10. Electrical transport

Freely movable charges, resulting from the excitation of donor, acceptor, or valence states, carry electrical current whenever subjected to an external electrical field. The free carriers are electrons and/or holes. In weak fields, the current is proportional to the electric field intensity (Ohm's law).

Quasiclassical approximation

Assume a gas of non-interacting electrons in a static external field described by the potential Φ. The probability amplitude of finding a carrier at the location r obeys the time-dependent Schroedinger equation

$$\left[H_0 - e\Phi(\vec{r}) \right] \psi(\vec{r},t) = i\hbar \frac{\partial}{\partial t} \psi(\vec{r},t) \ ,$$

(10.1)

where H_0 is one-electron Hamiltonian of the crystal without the electric field. For smooth changes of the external electric field on distances of the order of lattice constant, the effective mass approximation can be used, in analogy with the description of impurity states. Without loss of generality, we will treat the states close to the conduction band minimum, having the isotropic dispersion

$$E_c(\vec{k}) = E_c(0) + \frac{\hbar^2 \left|\vec{k}\right|^2}{2m^*} \ .$$

(10.2)

Using the reasoning that led to Eq. (7.16) for the stationary envelopes of Wannier function, we obtain here the time-dependent equation

$$\left[-\frac{\hbar^2}{2m^*} \Delta_{\vec{R}} - e\Phi(\vec{R}) \right] C(\vec{R},t) = \left[i\hbar \frac{\partial}{\partial t} - E_c(0) \right] C(\vec{R},t) \ .$$

(10.3)

The position of a wavepacket is influenced by the external field, in the quasiclassical approximation, it obeys the Newton equation of motion for the quasiparticle of the effective mass m*. The external force is given by the gradient of the potential, and leads to a constant acceleration in the static case. Without a resistance against the acceleration, the (drift) velocity and electrical current would increase without limits. In agreement with observations, we add a "damping term", or "collision term", to the equation of motion, compensating the acceleration due to the external field. Thus, the position of our (quasi)electron obeys the following equation of motion,

$$ m^* \frac{d^2\vec{r}}{dt^2} + \frac{m^*}{\tau} \frac{d\vec{r}}{dt} = -e\vec{E} \ , \tag{10.4} $$

where E is the intensity of the electric field (i.e., the gradient of potential) and τ is the "relaxation time"; it represents the mean time interval, needed to refresh the zero value of the electron drift velocity by collisions with the rest of the crystal. The second term in the left-hand side of Eq. (10.4) is called "relaxation" or "damping". After ending transient phenomena, the charge carrier acquires a constant drift velocity v_d, appended to the thermal velocity. The condition of the stationary state is evidently vanishing acceleration, i.e., the value of the drift velocity equal to

$$ \vec{v}_d = \left\langle \frac{d\vec{r}}{dt} \right\rangle = -\frac{e\tau}{m^*} \vec{E} \ . \tag{10.5} $$

The drift velocity and acceleration of a wave packet can also be treated in the following way: the transfer of energy is quantified as the group velocity of the wave packet,

$$ v_g = \frac{d\omega(k)}{dk} = \frac{1}{\hbar} \frac{dE(k)}{dk} \ . \tag{10.6} $$

The force F acting during the time dt increases the energy of the wave packet by

$$ dE(k) = Fv_g dt = \hbar v_g dk \ , \quad F = \hbar \frac{dk}{dt} \ . \tag{10.7} $$

Consequently, the acceleration is

$$\frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d^2E}{dkdt} = \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}F = \frac{F}{m^*} \ ,$$

(10.8)

with the use of the quadratic dispersion of Eq. (10.2).

