On the calculation of Hall factors for the characterization of electronic devices

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Abstract—In this work, a new method for the calculation of Hall factors is described. It is based on the interdependence with mobility components via the respective relaxation (scattering) times. The new method allows an accurate determination of mobility and carrier sheet concentration from Hall-effect measurements and can not only be applied to homogeneously doped substrates but also at the interfaces of electronic devices such as field-effect transistors. To demonstrate the general applicability of the method, we use it to predict the dependence of the Hall factor on dopant concentration in silicon and compare it with measured Hall factors reported in the literature.

Keywords—Hall factor, Hall measurements, relaxation (scattering) time, mobility, bulk silicon.

I. INTRODUCTION

Hall-effect measurements in combination with sheet resistivity measurements are well established to determine sheet concentration and mobility of charge carriers independently in semiconductors and metals. However, from the combination of the measured values one obtains an effective Hall mobility μ_H rather than the drift mobility μ of the majority charge carriers. The ratio of the two is called Hall factor or scattering factor and needs to be known a-priori for an accurate interpretation. It is common practice to assume that the Hall factor equals unity. From theory it is known that this is correct only in strong magnetic fields for which the condition $\mu B >> 1$ holds. For a magnetic field of B = 1 T, as an example, the mobility should be significantly higher than 10.000 cm^2/Vs . For lower fields and non-degenerate semiconductors, the Hall factor will depend on the particular mechanisms by which the charge carriers are scattered and this may depend in turn on material and measurement condition. A typical example where the assumption of a Hall factor equal to unity is not justified is the inversion channel of a MOSFET because of the rather low channel mobility. In consequence, when the Hall factor is ignored, the sheet concentration and mobility values extracted from Hall-effect measurements may be wrong by some 10% which is considerable for such devices.

In literature, various approaches have been presented to calculate transport properties and Hall factors. They are typically based on Monte Carlo methods or solutions of the Boltzmann transport equation taking the full band structure into account [1,2]. Despite being computationally demanding, they still need comparison with experiments and cannot be easily applied to general conditions in macroscopic devices. In this work we present a new method for the calculation of Hall factors. It is based on the fact that both Hall factor and mobility depend on the mechanisms by which the charge carriers are actually scattered. The links between the various mobility components and the Hall factor are the respective relaxation (scattering) times. A particular advantage of our method is that it can be easily applied for different materials under different measurement conditions. To show the applicability of the method, we calculated the Hall factors in bulk silicon as a function of doping concentration and compared them with the values reported in literature.

II. METHOD OF THE CALCULATION

The Hall factor r_{H0} is defined as the ratio of the Hall mobility to drift mobility and can be expressed in the relaxation time approximation through certain mean values of relaxation times:

$$r_{H0} = \frac{\mu_H}{\mu} = \frac{<\tau^2>}{<\tau>^2}$$
(1)

Therein, the parameter τ denotes the relaxation time, i.e. the mean free flight time between carrier collisions. In general, it will depend on the energy of the charge carriers. The squared brackets denote an averaging over the energy of the charge carriers. The inverse of the relaxation time $1/\tau$ is the average number of scattering events per unit time. For many scattering processes, the energy dependence of the relaxation time can be expressed as a simple power law:

$$\tau = aE^{-s} \tag{2}$$

where *a* and *s* are constants whose values depend on the involved types of scattering mechanisms. For example, for semiconductors with acoustic phonon or ionized impurity scattering, τ is proportional to $E^{-1/2}$ (*s* = 1/2) or to $E^{3/2}$ (*s* = -3/2), respectively [3].

