Optically detected cyclotron resonance investigations on 4*H* and 6*H* SiC: Band-structure and transport properties

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We present experimental data on the band-structure and high-mobility transport properties of 6*H* and 4*H*-SiC epitaxial films based on optically detected cyclotron resonance investigations. From the orientational dependence of the electron effective mass in 6*H*-SiC we obtain direct evidence for the camels back nature of the conduction band between the *M* and *L* points. The broadening of the resonance signal in 4*H*-SiC as a function of temperature is used to extract information on electron mobilities and to conclude on the role of the different scattering mechanisms. Under high microwave powers an enhancement of the electron effective mass is found which is explained by a coupling of the electrons with longitudinal optical phonons.

I. INTRODUCTION

We have recently reviewed on the cyclotron resonance (CR) determination of the electron effective masses in the three polytypes of SiC, 3*C*, 4*H*, and 6*H*.[1] For 3C SiC, CR experiments using far infrared radiation have been successfully demonstrated and allowed for a precise description of the conduction band minima at the *X* point.[2] Acoustic phonon scattering was the dominant electron scattering mechanism in the temperature range between 40 and 300 K.[3,4] Such data are still not available for the other two important polytypes, i.e., 4*H* and 6*H* SiC. While it was possible to resolve the complete anisotropy in the effective mass tensor of 4*H*,[5] for 6*H* only the anisotropy of the electron effective mass at two extremes, parallel and perpendicular to the ⟨0001⟩ direction could be established.[6] The experimental findings are in general agreement with theoretical calculations,[7–9] although fine details in the conduction band of 6H such as a camels back structure have escaped experiments. We have since then extended the CR experiments and it is now possible to present experimental evidence for the camels back nature. Also from temperature dependent measurements we were able to conclude on the nature of the scattering mechanisms at low temperatures. As in our recent experiments we used the optical detection of cyclotron resonance (ODCR). More details about the technique can be found in Refs. 10 and 11.

II. EXPERIMENTAL DETAILS

The 4*H*- and 6*H*-SiC epitaxial films were grown by the hotwall-chemical vapor deposition technique on off-axis substrates. The films were nominally undoped and *n* type with free carrier-densities between 2 and $5\times10^{14}\,\mathrm{cm}^{-3}$ and Hall mobilities around 1000 cm^2/Vs at room temperature. The sample thickness was 93 μm for the 4*H*-SiC film and varied from 15–35 μm for the 6*H*-SiC films.

For the determination of the electron effective mass and the transport properties optically detected cyclotron resonance experiments were conducted at a microwave frequency of 36 GHz. The sample was placed in the center of a cylindrical TE_{011} microwave cavity and immersed in superfluid helium at a temperature of $T=1.6$ K. A superconducting split coil magnet provided magnetic fields up to 4 Tesla. Excitation of the photoluminescence occurred with a HeCd laser at a wavelength of 325 nm (above band gap) and a power of $P=10$ mW. With an absorption coefficient of $\alpha=1200\,\mathrm{cm}^{-1}$ the average penetration depth of the laser was around 8 μm and only the luminescence of the film was excited.

For the detection of ODCR the microwave field was amplitude modulated and synchronous changes in the photoluminescence (PL) intensity were phase sensitively recorded by a lock-in amplifier.

III. RESULTS AND DISCUSSION

A. Cyclotron resonance on 4*H*-SiC

Figure 1 shows the luminescence spectrum of the 6*H*-SiC epitaxial film. The sharp lines are in part due to neutral donor bound exciton recombinations and the corresponding phonon replicas as well as phonon replicas of the free excitons. The broad band which is dominating in the spectrum originates from a donor-acceptor (D-A) pair emission. The residual donors and acceptors are nitrogen and boron, respectively. For the ODCR measurements the D-A pair band was used as a monitor. ODCR spectra for two different orientations of the magnetic field with respect to the *c* axis of the sample are shown in Fig. 2. The ODCR effect was weaker than that in the case of 4*H*-SiC resulting in a lower signal-to-noise ratio. With the magnetic field parallel to the *c* axis [Fig. 2(a)] the resonance is centered at 0.6222 T. From the line position one

