Determination of the electron effective-mass tensor in 4*H* SiC

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Experimental and theoretical results from studies of electron effective masses in 4*H* SiC are presented. Three principal values of the mass tensor are experimentally resolved by optical detection of cyclotron resonance, and are determined as $m(\mathrm{ML})=0.33\pm0.01m_0$, $m(\mathrm{M\Gamma})=0.58\pm0.01m_0$, and $m(\mathrm{MK})=0.31\pm0.01m_0$. These values are in good agreement with $m(\mathrm{ML})=0.31m_0$, $m(\mathrm{M\Gamma})=0.57m_0$, and $m(\mathrm{MK})=0.28m_0$, obtained from band-structure calculations based on the local density approximation to the density-functional theory using the linearized augmented plane-wave method. The conduction-band minimum is found to be at the *M* point of the Brillouin zone. [S0163-1829(96)03623-5]

With rapid developments of growth techniques, SiC has recently regained strong attention, owing not only to its potential technological importance for high-power, high-temperature, and high-frequency electronic devices, but also to its fascinating physical properties of polytypism. Differing in the stacking sequences of atomic layers, various SiC polytypes can be obtained ranging from zinc-blende structure of 3*C* SiC to different hexagonal crystal structures such as 6*H*, 4*H*, and 2*H* SiC. While the lowest band gap E_g of the most common SiC polytypes is known to be indirect, with E_g varying over a wide range for different polytypes, details about the band structures such as the position of the conduction-band minimum and effective-mass values near the band extrema are generally unknown. Such information is fundamental and crucial to the understanding of physical properties of the materials as well as to device modeling. Recently refined theoretical calculations on the band structures for several SiC polytypes have been performed.[1–4] The reliability of the approximations made in these calculations, however, awaits experimental examinations of the band-structure parameters. An exception can be seen in the calculations presented in Ref. 1, where the authors were aware of preliminary experimental results, which will be presented in detail in this paper. Cyclotron resonance (CR) has long been recognized as one of the most direct and accurate experimental tools for determination of effective masses m^* of carriers in semiconductors.[5] For a long period of time effective masses in the SiC polytypes have escaped a detailed study by CR due to a low carrier mobility μ (as a result of poor crystalline quality), since a successful CR requires $\omega\tau>1$. Here ω is the CR frequency and τ is the carrier scattering time, which enters the mobility in the relation $\mu=q\tau/m^*$. Only very recently high-quality SiC epilayers became available, which has made CR studies feasible. Electron effective masses and the physical properties near the conduction-band minimum in 3*C* SiC were obtained by a high-frequency CR technique,[6,7] where the high-frequency ω further facilitates achieving the CR conditions. The electron effective masses in 6*H* and 4*H* SiC were very recently determined by the optically detected CR (ODCR) technique.[8,9] ODCR fully exploits advantages of a much higher sensitivity due to the optical detection. Sensitive optical detectors in the visible and near infrared spectral range are largely available, so that CR can successfully be applied even for very thin SiC films. Furthermore, ODCR has the additional advantage of a much higher resolution, resulting from improved mobility due to photoneutralization of impurities.[10] However, these previous ODCR studies were not able to resolve and confirm the full anisotropy of the electron-mass tensors in 6*H* and 4*H* SiC, as predicted by theory,[1–4] due to a limited resolution. In this work, we report on a detailed ODCR study of the electron mass anisotropy in 4*H* SiC, taking advantages of a further improved resolution by optimizing experimental conditions. Three principal values of the mass tensor can now be resolved experimentally. These values are found to be in good agreement with our theoretically calculated values obtained from band-structure calculations based on the local density approximation (LDA) to the density functional theory, using the linearized augmented plane-wave (LAPW) method. The conduction-band minimum is shown to be at the *M* point of the Brillouin zone. A comparison of our results with other published theoretical calculations will also be given. The samples used were undoped 4*H* SiC epitaxial films grown on a (0001)-oriented 4*H* SiC substrate by the chemical vapor deposition technique. The *n*-type residual doping concentration is about 2×10^{14} cm^{-3}, and the thickness of the films is about 93 μm. The ODCR experiments were performed on a 36-GHz spectrometer, where the sample was immersed in superfluid helium at the center of a cylindrical TE_{011} microwave cavity. A magnetic field up to 4 T was supplied by a superconducting split coil magnet. Photoluminescence (PL) was excited by the 325-nm line of a HeCd laser (<10 mW) and was collected by a photomultiplier through a 1/4-m single grating monochromator. The change of PL intensity as a result of the amplitude-modulated microwave field was phase sensitively recorded by a lock-in amplifier, giving rise to the so-called ODCR signal. In Fig. 1 we display for easy reference the Brillouin zone of 4*H* SiC, where high symme-

