

Boltzmann Transportgleichung

Die Entwicklung von f_k als Funktion der Zeit aufgrund von Streuung, Diffusion und externen Feldern kann jetzt durch

$$\frac{df_k}{dt} = \frac{\partial f_k}{\partial t} \Big|_{\text{scatterings}}$$

Boltzmann Gleichung

beschrieben werden und die gesamte Ableitung durch

$$\frac{df_k}{dt} = \frac{\partial f_k}{\partial t} + \frac{\partial f_k}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial f_k}{\partial y} \frac{\partial y}{\partial t} + \frac{\partial f_k}{\partial z} \frac{\partial z}{\partial t} + \frac{\partial f_k}{\partial k_x} \frac{\partial k_x}{\partial t} + \frac{\partial f_k}{\partial k_y} \frac{\partial k_y}{\partial t} + \frac{\partial f_k}{\partial k_z} \frac{\partial k_z}{\partial t}$$

da

$$\mathbf{v} = \frac{\partial x}{\partial t} \mathbf{x} + \frac{\partial y}{\partial t} \mathbf{y} + \frac{\partial z}{\partial t} \mathbf{z} \text{ and } \frac{\partial k_x}{\partial t} \mathbf{k}_x + \frac{\partial k_y}{\partial t} \mathbf{k}_y + \frac{\partial k_z}{\partial t} \mathbf{k}_z = \frac{\mathcal{F}}{\hbar},$$

\mathbf{v} Geschwindigkeit, \mathcal{F} externe Kraft

und mit

$$\frac{\partial f_k}{\partial x} \mathbf{x} + \frac{\partial f_k}{\partial y} \mathbf{y} + \frac{\partial f_k}{\partial z} \mathbf{z} = \nabla_r f_k \text{ and } \frac{\partial f_k}{\partial k_x} \mathbf{k}_x + \frac{\partial f_k}{\partial k_y} \mathbf{k}_y + \frac{\partial f_k}{\partial k_z} \mathbf{k}_z = \nabla_k f_k,$$

erhalten wir

$$\frac{\partial f_k}{\partial t} + \mathbf{v} \cdot \nabla_r f_k + \frac{1}{\hbar} \mathcal{F} \cdot \nabla_k f_k - \frac{\partial f_k}{\partial t} \Big|_{\text{scattering}} = 0.$$

Boltzmann Transportgleichung

Der „Streuterm“ repräsentiert die Verteilungsfunktion aufgrund der Streuung zwischen den Elektronen und ihrer Umgebung

$$\frac{\partial f_k}{\partial t} \Big|_{\text{scattering}} = - \int [f_k(1 - f_{k'}) W_{k,k'} - f_{k'}(1 - f_k) W_{k',k}] dk',$$

Boltzmann Transportgleichung

$$\left. \frac{\partial f_k}{\partial t} \right|_{\text{scattering}} = - \int [f_k(1 - f_{k'})W_{k,k'} - f_{k'}(1 - f_k)W_{k',k}]dk',$$

Since the Boltzmann transport equation includes various nonequilibrium mechanisms, such as scattering, recombination, generation, drift, and diffusion, an exact solution for this equation is extremely difficult to obtain. Even approximate solutions require sophisticated numerical analyses, such as the Monte Carlo and drift-diffusion methods. One possible approximation is the relaxation time method, which assumes that the scattering term in Equation 5.110 can be replaced

$$\left. \frac{\partial f_k}{\partial t} \right|_{\text{collisions}} = - \frac{f_k - f_k^0}{\tau}, \quad \text{the relaxation time}$$

$$\frac{\partial f_k}{\partial t} + v \cdot \nabla_r f_k + \frac{1}{\hbar} \mathcal{F} \cdot \nabla_k f_k = - \frac{f_k - f_k^0}{\tau}.$$

in steady state, where $\frac{\partial f_k}{\partial t} = 0$,

$\frac{1}{\hbar} \nabla_k$ is simply $\frac{1}{m^*} \nabla_v$.

$$f_k = f_k^0 \left(1 - \frac{e\tau \mathcal{E}_x v_x}{k_B T} \right)$$

Geschwindigkeitsverteilungsfunktion im Gleich- und Nichtgleichgewicht

A plot of the nonequilibrium distribution function expressed in Equation 5.118 as a function of the drift velocity is shown in Fig. 5.19 for a free electron. For this plot, the temperature is assumed to be 300 K, the applied electric field is 5×10^5 V/cm, and the relaxation time (τ) is 0.4 ps.

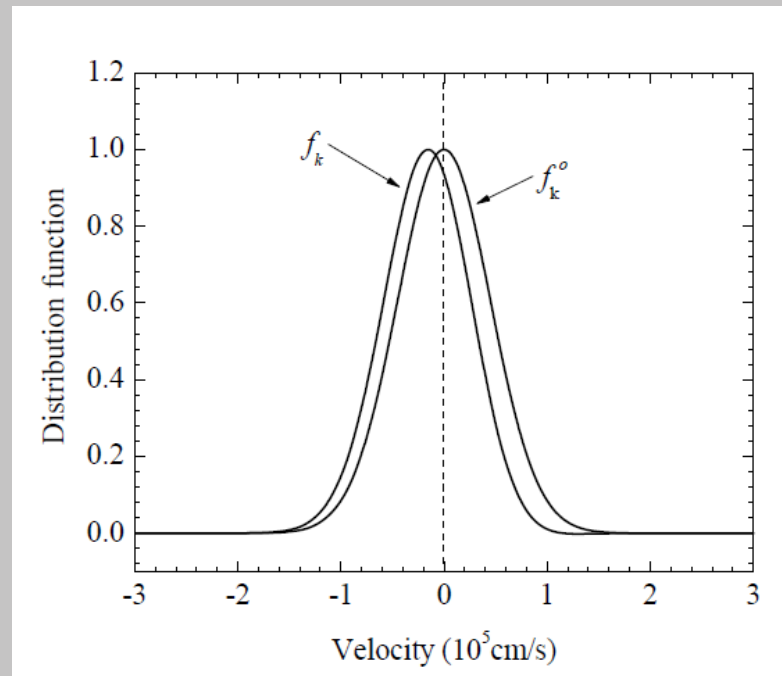


FIGURE 5.19 The distribution function plotted as a function of carrier velocity for equilibrium (f_k^0) and nonequilibrium (f_k) cases. Notice that the peak of f_k is shifted from $v_x = 0$.

