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Theoretical Models for the Electron Drift and Hall Mobility in N-Type 4H- and 6H-SiC

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For the successful development of a device simulator for SiC-based power and high temperature devices, it is crucial that we obtain a theoretical model that accurately describes the carrier mobility. The electron mobility in 4H- and 6H-SiC, the most widely used polytypes for device fabrication, depends strongly on the crystallographic direction of the traveling carriers due to the anisotropic structures of conduction bands, i. e., the device performance changes significantly depending on the configuration of the current channel. Recent Hall effect investigations have shown that the anisotropy of the Hall mobility can be as large as factor of 4.5 at room temperature. [1] While several experimental findings are available on the anisotropic conduction in hexagonal SiC polytypes [1-3], very little research has theoretically been done .

In this work we have constructed a theoretical model describing the drift and Hall mobility anisotropy in 4H- and 6H-SiC. The direction dependent effective masses have been estimated from the results of recent advanced band structure calculations. [4, 5] Although these band structure calculations predict rather complicated constant energy surfaces centered at M-points for 4H-SiC and 6H-SiC in the reciprocal space, we have assumed for both 4H- and 6H-SiC that there are six equivalent spheroidal constant energy surfaces centered exactly at M-points with each spheroidal having three different effective masses (m^*_l, m^*_{t1}, and m^*_{t2}) parallel to its three principle axes. The values of m^*_l, m^*_{t1}, and m^*_{t2} for 4H- and 6H-SiC are estimated from the parabolic fitting of the curvature of the conduction band minimum predicted by the theory. [4, 5] The values predicted in Ref. 4 agree especially well with the results of the recent ODCR measurements. [6]

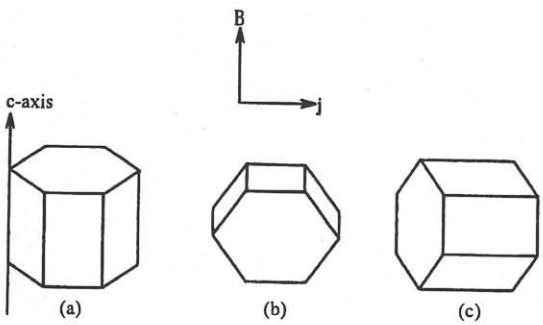

Fig. 1 Various configurations for the Hall measurements (a) [**j** ⊥ **c**, **B** // **c**], (b) [**j** ⊥ **c**, **B** ⊥ **c**], and (c) [**j** // **c**, **B** ⊥ **c**]

The electron Hall mobility for three distinct Hall measurement configurations has been calculated for 4H- and 6H-samples measured in Ref. 7 and 1, respectively. The three Hall geometries as shown in Fig.1 are (a) [**j** ⊥ **c**, **B** // **c**], (b) [**j** ⊥ **c**, **B** ⊥ **c**], and (c) [**j** // **c**, **B** ⊥ **c**] where **j** is the current direction, **B** is the magnetic field direction, and **c** is the direction of the c-axis of a hexagonal unit cell. The scattering mechanisms included in the mobility calculation were acoustic phonon intra- and inter-valley scattering, non-polar optical intra- and inter-valley scattering, and ionized impurity scattering. The effect of the band structure anisotropy on ionized impurity scattering, which turn out to be significant, has been also included. All parameters for the Hall mobility calculation is known except for the acoustic phonon deformation potential E_{ac}. We therefore obtain E_{ac} by fitting the experimentally measured Hall mobility in one of the three configurations, and used the same E_{ac} value for the remaining two configurations.

In Fig. 2 we show a comparison of our theoretical model with the experimentally measured electron Hall mobility in 6H-SiC of the nitrogen concentration 3.3×10^{16} cm^{-3} and the compensating acceptor concentration 1.0×10^{16} cm^{-3}. [1] The solid curves are results of our calculation including anisotropy and the dashed curves are the conventional model assuming isotropic bands. The effective masses $m^*_l=1.83$, $m^*_{t1}=0.75$, and $m^*_{t2}=0.24$ have been used based on the work of Persson and Lindefelt. [4] From the least square fitting of the experimental result shown in Fig. 2 (b), i. e., configuration [**j** ⊥ **c**, **B** ⊥ **c**], we obtain $E_{ac}=15$ eV, which is in the correct order of magnitude expected for this

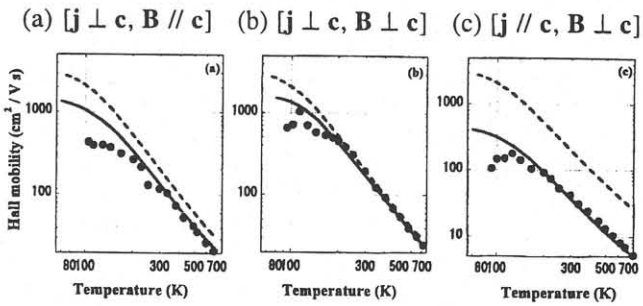

Fig. 2 The eletron mobility vs. temperature in 6H-SiC: theory with anisotropy (solid curves), theory without anisotropy (dashed curves), and experiments (•)