Current density, conductivity, mobility

The charge crossing a unit area per unit of time is called the current density, j; assuming the volume density of the carriers n, it is given by

$$\vec{j} = -ne\vec{v}_d = \frac{ne^2\tau}{m^*}\vec{E} \ .$$

(10.9)

Using the isotropic dispersion of Eq. (10.2), the proportionality factor between the current density and the electric field intensity is the scalar conductivity σ:

$$\vec{j} = \sigma\vec{E} \ , \quad \sigma = \frac{ne^2\tau}{m^*} \ .$$

(10.10)

In an anisotropic crystal, the directions of the current and field need not be the same; the conductivity is then represented by a matrix,

$$\vec{j} = \hat{\sigma}\vec{E} \ .$$

(10.11)

The conductivity is proportional to the square of the carrier charge (the current is proportional to the charge and velocity, which is also proportional to the charge via the force); consequently, the currents of carried by electrons and holes add up.

Since the carrier density in a semiconductor can depend strongly on temperature, a convenient quantity is the mobility μ:

$$\vec{v}_d = \mu \vec{E} \ . \tag{10.12}$$

The results shown above lead to the following relationship

$$\mu = \frac{e\tau}{m^*} \ . \tag{10.13}$$

The values of electron (e) and hole (h) mobility are typically different, leading to the total conductivity of

$$\sigma = e(n_e \mu_e + n_h \mu_h) \ . \tag{10.14}$$

Typical values of mobilities at room temperature are (in cm^2/Vs)

	electrons	holes
Si	1300	500
GaAs	8800	400

Boltzmann transport equation

The occupation probability of the band state of energy E_k in a crystal without external fields is given by the Fermi-Dirac statistics,

$$f_{\vec{k}}^{0} = \frac{1}{\exp\left(\dfrac{E_{\vec{k}} - E_F}{kT}\right) + 1} \quad,$$

(10.15)

where E_F is the Fermi energy (chemical potential). The presence of external field and scattering mechanisms changes the occupation probability; in a weak electric field (with a small intensity E), we retain only the linear term in the Taylor expansion of the change per unit time:

$$\left(\frac{df_{\vec{k}}}{dt}\right)_{\vec{E}} = \frac{df_{\vec{k}}^{0}}{dE_{\vec{k}}}\frac{dE_{\vec{k}}}{dt} = \frac{df_{\vec{k}}^{0}}{dE_{\vec{k}}}\left[\frac{d\vec{r}_{\vec{k}}}{dt} \cdot \left(-e\vec{E}\right)\right] = -\frac{df_{\vec{k}}^{0}}{dE_{\vec{k}}}\left(e\vec{v}_{\vec{k}} \cdot \vec{E}\right) \quad,$$

(10.16)

where v_k denotes the velocity of the wavepacket centered at r of the direct space and at the wave vector k in the reciprocal space.

After reaching a stationary situation, the probability of the occupation of one-electron states does not change in time; in the approximation of the relaxation time τ_k, we arrive to the following equality:

$$\frac{df_{\vec{k}}}{\tau_{\vec{k}}} = -\left(\frac{df_{\vec{k}}}{dt}\right)_{\vec{E}} \quad,$$

(10.17)

i.e.,

$$df_{\vec{k}} = \frac{df_{\vec{k}}^{0}}{dE_{\vec{k}}}e\tau_{\vec{k}}\left(\vec{v}_{\vec{k}} \cdot \vec{E}\right) \quad.$$

(10.18)

Using Eq. (10.15), we arrive at the following relation for the current density ("Ohm's law "):

$$\vec{j} = \int_{BZ} e\vec{v}_{\vec{k}} \left(f_{\vec{k}}^0 + df_{\vec{k}} \right) d^3\vec{k} = e^2 \int_{BZ} \tau_{\vec{k}} \vec{v}_{\vec{k}} \frac{df_{\vec{k}}^0}{dE_{\vec{k}}} \left(\vec{v}_{\vec{k}} \cdot \vec{E} \right) d^3\vec{k} \ . \tag{10.19}$$

