```
#########################################################################
#################
# This is a model file for an AlGaN/GaN HEMT
# Material and material properties
# adding: GaN, AlGaN, AlN, SiC, nitride, metal
# Ohmic and Schottky contacts
#########################################################################
#################

#-------global constants-----------------------------------------------------
set k 1.38066e-23
set q 1.60218e-19
set T 300.0
set Vt [expr ($k*$T/$q)]   ;#thermal voltage
set eps0 8.854e-14    ;#permittivity of free space
#--------------------------------------------------------------------------------

#creating all the materials we need to have (GaN, AlGaN, AlN, SiC, nitride, metal)

#-------------------nitride and metal-------------------------------------------------

mater add name=Nitride
mater add name=Metal
        # Electrons and holes are not solved for in the nitride or metal so only the relative permittivity
needs to be given
        pdbSetDouble Nitride DevPsi RelEps 7.0
        pdbSetDouble Metal DevPsi RelEps 5.0e6
mater add name=Electrolyte
        pdbSetDouble Electrolyte DevPsi RelEps 78.0

        mater add name=GaO
        pdbSetDouble GaO DevPsi RelEps 78.0

        mater add name=GaO2
        pdbSetDouble GaO2 DevPsi RelEps 7.0

#----------------------GaN-----------------------------------------------------
mater add name=GaN

   #set GaN relative permittivity
   pdbSetDouble GaN DevPsi RelEps 8.9

   #set GaN electron affinity
   pdbSetDouble GaN Affinity 3.1

   #set Bandgap according to Eric Heller info
   pdbSetDouble GaN Eg (3.51-(7.7e-4*Temp*Temp)/(600+Temp))

   #set Ev and Ec for GaN
   pdbSetDouble GaN Hole Ev "((-[pdbGetDouble GaN Affinity])-([pdbGetDouble GaN Eg])+(DevPsi))"
```

```
pdbSetDouble GaN Elec Ec "((-[pdbGetDouble GaN Affinity])+(DevPsi))"

pdbSetDouble GaN Hole Nv (4.6e19*sqrt(Temp*Temp*Temp/2.7e7))
pdbSetDouble GaN Elec Nc (2.3e18*sqrt(Temp*Temp*Temp/2.7e7))

        #------------------Mobility----------------------------------------------------------------
#set low field electron mobility via analytical expression from Farahmand for low field mobility
#paramters for GaN for low field mobility from Farahmand
pdbSetDouble GaN Elec mumin 295.0
pdbSetDouble GaN Elec mumax 1460.7
pdbSetDouble GaN Elec alpha 0.66
pdbSetDouble GaN Elec beta1 -1.02
pdbSetDouble GaN Elec beta2 -3.84
pdbSetDouble GaN Elec beta3 3.02
pdbSetDouble GaN Elec beta4 0.81
pdbSetDouble GaN Elec Nref 1e17

set Gmumin ([pdbGetDouble GaN Elec mumin])
set Gmumax ([pdbGetDouble GaN Elec mumax])
set Glowalpha ([pdbGetDouble GaN Elec alpha])
set Gbeta1 ([pdbGetDouble GaN Elec beta1])
set Gbeta2 ([pdbGetDouble GaN Elec beta2])
set Gbeta3 ([pdbGetDouble GaN Elec beta3])
set Gbeta4 ([pdbGetDouble GaN Elec beta4])
set GNref ([pdbGetDouble GaN Elec Nref])

#build equation for low field mobility
set Gseg1 "$Gmumin*(1*exp(log(Temp/300)*($Gbeta1)))"