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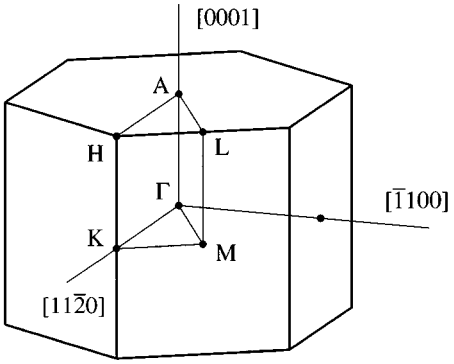

FIG. 1. The Brillouin zone of 4*H* SiC, with high symmetry points in *k* space and the directions corresponding to the three main crystallographic axes in real space.

try points in *k* space and the directions corresponding to the three main crystallographic axes in real space are indicated. In Fig. 2 we show ODCR spectra taken at 1.6 K when the magnetic field *B* is oriented along these axes of the 4*H* SiC lattice. They were obtained by monitoring a PL band at about 2.4 eV due to residual donor-acceptor pair recombination. The ODCR signal corresponds to an increase in the PL intensity by about 10 % at the highest microwave power available (200 mW). Such a high microwave power, however, considerably broadens the CR lines. To improve the resolution, the ODCR spectra such as those shown in Fig. 2 were typically taken at 20-dB attenuation of the microwave power. Since the PL band merely provides a medium for detecting CR without affecting the CR process itself, the details of the PL emission are beyond the scope of the present work and will not be discussed further.

As can be seen in Fig. 2(a), a single CR line was observed

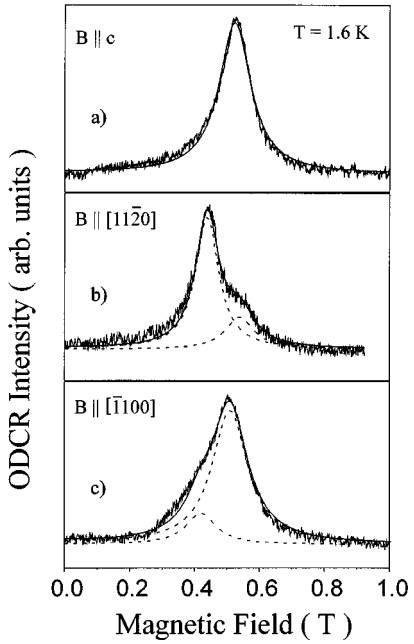

FIG. 2. ODCR spectra taken at 1.6 K when the magnetic field *B* is oriented along the three main crystallographic axes of 4*H* SiC lattice. The dashed curves represent deconvoluted CR lines and the solid curves sum up the deconvoluted CR lines.