Einfluss eines elektrischen Feldes auf die Verteilungsfunktion

The nonequilibrium distribution function can also be realized by shifting the wave vector \mathbf{k} by $e\tau\mathcal{E}/\hbar$. This can be accomplished by considering the distribution function for electrons in a parabolic band at equilibrium,

By setting the Fermi energy to zero, $E_k = \frac{\hbar^2 k^2}{2m}$, and by replacing \mathbf{k} with $\mathbf{k} - e\tau\mathcal{E}/\hbar$, one can obtain the distribution function for the nonequilibrium case as shown in Fig. 5.20. If the applied electric field is along the x -direction, the distribution will shift only for k_x . In equilibrium, there is a net cancellation between positive and negative momenta, but when an electric field is applied, there is a nonzero net shift in the electron momenta given by $\delta\mathbf{p} = \hbar\delta\mathbf{k} = -e\tau\mathcal{E}$.

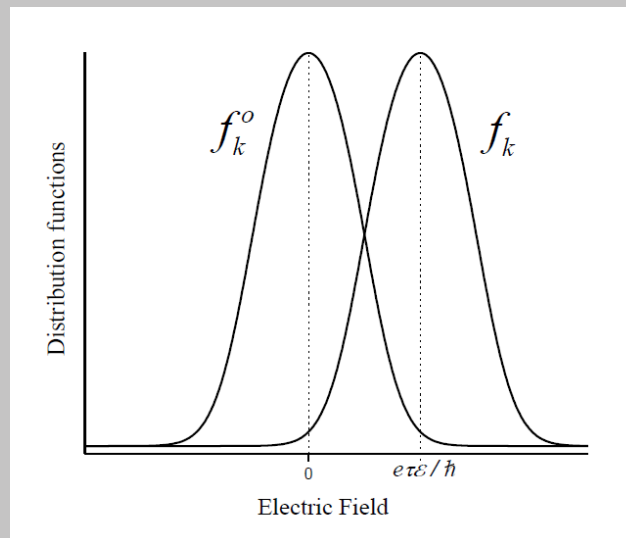


FIGURE 5.20 The displaced distribution function shows the effect of an applied electric field.

Herleitung der Transportkoeffizienten mit der BTG

The relaxation time depends on various scattering mechanisms. This relaxation time depends on the energy and mass of the scattered particles (e.g., electron) according to the following relation:

$$\tau = \tau_0 (m^*)^\alpha (E)^\beta,$$

where τ_0 is a constant and α and β are constants that characterize the scattering mechanism, which depend on the type of scattering mechanism. For example, $\alpha = 1/2$ and $\beta = 3/2$ for electron-ionized impurity scattering, while alloy scattering yields $\alpha = -1/2$ and $\beta = -3/2$.

$$m^* v = \hbar k$$

$$-v \cdot \nabla_r f_k + \frac{e}{m^*} (\mathcal{E} + v \times B) \cdot \nabla_v f_k = \frac{f_k - f_k^0}{\tau}.$$

$$f_k = f_k^0 - v \cdot Q(E) \frac{\partial f_k^0}{\partial E},$$

where $Q(E)$ is an unknown vector function that depends only on the energy of the electron (E).

Herleitung der Transportkoeffizienten mit der BTG

For the small perturbation case, in which $(f_k - f_k^0) < 1$,

To obtain a solution for $Q(E)$, let us assume that the applied electric field and temperature gradient lie in the x - y plane, while the magnetic field is applied along the z -direction. The x and y components of $Q(E)$ are

Hall

Seebeck

$$Q_x(E) = \frac{\tau \left(-e\mathcal{E}_x + \frac{(E_F - E)}{T} \frac{\partial T}{\partial x} \right) - \omega_c \tau^2 \left(-e\mathcal{E}_y + \frac{(E_F - E)}{T} \frac{\partial T}{\partial y} \right)}{1 + \omega_c^2 \tau^2}$$

$$Q_y(E) = \frac{\tau \left(-e\mathcal{E}_y + \frac{(E_F - E)}{T} \frac{\partial T}{\partial y} \right) + \omega_c \tau^2 \left(-e\mathcal{E}_x + \frac{(E_F - E)}{T} \frac{\partial T}{\partial x} \right)}{1 + \omega_c^2 \tau^2},$$

where ω_c is the cyclotron angular frequency (eB_z/m^*).

$$f_k = f_k^0 - \mathbf{v} \cdot \mathbf{Q}(E) \frac{\partial f_k^0}{\partial E},$$

Elektrische Leitfähigkeit und Beweglichkeit in n-type Halbleiter

$$J_x = -en v_x = -e \int_0^{\infty} v_x f(E) g^{3D}(E) dE,$$

$$f(E) = (f_k - f_k^0) = -v \cdot Q(E) \frac{\partial f_k^0}{\partial E},$$

$$g^{3D}(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E},$$

$$Q_x(E) = -\tau e \mathcal{E}_x \\ Q_y(E) = -\tau e \mathcal{E}_y.$$

$$J_x = -en v_x = e \int_0^{\infty} v_x^2 Q(E) \frac{\partial f_k^0}{\partial E} g^{3D}(E) dE = -e^2 \mathcal{E}_x \int_0^{\infty} \tau v_x^2 \frac{\partial f_k^0}{\partial E} g^{3D}(E) dE$$

$$v_x^2 = v_y^2 = v_z^2 = \frac{2E}{3m^*}$$

$$\frac{\partial f_k^0}{\partial E} = -\frac{f_k^0}{k_B T}$$

$$= \frac{2e^2 \mathcal{E}_x}{3m^* k_B T} \int_0^{\infty} \tau E g^{3D}(E) f_k^0 dE,$$