set Gseg2 "($Gmumax-$Gmumin)*(1*exp(log(Temp/300)*($Gbeta2)))"
set Gseg3 "$GNref*(1*exp(log(Temp/300)*($Gbeta3)))"
set Gseg4 "((abs(Doping)+1)/$Gseg3)";     #modified to include ionized donor or acceptor traps
set Gseg5 "$Glowalpha*(1*exp(log(Temp/300)*($Gbeta4)))"
set Gseg6 "1*exp(log($Gseg4)*($Gseg5))"
set Gseg7 "1+$Gseg6"
set Gseg8 "($Gseg2)/($Gseg7)"

pdbSetDouble GaN Elec lowfldmob "($Gseg1)+($Gseg8)"

#parameters and expression for high field mobility using Eric Heller's equations
set Gvsat "3.3e7-(3.0e6*(Temp/300))"
set Gbeta "0.85*(exp(log(Temp/300)*(0.4)))"
set GEfield "abs(dot(DevPsi,y*1e-4))+1"

set G1 "((([pdbGetDouble GaN Elec lowfldmob])*($GEfield))/($Gvsat))"
set G2 "(exp(log($G1)*($Gbeta)))"
set G3 "(1+($G2))"
set G4 "(1/$Gbeta)"
set G5 "(exp(log($G3)*($G4)))"

set Ghigh "(([pdbGetDouble GaN Elec lowfldmob])/($G5))"
```

```
    pdbSetDouble GaN Elec mob $Ghigh

    #set parameters for GaN High Field mobility from Farahmand (not used right now)
    pdbSetDouble GaN Elec alpha 6.1973
    pdbSetDouble GaN Elec n1 7.2044
    pdbSetDouble GaN Elec n2 0.7857
    pdbSetDouble GaN Elec Ecmob 220893.6
    pdbSetDouble GaN vsat 1.9064e7
    pdbSetDouble GaN vsat (2.7e7/(1+0.8*exp(Temp/600)))

    #set electron mobility via analytical expression from Farahmand for high field mobility
    set Glowfldmob ([pdbGetDouble GaN Elec lowfldmob])
    set Ghighalpha ([pdbGetDouble GaN Elec alpha])
    set Gn1 ([pdbGetDouble GaN Elec n1])
    set Gn2 ([pdbGetDouble GaN Elec n2])
    set GEcmob ([pdbGetDouble GaN Elec Ecmob])
    set Gvsat ([pdbGetDouble GaN vsat])
    set GEfield1 "abs(dot(DevPsi,y*1.e-4))+1"

    set GEfield_EcRatio1 "(($GEfield1)/($GEcmob))"
    set GEn1_1 "(exp(log($GEfield1)*($Gn1-1)))"
    set GEn1_3 "(exp(log($GEcmob)*($Gn1)))"
    set GEn1_2 "(exp(log($GEfield_EcRatio1)*($Gn1)))"
    set GEn2_1 "(exp(log($GEfield_EcRatio1)*($Gn2)))"
    set num1 "($Glowfldmob+($Gvsat*(($GEn1_1)/($GEn1_3))))"
    set denom1 "(1.0+($Ghighalpha*($GEn2_1))+($GEn1_2))"
    #set testmob1 "($num1)/($denom1)"

    #set hole mobility as constant
    pdbSetDouble GaN Hole mob 100

    #pdbSetDouble GaN Elec mob 440
        #-------------------------------------------------------------------------------------------

        #----------------------GaN2-----------------------------------------------------
mater add name=GaN2

    #set GaN relative permittivity
    pdbSetDouble GaN2 DevPsi RelEps 8.9

    #set GaN electron affinity
    pdbSetDouble GaN2 Affinity 3.1

    #set Bandgap according to Eric Heller info
    pdbSetDouble GaN2 Eg (3.51-(7.7e-4*Temp*Temp)/(600+Temp))

    #set Ev and Ec for GaN
    pdbSetDouble GaN2 Hole Ev "((-[pdbGetDouble GaN2 Affinity])-([pdbGetDouble GaN2 Eg])+(DevPsi))"
    pdbSetDouble GaN2 Elec Ec "((-[pdbGetDouble GaN2 Affinity])+(DevPsi))"

    pdbSetDouble GaN2 Hole Nv (4.6e19*sqrt(Temp*Temp*Temp/2.7e7))
```

```