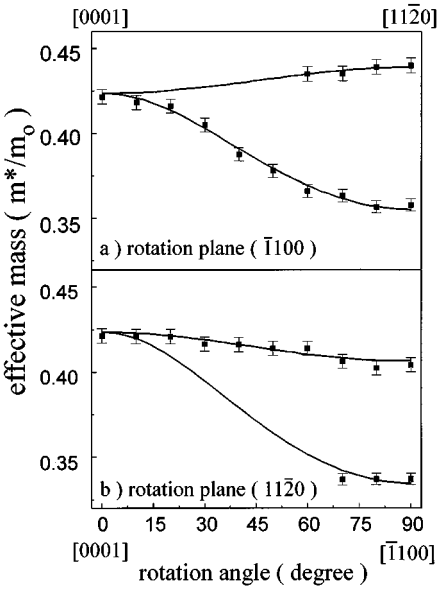

FIG. 3. Angular dependence of the ODCR spectra by rotating *B* (a) in the $(\bar{1}100)$ plane or (b) in the $(11\bar{2}0)$ plane. The experimental data are given by the full squares and the fitting curves by using Eq. (1) are shown by the drawn lines, taking into account all possible inequivalent electron valleys with respect to the magnetic field direction.

when *B* was along the [0001] direction (i.e., the *c* axis), giving rise to a combined electron effective mass in the basal plane $m^*(\Gamma\text{-}M\text{-}K)=0.425m_0$. The ODCR spectra shown in Figs. 2(b) and 2(c) obtained for the two crystallographic axes in the basal plane are quite different from Fig. 2(a), confirming the previously reported anisotropy of the electron mass parallel and perpendicular to the *c* axis.[9] Moreover, the ODCR spectrum taken when $B||[\bar{1}100]$ [Fig. 2(c)] clearly differs from that when $B||[11\bar{2}0]$ [Fig. 2(b)]. This provides unambiguous evidence on an additional anisotropy of the electron mass in the basal plane, which could not be revealed in the previous studies[9] due to a lower resolution. Two combined electron mass values can be obtained when $B||[\bar{1}100]$ and $B||[11\bar{2}0]$, with the aid of a deconvolution analysis of the ODCR spectra assuming a Lorenzian line shape. These two mass values arise from two sets of inequivalent orientation of the mass tensor from different electron valleys, with respect to the direction of *B*. To fully resolve the anisotropy of the mass, a detailed angular dependent study of the ODCR spectra was carried out by rotating *B* in the $(\bar{1}100)$ plane or in the $(11\bar{2}0)$ plane. The results are summarized in Fig. 3, and were analyzed by using a general expression for the cyclotron effective mass:

$$m^*=\left[\frac{m_1m_2m_3}{m_1H_1^2+m_2H_2^2+m_3H_3^2}\right]^{1/2}, \qquad (1)$$

where $H_{1,2,3}$ are the direction cosines of the magnetic field direction with the principal axes of the mass tensor. The three principal mass values are determined from a best fit to the experimental data as $m_3=m(ML)=0.33\pm0.01m_0$, $m_1=m(M\Gamma)=0.58\pm0.01m_0$, and $m_2=m(MK)=0.31\pm0.01m_0$. The principal directions of the mass tensor are indicated in Fig. 1. Even though these ODCR results are

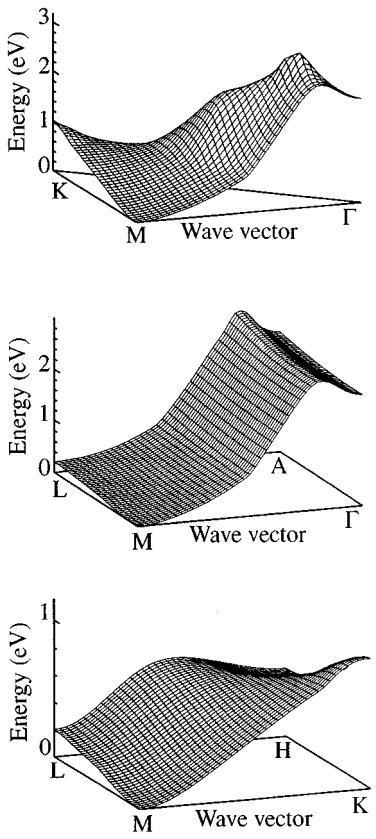

FIG. 4. Energy diagrams near the conduction-band minimum in three high symmetry planes in k space (see Fig. 1), which contain the M point.