We will proceed with using non-degenerate electro gas with the quadratic dispersion of Eq. (10.2); neglecting the unity in the denominator of the Fermi-Dirac statistics (10.15) leads to the classical Boltzmann statistics,

$$f_{\vec{k}}^0 = \exp\left(\frac{E_F - E_{\vec{k}}}{kT} \right) = \exp\left(\frac{E_F - E_c(0)}{kT} \right) \exp\left(-\frac{\hbar^2}{2m^* kT} \left(k_x^2 + k_y^2 + k_z^2 \right) \right) \ . \tag{10.20}$$

The dense set of allowed values of k will be treated as (quasi)continuum; the" Gaussian profile" of Eq. (10.20) has the following dispersion in all of the three directions of the reciprocal space,

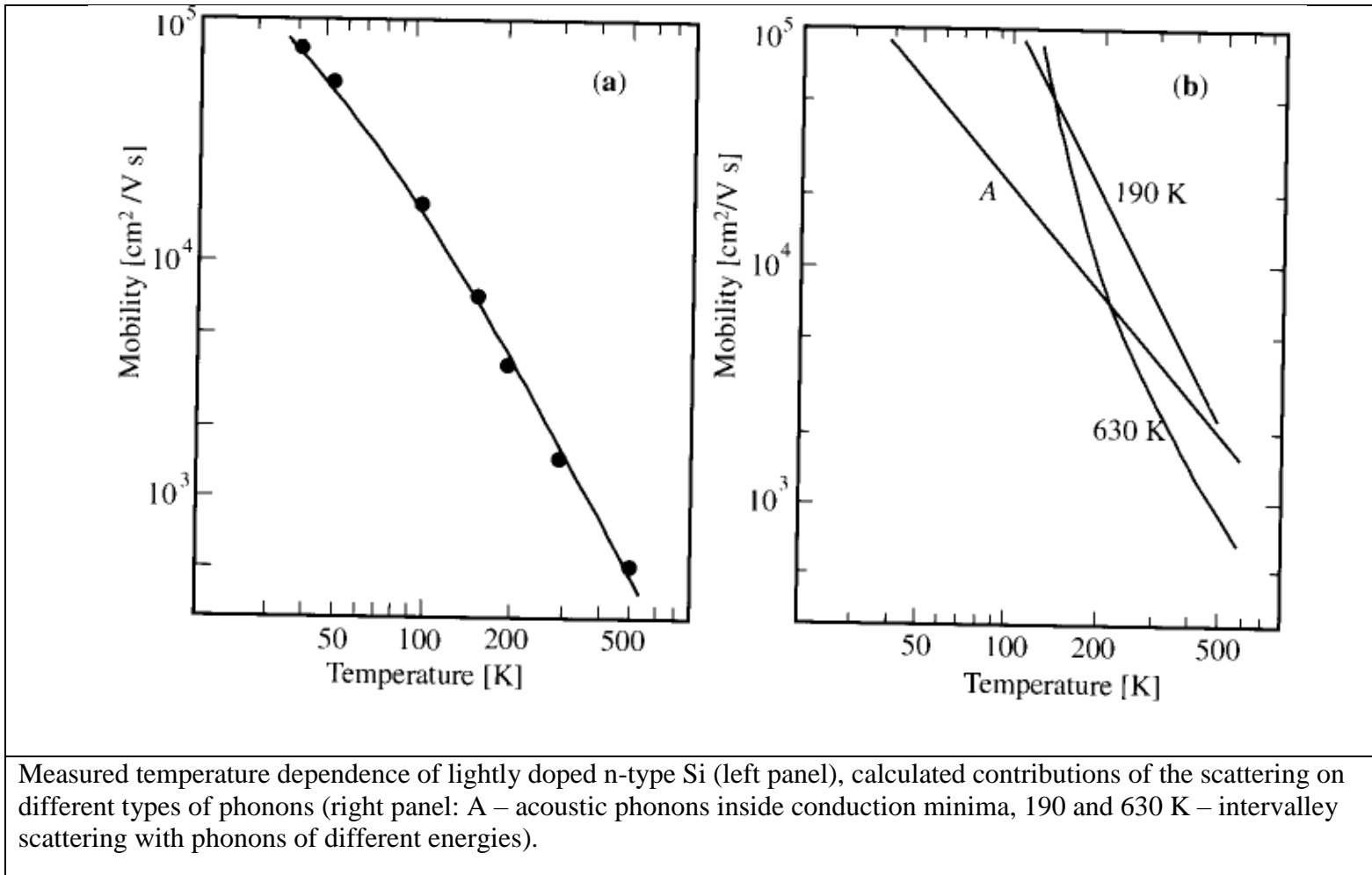$$D(k_x) = D(k_y) = D(k_z) = \frac{m^* kT}{\hbar^2} \ . \tag{10.21}$$