Leitfähigkeit und Hallkoeffizient

$$\frac{\partial f_k^0}{\partial E} = -\frac{f_k^0}{k_B T}$$

$$\sigma = \frac{J_x}{E_x} = \frac{2e^2}{3m^*k_B T} \int_0^\infty \tau E g^{3D}(E) f_k^0 dE = \frac{2ne^2}{3m^*k_B T n} \int_0^\infty \tau E g^{3D}(E) f_k^0 dE$$

$$E = \frac{3}{2} k_B T$$

$$n = \int_0^\infty g^{3D}(E) f_k^0 dE$$

$$= \frac{ne^2}{m^*} \frac{\int_0^\infty \tau E g^{3D}(E) f_k^0 dE}{\int_0^\infty \left(\frac{3k_B T}{2}\right) g^{3D}(E) f_k^0 dE} = \frac{ne^2}{m^*} \frac{\int_0^\infty \tau E^{3/2} f_k^0 dE}{\int_0^\infty E^{3/2} f_k^0 dE} = \frac{ne^2 \langle \tau \rangle}{m^*}$$

$$\langle \tau \rangle = \frac{\int_0^\infty \tau E^{3/2} f_k^0 dE}{\int_0^\infty E^{3/2} f_k^0 dE}$$

$$R_H = \frac{E_y}{J_x B_z} \Big|_{J_y=0} = -\left(\frac{3k_B T}{2e}\right) \frac{\int_0^\infty \tau^2 E g^{3D} F(E) f_k^0 dE}{\left[\int_0^\infty \tau E g^{3D} F(E) f_k^0 dE\right]^2} = -\frac{1}{en} \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2}$$

$$r = \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2}$$

Für einen Streuprozess

$$\tau(E) = \tau_0 E^\beta.$$

$$\langle \tau \rangle = \tau_0 \frac{\int_0^\infty E^{\beta+3/2} e^{-(E-E_F)/k_B T} dE}{\int_0^\infty E^{3/2} e^{-(E-E_F)/k_B T} dE} = \tau_0 (k_B T)^\beta \frac{\Gamma(\frac{5}{2} + \beta)}{\Gamma(\frac{5}{2})},$$

$$\sigma = \frac{ne^2 \tau_0}{m^*} (k_B T)^\beta \frac{\Gamma(\frac{5}{2} + \beta)}{\Gamma(\frac{5}{2})},$$

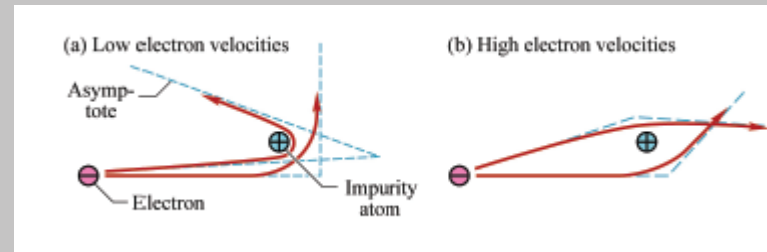
$$\mu_n = \frac{e \tau_0}{m^*} (k_B T)^\beta \frac{\Gamma(\frac{5}{2} + \beta)}{\Gamma(\frac{5}{2})}.$$

$$\mu_H = \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2} \mu,$$

$$R_H = \left. \frac{E_y}{J_x B_z} \right|_{J_y=0} = - \left(\frac{3k_B T}{2e} \right) \frac{\int_0^\infty \tau^2 E g^{3D} F(E) f_k^0 dE}{\left[\int_0^\infty \tau E g^{3D} F(E) f_k^0 dE \right]^2} = - \frac{1}{en} \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2}.$$

Hall factor, r , $r = \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2}.$

Streuung



$$\sigma_t = 2\pi \int_0^\pi \sigma(\theta') (1 - \cos \theta') \sin \theta' d\theta',$$

$$\sigma(\theta') = \frac{V^2 k'^2 |W_{k,k'}|^2}{(2\pi \hbar v_{k'})^2},$$

where V is the volume of the crystal, $W_{k,k'}$ is the transition matrix element for the particle that is scattered from state k to state k' , and $v_{k'}$ is the particle velocity in state k' . For elastic collisions, both momentum and energy are conserved, which means that $v_k = v_{k'}$ and $k = k'$. Derivations of the mobility and scattering

Streuung

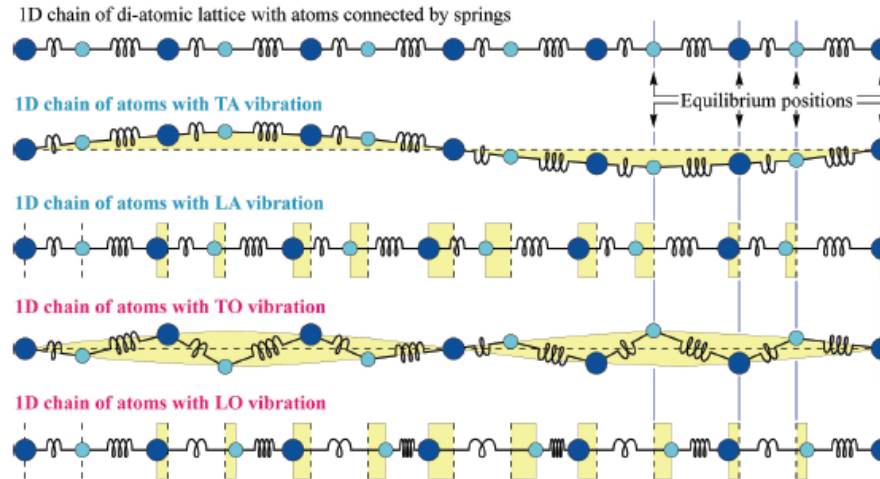


Fig. 19.6. Four vibrational modes of a one-dimensional di-atomic lattice, namely the transverse acoustical (TA), longitudinal acoustical (LA), transverse optical (TO), and longitudinal optical (LO) vibrational mode.

