (110)-pinnan miehittämättömät tilat joilla on kontribuutiota STM-kuviin (a) Alin miehittämätön tila. (b) Dangling bond -tila, energia 0,6eV. (c) Resonanssitala, energia 1,05 eV. (d),(e),(f) Tilojen aaltofunktiot.