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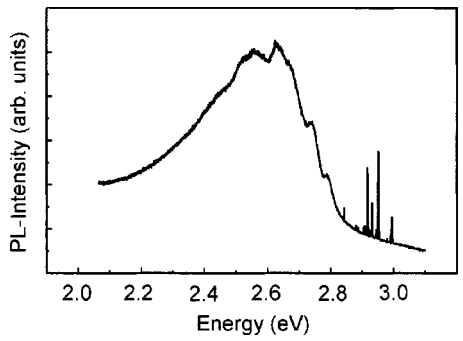

FIG. 1. Photoluminescence spectrum of the 6H-SiC sample at 1.6 K (by the HeCd laser excitation at 325 nm, $P=10$ mW).

calculates an effective mass in the basal plane of $m^*_{M\text{-}K}=0.485m_0$. From an analysis of the CR linewidth the scattering time τ was determined to be 5.3×10^{-11} s and hence the corresponding mobility $\mu=1.8\cdot10^5$ cm^2/Vs. As in the case of 4H-SiC one expects an anisotropic mass (tensorial mass) and therefore angular dependent measurements were performed with rotations of the magnetic field in the $(11\bar{2}0)$ and $(1\bar{1}00)$ planes. In both cases the resonance was only observable up to angles of 60° [see Fig. 2(b)] and its field position at this angle was within experimental error identical. This corresponds to spheroidal energy surfaces, which are oriented parallel to the c-axis. This result is in agreement with Raman experiments,[12] which indicate that the conduction band minimum is along the M-L direction. Similar conclusions have been derived from exciton spectroscopy.[13,14]

A complete angular dependence for a rotation in the $(1\bar{1}00)$ plane is shown in Fig. 3. For comparison the effective masses determined at 9 GHz for parallel and perpendicular orientations are shown in full circles.

In order to determine the mass parallel to c axis, $m^*_\parallel$, a fit to the data points was performed. Under the assumption of an isotropic mass within the basal plane the mass is given by

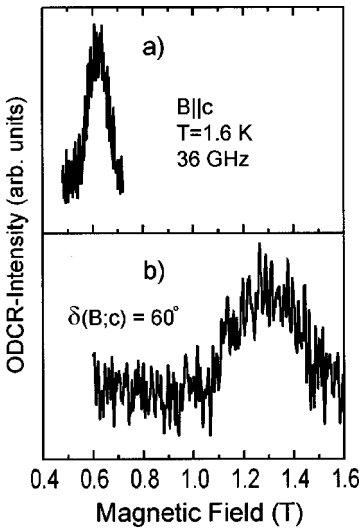

FIG. 2. Optically detected cyclotron resonance of 6H-SiC at 36 GHz and $T=1.6$ K for an orientation of the magnetic field parallel to the c axis (a) and for an angle 60 degrees between the c axis and the magnetic field (b).

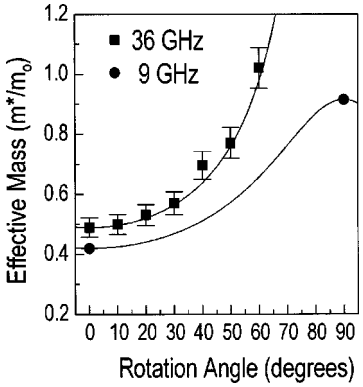

FIG. 3. Orientational dependence of the electron effective mass m^* in units of m_0 in 6H-SiC at $T=2$ K by rotating the sample in the $(1\bar{1}00)$ plane. The zero degree in angle corresponds to $\bar{B}\|\bar{C}$. The experimental data are given by full squares and circles, the drawn line is a fit using Eq. (1) and the values of Table I.

$$m^*=\left[\left(\frac{\cos^2\Theta}{m_\perp^{*2}}\right)+\left(\frac{\sin^2\Theta}{m_\perp^* m_\parallel^*}\right)\right]^{-1/2},$$

where Θ is the angle between the magnetic field B and the c axis. The resulting values are given in Table I. One notes that the perpendicular mass is about 15% higher for the 36 GHz measurements. Even more astonishing is that the parallel mass has an infinite value, but was 2 in the 9-GHz experiments.[6] In order to understand this surprising behavior we take a closer look to the band structure in the light of recent theoretical calculations (see also Fig. 4). Lambrecht and Segall[8] derived for the masses in the hexagonal plane two values $m^*_{M\Gamma}=0.77m_0$ and $m^*_{MK}=0.24m_0$. In the c direction the value m^*_{ML} is $1.42m_0$. The minimum of the conduction band is in the direction M to L midway between both symmetric points. This results in six equivalent energy ellipsoids. Through the three equivalent M-points two valleys are connected with a barrier of 9.5 meV in between, a ''camels back''-structure (see Fig. 4). For the cyclotron mass in the basal plane one hence obtains $m^*=\sqrt{m^*_{M\Gamma}\cdot m^*_{MK}}=0.429m_0$ in good agreement with the experimental result of Son *et al.*[6]