For isotropic dispersion relations, the directions of the electric field intensity, drift velocity, and current density coincide. The scalar conductivity can be found by performing the integration in Eq. (10.19), transferred to the integration over energy using the density of states. The latter (per unit volume, assuming the spin degeneracy) results from Eq. (2.18) as

$$\frac{D(E)}{V} = \frac{\left(2m^* \right)^{3/2}}{2\pi^2 \hbar^3} \sqrt{E - E_c} \ \text{ for } E > E_c. \tag{10.22}$$

Using this density of states in Eq. (10.19) provides the following formula for the scalar conductivity:

$$\sigma = \frac{e^2}{3\pi^2 m^* kT} \int_0^\infty \tau(E) v^2(E) D(E) dE \ .$$

(10.23)

We can therefore improve the predictions of conductivity by including specific energy-dependence of the involved scattering processes.

Measured temperature dependence of lightly doped n-type Si (left panel), calculated contributions of the scattering on different types of phonons (right panel: A – acoustic phonons inside conduction minima, 190 and 630 K – intervalley scattering with phonons of different energies).
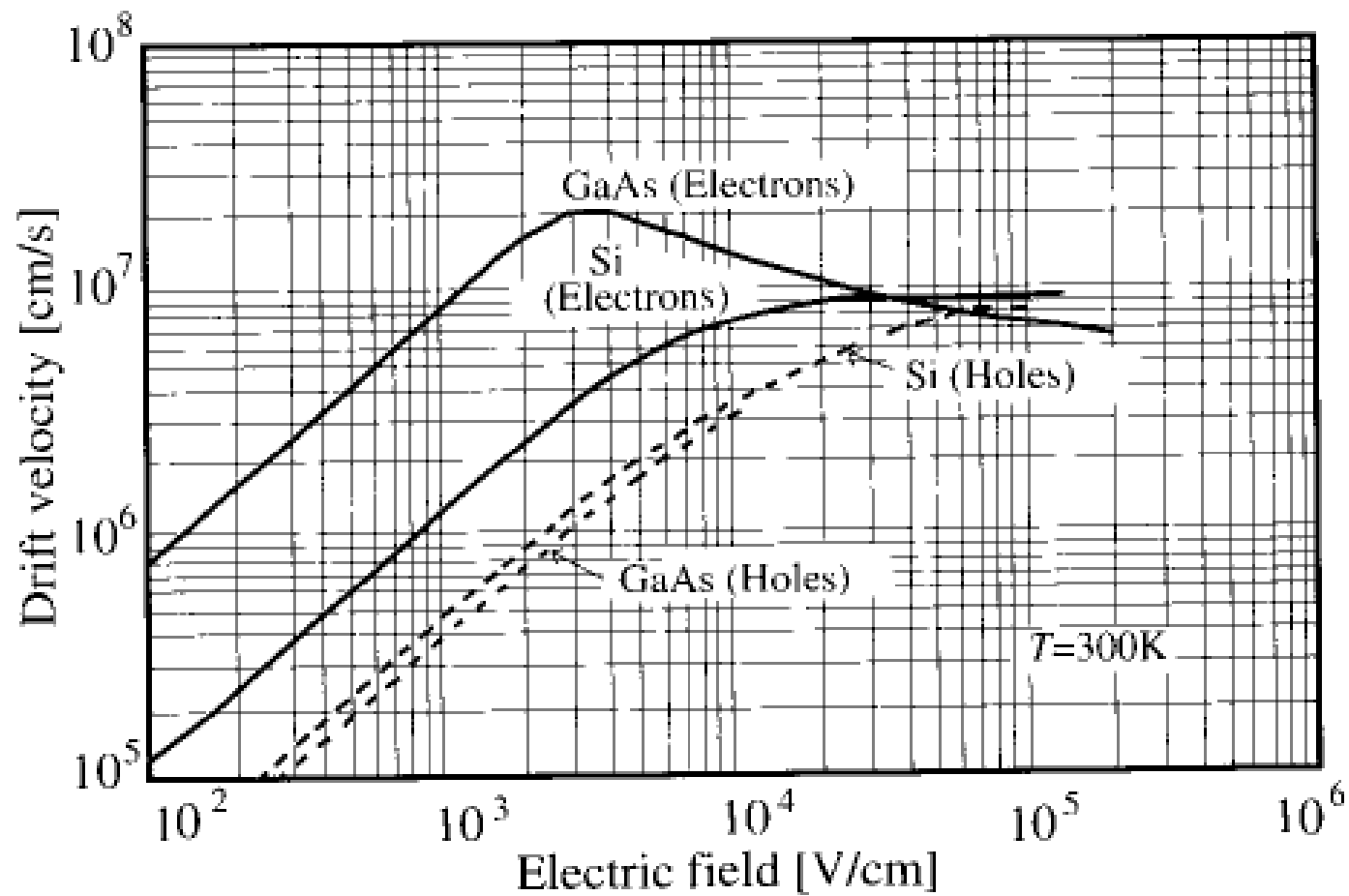
Note the substantial shortening of the scattering time in Eq. (10.13) with increasing temperature.
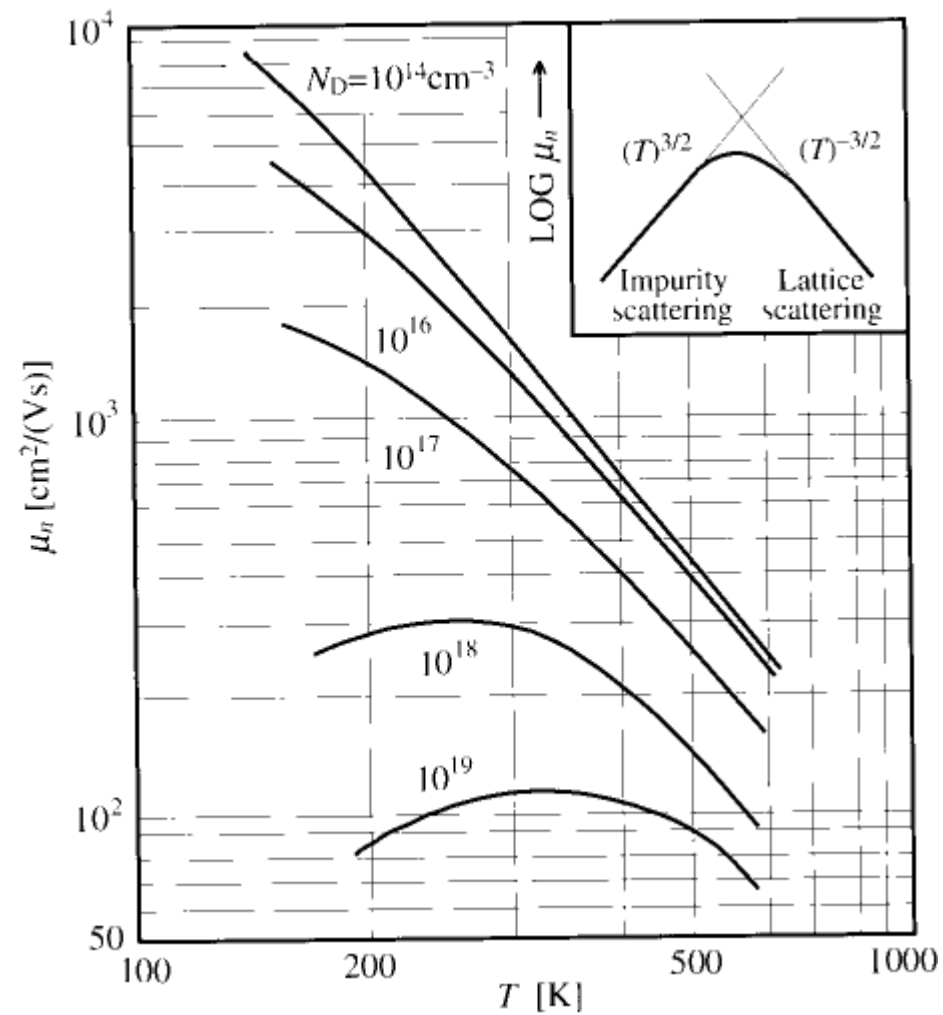
Temperature dependence of mobility of the n-type Si pro different donor concentrations.
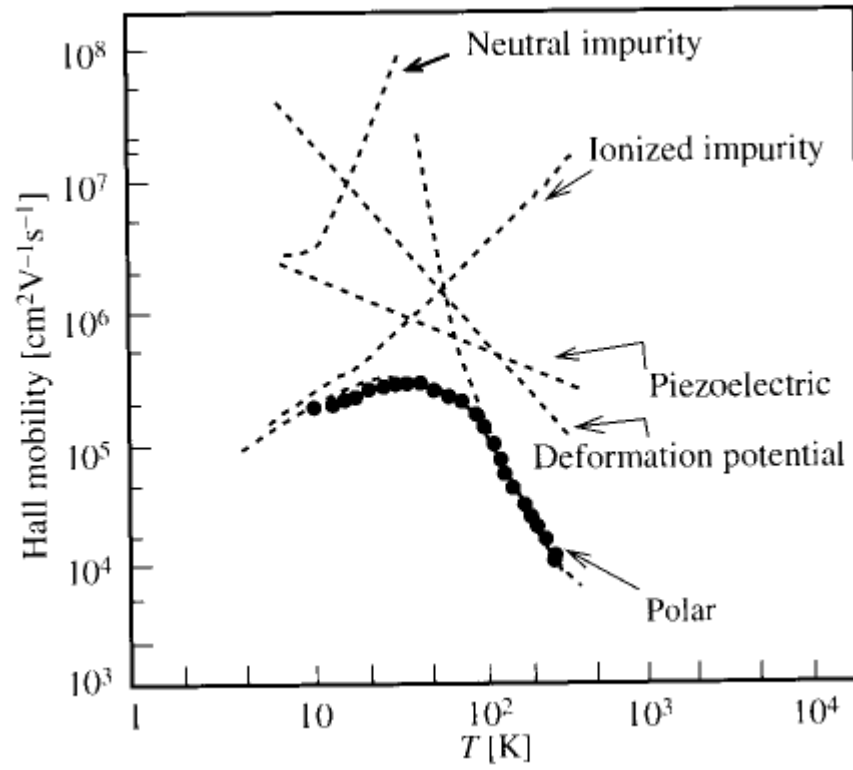
Temperature dependence of the mobility of n-type GaAs and contributions of different scattering mechanisms.

