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ELECTRON DRIFT MOBILITY OF DEGENERATE SEMICONDUCTORS DUE TO IONIZED IMPURITY SCATTERING – PHASE III

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Pendragon Corporation

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Final Report

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14. ABSTRACT
Analysis of electron drift mobility of degenerate semiconductors due to ionized impurities and electron drift mobility of degenerately doped zinc oxide (ZnO).

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1. Objective

In the first phase of this three-phase effort, a new theoretical treatment of the electron mobility due to ionized-impurity scattering in degenerate semiconductors was introduced. In the second phase, the accuracy of the new theory was verified by the use of several methods, both analytical and numerical.[1,2] The main objective of the present work, the third and final phase, is to develop a computer program based upon the new theory so that it can be applied it to experimental data on ZnO measured by the Air Force Research Laboratory[3] in order to understand the fundamental electronic behavior of this material and its potential for particular applications.

2. Hall Effect Measurements

Typically, electrical characterization of semiconductor materials is carried out by means of experimental measurements using the Hall Effect in a uniform magnetic field.[4] Hall Effect measurements give values for the carrier mobility μ and the sheet carrier concentration, which latter is the product of the layer thickness and the uniform carrier concentration n. The resulting Hall mobility, which is identical with drift mobility *for degenerate materials*, is independent of the thickness of the sample. Provided the voltmeter used for the measurements responds *linearly*, the resulting mobility values simply vary inversely with the strength of the magnetic field. In fact, the reciprocal of the dimensions of mobility ($m^2/V/s$) are identical to the dimensions of the magnetic field (Tesla).[5] Therefore, the accuracy of the mobility values determined by the Hall Effect are set by the accuracy with which the magnetic field is known.

In the present work, the accuracy of the experimental magnetic field and the Hall Effect measurements are not known but are thought to be within a few percent, probably within ±2%. Therefore, throughout this work, comparisons between theoretically calculated mobility and experimental mobility values are regarded as significant only to within ±2%, as estimated by the accuracy of the experimental data. Calculations of theoretical mobility values are carried out to better than 0.2%.

3. Fundamental Equations

The theoretical electron mobility due to ionized-impurity scattering for n-type semiconductors is given by the following equations, which were developed in Phase I of this work.[1] Experimental measurements give the value of the electron concentration, which for degenerate conditions is given by

$$n = k_F^3 / 3\pi^2 = \int (k/\pi)^2 f dk \tag{1}$$

where k_F is the magnitude of the momentum wave vector at the Fermi Level E_F and

$$E_F = \hbar^2 k_F^2 / 2m - E_g \left[1 - \sqrt{1 + 2\hbar^2 k_F^2 (m/m^* - 1)/mE_g} \right] / 2 \tag{2}$$

The free electron mass is m, $\hbar$ is the reduced Planck constant, the energy gap is E_g, and the effective mass at the bottom of the conduction band is m^*, the latter two being input material parameters used for the theoretical calculations.

In this work, the degeneracy ratio is defined as the ratio of the Fermi Level to the thermal energy, $E_g/\kappa T$. A degenerate semiconductor will be taken to have a degeneracy ratio greater than 12. This criterion gives theoretical accuracies within about 0.2%.

The Fermi-Dirac Probability Distribution Function f fundamentally defines the Fermi Level.

$$f = 1/[e^{(E-E_F)/\kappa T} + 1] \tag{3}$$

Thus, given the electron concentration from Hall Effect measurements and the two material parameters from the scientific literature[6], the momentum wave vector and the Fermi Level can be calculated from eqs. (1) and (2). These results are then used to calculate the mobility.

The electron mobility μ_{ii} due to ionized-impurity scattering in degenerate semiconductors is given by

$$\mu_{ii} = \frac{8\pi^3 \varepsilon_s^3 \hbar^5 k_F^2 \beta_F^2}{e^5 m^3 d_F^3 N [D_F \cdot \ln(1 + 4k_F^2/\beta_F^2) - B_F]} \tag{4}$$