For the mass parallel to the c-axis the nonparabolicity of the conduction band plays a key role. Lambrecht and Segall[8] predicted that the mass will increase from 1.1 to 2.0 (maximum energy at the barrier height) depending on the electron energy. Similar results were obtained by Person and Lindfeldt.[9] According to their calculations the minimum of the conduction band is at 0.4 times the distance between the M and L point. The barrier height is 5.3 meV. For the masses see Table I.

With this information we are able to explain the results of Fig. 3. According to Son *et al.*[6] the ODCR measurements at 9 GHz were conducted with a microwave power of 100 mW. Depending on the quality factor of the resonator the microwave electric field can reach values up to 10^2 V/cm. With a scattering time of $\tau=10^{-11}$ s the carriers can gain 10 meV in energy which is close to the barrier height and the mass of $2.0m_0$ is in agreement with the theoretical values.

The ODCR measurement at 36 GHz used 200 mW (2×10^2 V/cm). The electron energy is approximately 40 meV using the τ of 5×10^{-11} s and a mass of $2m_0$. The

TABLE I. Effective electron masses in 6*H*-SiC from experiment and theory.

	Experimental values		Theoretical values		
Effective masses in units of m_0	Ref. 6 9 GHz	This work 36 GHz	Ref. 7	Ref. 8	Ref. 9
$m^*_{M\Gamma}=m^*_{\perp 1}$	0.42	0.485	0.77	0.51	0.81
$m^*_{MK}=m^*_{\perp 2}$	0.42	0.485	0.24	0.3	0.25
$m^*_{ML}=m^*_{\parallel}$	2.0	∞	1.42	0.71	2.07

energy would hence be four times higher than the barrier and an infinite mass would be plausible.

B. Scattering processes and hot electron effects

In contrast to conventional cyclotron resonance where the absorption of far infrared or microwave irradiation is detected, in ODCR intensity changes in the photoluminescence are measured. One essential question is, therefore, how the carriers interact on the optical recombination processes. Two different mechanisms have been discussed (i) impact ionization of shallow donors, bound excitons, or free excitons[10,15–17] and (ii) thermal effects,[18] where the energy of the carriers is transferred to the lattice. The latter changes the lattice temperature and thereby the luminescence intensity. Sometimes one can not distinguish between both processes since they depend on microwave power, temperature and the optical excitation power. For more details see Refs. 10, 15–18.

Also the resonance line shape is influenced by the experimental conditions. With increasing microwave power the resonance broadens and the $\omega\tau$-product decreases from 8 to 1.5 (see Fig. 5). In order to deduce the mobility from the resonance half width low microwave powers have to be used. An interesting effect occurs for microwave powers higher than 100 mW (see Fig. 5)—a dip in the resonance line. It will be explained by interaction of hot carriers with optical phonons (see below).

For the determination of the carrier mobility we performed temperature dependent ODCR measurements at 36 GHz at a microwave power of 10 mW. The scattering time deduced from the resonance halfwidth and the mobility calculated according to

$$\mu=\frac{e\tau}{m^*}. \tag{1}$$

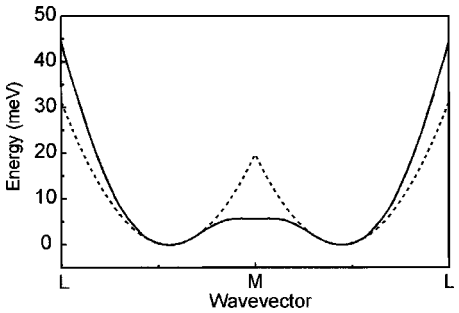

FIG. 4. Schematic energy dispersion near the conduction band minima in 6*H*-SiC along the *ML* direction with a camels back structure. The dashed line shows a parabolic approximation.