The values of the averages $\langle \tau \rangle$ and $\langle \tau^2 \rangle$ can be calculated analytically as long as the relaxation time can be expressed in the form of a power law. They take the form

$$<\tau>=\frac{a(kT)^{-s}\,\Gamma(\frac{s}{2}-s)}{\Gamma(\frac{s}{2})},\tag{3}$$

$$<\tau^{2}>=\frac{a^{2}(kT)^{-2s}\Gamma\left(\frac{5}{2}-2s\right)}{\Gamma\left(\frac{5}{2}\right)}$$
(4)

with k standing for Boltzmann's constant, T temperature, and $\Gamma(n)$ the gamma function defined as:

$$\Gamma(n) \equiv \int_{0}^{\infty} x^{n-1} e^{-x} dx$$
 (5)

In accordance with (1), it follows from the expressions above that the Hall factor becomes $r_{H0} = 1.18$ for acoustic phonon scattering and $r_{H0} = 1.93$ for ionized impurity scattering. It was also suggested by Erginsoy [4] that the relaxation time for scattering at neutral impurities is independent of the energy of the charge carriers (s = 0). For such a mechanism dominating at extremely low temperature or for heavily doped semiconductors, the Hall factor becomes $r_{H0} = 1$. In summary, depending on the actual scattering mechanism, values of the Hall factor r_{H0} may vary between 1 and 1.93.

In a real electronic device, several charge scattering mechanisms are usually involved in parallel. In order to calculate the Hall factor from (1), we need to determine the values of $\langle \tau \rangle$ and $\langle \tau^2 \rangle$ for such conditions. This can be done by accounting these several scattering mechanisms when averaging relaxation times over energy. As suggested by Iwata [5], the various scattering mechanisms can be combined in the form

$$<\tau>=\frac{\int_{0}^{\infty} \frac{x^{3/2} e^{-x} dx}{\sum_{i} \tau_{i}^{-1}}}{\int_{0}^{\infty} x^{3/2} e^{-x} dx}$$
(6)

$$<\tau^{2}> = \frac{\int_{0}^{\infty} \frac{x^{3/2} e^{-x} dx}{[\Sigma_{i} \tau_{i}^{-1}]^{2}}}{\int_{0}^{\infty} x^{3/2} e^{-x} dx}$$
(7)

where x stands for ε/kT with ε denoting the kinetic energy of an electron and the index *i* the particular scattering mechanism.

To apply (6) and (7) to certain experimental conditions, we have to know the relaxation times for each of the scattering mechanisms and their dependence on the energy of the charge carriers under investigation. For example, for measurements in a MOS structure, only scattering of the prevalent charge carriers in the inversion layers should be considered. A peculiarity of Hall-effect measurements in MOS structures is scattering at interface defects which is largely negligible for measurements on bulk semiconductor samples. This difference in the measurement conditions can manifest itself in different Hall-factor values. The new method for the calculation of Hall factors presented in this work allows us to master the complexity of the necessary calculations. As indicated above, it takes advantage of the interdependence of the scattering time with mobility. In general, the electron mobility in a semiconductor can be expressed as:

$$\mu_e = \frac{e < \tau >}{m_e^*} \tag{8}$$

where $\langle \tau \rangle$ is the mean relaxation time that may contain the contributions from several scattering processes, *e* denotes

elementary charge, and m_e^* stands for the effective electron mass. It is further assumed that the scattering events are independent of each other so that neither of the τ_i is affected by other scattering process. The contributions of the individual scattering times τ_i to the global scattering time τ can then be combined in the form

$$\frac{1}{\tau} = \sum_{i} \frac{1}{\tau_i}.$$
(9)

Since the electron mobility is proportional to τ , (9) can be rewritten in terms of the mobility components μ_i associated with the various scattering mechanisms. The result,

$$\frac{1}{\mu} = \sum_{i} \frac{1}{\mu_i},\tag{10}$$

is known as the Matthiessen's rule. From (8) we see that relaxation time and electron mobility differ only by a constant factor of e/m_e^* . Having the possibility to calculate specific mobility components μ_i , the components of scattering time τ_i associated with these mechanisms can be easily found. If a power-law dependence of the relaxation time on the electron energy can be assumed, the unknown constant *a* in (2) can be calculated from (3) and (8). Given *a*, the energy dependence of the relaxation time for *i*th scattering component can be derived as:

$$\tau_i(E) = \frac{\mu_i m_e^* \Gamma\left(\frac{5}{2}\right) E^{-s_i}}{e(kT)^{-s_i} \Gamma\left(\frac{5}{2} - s_i\right)}$$
(11)

