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Electric field dependence of the electron mobility in bulk wurtzite ZnO

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Abstract. **The electric field dependence of the electron mobility in bulk wurtzite zinc oxide (ZnO) material is studied. The low-field electron mobility is calculated as a function of doping concentration and lattice temperature. The results show that above nearly 50 K the electrical conduction is governed by activation through the bulk material and the conduction is then influenced by both lattice and impurity scattering mechanisms. The high-field characteristics are also considered. The transition between the low-field and high-field regions is specified. The negative differential mobility for bulk ZnO at room temperature is observed at electric fields above 280 kV/cm.**

Keywords. **Electron drift velocity; low-field mobility; saturation velocity.**

1. Introduction

Recently, zinc oxide (ZnO) semiconductor has received a great attention for electronic and optoelectronic applications because of its noticeable advantages over GaN and other III-nitrides. ZnO has unique properties with possible application to ultraviolet light emitters, gas sensors, surface acoustic wave devices and transparent electronics (Ozgur *et al* 2005).

A distinguished characteristic of ZnO, compared with many other direct gap semiconductors, is the large intervalley separation which is approximately 3·23 eV, while this is 330 meV in GaAs and 2·25 eV in GaN. This may lead to a use of a simple analytical nonparabolic approximation for the conduction band around the centre of the Brillouin zone even at moderately high electric field up to several hundred kV/cm (Goano *et al* 2007).

The electron mobility in bulk ZnO as a function of electric field is important parameter for device design and analysis. At low-field level, the bulk sample carriers are almost in equilibrium with the lattice vibrations and the low-field mobility is mainly affected by phonon and Coulomb scattering (Schroder 1987). At higher electric fields, mobility becomes field-dependent parameter.

There are many theoretical models to describe the low-field mobility for bulk materials. Those include the constant mobility model, Caughey and Thomas (1967) model and Arora model (Arora *et al* 1982). In such models, the low-field mobility is temperature- and doping-concentration-dependent. On the other hand, Dorkel and Letureq (1981) presented a model, where the dependence on the carrier–carrier scattering was considered in the low-field mobility formulation. Klaassen (1992) model provided unified description of majority and minority carrier mobility, where the effects of lattice scattering, screened Coulomb charges, carrier–carrier scattering and impurity clustering effects at high concentrations are considered.

In this paper, the electric-field dependent electron mobility in bulk wurtzite ZnO is studied. The low-field electron mobility, as a function of doping concentration and lattice temperature, is computed. High-field electron mobility and the electron saturation velocity are also studied. The transition between the low-field and high-field regions is determined.

2. Theory

The low-field mobility models are best understood by starting with the modelling approach of Caughey and Thomas (1967),

$$\mu_0 = \mu_{\min} + \frac{\mu_{\max} - \mu_{\min}}{1 + (N/C)^{\alpha}}, \tag{1}$$

where C and α are fitting parameters, N the total doping density and $\mu_{\max}$ and $\mu_{\min}$ the 'maximum–minimum' behaviour of the mobility.

To match the experimental findings, at doping levels greater than 5×10^{19} cm^{-3}, Masetti *et al* (1983) assumed that:

$$\mu_0 = \mu_{\min} + \frac{\mu_{\max} - \mu_{\min}}{1 + (N/C_1)^{\alpha_1}} - \frac{\mu_1}{1 + (C_2/N)^{\alpha_2}}, \tag{2}$$

where μ_1, C_1, C_2, α_1 and α_2 are new fitting parameters.

According to Arora (Arora *et al* 1982), the temperature (T) and ionized impurity concentration (N_i) dependence of the low-field mobility is given by:

$$\mu_0 = \mu_{om} + \frac{\mu_d}{1 + (N_i/N_0)^{r}}, \tag{3}$$

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where

$$\mu_{om} = r_m \left(\frac{T}{T_0}\right)^{\alpha_m}, \qquad \mu_d = r_d \left(\frac{T}{T_0}\right)^{\alpha_d},$$
$$N_0 = r_N \left(\frac{T}{T_0}\right)^{\alpha_N}, \qquad r = r_a \left(\frac{T}{T_0}\right)^{\alpha_a}, \tag{4}$$

with $T_0 = 300\,\mathrm{K}$ and the quantities $r_m, r_d, r_N, r_a, \alpha_m, \alpha_d, \alpha_N$ and α_a are fitting parameters.