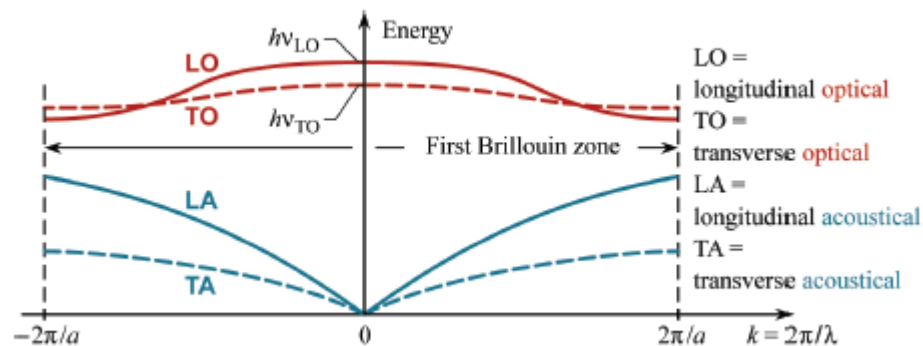


Fig. 19.7. Phonon dispersion relation in di-atomic lattice.

Streumechnismen (3-dim)

Scattering from an Ionized Impurity

$$\frac{1}{\tau_i} = \frac{e^4 N_i \ln \left[\frac{8m^* E \epsilon_0 k_B T}{\hbar^2 e^2 n'} \right]}{16\pi (2m^*)^{1/2} \epsilon^2 \epsilon_0^2 E^{3/2}}$$

$$\mu_i = \frac{e \langle \tau_i \rangle}{m^*} = \frac{64 \sqrt{\pi} \epsilon^2 \epsilon_0^2 (2k_B T)^{3/2}}{N_i e^3 (m^*)^{1/2} \ln \left[\frac{12m^* (k_B T)^2 \epsilon_0}{\hbar^2 e^2 n'} \right]}$$

Scattering from a Neutral Impurity

$$\frac{1}{\tau_{ni}} = \frac{80\pi \epsilon \epsilon_0 N_n \hbar^3}{m^{*2} e^2}$$

$$\mu_{ni} = \frac{e \tau_{ni}}{m^*} = \frac{m^* e^3}{80\pi \epsilon \epsilon_0 N_n \hbar^3}$$

Scattering from Acoustic Phonons: Deformation Potential

$$\tau_{dp} = \frac{\pi \hbar^4 C_1}{\sqrt{2} (m^*)^{3/2} k_B T E_1^2 E^{1/2}}$$

$$\mu_{dp} = \frac{e \langle \tau_{dp} \rangle}{m^*} = \frac{2\sqrt{2} \pi e \hbar^4 C_1}{3 (m^*)^{5/2} (k_B T)^{3/2} E_1^2}$$

$$C_1 = (C_{11} + C_{12} + C_{44})/2 = \rho v_s^2$$

Scattering from Acoustic Phonons: Piezoelectric Potential

$$\tau_{pz} = \frac{2\sqrt{2} \pi \hbar^2 \epsilon \epsilon_0}{e^2 (m^*)^{1/2} k_B T P^2 E^{1/2}}$$

$$\mu_{pz} = \frac{e \langle \tau_{pz} \rangle}{m^*} = \frac{2\sqrt{2} \pi \hbar^2 \epsilon \epsilon_0}{3 (m^*)^{3/2} e P^2 (k_B T)^{1/2}}$$

Optical Phonon Scattering: Polar and Nonpolar

$$\tau_{po} = \frac{2\sqrt{2} \pi \hbar^2 (e^{T_{po}/T} - 1) \chi(T_{po}/T) E^{1/2}}{e^2 (m^*)^{1/2} (k_B T_{po}) (\epsilon_\infty^{-1} - \epsilon^{-1}) \epsilon_0}$$

$$\mu_{pz} = \frac{e \langle \tau_{po} \rangle}{m^*} = \frac{2\sqrt{2} \pi \hbar^2 (e^{T_{po}/T} - 1)}{e (m^*)^{3/2} (k_B T_{po})^{1/2} (\epsilon_\infty^{-1} - \epsilon^{-1}) \epsilon_0}$$

$$\tau_{npo} = \frac{2\sqrt{2} \pi \rho \hbar^3 \omega_0}{D_0 (m^*)^{3/2} n_0 [\sqrt{E + \hbar \omega_0} + \mathcal{H}(E - \hbar \omega_0) (n_0 + 1) n_0^{-1} \sqrt{E - \hbar \omega_0}]}$$

$$n_0 = 1 / [\exp(\hbar \omega_0 / k_B T) - 1]$$

$$\mu_{npo} = \frac{2\sqrt{2} \pi \rho \hbar^4 \omega_0^2 e}{3 D_0^2 (m^*)^{5/2} (k_B T)^{3/2}} \quad \text{for } k_B T \gg \hbar \omega_0$$

$$\mu_{npo} = \frac{\pi \rho \hbar^4 e \sqrt{2} \hbar \omega_0}{D_0^2 (m^*)^{5/2} n_0} \quad \text{for } k_B T \ll \hbar \omega_0$$

Streumechnismen (3-dim)

Scattering from Short-Range Potentials

Scattering from Dislocations

the dislocation line is cylindrical with a radius R and length L .

$$\tau_{\text{dis}} = \frac{3}{8N_d R v}$$

$$\mu_{\text{dis}} = \frac{e(\tau_{\text{dis}})}{m^*} = \frac{3e}{8N_d R} \frac{1}{\sqrt{3m^*k_B T}} \cdot \frac{4\sqrt{2}}{3\sqrt{\pi}} \approx \frac{3e}{8N_d R} \frac{1}{\sqrt{3m^*k_B T}}$$

Scattering from δ -Function and Alloy Potentials

$$V = V_\delta E_\delta \delta(\mathbf{r} - \mathbf{r}_0)$$

$$\tau_\delta = \frac{\pi}{\sqrt{2}} \frac{\hbar^4}{N V_\delta^2 E_\delta^2 (m^*)^{3/2} E^{1/2}}$$

$$\mu_\delta = \frac{2\sqrt{2}\pi}{3} \frac{e\hbar^4}{N V_\delta^2 E_\delta^2 (m^*)^{5/2} (k_B T)^{1/2}}$$

$$N V_\delta^2 E_\delta^2 = V_c x(1-x) E_{AB}^2$$

$$\mu_{\text{al}} = \frac{2\sqrt{2}\pi}{3} \frac{e\hbar^4}{V_c E_{AB}^2 x(1-x) (m^*)^{5/2} (k_B T)^{1/2}}$$