Here we determine only the mobility in the basal plane. We assume that Mathiesen's rule is valid

$$\frac{1}{\tau}=\sum_i \frac{1}{\tau_i} \tag{2}$$

and the total scattering time is the sum of the individual scattering processes.[19] The data are shown in Fig. 6 as full squares. In addition the value from Hall effect measurements[20] at room temperature is shown (full triangle). The mobility increases slightly up to a temperature of 9 K and then steadily decreases up to 22 K. Above 22 K the ODCR signal has vanished in the noise. This behavior can be described by three main scattering processes [see, e.g., Refs. 19 and 21]—scattering by impurities, where one has to distinguish between neutral and ionized impurities and scattering by acoustical phonons dominating at higher temperatures (see Fig. 6, dashed lines). In most semiconductors scattering by impurities is dominating at a low temperature. For the scattering by neutral impurities with a concentration N we have the following relation

$$\mu=\frac{e}{20a_B\hbar}\frac{m^*/m_0}{\varepsilon N}, \tag{3}$$

with the Bohr radius a_B and the dielectric constant ε.

For scattering by ionized impurities we used the relation from Brooks and Herring,[22] which gives good results for

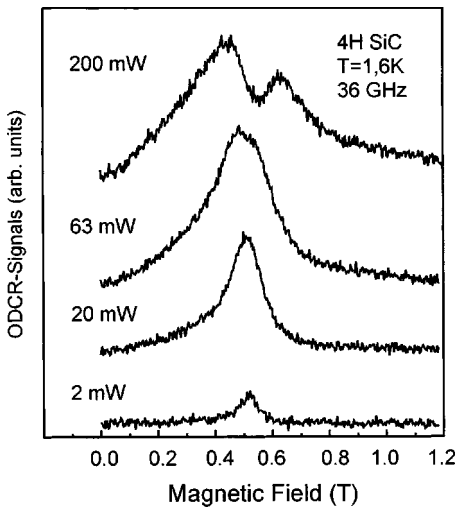

FIG. 5. Microwave power-dependent ODCR measurements of 4*H*-SiC (a) at microwave frequency of 36 GHZ. The magnetic field was parallel to the *c* axis.

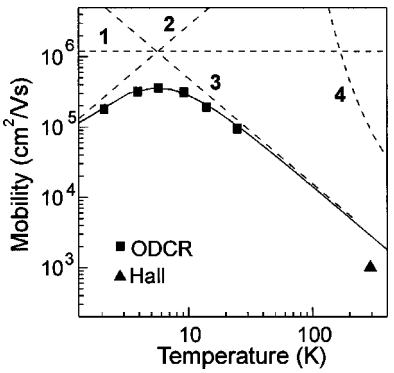

FIG. 6. Mobility in 4*H*-SiC as a function of temperature. Full squares are the data from ODCR, the triangle is from Hall effect measurements at room temperature. The dashed lines are calculated mobilities for scattering at neutral (1) and ionized (2) impurities, the influence of the acoustic deformation potential (3) and polar optical (4) scattering. The drawn line takes into account all four processes.

low-carrier densities and not too high-carrier velocities. If one assumes that the impurities concentration N_I is constant, we obtain for the mobility

$$\mu = \frac{2^{7/2}(4\pi\varepsilon\varepsilon_0)^2(k_BT)^{3/2}}{\pi^{3/2}Z^2e^3(m^*/m_0)^{1/2}N_I[\ln(1+\beta^2)-0{,}434\beta^2/(1+\beta^2)]}, \tag{4}$$

with

$$\beta = 2\frac{(m^*/m_0)}{\hbar}\left(\frac{2}{m^*/m_0}3k_BT\right)^{1/2}L_D$$

$$\text{and } L_D = \sqrt{\frac{k_BT\varepsilon\varepsilon_0}{e^2n}}.$$

N_1 is the total concentration of impurities in the crystal, L_D is the Debeye screening length with the parameter *n*, which gives the concentration of free carriers. All other symbols have their usual meanings. The scattering by acoustic phonons is given by

$$\mu = \frac{2\sqrt{2\pi}}{3}\frac{e\hbar^4c_l}{(m^*/m_0)^{5/2}(k_B)^{3/2}\varepsilon_{ac}^2}T^{-3/2}, \tag{5}$$

c_1 is the longitudinal elastic modulus, $6\times10^{12}\,\mathrm{dyn/cm^2}$ and $\varepsilon_{ac}=20\,\mathrm{eV}$ the deformation potential.