The high-field electron characteristics are well understood by studying the relationship between the drift velocity $v(E)$ and the electric field. By the aid of Arora model, one can write

$$v(E) = \frac{\mu_0 E + v_{sat}\,(E/E_c)^{\beta_1}}{1 + (E/E_c)^{\beta_1} + a\,(E/E_c)^{\beta_2}}, \tag{5}$$

where μ_0 is the temperature- and doping-dependent low-field electron mobility given from (3), v_{sat} the saturation velocity, E_c the critical field corresponding to the maximum steady state velocity and a, β_1, β_2 the fitting parameters.

The temperature dependence of the drift velocity is properly specified by considering the model which suggested that the fitting parameters could be modified to be temperature-dependent according to the equation (Yang *et al* 2010)

$$\mathrm{par}(T) = \mathrm{par}(300) \times \left[a + bT + cT^2\right], \tag{6}$$

where par(300) is a parameter at $T = 300\,\mathrm{K}$ and a, b and c are constants.

3. Results and discussion

Calculations of the low-field electron mobility and high-field electron characteristics as a function of temperature and doping concentration for bulk wurtzite ZnO were carried out according to (3) and (4). The numerical values of the parameters used in the calculations are given in table 1.

Table 1. Parameters used in the field-dependent electron mobility calculations using (3) and (4) for bulk wurtzite ZnO (extracted from Furno *et al* 2008).

Parameter	Value
r_m	98·92 $\mathrm{cm^2/V{\cdot}s}$
r_d	304·1 $\mathrm{cm^2/V{\cdot}s}$
r_N	$1{\cdot}92 \times 10^{17}\,\mathrm{cm^{-3}}$
r_a	1·058
α_m	−0·698
α_d	−3·386
α_N	2·718
α_a	−0·125
E_c	290 kV/cm
a	2·4
β_1	4·5
β_2	0·85

Figure 1 shows the low-field electron mobility *vs* temperature for ZnO in a temperature range from 10 to 400 K. The mobility was calculated at different values of donor concentration from 3×10^{16} up to 5×10^{17} $\mathrm{cm^{-3}}$. In figure 1, two main regions can be distinguished. In temperature range, between 10 and approximately 50 K (the value depends on the carrier concentration), the electron mobility increases with the increase of temperature. The second range is from 50 up to 400 K in which the mobility decreases with the elevation of temperature.

Above approximately 50 K, the conduction is assumed to be dependent on the activation processes of electrons between donor sites and the conduction band. In that range of temperature, scattering of electrons determines the mobility behaviour. Scattering by acoustic and optical phonons are probably the dominant processes at higher temperatures, while at lower temperatures, the ionized impurity scattering process might be the dominant one.

Below 50 K, the mobility data are assumed to be determined by both band and hopping conduction (Look *et al* 1998). The experimental data of low-field mobility on bulk wurtzite ZnO at carrier concentration 6×10^{16} $\mathrm{cm^{-3}}$ shows that the critical temperature between the two types of conduction is about 40 K, which may be considered in a good agreement with our calculations (Bertazzi *et al* 2009).

In order to study the temperature-dependent electronic behaviour, the low-field mobility is plotted as a function of T for temperatures above 100 K at some selected values of the donor concentration, see figure 2. Experimental Hall mobility data extracted from Bellotti and Bertazzi (2007) are also included as well as results from Monte Carlo simulation (ABMC) data from Furno *et al* (2008). Inspection of figure 2 reveals that the present calculated results fit well with the experimental results of Bellotti and Bertazzi (2007).

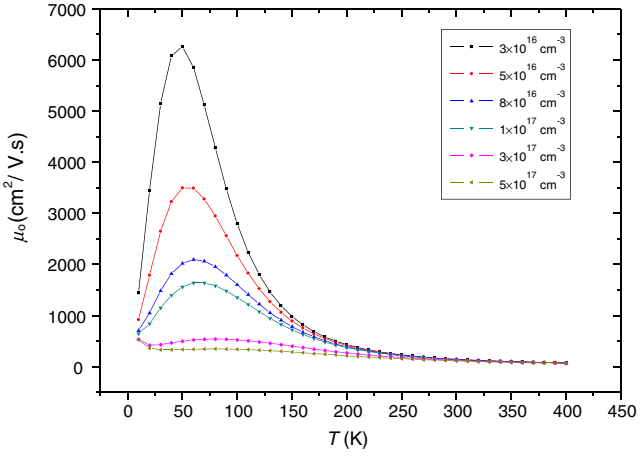

Figure 1. Low-field electron mobility vs temperature for ZnO in a temperature range from 10 up to 400 K. The curves are calculated at different values of donor concentration from 3×10^{16} up to 5×10^{17} $\mathrm{cm^{-3}}$. Peak mobilities are noticed at approximately 50 K (the value depends on the carrier concentration).