Literatur: O. Manasreh „Introduction to nanomaterials and devices“
D.C. Look „Electrical characterization of GaAs materials and devices“

Scattering from Dipoles

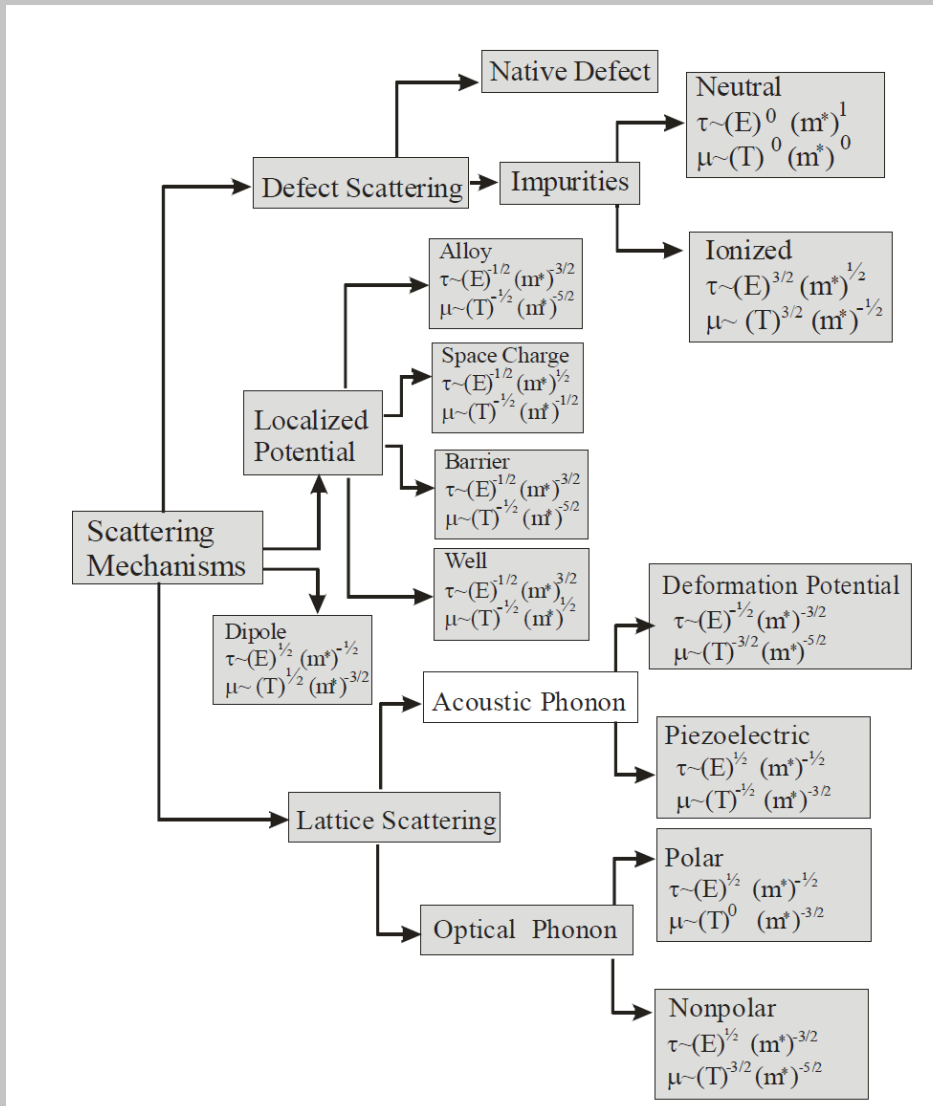
When acceptor and donor atoms in semiconductors are close together, they scatter electrons as a dipole instead of as individual monopoles.

$$\tau_{\text{dipole}} = \frac{2\sqrt{2}\pi 3\hbar^2 \epsilon_0^2 \epsilon^2 E^{1/2}}{(m^*)^{1/2} e^2 N q_d^2}$$

$$\mu_{\text{dipole}} = \frac{2^{9/2} \sqrt{\pi} \hbar^2 \epsilon_0^2 \epsilon^2 (k_B T)^{1/2}}{(m^*)^{3/2} e N q_d^2}$$

$$\mu_{\text{dipole}} = 3.57 \times 10^7 \frac{T^{1/2}}{\{l(\text{cm})\}^2 N(\text{cm}^{-3})} \text{ cm}^2/\text{V/s.}$$

Streumechnismen (3-dim)



$$\tau = \tau_0 (m^*)^\alpha (E)^\beta,$$

Streumechnismen (3-dim)