The static dielectric permittivity (the third, and last, material parameter) is ε_S and the fundamental charge is e. The effective concentration of scattering centers is given by the concentrations of single donors N_d, single acceptors N_a, and double acceptors N_{aa}.[7]

$$N = N_d + N_a + 4N_{aa} \tag{5}$$

The remaining quantities in eq. (4) are[8]

$$\beta_F^2 = \frac{e^2(2m)^{3/2}}{2\pi^2\varepsilon_s\hbar^3}\cdot\left[E_F + E_g m/2m^* - \sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F+E_g)}\right]^{1/2} \times \left[1 - \frac{(m/m^* - 1)E_g/2}{\sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F+E_g)}}\right] \tag{6}$$

and

$$1/d_F = 1 + (m/m^* - 1)/\sqrt{1 + 2\hbar^2 k_F^2 (m/m^* - 1)/mE_g} \tag{7}$$

$$D_F = 1 + (2\beta_F^2 c_F^2/k_F^2) + (3\beta_F^4 c_F^4/4k_F^4) \tag{8}$$

$$B_F = [4k_F^2/\beta_F^2 + 8(1 + 2k_F^2/\beta_F^2)c_F^2 + 6(1 + \beta_F^2/2k_F^2 - 4k_F^2/3\beta_F^2)c_F^4]/(1 + 4k_F^2/\beta_F^2) \tag{9}$$

where

$$c_F^2 = 1/2 - 1/2\sqrt{1 + 2\hbar^2 k_F^2 (m/m^* - 1)/mE_g} \tag{10}$$

Therefore, given the three material parameters from the literature[6] as input data and the electron concentration from Hall measurements, the mobility can be calculated from eq. (4) when values are assumed for the acceptor concentrations. Hence, the only unknowns are the acceptor concentrations (since $N_d = n + N_a + 2N_{aa}$), which can then be determined by comparisons between experimental and theoretical mobility values.

4. Fortran Program Code

Calculations of the theoretical electron mobility due to ionized-impurity scattering in degenerate n-type semiconductors are carried out using the following Fortran computer program entitled "MuiiDegen." Lines are numbered as LL1 etc.