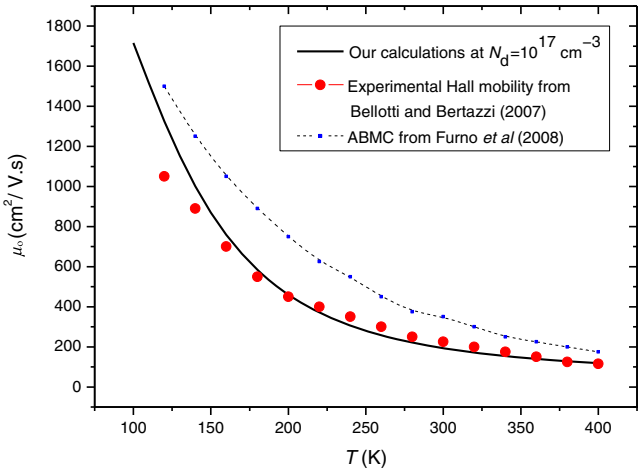

Figure 2. Low-field electron mobility at temperatures above 100 K for bulk wurtzite ZnO calculated at donor concentration of 10^{17} cm^{-3} (solid line). The calculated results are compared to experimental work from Bellotti and Bertazzi (2007) (symbols) and Monte Carlo simulation from Furno *et al* (2008) (dashed line).

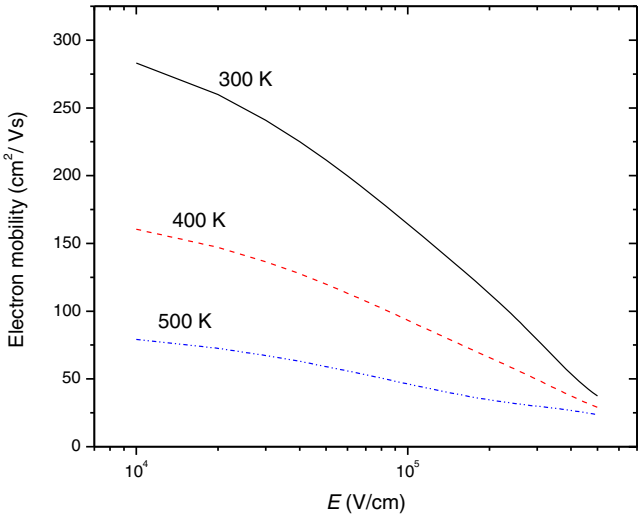

Figure 3. Electron mobility vs electric field at temperatures 300, 400 and 500 K for bulk wurtzite ZnO.

The room temperature (300 K) electron mobility extracted from figure 1 was 200 cm^2/V·s. This result is close to the value of 205 cm^2/V·s which is reported by Bellotti and Bertazzi (2007) and Furno *et al* (2008).

The electron mobility of bulk ZnO was investigated with the variation of the electric field strength up to 500 kV/cm. Figure 3 represents the change of the electron mobility vs the electric field at different temperatures: 300, 400 and 600 K. It is evident from figure 3 that the mobility is field-dependent and it decreases with increase in the electric field. This is probably due to increased lattice scattering at higher carrier energies gained by the field.