kind of material. The deviation between experiment and calculation in the low temperature region may be due to the effect of hopping conduction in experimentally determined mobility. The main result of our work is the comparison between theory and experiments shown in Fig. 2 (a) and (c). Using the same value of E_{ac}=15 eV as obtained in Fig. 2 (b), the adjustable-parameter-free calculation of the Hall mobility for configurations [**j** ⊥ **c**, **B** // **c**] and [**j** // **c**, **B** ⊥ **c**] agree very well with the experiments. The contribution of the various scattering mechanisms for [**j** // **c**, **B** ⊥ **c**] is shown in Fig. 3. It is also possible to represent the Hall mobility anisotropy using the masses reported in Ref. 5, though the agreement with the experiment is not as good as the one shown in Fig. 2. It is found that the Hall mobility anisotropy is sensitive especially to the value of m^*_l. Since the value of m^*_l found in ODCR measurements [6] was closer to the one proposed in Ref. 4 than the one in Ref. 5, it is understandable that we obtain better agreement with the experiment using the masses predicted by Persson and Lindefelt.

A similar calculation of the electron Hall mobility for 4H-SiC [**j** ⊥ **c**, **B** // **c**] is shown in Fig. 4. The nitrogen and compensating acceptor concentrations are 7.0×10^{15} cm^{-3} and 1.3×10^{15} cm^{-3}, respectively. The experimental data have been taken from Ref. 7. The parameters needed for the relaxation time calculation due to various scattering mechanisms have been determined independently from the fitting of the mobility in a high purity 4H-SiC epitaxial film given in Ref. 8. Our results, based on the no-adjustable parameter calculation, agree very well with the experiment.

Up to now we have shown our calculation of the Hall mobility rather than the drift mobility since most of the experimentally determined mobility so far published was measured by the Hall effect. Very recently the Hall factor r_H which relates the Hall mobility μ_H to the drift mobility μ_d through $\mu_H=r_H\mu_d$ has been measured for 4H-SiC experimentally by Rutsh et. al. [7] In Fig. 4 we compare our calculation of r_H as a function of temperature with experimentally determined r_H reported in Ref. 9. The values of the calculation stay within 15% of the experiment through out the temperature region investigated. Our model, therefore, is very useful for the calculation of the both drift and Hall mobilities in hexagonal SiC.

References

1. M. Schadt, G. Pensl, R. P. Devaty, W. J. Choyke, R. Stein, and D. Stephani, Appl. Phys. Lett., **65** (1994).
2. G. Bosch. J. Phys. Chem. Solids, **27**, 795 (1966).
3. G. A. Lomakina and Yu. A. Vodakov, Sov. Phys. Solid State **15**, 83 (1973).
4. C.Persson and U.Lindefelt,Phys.Rev.B, **54**,10257 (1996).
5. W. R. L. Lambrecht and B. Segall, Phys. Rev. B, **52**, R2249 (1995)
6. N. T. Son et al. Appl. Phys. Lett. **65**, 3209 (1994); Appl. Phys. Lett., **66**, 1074 (1995).
7. G. Rutsch, *et. al.*, Materials Science Forum **264-268**, 517 (1998).
8. W. J. Choyke and G. Pensl, MRS Bulletin, **22**, 25 (1997).

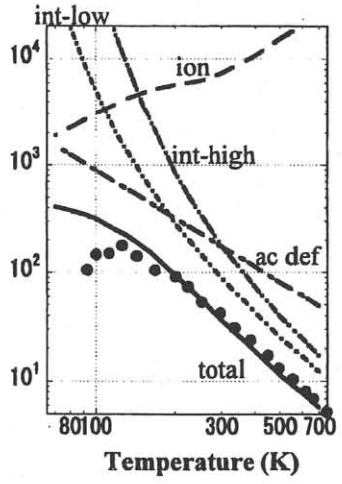

Fig. 3 The contribution of various scattering mechanisms in 6H-SiC for [**j** // **c**, **B** ⊥ **c**]: acoustic phonon deformation potential (ac def), high and low intervalley (int-high and int-low) and ionized impurity (ion) scatterings

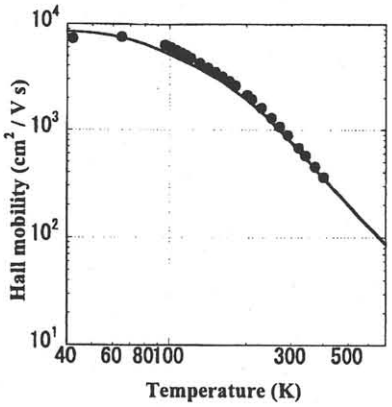

Fig. 4 The eletron mobility vs. temperature in 4H-SiC: theory with anisotropy (solid curve) and experiments (•).

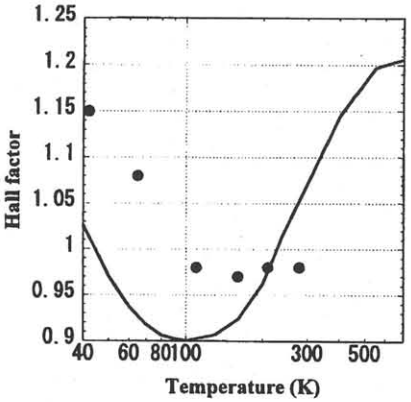

Fig. 5 The Hall factor r_H vs. temperature in 4H-SiC: theory with anisotropy (solid curve) and experiments (•).