Note: This listing has been edited for presentation purposes; it cannot be substituted for the actual source code.

```
LL1  PROGRAM MuiiDegen
LL2     * Ionized-Impurity Degenerate Mobility Calculations
LL3     * D. L. Rode, Pendragon Corporation, Feb. 10, 2019
LL4     * Calculate kF, BetaF, Fermi Level, and Muii from
LL5     * Phase I Final Report Formulas (15), (16), (18), (20)
LL6     * for Degenerate Electron-Concentration Conditions
LL7     CHARACTER U*72
LL8     CHARACTER*1 CF(3),CG(3),CH(72)
LL9  REAL E, EM, EPS0, HBAR, PIR, EPSK, EGEV, EMSTAR,
LL10        1CCN, CONC, EG, KF, EPSS, EFEV, BETA, BETA2, CNA, CNAA,
LL11        2CONA, CONAA, ND, NOD, NN, RDF, CF2, DF, BF, MCON, MUII
LL12 INTEGER I
LL13 90 FORMAT(///3X,72A1)
LL14 91 FORMAT(3X,72A1)
LL15 92 FORMAT(3X,3A1,66X,3A1)
LL16 93 FORMAT(3X,3A1,22X,'SEMICONDUCTOR ELECTRON',22X,3A1)
LL17 94 FORMAT(3X,3A1,24X,'TRANSPORT ANALYSIS',24X,3A1)
LL18 95 FORMAT(3X,3A1,25X,'version MuiiDegen',24X,3A1)
LL19 96 FORMAT(3X,3A1,16X,'Dan Rode, Pendragon Corporation',15X,3A1)
LL20 97 FORMAT(3X,3A1,31X,'2018',31X,3A1)
LL21 DO 84 I=1,3
LL22 CF(I)='*'
LL23 CG(I)='*'
LL24 84 CONTINUE
LL25 DO 85 I=1,72
LL26 CH(I)='*'
LL27 85 CONTINUE
LL28 WRITE(6,90) CH
LL29 WRITE(6,91) CH
LL30 DO 86 I=1,2
LL31 WRITE(6,92) CF,CG
```

```
LL32  86 CONTINUE
LL33  WRITE(6,93) CF,CG
LL34  WRITE(6,94) CF,CG
LL35  WRITE(6,92) CF,CG
LL36  WRITE(6,95) CF,CG
LL37  WRITE(6,92) CF,CG
LL38  WRITE(6,96) CF,CG
LL39  WRITE(6,97) CF,CG
LL40  DO 87 I=1,2
LL41  WRITE(6,92) CF,CG
LL42  87 CONTINUE
LL43  DO 88 I=1,2
LL44  WRITE(6,91) CH
LL45  88 CONTINUE
LL46  OPEN(UNIT=13,FILE='Muii_OUT.doc',POSITION='APPEND')
LL47  WRITE(6,1)
LL48  1 FORMAT('ENTER IDENTIFYING TEXT ON ONE LINE:')
LL49  READ(5,2) U
LL50  2 FORMAT(A72)
LL51  WRITE(13,18) U
LL52  18 FORMAT(/,A72)
LL53  WRITE(6,12)
LL54  12 FORMAT('ENTER Dielectric K, Energy Gap-eV, Eff. Mass')
LL55  READ(5,*) EPSK, EGEV, EMSTAR
LL56  MCON=2.8141E-13*EPSK*EPSK*EPSK
LL57  WRITE(13,14)
LL58  14 FORMAT(' Dielectric_K, Energy Gap-eV, Eff._Mass')
LL59  WRITE(13,15) EPSK, EGEV, EMSTAR
LL60  15 FORMAT(1PE11.3,',',1PE11.3,',',1PE11.3)
LL61  WRITE(13,16)
LL62  16 FORMAT(' e_Conc./cc, Muii,Nd,       Na,      Naa')
LL63  E=1.60218E-19
LL64  EM=9.10939E-31
LL65  EPS0=8.85419E-12
LL66  HBAR=1.05457E-34
LL67  PIR=4*ATAN(1.0)
LL68  EG=E*EGEV
LL69  EPSS=EPS0*EPSK
LL70  89 CONTINUE
LL71  WRITE(6,4)
```

```
LL72  4 FORMAT('ENTER Concs./cc: n, Na, Naa --Enter Zero To End')
LL73  READ(5,*) CCN, CNA, CNAA
LL74  IF(CCN.LT.1.0) GO TO 83
LL75  WRITE(6,16)
LL76  CONC=1.0E+6*CCN
LL77  CONA=1.0E+6*CAN
LL78  CONAA=1.0E+6*CNAA
LL79  ND=CCN+CNA+2.0*CNAA
LL80  NOD=1.0E+6*ND
LL81  NN=NOD+CONA+4.0*CONAA
LL82  KF=EXP(LOG(3.0*PIR*PIR*CONC)/3.0)
LL83  EFEV=(HBAR*KF/E)*HBAR*KF/2.0/EM-EGEV/2.0
LL84  EFEV=EFEV+EGEV*SQRT(1+2*(HBAR*KF/EG)*(HBAR*KF/EM)*(1/EMSTAR-1))/2
LL85   BETA=(E*SQRT(2*EM)/HBAR)*(E*SQRT(2*EM)/HBAR)*(E*SQRT(2*EM)
LL86     1/HBAR)/2/PIR/PIR/EPSS/SQRT(E)
LL87   BETA2=SQRT((EFEV+EGEV/2.0/EMSTAR)*(EFEV+EGEV/2.0/EMSTAR)-
LL88     1EFEV*(EFEV+EGEV))
LL89   BETA2=BETA*SQRT(EFEV+EGEV/2/EMSTAR-BETA2)*(1-(1/EMSTAR-1)*EGEV/2
LL90     1/BETA2)
LL91   BETA=SQRT(BETA2)
LL92   RDF=SQRT(1.0+2.0*(HBAR/EM)*KF*KF*HBAR*(1.0/EMSTAR-1.0)/EG)
LL93   CF2=0.5-0.5/RDF
LL94   RDF=1.0+(1.0/EMSTAR-1.0)/RDF
LL95   DF=1.0+BETA2*CF2*(2.0+3.0*BETA2*CF2/4.0/KF/KF)/KF/KF
LL96   BF=KF*KF/BETA2
LL97   BF=(4.0*BF+8.0*(1.0+2.0*BF)*CF2+6.0*(1.0+0.5/BF-BF/0.75)*
LL98     1CF2*CF2)/(1.0+4.0*BF)
LL99   MUII=MCON*RDF*RDF*RDF*KF*KF*BETA2/NN/(DF*LOG(1.0+4.0*KF*KF/
LL100    1BETA2)-BF)
LL101  WRITE(6,6) CCN, MUII, ND, CNA, CNAA
LL102  WRITE(13,6) CCN, MUII, ND, CNA, CNAA
LL103  6 FORMAT(1PE10.3,',',1PE10.3,',',1PE10.3,',',1PE10.3,',',1PE10.3)
LL104  GO TO 89
LL105  83 CLOSE(13)
LL106  END PROGRAM MuiiDegen
```

5. Line-by-Line Description of the Fortran Code

The following is a line-by-line description of the MuiiDegen Fortran computer program, which implements eq. (4) for electron mobility due to ionized impurities (*only*).