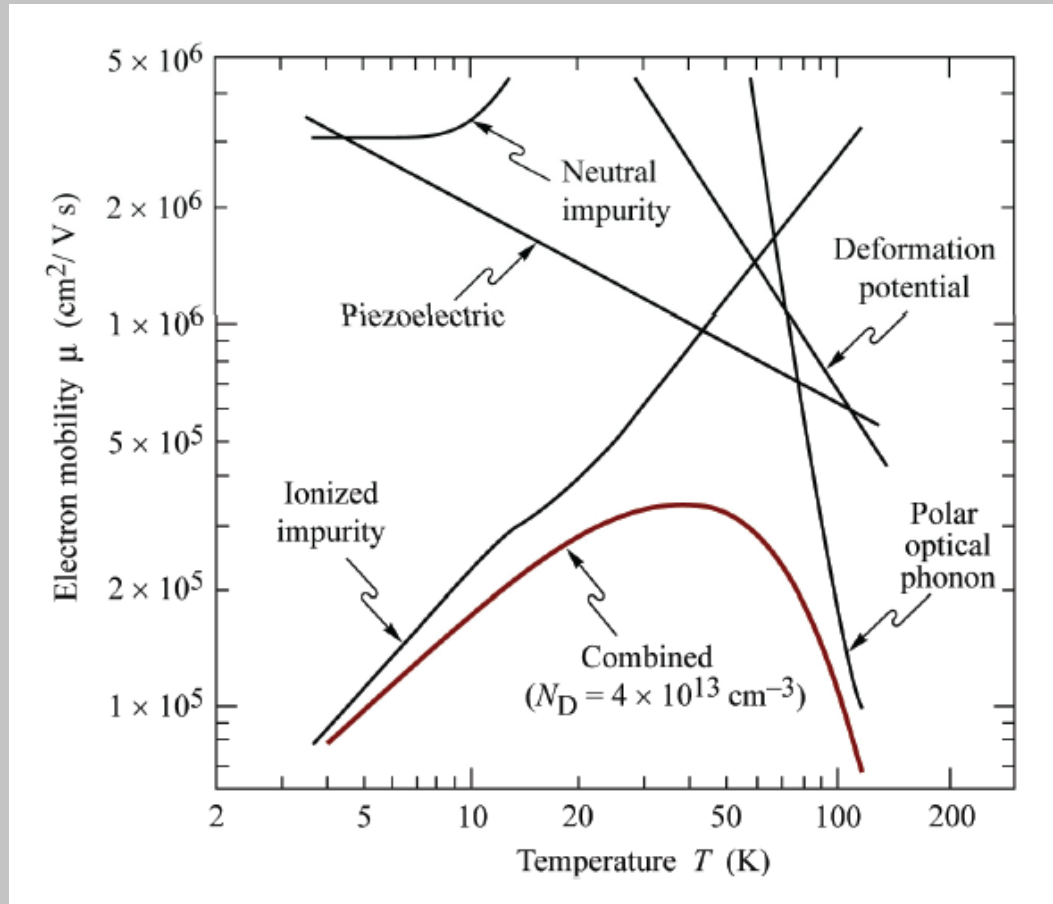


Fig. 19.9. Calculated electron mobilities due to different scattering mechanisms and combined mobility inferred from Matthiessen's rule in high purity GaAs ($N_D = 4 \times 10^{13} \text{ cm}^{-3}$) as a function of temperature (after Wolfe et al., 1970).

Matthiessen's rule