consistent with a location of the conduction-band minimum to be at the M point, a precise determination cannot be achieved solely from the ODCR study. To give better insight of the location of the conduction-band minimum, we have performed a parallel theoretical investigation of the electron mass by band-structure calculations in 4H SiC. The calculations are based on the LDA to the density functional theory, using all-electron potentials, by the LAPW method. In Fig. 4 the energy band diagrams are shown in three high symmetry planes in k space (see Fig. 1), which contain the M point. It is clear that the conduction-band minimum is indeed at the M point. This is further confirmed by performing a close-up study of the energy band in the nearest vicinity of the M point, not only limited to the high symmetry planes. We failed to observe any possible small displacement of the band minimum from the M point. The calculated mass values at the M point are given in Table I, which are in a good agreement with the experimental results from this work. The two mass values obtained when $B||[\bar{1}100]$ and $B||[11\bar{2}0]$ [Figs. 2(b) and 2(c)] can now be attributed to two pairs of inequivalent electron valleys with respect to the magnetic field direction. When $B||[0001]$ [Fig. 2(a)], all three pairs of electron valleys are equivalent, resulting in a single CR peak as observed experimentally. Band-structure calculations, done by other groups,[1–4] confirm the position of the conduction-band minimum, even though results were only presented in the symmetry directions. It should also be pointed out that our calculated values of the electron effective masses agree with earlier calculations. In comparison with Refs. 1 and 3 the

TABLE I. A summary of the electron effective mass values obtained in this work from the ODCR experiments and our band-structure calculations.

The principal values of the electron mass tensor	From the ODCR experiments	From the band-structure calculations
$m(ML)$	$0.33\pm0.01m_0$	$0.31m_0$
$m(M\Gamma)$	$0.58\pm0.01m_0$	$0.57m_0$
$m(M\mathrm{K})$	$0.31\pm0.01m_0$	$0.28m_0$

deviations are at most 15%, whereas significant difference can be found from the results in Refs. 2 and 4. In the latter references it seems that, in view of the experimental results, the inclusion of quasiparticle corrections changes the results for the worse. The electron masses obtained in this work deviate considerably from those deduced from the analysis of the far-infrared absorption of the shallow N donors.[11] The latter is believed to suffer from a too simple model of the analysis, which is only strictly valid for cubic crystals. In fact good agreement was found in 3C SiC between the electron mass values from CR and from the analysis of the effective-mass donor transitions.[12] A more sophisticated theory is, however, required in the case of 4H SiC for a reliable analysis of the far-infrared absorption of the shallow N donors, based on the recently improved understanding of the band structure. The results from this work are in line with the results of Ref. 1 and are expected to contribute in resolving the controversy. The results can also explain the peculiarity in the anisotropy of the Hall mobility in 4H SiC,[13] where a higher electron mobility along the c axis than that in the basal plane (just opposite to the situation in 6H and 15 R SiC) can now be understood as being due to a smaller electron mass along the c axis as compared to the averaged in-plane mass. In conclusion, we have directly determined the electron effective mass tensor in 4H SiC by the ODCR technique. Three principal values of the mass tensor are experimentally resolved as $m(ML)=0.33\pm0.01m_0$, $m(M\Gamma)=0.58\pm0.01m_0$, and $m(MK)=0.31\pm0.01m_0$. Very good agreement has been found between the experimental results and the theoretical mass values $m(\mathrm{ML})=0.31m_0$, $m(\mathrm{M}\Gamma)=0.57m_0$, and $m(\mathrm{MK})=0.28m_0$ obtained from our band-structure calculations. A careful examination of the band-structure has led to the conclusion that the conduction-band minimum is at the M point of the Brillouin zone. The results from this work can account for peculiarities arising from the previously reported transport measurements and can contribute to a better understanding of the far-infrared absorption of the shallow donors in 4H SiC.

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