In the listing below, the Output Unit is a file titled "Muii_OUT.doc" in the root directory. Also in the root directory may appear a text file titled "MuiiDegen output." This is a detailed activity report of the most recent use of the Fortran program; to it may be appended previous activity so it can be used to track usage history.

LL1	Program Title
LL2	Comment
LL3	Comment
LL4	Comment
LL5	Comment
LL6	Comment
LL7	Comment
LL8	Declaration
LL9	Declaration
LL10	Declaration
LL11	Declaration
LL12	Declaration
LL13	Format Statement
LL14	Format Statement
LL15	Format Statement
LL16	Format Statement
LL17	Format Statement
LL18	Format Statement
LL19	Format Statement
LL20	Format Statement
LL21	Construct Banner
LL22	Construct Banner
LL23	Construct Banner
LL24	Construct Banner
LL25	Construct Banner
LL26	Construct Banner

LL27 Construct Banner
LL28 Construct Banner
LL29 Write Banner
LL30 Write Banner
LL31 Write Banner
LL32 Write Banner
LL33 Write Banner
LL34 Write Banner
LL35 Write Banner
LL36 Write Banner
LL37 Write Banner
LL38 Write Banner
LL39 Write Banner
LL40 Write Banner
LL41 Write Banner
LL42 Write Banner
LL43 Write Banner
LL44 Write Banner
LL45 Write Banner
LL46 Open Output Unit
LL47 Write Input Instruction
LL48 Format Input Instruction
LL49 Read Sample Identification Information
LL50 Format Sample Identification Information
LL51 Write Sample Identification Information to Output Unit
LL52 Format Sample Identification Information
LL53 Write Input Material Parameter Instruction
LL54 Format Input Material Parameter Instruction
LL55 Read Input Material Parameters
LL56 Constant Factor for Mobility $MCON = 8 \times 10^4 \pi^3 \varepsilon_s^3 \hbar^5 / e^5 m^3$
LL57 Write Input Material Parameter Instruction
LL58 Format Input Material Parameter Instruction
LL59 Write Input Material Parameters to Output Unit
LL60 Format Input Material Parameters to Output Unit

LL61 Write Input Parameter Header to Output Unit
LL62 Format Input Parameter Header to Output Unit
LL63 Fundamental Charge e
LL64 Electron Mass m
LL65 Vacuum Permittivity ε_o
LL66 Reduced Planck's Constant
LL67 π
LL68 Energy Gap in Joules
LL69 Low-Frequency, Static Permittivity ε_s
LL70 Continuation Statement
LL71 Write Input Material Parameter Instruction
LL72 Format Input Material Parameter Instruction
LL73 Read Input Material Parameters
LL74 Conditional Branch to END Program
LL75 Write Input Parameter Header
LL76 Electron Concentration per cubic meter
LL77 Single Acceptor Concentration per cubic meter
LL78 Double Acceptor Concentration per cubic meter
LL79 Single Donor Concentration per cubic cm
LL80 Single Donor Concentration per cubic meter
LL81 Ionized-Impurity Scattering Strength Concentration
LL82 Degenerate Fermi Momentum k_F
LL83 Dummy Fermi Level Statement
LL84 Fermi Level E_F in eV
LL85 Dummy Screening Length
LL86 Dummy Screening Length
LL87 Dummy Screening Length
LL88 Dummy Screening Length
LL89 Cetnar-Rode Screening Length Square
LL90 Cetnar-Rode Screening Length Squared
LL91 Cetnar-Rode Screening Length
LL92 Dummy Variable for Wave Function Admixture
LL93 Wave Function Admixture c_F^2