It should be noted that these formulas are valid for nondegenerate semiconductors with a single-valley spherical energy band. For multi-valley semiconductors, such as Si, SiC and Ge, the expression for the Hall factor has to be modified. For this purpose, the Hall factor given by (1) for the singlevalley model is multiplied by a constant a_0 that accounts for the anisotropy of the effective electron mass. Thus, the Hall factor for the case of a multiple conduction valley semiconductor can be expressed in the form [6]

$$r_H = r_{H0}a_0 \tag{12}$$

where r_{H0} is the scattering factor given by (1) for single-valley semiconductors assuming isotropic model, and a_0 is known as the "Hall mass factor" or anisotropy factor of the Hall-effect. The latter is given by [6]

$$a_0 = \frac{3K(K+2)}{(2K+1)^2} \tag{13}$$

with *K* being the ratio of longitudinal and transverse effective masses of the electrons. For Si, SiC and Ge, the Hall mass factor a_0 takes values of 0.87, 0.98 and 0.785, respectively.

Using (6) - (11), and assuming the concurrent action of different scattering mechanisms, the Hall factor can be easily determined and corrected with the anisotropy model given in (12).

III. HALL FACTOR IN BULK SILICON

To check the feasibility of our new method for the calculation of Hall factors, we applied it to the calculation of the Hall factor in bulk silicon, which was extensively investigated in the literature. Specifically, we investigated the dependence of the Hall factor in *n*-type silicon at room temperature on the doping concentration. For this purpose, we performed simulations of electronic transport in phosphorus-doped silicon samples for the range of phosphorus concentration from 1×10^{17} cm⁻³ to 2×10^{20} cm⁻³. Given bulk silicon, we assumed that the mobility is determined by Coulomb scattering on ionized impurities and by bulk phonon scattering. To model the mobility component due to bulk phonon scattering, a constant mobility of $\mu_{ph} = 1417 \text{ cm}^2/\text{Vs}$ at T = 300 K was adopted from the work of Lombardi et al. [7]. The mobility component due to charged impurity scattering was calculated using the Arora model as implemented in TCAD Sentaurus. It can be described by [8]

$$\mu_{dop} = \mu_{min} + \frac{\mu_d}{1 + (\frac{N_D}{N_0})^{A^*}}$$
(14)

with N_D standing for the donor concentration and μ_{min} , μ_d , N_0 and $A^* > 0$ for some given parameters of the model. To predict the dependence of the Hall factor on the dopant concentration, we started with an analysis of (14). It is clear from the functional dependence that the doping-related component will strictly decrease with an increasing doping concentration. This is shown also in Fig. 1. It can be interpreted as an increase of the number of scattering centers in the bulk with an increasing dopant concentration, leading further to a monotonic increase of Coulomb scattering. Keeping in mind that the Hall factor is $r_{H0} = 1.18$ for the limiting case of exclusive acoustic phonon scattering and $r_{H0} = 1.93$ for the exclusive case of ionized impurity scattering, one expects also an increase of the Hall factor with doping concentration. On the other hand, several groups found experimentally that the Hall factor in n-type silicon increases with donor concentrations but only until a doping level of about 3×10^{18} cm⁻³ [9-13]. With a further increase of doping concentration, the Hall factor decreases and, for doping concentrations exceeding 10²⁰ cm⁻³, the Hall factor approaches the theoretical value of $r_H = 0.87$ [11]. This value of r_H results from $r_{H0} = 1$ in (12) with the anisotropy of the electron mass in silicon taken into consideration. It is important here to point out that a value of $r_{H0} = 1$ indicates that the semiconductor has already become degenerate. Vice versa, the reduction of the Hall factor can be taken as an indication that the importance of scattering at charged impurities decreases at sufficiently high doping levels. The apparent contradiction between the Hall factor found experimentally and predicted by our model can be reconciled by noting that the effect of the screening due to the presence of majority charge carriers has not been accounted for. This kind of screening is expected at very high doping levels at which doping acts not only as a source of Coulomb scattering at ionized impurities but simultaneously reduces it due to the increase in the concentration of majority carriers.



