Diamond & Related Materials 23 (2012) 23–27

Contents lists available at SciVerse ScienceDirect

Diamond & Related Materials

journal homepage: www.elsevier.com/locate/diamond

Charge carrier mobility in gallium nitride

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ARTICLE INFO

Article history:
Received 16 September 2011
Received in revised form 14 December 2011
Accepted 20 December 2011
Available online 28 December 2011

Keywords:
Gallium nitride
Defects
Defect characterization

ABSTRACT

The processes of the charge carrier scattering on the short-range potential caused by interaction with polar and nonpolar optical phonons, piezoelectric and acoustic phonons, static strain, neutral and ionized impurities in wurtzite n-GaN with impurity concentration 1.1×10^{16} cm$^{-3}\div1.9\times10^{18}$ cm^{-3} and in wurtzite p-GaN with impurity concentration 1.9×10^{19} cm$^{-3}\div2.6\times10^{20}$ cm^{-3} are considered. The temperature dependences of electron mobility in the range $15\div500$ K and hole mobility in the range $100\div1000$ K are calculated.

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1. Introduction

Gallium nitride is one of the semiconducting materials which finds a wide application in high temperature, high frequency and radiation hardness devices. Further progress in the design and optimization of GaN-based devices requires a thorough adequate approximation of the material parameters. One of the important material parameters is the charge carrier mobility. Experimental data of the dependence of electron and hole mobility on temperature and doping concentration have been reported in [1–13]. Theoretical analysis of this data was carried out by iterative method [14–16], variational method [17,18] and Monte Carlo method [19]. The common feature of these methods is the using of the long-range charge carrier scattering models for the description of the transport phenomena in this semiconductor. In these models it is supposed that either the charge carrier interacts with all the crystal (electron–phonon interaction) or it interacts with the defect potential of the impurity the action radius of which is equal to ~10–1000 a_0 (a_0 — lattice constant). However, such an assumption has next contradictions: a) it contradicts the special relativity according to which the charge carrier would interact only with the neighboring crystal region; b) it contradicts the atomistic hypothesis according to which the charge carrier interacts (and transfers the energy respectively) only with one atom but not simultaneously with many atoms which are situated in different points of space. Besides for defects with the interaction energy $U\approx1/r^n$ (n = 1,2) on distances ~*10* a_0 the potential becomes the magnitude of the second order while all mentioned above scattering models are considered in the first (Born) approximation. From the other side in [20–22] the short-range models of charge carrier scattering in $A^{II}B^{VI}$ solid solutions were proposed in which the above mentioned shortcomings were absent. It has been supposed there that the carrier interacts with the defect potential only within the limits of one elementary cell, i.e. the interaction radius of the short-range potential is founded in a form $R=\gamma\, a_0$ (a_0 — lattice constant, γ — the respective adjusting parameters). The aim of the present paper is to use this approach for description of the charge carrier scattering processes on the various types of crystal defects in gallium nitride.

2. Theory

All above-mentioned short-range scattering models describe the transport phenomena in zinc blende semiconductors. In order to apply these models for wurtzite GaN it is necessary to embed the following modifications in formulas for carrier transition probability: a) the volume of the elementary cell of zinc blende structure $V_{ZB}=a_0^3/4$is replaced by the volume of the elementary cell of wurtzite structure $V_W=a_0^2\ c_0\sqrt{3}/2$(a_0;c_0– lattice constants of hexagonal structure); and b) during integration over the charge carrier wave vector the lattice constant of zinc blende structure a_0 is replaced by expression $(a_0+c_0)/2$. Taking this into account the carrier transition probability from state k to state k' caused by the interaction with polar optical (PO), nonpolar optical (NPO), piezoelectric (PZ — piezooptic (POP) and piezoacoustic (PAC)), acoustic (AC) phonons, static strain (SS) potential, ionized (II) and neutral (NI) impurity can be obtained [20–22]. It must be noticed that the strong power dependence of parametersγ_{PO},γ_{PZ},γ_{II} sharply limits the choice opportunities of their numerical values.