LL94 Reciprocal of E-k Jacobian d

LL95 D_F Factor in Ionized-Impurity Scattering Rate

LL96 Dummy B_F Factor in Ionized-Impurity Scattering Rate

LL97 B_F Factor in Ionized-Impurity Scattering Rate

LL98 B_F Factor in Ionized-Impurity Scattering Rate

LL99 Electron Drift Mobility Due to Ionized Impurities

LL100 Electron Drift Mobility Due to Ionized Impurities

LL101 Write Output Mobility and Doping Parameters

LL102 Write Mobility and Doping Parameters to Output Unit

LL103 Format Mobility and Doping Parameters to Output Unit

LL104 GO TO Statement to Enter More Input Data

LL105 Close Output Unit

LL106 End Program

6. How to use the Fortran Program MuiiDegen

To use the Fortran program MuiiDegen, open the MuiiDegen application and respond to the prompts as follows.

ENTER IDENTIFYING TEXT ON ONE LINE

> Enter an arbitrary alphanumeric string up to 72 characters in length.
> For example, ZnO Sample No. 122345

ENTER Dielectric K, Energy Gap-eV, Eff. Mass

> Enter numerical values for the static dielectric constant $Ks = \varepsilon_s/\varepsilon_o$, the energy gap E_g in eV units, and the effective mass ratio m^*/m, each separated by a space character. For example, 8.12 3.43 0.328

ENTER Concs./cc: n, Na, Naa --Enter Zero To End

> Enter numerical values for the electron concentration n from Hall measurement, the single acceptor concentration N_a, and the double acceptor concentration N_{aa} in 1/cc units, each separated by a space character.
> For example, 1.11E21 2.3E19 2.05E20
> (The single donor concentration is calculated automatically.)

MuiiDegen output appears as
> e_Conc./cc, Muii, Nd, Na, Naa

These data include re-stated input concentrations and the computed electron mobility. For example, using the above data the output is

> 1.110E+21, 3.078E+01, 1.543E+21, 2.300E+19, 2.050E+20

Here, the second and third numbers give mobility equal to 30.78 $cm^2/V/s$ and the calculated donor concentration equal to 1.543E21/cc.

MuiiDegen responds with
ENTER Concs./cc: n, Na, Naa --Enter Zero To End

You may enter more data, or EXIT the program by any suitable means.

Output data are also written to a file named “Muii_OUT.doc”. Here is an example.

```
ZnO
Dielectric_K,EnergyGap-eV,Eff._Mass
8.120E+00,3.430E+00,3.400E-01
e_Conc./cc,Muii,Nd,Na,Naa
1.000E+19,2.026E+02,1.000E+19,0.000E+00,0.000E+00
1.000E+20,1.092E+02,1.000E+20,0.000E+00,0.000E+00
1.000E+21,6.496E+01,1.000E+21,0.000E+00,0.000E+00
1.000E+22,3.648E+01,1.000E+22,0.000E+00,0.000E+00
1.000E+23,1.921E+01,1.000E+23,0.000E+00,0.000E+00
```

The above output can be inserted into an Excel Spreadsheet as a .csv file, by use of the IMPORT command, which places the data in a format suitable for graphing or for further analysis. A complete activity report, entitled “MuiiDegen output,” may also appear in the root directory to which may be appended previous activity, allowing for tracking of historical usage. This file also contains all of the details of the input material parameters used for the calculation.

7. Comparison with Earlier Work using SETA

It may be well to discuss here an illustration of the importance of the present treatment of the problem of electron transport, particularly under degenerate conditions.

For this comparison, the material parameters of uncompensated, degenerate ZnO are used. Figure 1 shows results for electron mobility at T = 60K where it is anticipated on physical grounds that the mobility should smoothly decline as the electron concentration increases, as shown by the solid curve which represents eq. (4) of the present work. Clearly, the Semiconductor Electron Transport Analysis (SETA) results (dashed curve) fail badly for the larger concentrations. One may observe that whenever SETA fails, at the maxima, it under-represents the electron scattering rate. This is thought to be due to the method of numerical integration, even using 5000 integration increments, over the perturbation probability distribution function.[1] These results give some confidence in MuiiDegen.