Polar optical scattering has been neglected. Due to the high Debye temperature of 1200 K it contributes only at temperatures above room temperature. Using the equations one is able to calculate the total mobility and fit it to the measured data. The necessary parameters which enter into the equations are only partly known for 4*H*-SiC. For the neutral impurity scattering the concentration of impurities enters. From the Hall effect measurements the donor concentration was determined to be $2\times10^{14}\,\mathrm{cm^{-3}}$, a possible compensation by acceptors was not considered. In order to reach the high mobility, the impurity concentration must be less than $5\times10^{14}\,\mathrm{cm^{-3}}$. It is difficult to estimate the contribution of ionized impurities, since the total number as well as the free carrier concentration has to be known. Free carriers are mainly generated by optical excitation. With a laser power of 10 mW and an average lifetime of $10^{-6}\,\mathrm{s}$ one calculates a concentration of $n=1\times10^{15}\,\mathrm{cm^{-3}}$.

Taking the number of ionized impurities as a free parameter one obtains a value of $1\times10^{13}\,\mathrm{cm^{-3}}$ from a fit to the data. This corresponds to an average distance between the scattering centers of approximately 300 nm. With a cyclotron radius $\sqrt{\hbar/eB}=35\,\mathrm{nm}$ only a fraction of the electrons would be scattered by ionized impurities. Nevertheless it is the dominating scattering process for $T<10\,\mathrm{K}$. For temperatures $T>15\,\mathrm{K}$ the mobility is determined by acoustic deformation potential scattering. Also the mobility at room temperature fits to this behavior. Due to the contacts and averaging over a whole sample the Hall mobilities are always lower than mobilities from cyclotron resonance.

If an electric field acts on free conduction electrons, the thermal equilibrium between the carriers and the lattice is disturbed. This is the case when the gain in energy through the external field is not completely transferred to the lattice. The energy distribution of the electrons is then described by an electron temperature T_e, which is higher than the lattice temperature. In general the momentum relaxation time τ depends on the carrier energy. The mobility is hence a function of the electron temperature T_e and depends on the applied field strength. For thermal electrons the scattering by the acoustic deformation potential is an elastic process. If carriers are accelerated in an external field one can distinguish two regions.[19] If the drift velocity of the carriers v_e is smaller than the speed of the sound u_l in the material ($v_e=\mu_0\mathbf{E}\ll u_l$) the mobility is

$$\mu = \frac{\mu_0}{\sqrt{1+\frac{3\pi}{32}\left(\frac{\mu_0\mathbf{E}}{u_l}\right)^2}}. \tag{6}$$

If $v_e=\mu_0\vec{E}\gg u_l$ holds, one obtains for the mobility:

$$\mu = \left(\frac{3\pi}{32}\right)^{1/4}\sqrt{\frac{\mu_0\mu_l}{\mathbf{E}}}. \tag{7}$$

This is the ''hot-electron'' case.

Carriers can also interact with optical phonons. In polar materials hot electrons can excite optical phonons. To do so they must gain sufficient energy in the electric field of the resonator to reach within the scattering time τ the energy of $\hbar\omega_{\mathrm{LO}}$ of an optical phonon.

$$\hbar\omega_{\mathrm{LO}} = \frac{e^2\mathbf{E}^2}{2m^*}\tau^2. \tag{8}$$

For a scattering time of $2\times10^{-11}\,\mathrm{s}$ and a phonon energy of 120 meV in SiC the field strength must be $\mathbf{E}=130\,\mathrm{V/cm}$.

The dependence of the mobility on the electric field is given by[23]

$$\mu = \frac{\sqrt{\frac{2\hbar\omega_{\mathrm{LO}}}{m^*}}}{\mathbf{E}}. \tag{9}$$

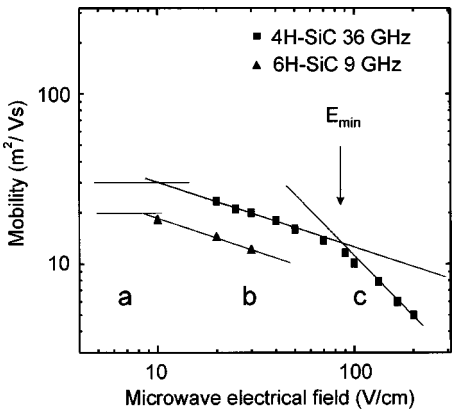

FIG. 7. Influence of the microwave electric field on the carrier mobility for 6*H*-SiC (full triangles) and 4*H*-SiC (full squares) at $T=1.6$ K (a, b, and c refer to different interaction mechanisms, for details see text).