$$\frac{1}{\mu} = \frac{1}{\mu_{AC}} + \frac{1}{\mu_{OP}} + \frac{1}{\mu_{II}} + \frac{1}{\mu_{NI}} + \dots$$

$$\frac{1}{\mu} = \sum_i \frac{1}{\mu_i}$$

Streumechnismen (2-dim)

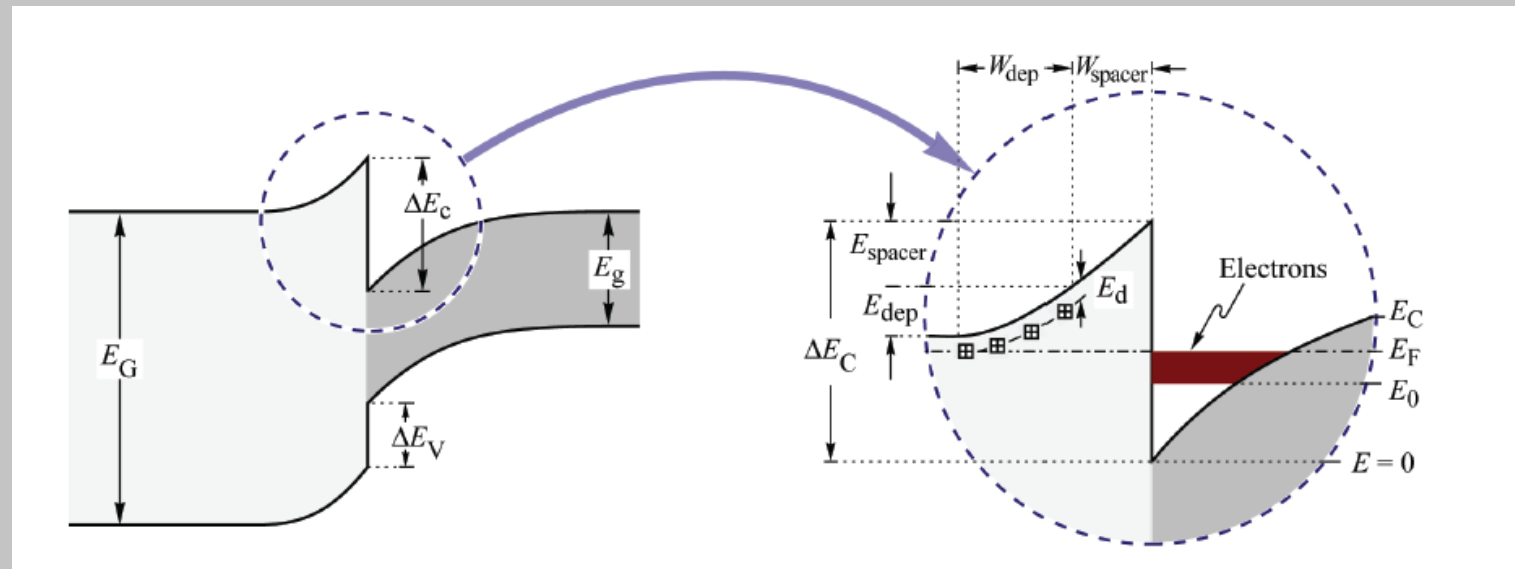
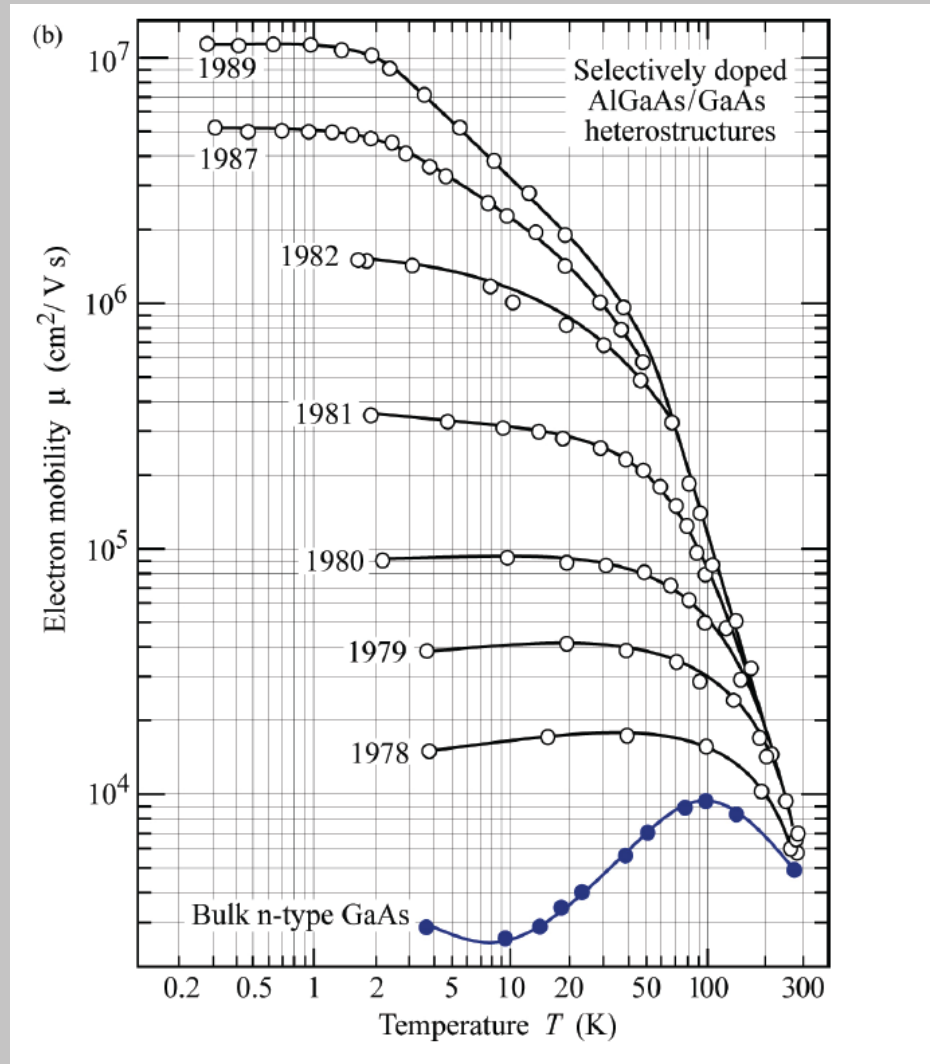
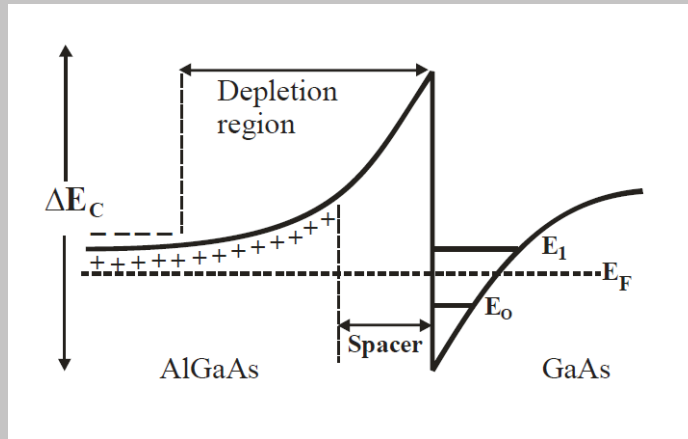