Drift velocity of electrons and holes in GaAs and Si vs. external electric field.

Metal-Insulator Transition (MIT) in heavily doped semiconductors

definition using the direct-current (dc) conductivity:

$$\sigma(T) > 0 \quad \text{for} \ \ T \to 0 \ ... \ \text{metal,}$$
$$\sigma(0) = 0 \qquad\qquad\quad ... \ \text{insulator.}$$

(10.24)

Examples of Si:P, from Loehneysen 1998
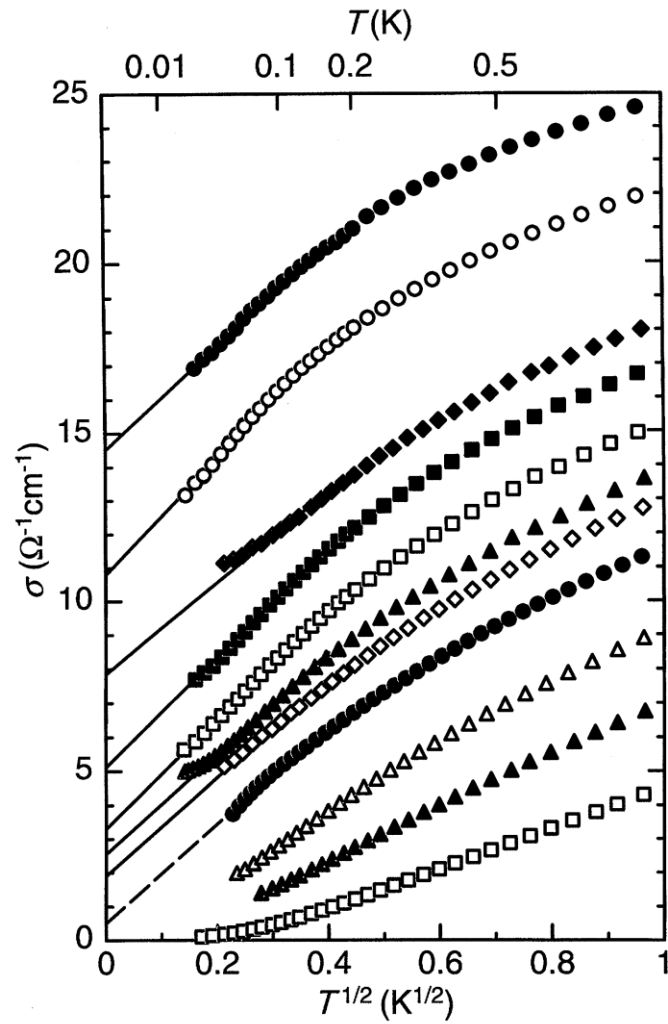
Figure 1. Electrical conductivity σ versus $\sqrt{T}$ of Si:P close to the MIT. P concentrations (in 10^{18} cm^{-3}) are from top to bottom: 3.69, 3.67, 3.63, 3.60, 3.58, 3.56, 3.55, 3.52, 3.50, 3.45, 3.38 (after Stupp *et al.* 1993).
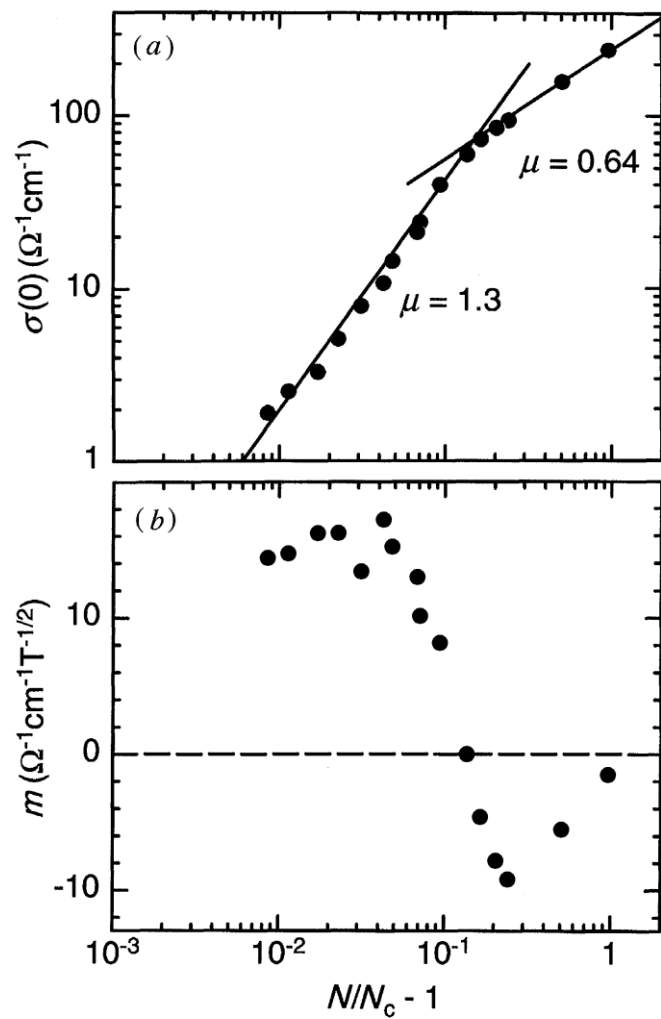
Figure 2. (a) $\sigma(0) = \sigma(T \to 0)$ and (b) $m = \mathrm{d}\sigma/\mathrm{d}\sqrt{T}$ versus reduced concentration $N/N_c - 1$, with $N_c = 3.52 \times 10^{18} \mathrm{cm}^{-3}$ (after Stupp *et al.* 1993).