The conduction band is assumed to be nonparabolic, spherical and according to Kane's model is employed in the form:

$$\frac{\hbar^2k^2}{2\ m_n}=\varepsilon\ (1+\alpha\ \varepsilon), \tag{1}$$

where the nonparabolicity coefficient α is given by $\alpha=\frac{1}{E_g}\left(1-\frac{m_n}{m_0}\right)^2$, m_0– the free electron mass.

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doi:10.1016/j.diamond.2011.12.018

The valence band is assumed to be parabolic and spherical. The hole effective mass is not well known for GaN — it demonstrates a wide range of numerical values: $m_h = 0.59\ m_0$ [23]; $m_h = 0.8\ m_0$ [24]; $m_h = 1.1\ m_0$ [25]; $m_h = 1.4\ m_0$ [26]; $m_h = 2.2\ m_0$ [27]. The value $m_h = 1.4\ m_0$ was used in these calculations because it yields the best agreement with experimental data. The next parameter which is unknown for GaN is the optical deformation potential $E_{NPO}(d_0$– for conduction band electrons). To estimate its value let's use the fact that for conduction band of the zinc blende GaP, GaAs, GaSb it is equal 28.9, 36,4 and 32.3 eV respectively [28]. Therefore for gallium nitride the value $d_0 = 29$ eV was chosen. The hole scattering on NPO and AC phonons was described on the basis of the effective deformation potentials defined in [29–32]:

$$E_{NPO} = \frac{M_{Ga} + M_N}{2(M_{Ga}M_N)^{1/2}} \left[\frac{C_t\left(\frac{C_l}{C_t} + 2\right)}{2\rho\ \omega_{LO}^2 \left(\frac{a_0 + c_0}{2}\right)^2} \right]^{1/2} d_0; \tag{2}$$

$$E_{AC} = \frac{C_l/C_t + 2}{6\ C_l/C_t} \left[a^2 + \frac{C_l}{Ct}\left(b^2 + \frac{d^2}{2}\right) \right], \tag{3}$$

where a, b, and d — the fundamental valence band deformation potentials; C_l and C_t — the spherically averaged elastic coefficients of wurtzite structure given by [33]:

$$C_x = C_{11} + C_{33} - 2\ C_{13} - 4\ C_{44}\ ;\ C_l = \frac{1}{3}(2\ C_{11} + C_{33}) - \frac{2}{15}C_x\ ;\ C_t = C_{44} + \frac{2}{15}C_x. \tag{4}$$

The values a, b, and d for GaN are absent in literature. To estimate their quantities the same method as described above for d_0 was used on the base of data presented in [28]. Therefore for gallium nitride one can obtained: $a = -8.9$eV; $b = -1.8$eV; $d = -4.7$eV. The other material parameters used for calculation are listed in Table 1.

Table 1
Parameters of wurtzite GaN used in calculations.

Material parameter	Value
Lattice constant, a_0 (m)	3.189×10^{-10} [a]
c_0 (m)	5.185×10^{-10} [a]
Energy gap, E_g (eV)	$3.503 - 5.08 \times 10^{-4}\ T^2/(T + 996)$ [a, b]
Electron effective mass, m_n / m_0	0.22 [c,d]
Hole effective mass, m_h / m_0	1.4 [e]
Density, ρ_0 (gm cm^{-3})	6.1 [f]
Sound velocity, c (m s^{-1})	6.59×10^3 [f]
Optical deformation potential, d_0 (eV)	29 [g]
Valence band deformation potentials,	
a (eV)	−8.9 [g]
b (eV)	−1.8 [g]
d (eV)	−4.7 [g]
Acoustic deformation potential (conduction band), E_{AC} (eV)	9.2 [c,d]
Elastic constants ($\times 10^{11}$, N m^{-2}):	
C_{11}	3.9 [h]
C_{13}	1.06 [h]
C_{33}	3.98 [h]
C_{44}	1.05 [h]
Optical phonon energy, (meV)	91.2 [d, i]
Piezoelectric tensor component, e_{14} (C m^{-2})	0.5 [c, i]

[a] Ref.[34].
[b] Ref.[35].
[c] Ref.[14].
[d] Ref.[18].
[e] Ref.[26].
[f] Ref.[36].
[g] Estimated value.
[h] Ref.[8].
[i] Ref.[19].