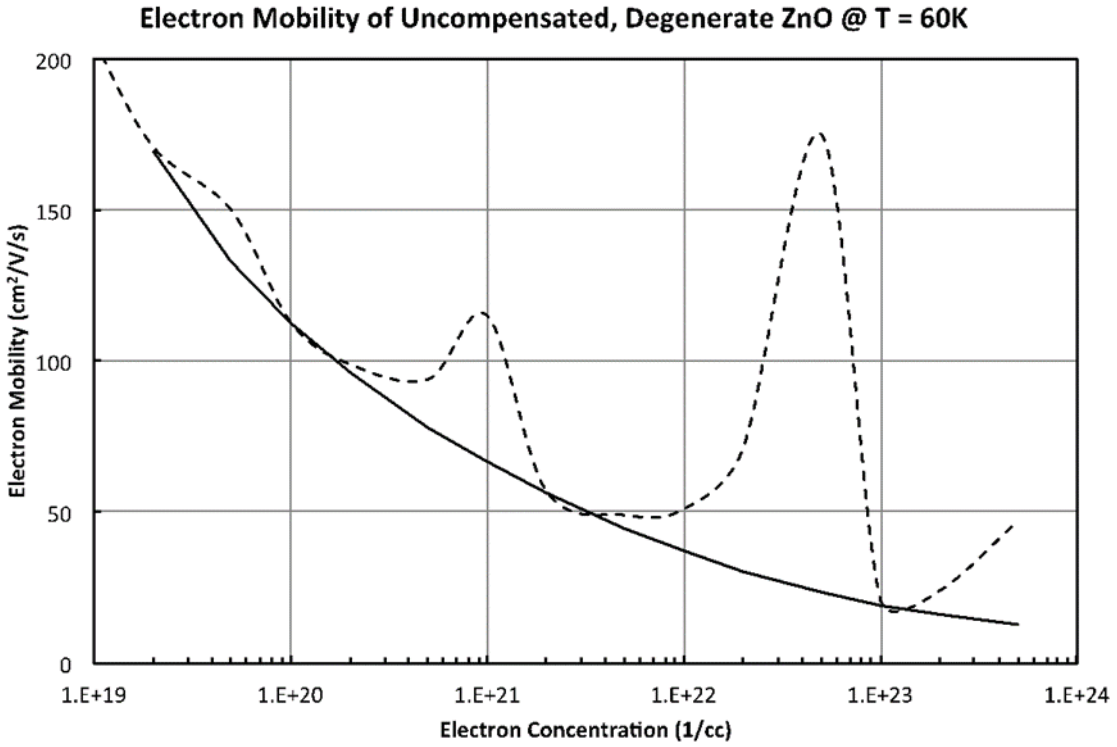

Figure 1: Comparison is shown of Calculated Electron Mobility using SETA (dashed curve) *versus* using eq. (4) of the Present Work

8. Analysis of Experimental Data

Cetnar[9] and Look[10] have kindly provided experimental data for the following work.

Electrical characterization of degenerate, Ga-doped ZnO was carried out using Hall Effect measurements to determine the electron mobility and the sheet carrier concentration. The bulk carrier (electron) concentration *n* must be determined by dividing the sheet carrier concentration by the thickness of the sample. Sample thicknesses fall within the range of 278 to 578 nanometers. The accuracy of the thickness measurements is not stated but is expected to be a small number of nanometers, so carrier concentration accuracies may be within perhaps one or two percent. Electron mobility accuracies are also estimated to be within one or two percent. So, for example, the T = 33.9K mobility figure shown below, 34.3, may be interpreted as something between 34.0 and 34.6, at best.

Consider data[9] for Sample No. G3ZO-313. This is a Ga-doped ZnO sample 575.5nm thick. Donors are singly ionized, and acceptors are doubly ionized.

Reference: Sample No. G3ZO-313 15Jan14
Measurements by T. A. Cooper

Fit of experimental mobility to MuiiDegen calculated mobility:

T = 33.9K, n = 8.84E20, experimental mobility μ = 34.3 $cm^2/V/s$
MuiiDegen N_d = 1.18E21, N_{aa} = 1.480E20, calculated μ theor. = 34.79
MuiiDegen N_d = 1.19E21, N_{aa} = 1.530E20, calculated μ theor. = 34.21
MuiiDegen N_d = 1.20E21, N_{aa} = 1.580E20, calculated μ theor. = 33.65

Or, adjusting *n*,

T=33.9K, n = 8.85E20, experimental mobility μ = 34.3 $cm^2/V/s$
MuiiDegen calc. N_d = 1.18E21, N_{aa} = 1.475E20, calculated μ theor. = 34.86
MuiiDegen calc. N_d = 1.19E21, N_{aa} = 1.525E20, calculated μ theor. = 34.28
MuiiDegen calc. N_d = 1.20E21, N_{aa} = 1.575E20, calculated μ theor. = 33.72

As another example, electron mobility data for the ZnO sample of Look[10] shows electron mobility from T = 20 K to 300K (see Table 1). No accuracy or error limits are stated.