The high–field electron mobility characteristics can be understood by determining the electron drift velocity, $v(E)$

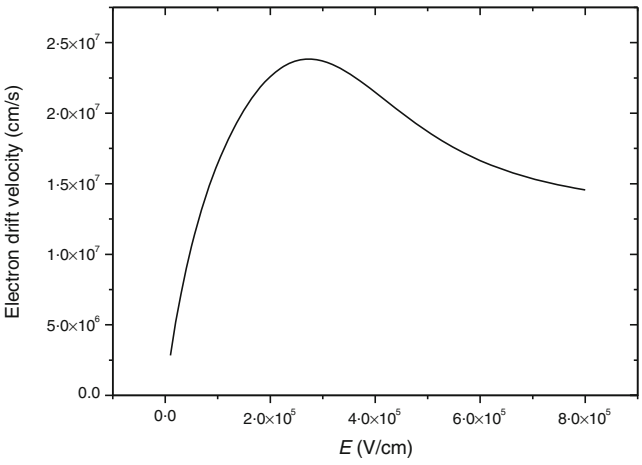

Figure 4. Electron drift velocity vs electric field at room temperature for bulk wurtzite ZnO.

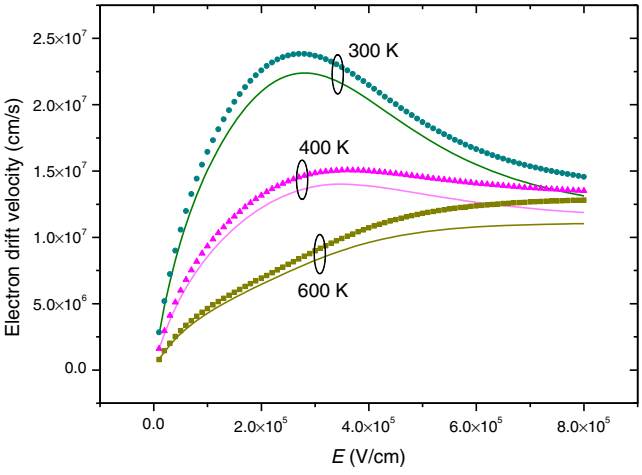

Figure 5. Electron drift velocity vs electric field at 300, 400 and 600 K for bulk wurtzite ZnO. The lines represent our calculations using Yang *et al* (2010) model and symbols represent calculations using Arora *et al* (1982) model.

as a function of the electric field. Equation (5) is used to calculate the drift velocity with the variant electric field. Figure 4 shows the dependence of the drift velocity on the electric field at room temperature. The dependence of $v(E)$ on the electric field presents a dual-slope behaviour, similar to that observed in GaN and other III-nitrides (Bellotti *et al* 2001). Inspection of figure 4 reveals that there is a negative differential mobility (NDM) at room temperature observed at electric fields above 280 kV/cm. This value can be considered as a distinguished point between the low- and the high-field characteristics.

In order to examine the model suggested that the parameters are all temperature-dependent (6) as introduced by Yang *et al* (2010). Figure 5 demonstrates the electron drift velocity calculated using this model compared to that calculated from (5). The numerical values used in the

Table 2. Parameters used in the temperature-dependent high field characteristics calculations using the Yang model for bulk wurtzite ZnO (Yang *et al* 2010).

Parameters	a	b	c
E_c	0·521	$1{\cdot}944\times10^{-3}$	$-1{\cdot}175\times10^{-6}$
v_{sat}	1·581	$-2{\cdot}431\times10^{-3}$	$1{\cdot}35\times10^{-6}$
a	3·086	$-9{\cdot}823\times10^{-3}$	$9{\cdot}608\times10^{-6}$
β_1	0·9611	$6{\cdot}297\times10^{-3}$	$-2{\cdot}358\times10^{-7}$
β_2	0·6687	$1{\cdot}223\times10^{-3}$	$-3{\cdot}475\times10^{-7}$

calculations are listed in table 2. In the figure, the lines show the calculations using Yang model and the symbols are due to Arora model (5). The same trends can be observed.

At high electric fields, the electron drift velocity decreases due to increased intra- and inter-valley scattering. It is reported that the electron population of ZnO in the Γ-valley is high (Arabshahi *et al* 2009). Then, the velocity is influenced by scattering processes at high electric fields. The effect of the field then becomes more dominant than the effect of temperature and consequently, it becomes temperature independent.

4. Conclusions

The low-field electron mobility is carried out as a function of temperature from 10 to 400 K at different doping concentrations. The results show that above nearly 50 K, the conduction is influenced by both lattice and impurity scattering mechanisms. The dependence of the electron mobility on the electric field shows a maximum electron drift velocity at electric field around 280 kV/cm. This probably determines the distinct value between low-field and high-field regions and then the negative differential mobility is observed at electric fields above 280 kV/cm.

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