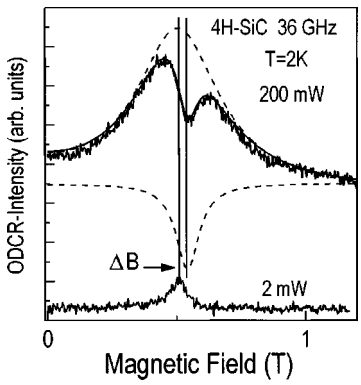

FIG. 8. ODCR measurements of 4*H*-SiC at microwave powers of 2 and 200 mW. The measurement at 200 mW is a superposition of two signals with different signs. Note the difference in magnetic field positions.

The field strength in the resonator is proportional to the square root of the applied microwave power. As can be seen in Fig. 5 with increasing microwave powers the half width of the cyclotron resonance increases, and hence the scattering time decreases. In Fig. 7, the mobility as a function of the microwave electric field is shown. There are three different regimes (a,b,c). For the region (a), where according to Eq. (6) one expects only a small decrease in the mobility ($\mathbf{E} \leqslant 10$ V/cm) no experimental data are available. ODCR could be observed starting from 1 mW corresponding to $\mathbf{E} = 20$ V/cm at 36 GHz and $\mathbf{E} = 10$ V/cm at 9 GHz. The velocity of the carriers is such that $v_e \gg u_l$. For the region (b) we find a slope of $-\frac{1}{2}$, which is expected according to Eqs. (6) and (7) $(1/\sqrt{\mathbf{E}})$. There is no difference for 6*H*-SiC and 4*H*-SiC.

For microwave powers above 140 V/cm the slope changes and it shows the behavior on the electric field from Eq. (9) $(1/\mathbf{E})$. This could be verified only for 4*H*-SiC, since in the 9-GHz resonator field strength above 100 V/cm could not be reached.

As mentioned above for microwave powers above 100 mW there is a dip in the resonance. It is caused by a second resonance, which is seen as a decrease in the luminescence intensity. It is slightly shifted to higher magnetic field as can be seen more clearly in Fig. 8. Here, we compare two ODCR signals at 2 and 200 mW. The measured curve at 200 mW can very well be accounted for by a superposition of two Lorentzian curves with different signs. The position of the negative signal is shifted by 0.03 T from the positive one. It means an increase in mass from $m^* = 0.425 m_0$ to $m^* = 0.45 m_0$. Its halfwidth amounts to $\frac{1}{4}$ and its area $\frac{1}{7}$ of the positive signal. A similar phenomenon was found in ZnSe (Ref. 24) and explained by coupling of electrons with LO phonons. When interacting with LO phonons of the lattice the electron must be treated as a polaron. Connected to it is an increase of the mass. The polaron mass m_p is

$$m_p = \approx (1 + \alpha/6) m^*. \tag{10}$$

With a coupling constant α of 0.3 the mass enhancement is approximately 5% as found experimentally. Other effects such as nonparabolicity of the conduction band have not been observed. This is in general agreement with band-structure calculations,[25] which predict a parabolic conduction band up to 200 meV above the bottom.

IV. SUMMARY

Photoluminescence and optically detected cyclotron resonance experiments have been performed on 4*H*- and 6*H*-SiC epitaxial films grown by the hotwall-chemical vapor deposition technique. From the ODCR experiments on 6*H*-SiC at 36 GHz we obtain direct evidence for the camels back nature of the conduction band. The minimum is located between the *M* and the *L* point. Our experimental findings are in agreement with theoretical predictions.[8,9,26] From temperature dependent ODCR experiments in 4*H*-SiC we extract information on electron mobility and on the contributions of different individual scattering processes to it. For temperatures $T > 15$ K the mobility is determined by acoustic deformation potential scattering, which also explains the mobility at room temperature. By a variation of the microwave power and films the microwave electric field the interaction of ''hot'' (nonthermal) electrons with the longitudinal optical phonon could be studied.

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