Table 1. Electron Mobility Data

T	Mobility DCL	T	Mobility DCL
[K]	[cm2/V/s]	[K]	[cm^2/V/s]
20	46.88	160	45.25
40	46.79	180	44.56
60	46.67	200	43.93
80	46.60	220	43.11
100	46.42	240	42.29
120	46.18	260	41.52
140	45.76	280	40.72

Reference: D. C. Look,[10] Ga-doped ZnO Electron Mobility Data 190129

The low temperature mobility is about 46.8, as shown in the Table, and the experimental value of the carrier concentration is $n = 1.12 \times 10^{21}$ / *cc*. Assuming material parameters: $E_g = 3.43$, m* = 0.328, and K = 8.12 with, $N_d = 1.27 \times 10^{21}$ / *cc*, and $N_{aa} = 7.5 \times 10^{19}$ / *cc*, gives T = 20K MuiiDegen mobility 47.01. Using $N_d = 1.26 \times 10^{21}$ / *cc* and $N_{aa} = 8.0 \times 10^{19}$ / *cc* and gives T = 20K MuiiDegen mobility 46.13. *versus* the experimental result, 46.8. These results show a remarkably low level of dopant compensation.

An excellent series of data is given by Look *et al.*[7] in their Figure 1. The low-temperature data are analyzed below. The theoretical calculations agree with experimental data within about 1% at the lower temperatures for the ZnO samples as follows.

a) Un-annealed Sample

Assuming material parameters: Eg = 3.43, m* = 0.328, and K = 8.12 with $n = 1.11 \times 10^{21}$ / *cc*, $N_d = 1.51 \times 10^{21}$ / *cc*, and $N_{aa} = 2.00 \times 10^{20}$ / *cc* gives T = 20K MuiiDegen mobility 31.75 *versus* experimental result 32.0.

b) 450°C Annealed Sample

Assuming material parameters: Eg = 3.43, m* = 0.328, and K = 8.12 with $n = 9.99 \times 10^{20}$ / *cc*, $N_d = 1.20 \times 10^{21}$ / *cc*, and $N_{aa} = 1.05 \times 10^{20}$ / *cc* gives T = 20K MuiiDegen mobility 41.46 *versus* experimental result 41.8.

c) 500°C Annealed Sample

Assuming material parameters: Eg = 3.43, m* = 0.328, and K = 8.12 with $n = 1.02 \times 10^{21}$ / *cc*, $N_d = 1.15 \times 10^{21}$ / *cc*, and $N_{aa} = 6.50 \times 10^{19}$ / *cc* gives T = 20K MuiiDegen mobility 48.72 *versus* experimental result 49.0.

d) 600°C Annealed Sample

Assuming material parameters: Eg = 3.43, m* = 0.328, and K = 8.12 with $n = 7.51 \times 10^{20}$ / *cc*, $N_d = 8.50 \times 10^{20}$ / *cc*, and $N_{aa} = 5.10 \times 10^{19}$ / *cc* gives T = 20K MuiiDegen mobility 51.35 *versus* experimental result 51.5.

These results agree fairly well with those of Look *et al.* Generally, the estimated donor concentrations agree within 5% and the acceptor concentrations agree within 60%, but, of course, with the acceptor concentrations we are dealing with rather small numbers.

It may also be mentioned that for these data, the difference between theory and experiment consistently shows experiment is less than theory from low-to-high temperature by about 1.6%. Might this be due to compressive strain due to substrate thermal expansion mismatch, or to higher lying conduction band minima?

9. Conclusion

In summary, electron transport calculations using the new MuiiDegen Fortran computer program show excellent agreement, within 1%, with experimental results on degenerately doped ZnO. This new capability gives the important advantage of stable numerical calculations for electron concentrations well beyond those of the SETA Fortran program. It does not include the temperature dependence of the electron mobility, but it does incorporate wave function admixture and conduction band non-parabolicity.

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