Fig. 1. Bulk mobility in silicon as a function of phosphorus concentration.

To account for the screening of ionized impurities by majority carriers, we have to adapt our model accordingly. The suggested modification for the degenerate case is based on an analogy between screened ionized impurities and neutral impurities. At sufficiently low dopant concentration, the distances between the ionized impurities are sufficiently large so that the free electrons can be considered to exist separately from them. As the impurity concentration and with it the concentration of free electrons increases, electrons will spend on their paths more and more time in the vicinity of ionized impurities. For very high dopant concentrations, impurities will find themselves surrounded by alternating electrons which compensate their charge. In terms of the power-law energy dependence of the relaxation times, the power index s in (2) should change accordingly from the value of -3/2 typical for ionized impurity scattering to the value of 0 that is valid for the scattering on the neutral centers. Evidence from the measurements of Hall factors indicates that this decrease happens at a doping level exceeding about 3×10^{18} cm⁻³ which corresponds closely to the Mott transition [14]. To include the effect in our Hall-factor calculation, based on the reasoning above, we model the predicted dependence of the power index s on doping concentration N_i empirically in the form

$$s = 1.5 \times \left(\frac{1}{1 + \left(\frac{3 \times 10^{19}}{N_i}\right)^{1.2}} - 1\right)$$
(15)

A graphical representation of this relationship can be found in Fig. 2. In accordance with (15), the power index *s* changes from -3/2 to 0 when dopant concentration grows from zero to infinity. At low dopant densities, when scattering at ionized centers is dominant, *s* has its minimum equal to -3/2. With increasing screening, the importance of Coulomb scattering will decrease, which is reflected in the increase of the constant *s*. Finally, at high doping levels around 2×10^{20} cm⁻³, the scattering is similar to that at neutral impurities, which is reflected in the tendency of *s* towards the value of 0.



Fig. 2. The dependence of the power index s for Coulomb scattering on dopant density including screening.

In accordance with the method presented in the previous section, taking the mobility degradation due to phonon and Coulomb scattering in the phosphorus-doped silicon bulk material and introducing the effect of screening at high doping levels discussed above into account, the Hall factor in the bulk Si was calculated as a function of dopant concentrations. The results of this calculation are shown in Fig. 3 in comparison with the measurements reported in the literature for Si [9-13].



Fig. 3. The electron Hall factor against phosphorus doping concentration in silicon.

In accordance with the predictions of our method, the Hall factor in bulk silicon increases up to a doping level of 4×10^{18} cm⁻³. When the phosphorus concentration increases further, the screening of the ionized impurities by the majority charge carriers sets in and leads to a continuous reduction of r_H towards a value of 0.87 when the dopant density reaches a value of 2×10^{20} cm⁻³.

For a correct interpretation of the results, we also present in Fig. 3 typical error bars of these measurements which are about 12% and independent of doping level. It should be noted our calculated values are within the experimental error of nearly all experimental data points. The excellent agreement between calculations and experimental results confirms the validity of our new method for the calculation of Hall factors and allows us to apply this method further to electronic devices for which the additional complication by the interface imposes conventional approaches.

V. SUMMARY

In this work a new method for the calculation of Hall factors has been presented which is based on its interdependence with mobility via the relaxation (scattering) time. The method was validated by applying it to the dopant dependence in bulk silicon and comparing the calculated values to the experiments available. The simplicity of the method suggested allows to apply it further to the interpretation of Hall-effect measurements on electronic devices like MOSFETs where the presence of the interface to the gate oxide poses an additional severe complication.

ACKNOWLEDGMENT

This work has been carried out in the framework of the project MobiSiC (Mobility engineering for SiC devices) and supported by the Program Inter Carnot Fraunhofer (PICF 2010) by BMBF (Grant 01SF0804) and ANR.

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