An improved electron mobility model for wurtzite ZnO

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Abstract

An improved analyticl model for the electron mobility in wurtzite ZnO is developed. The numerical results of Monte Carlo transport simulations in previous literature have been evaluated and referred as the basis for the model development. The improved model describes properly the variation of the field-dependent mobility with carrier concentration and temperature, not only for room temperature but also for temperatures considerably higher than 300K, showing good agreements with previous results.

1. Introduction

Recently, ZnO has attracted much attention not only as a suitable closely lattice-matched substrate for GaN but also as a potentially useful optoelectronic material in its own right[1]. However, no preexisting analytical mobility model provides a satisfactory description of the field dependence of the Monte Carlo calculated ZnO mobility. It is the purpose of this work to provide an complete and reasonable description of the electron mobility in wurtzite ZnO for device simulations and designs.

2. Low-field mobility for ZnO

In this paper, the MC based model proposed by Enrico Furno, et al. is introduced [2].

\[
\mu_0 = \mu_{\text{min}} \left( \frac{T}{300} \right)^{r_{\text{min}}} + \frac{\mu_d \left( \frac{T}{300} \right)^{r_d}}{1 + \left( \frac{N_{\text{d}}}{N_{\text{ref}}} \right)^{a_1 \left( \frac{T}{300} \right)^{q_1}}}
\]

where \(\mu_0\) is the low-field mobility for ZnO, \(\mu_{\text{min}}, \mu_d, N_{\text{ref}}, a_1, r_{\text{min}}, r_d, r_{\text{ref}}\) and \(r_{\text{al}}\) are fitting parameters.

Table 1. Low-field mobility parameters for ZnO [2]

<table>
<thead>
<tr>
<th>Par</th>
<th>(\mu_{\text{min}}) (cm/V.s)</th>
<th>(\mu_d) (cm/V.s)</th>
<th>(N_{\text{ref}}) ((10^{17} \text{cm}^{-3}))</th>
<th>(a_1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>98.92</td>
<td>304.1</td>
<td>1.923</td>
<td>1.058</td>
</tr>
<tr>
<td>Par</td>
<td>(r_{\text{min}})</td>
<td>(r_d)</td>
<td>(r_{\text{ref}})</td>
<td>(r_{\text{al}})</td>
</tr>
<tr>
<td>Value</td>
<td>-0.698</td>
<td>-3.386</td>
<td>2.718</td>
<td>-0.125</td>
</tr>
</tbody>
</table>

3. High-field mobility for ZnO

The modeling of high-field electron mobility has been the most critical part of the entire model development [6]. The experimental database for high electric field domain for ZnO is quite limited. Hence,
the numerical results of MC simulations have been used to develop our model for the high-field electron mobility[1,7,8].

a) In this context, an approximated expression suited to model such velocity-field characteristics is given [9] as:

\[ V(E) = \frac{\mu_0 E + V_s\left(\frac{E}{E_c}\right)^{n_1}}{1 + a\left(\frac{E}{E_c}\right)^{n_2} + \left(\frac{E}{E_c}\right)^{n_1}} \]  

(2)

where \( \mu_0 \) is the low-field mobility determined by Eq.(1). \( E_c, V_s, a, n_1 \) and \( n_2 \) are fitting parameters.

Up to now, the low-field mobility is the only quantity in Eq. (2) showing a temperature dependence. This is not sufficient to properly model the temperature dependence of the velocity-field characteristics. Thus a temperature dependence of the fitting parameters is introduced by

\[ \text{Par}_T = \text{Par}_{300K} \left[a + bT + cT^2\right] \]  

(3)

where \( \text{Par}_T \) is the parameter of interest (\( E_c, V_s, a, n_1, n_2 \) in Eq. (2) ) and \( a, b, \) and \( c \) are constants that have to be determined by fitting.

b) The Monte Carlo results for 300K shown in Fig.2 constitute the data base for model development.

The modeled 300K low-field mobility (obtained by Eq. (1)) has been fixed during fitting. By a fitting procedure the parameters \( V_s, E_c, a, n_1, n_2 \) from Eq. (2) have been ascertained. The determined parameters in the model are list in Table 2.

Table 2. 300K parameters of high-field mobility for ZnO (\( N_d=10^{17}\) cm\(^{-3}\))

<table>
<thead>
<tr>
<th>( E_c ) (kV/cm)</th>
<th>( V_s ) (10(^7) cm/s)</th>
<th>a</th>
<th>n(_1)</th>
<th>n(_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>287.5</td>
<td>1.109</td>
<td>2.555</td>
<td>4.283</td>
<td>0.8028</td>
</tr>
</tbody>
</table>

c)The final step was to include the temperature dependence of the high-field transport in the model for ZnO. In [1,7,8] Monte Carlo transport simulations for temperatures ranging from 100K to 600K have been carried out. The results of these calculations have been used to estimate the temperature dependence of the parameters \( E_c, V_s, a, n_1, n_2 \) according to Eq. (2). The obtained constants \( a, b \) and \( c \) are shown in the Table 3.

![Fig.3 300K, 450K and 600K velocity-field relation curves for ZnO (\( N_d=10^{17}\) cm\(^{-3}\))](image)

Fig.3 shows the velocity-field characteristics calculated for ZnO for temperature 300K, 450K and 600K. The modeled velocity-field curves in Fig.3 show how the proposed model describes the effect of elevated temperatures on the high-field transport and the same trends as the Monte Carlo results from [1,7,8]. The drift velocity decreases with increasing temperature due to the increased total scattering rate. In addition, this increased relaxation of electron energy and momentum results in a higher threshold field to heat the electrons in order for them to scatter to the satellite valleys. Thus, the threshold field increases with temperature while the peak drift velocity decrease.
Fig. 3 also shows the velocity-field characteristics calculated from model [2]. This model also applies Eq. (2). Contrary to the present model, however, only the low-field mobility is assumed to be temperature dependent, while the parameters $E_c$, $V_s$, $a$, $n_1$ and $n_2$ are constants, do not vary with the temperature. Clearly the high-field transport at elevated temperatures is not described correctly by the model [2].

### Table 3 The temperature dependence parameters of high-field mobility for ZnO

<table>
<thead>
<tr>
<th>Par</th>
<th>$E_c$</th>
<th>$V_s$</th>
<th>$a$</th>
<th>$n_1$</th>
<th>$n_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>0.5216</td>
<td>1.581</td>
<td>3.086</td>
<td>0.9611</td>
<td>0.6687</td>
</tr>
<tr>
<td>b,K$^{-1}$</td>
<td>$1.944 \times 10^3$</td>
<td>$-2.431 \times 10^3$</td>
<td>$-9.823 \times 10^3$</td>
<td>$6.297 \times 10^3$</td>
<td>$1.223 \times 10^3$</td>
</tr>
<tr>
<td>c,K$^{-2}$</td>
<td>$-1.175 \times 10^6$</td>
<td>$1.35 \times 10^9$</td>
<td>$9.608 \times 10^6$</td>
<td>$-2.358 \times 10^7$</td>
<td>$-3.475 \times 10^7$</td>
</tr>
</tbody>
</table>

### 4. Conclusion

In this paper, an improved electron mobility model for bulk wurtzite ZnO has been developed. The model is based on a large number of MC results published in the open literatures. The improved model describes properly the dependence of the mobility on electron concentration, temperature and field for a wider range of temperature than before. It consists of simple analytical equations and can be easily incorporated in a numerical device simulator to design and optimize different ZnO device structures.

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### 5. References