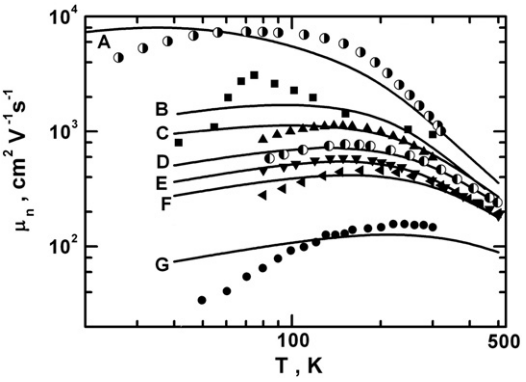

Fig. 1. The temperature dependence of electron mobility in GaN crystals with different impurity concentration. Experiment — Ref. [3,5,12,13].

The calculation of the conductivity tensor components was made on the base of the formalism of a precise solution of the stationary Boltzmann equation [37]. Using this formalism one can obtain additional fitting parameter $\gamma_{SS}N_{SS}$ (we put $\gamma_{SS} = 1$) for SS-scattering mode.

3. Comparison of theory and experiment

A comparison of the theoretical temperature dependences of the electron mobility $\mu_n(T)$ was made with the experimental data presented in [3,5,12,13]. The doping level in examined samples varied from 1×10^{16} cm^{-3} to 1.9×10^{18} cm^{-3}. The Fermi level was calculated from the charge neutrality equation for n-type, wide-band gap semiconductor (intrinsic ionization is neglected) with donors and compensated acceptors given by:

$$n + N_A = \frac{N_{D1}}{1 + 2\exp\left(\frac{F - E_{D1}}{k_B T}\right)} + \frac{N_{D2}}{1 + 2\exp\left(\frac{F - E_{D2}}{k_B T}\right)}, \tag{5}$$

where N_{D1}, N_{D2}, N_A, E_{D1}, E_{D2}– the donors ,acceptors concentration and donor ionization energies respectively which defined in [5,12,13].

For sample with unknown doping concentration [3] the Fermi level was calculated from neutrality equation $n = 1/eR_{exp}$ (R_{exp}– experimental value of Hall coefficient).

The theoretical $\mu_n(T)$ curves are presented in Fig. 1. The obtained electron scattering parameters for different scattering modes are listed in Table 2. It is seen that the theoretical curves well agree with experimental data in all investigated temperature range except the sample with maximum doping level (curve G).

To estimate the role of the different scattering mechanisms in Fig. 2a–c the dotted lines represent the appropriate dependences. For the samples A and E with low (~10^{16} cm^{-3}) and average (~10^{17} cm^{-3}) value of impurity concentration the main scattering mechanism at low temperature (T<70 K) is static strain scattering

Table 2
Parameters γ for different scattering modes (electrons).

Sample	γ_{PO}	γ_{PZ}	γ_{II}	$\gamma_{SS}\ N_{SS} \times 10^{14}$ (cm^{-3})
A [a]	0.90	0.44	1.0	1.0
B [b]	0.93	0.44	1.0	8.0
C [c]	0.90	0.44	1.0	10.0
D [d]	0.90	0.44	1.0	22.0
E [d]	0.93	0.44	1.0	32.0
F [d]	0.90	0.44	1.0	40.0
G [c]	0.90	0.44	1.0	160.0

[a] Ref.[13].
[b] Ref.[3].
[c] Ref.[12].
[d] Ref.[5].

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