Electron mobility in graphene

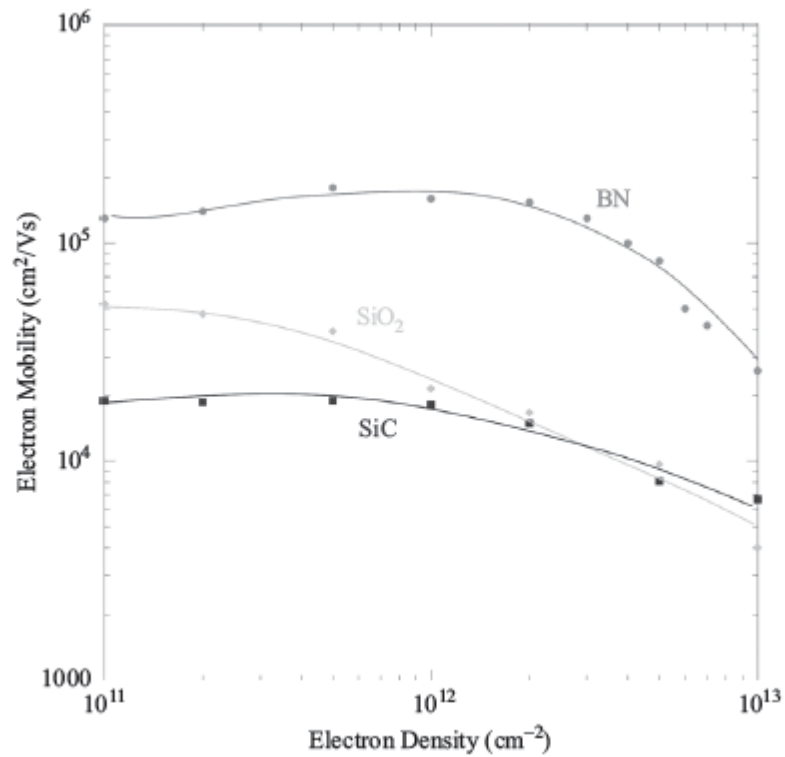depends on substrate (from Ferry2013)

Figure 5.1. The 300 K mobility in graphene, on several different substrates, as a function of the electron density.