Fig. 20.4. Band diagram of a selectively doped heterostructure consisting of a doped wide-gap semiconductor and an undoped narrow-gap semiconductor. Due to the lower conduction band energy, electrons transfer from their parent donors to the narrow-gap semiconductor.

Stromechnismen (2-dim)



Streumechnismen und Einfluss des Spacers

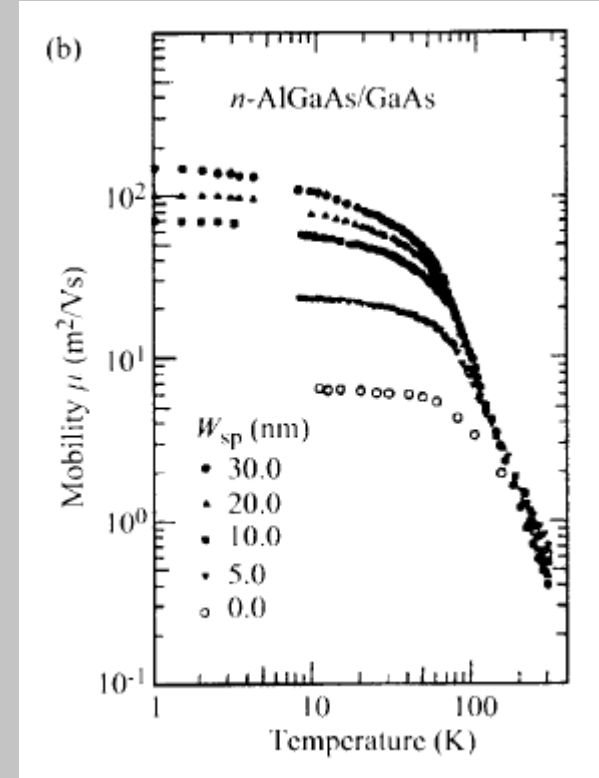
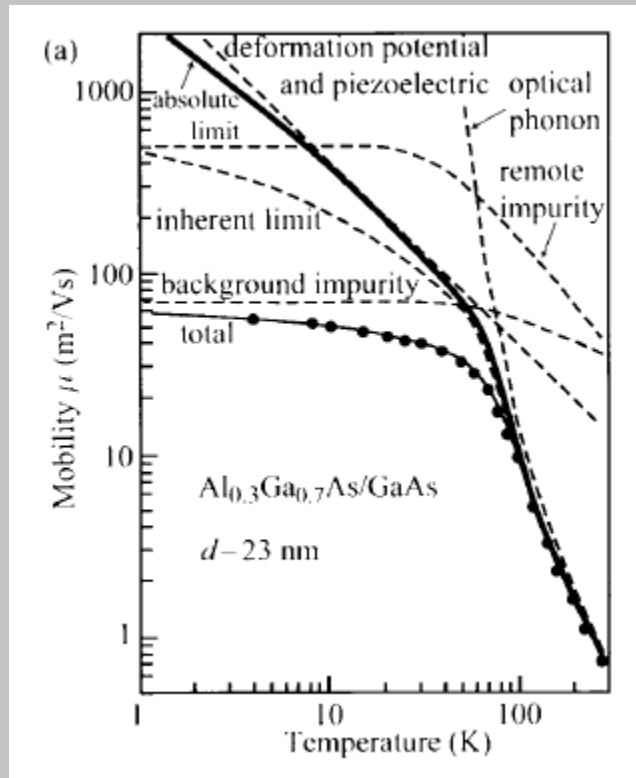
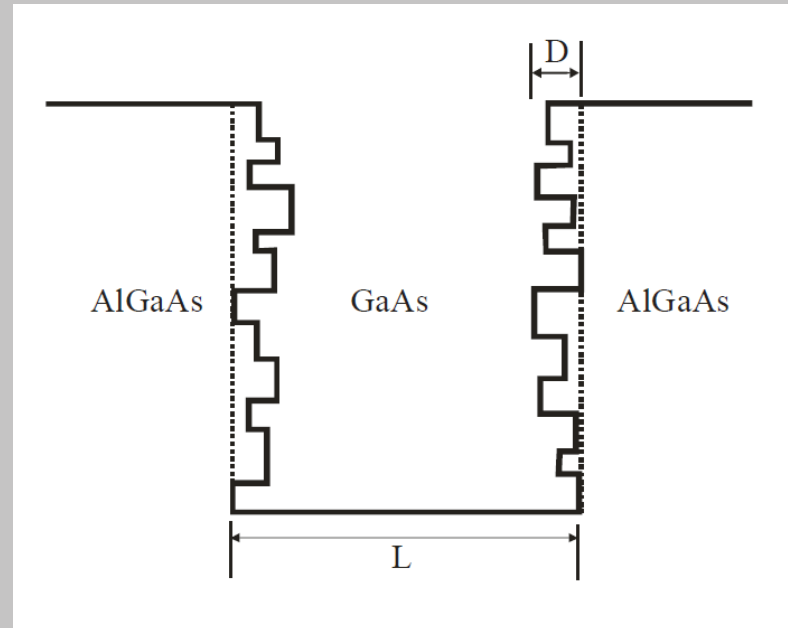


Fig. 10.20 (a) Influence of various scattering mechanisms on the mobility of a GaAs/AlGaAs heterostructure. (Reprinted with permission from Walukiewicz *et al.*, 1984. Copyright 1984 by the American Physical Society.) (b) Mobilities of electrons in modulation doped GaAs/AlGaAs heterostructures with varying spacer layer thickness W_{sp} . (Solomon *et al.*, 1984).

Streuung an Interface-Rauhigkeit



For a GaAs/AlGaAs quantum well numerical calculation, let us set $L = 125 \text{ \AA}$, $m^* = 0.067m_0$, $D/L = 0.03$, and $\lambda/L = 0.2$. For a carrier concentration of $10^{12}/\text{cm}^2$, the Fermi wave vector is $k_F = \sqrt{2\pi n_s} = 2.5 \times 10^6 \text{ cm}^{-1}$ and $\lambda k_F = 0.62$. For a screening length of $k_{sc} = 2/a^* = 2/100 \text{ \AA}$, we obtain $k_{sc}/k_F = 0.798$. Assuming that $\theta < 1$, we obtain for the integral an absolute value of 0.205. E_1 is obtained for the first subband as 35.99 meV. Substituting these values in Equation 5.177, we obtain $\tau_{p,1} = 3.97 \times 10^{-11} \text{ s}$. The mobility associated with this scattering time is seen to be $\mu_{p,1} \approx 1.04 \times 10^6 \text{ cm}^2/\text{V/s}$. If the 2π in the integral is dropped, the mobility reduces to $\mu_{p,1} \approx 1.7 \times 10^5 \text{ cm}^2/\text{V/s}$. Scattering from the interface roughness in quantum structures can dominate many scattering mechanisms at low temperatures.

Interface roughness

In Fig. 5.24, the interface roughness between GaAs and AlGaAs is presented as a variation of the well thickness. The ideal interfaces are shown as dotted lines in the figure. If the average fluctuation of the GaAs well is taken as D and the spatial correlation of the roughness is described by a correlation length, λ , the electron momentum relaxation time for an infinite quantum well is derived (Mitin *et al.*) as

$$(\tau_{p,n})^{-1} = \frac{4\pi m^* D^2 \lambda^2 E_n^2}{\hbar^3 L^2} \cdot \int_0^{2\pi} \frac{1}{2\pi} \frac{(1 - \cos \theta)}{\left[1 + \frac{k_{sc}}{2k_F} \sin \frac{\theta}{2}\right]^2} \exp\left\{-\lambda^2 k_F^2 \sin^2 \frac{\theta}{2}\right\} d\theta,$$

where L is the width of the quantum well, k_F is the Fermi wave vector, and k_{sc} has been defined previously as the screening length given as $k_{sc} = 2/a^*$, (where a^* is the bulk effective Bohr radius, which is $\sim 100 \text{ \AA}$ for GaAs), and E_n is the quantized energy levels, which are given as $E_n = \hbar^2 \pi^2 n^2 / (2m^* L^2)$ for $n = 1, 2, 3, \dots$. The relaxation time for the first subband ($n = 1$) can be written as

$$(\tau_{p,1})^{-1} = \frac{2\pi^3 D^2 \lambda^2 E_1}{\hbar L^4} \cdot \int_0^{2\pi} \frac{1}{2\pi} \frac{(1 - \cos \theta)}{\left[1 + \frac{k_{sc}}{2k_F} \sin \frac{\theta}{2}\right]^2} \exp\{-\lambda^2 k_F^2 \sin^2 \frac{\theta}{2}\} d\theta.$$