pdbSetDouble GaN2 Elec Nc (2.3e18*sqrt(Temp*Temp*Temp/2.7e7))

        #------------------Mobility----------------------------------------------------------------
#set low field electron mobility via analytical expression from Farahmand for low field mobility
#paramters for GaN for low field mobility from Farahmand
pdbSetDouble GaN Elec mumin 295.0
pdbSetDouble GaN Elec mumax 1460.7
pdbSetDouble GaN Elec alpha 0.66
pdbSetDouble GaN Elec beta1 -1.02
pdbSetDouble GaN Elec beta2 -3.84
pdbSetDouble GaN Elec beta3 3.02
pdbSetDouble GaN Elec beta4 0.81
pdbSetDouble GaN Elec Nref 1e17

set Gmumin ([pdbGetDouble GaN Elec mumin])
set Gmumax ([pdbGetDouble GaN Elec mumax])
set Glowalpha ([pdbGetDouble GaN Elec alpha])
set Gbeta1 ([pdbGetDouble GaN Elec beta1])
set Gbeta2 ([pdbGetDouble GaN Elec beta2])
set Gbeta3 ([pdbGetDouble GaN Elec beta3])
set Gbeta4 ([pdbGetDouble GaN Elec beta4])
set GNref ([pdbGetDouble GaN Elec Nref])

#build equation for low field mobility
set Gseg1 "$Gmumin*(1*exp(log(Temp/300)*($Gbeta1)))"
set Gseg2 "($Gmumax-$Gmumin)*(1*exp(log(Temp/300)*($Gbeta2)))"
set Gseg3 "$GNref*(1*exp(log(Temp/300)*($Gbeta3)))"
set Gseg4 "((abs(Doping)+1)/$Gseg3)";     #modified to include ionized donor or acceptor traps
set Gseg5 "$Glowalpha*(1*exp(log(Temp/300)*($Gbeta4)))"
set Gseg6 "1*exp(log($Gseg4)*($Gseg5))"
set Gseg7 "1+$Gseg6"
set Gseg8 "($Gseg2)/($Gseg7)"

pdbSetDouble GaN2 Elec lowfldmob "($Gseg1)+($Gseg8)"

#parameters and expression for high field mobility using Eric Heller's equations
set Gvsat "3.3e7-(3.0e6*(Temp/300))"
set Gbeta "0.85*(exp(log(Temp/300)*(0.4)))"
set GEfield "abs(dot(DevPsi,y*1e-4))+1"

set G1 "((([pdbGetDouble GaN Elec lowfldmob])*($GEfield))/($Gvsat))"
set G2 "(exp(log($G1)*($Gbeta)))"
set G3 "(1+($G2))"
set G4 "(1/$Gbeta)"
set G5 "(exp(log($G3)*($G4)))"

set Ghigh "(([pdbGetDouble GaN Elec lowfldmob])/($G5))"

pdbSetDouble GaN2 Elec mob $Ghigh

#set parameters for GaN High Field mobility from Farahmand (not used right now)
```

```
   pdbSetDouble GaN Elec alpha 6.1973
   pdbSetDouble GaN Elec n1 7.2044
   pdbSetDouble GaN Elec n2 0.7857
   pdbSetDouble GaN Elec Ecmob 220893.6
   pdbSetDouble GaN vsat 1.9064e7
   pdbSetDouble GaN vsat (2.7e7/(1+0.8*exp(Temp/600)))

   #set electron mobility via analytical expression from Farahmand for high field mobility
   set Glowfldmob ([pdbGetDouble GaN Elec lowfldmob])
   set Ghighalpha ([pdbGetDouble GaN Elec alpha])
   set Gn1 ([pdbGetDouble GaN Elec n1])
   set Gn2 ([pdbGetDouble GaN Elec n2])
   set GEcmob ([pdbGetDouble GaN Elec Ecmob])
   set Gvsat ([pdbGetDouble GaN vsat])
   set GEfield1 "abs(dot(DevPsi,y*1.e-4))+1"

   set GEfield_EcRatio1 "(($GEfield1)/($GEcmob))"
   set GEn1_1 "(exp(log($GEfield1)*($Gn1-1)))"
   set GEn1_3 "(exp(log($GEcmob)*($Gn1)))"
   set GEn1_2 "(exp(log($GEfield_EcRatio1)*($Gn1)))"
   set GEn2_1 "(exp(log($GEfield_EcRatio1)*($Gn2)))"
   set num1 "($Glowfldmob+($Gvsat*(($GEn1_1)/($GEn1_3))))"
   set denom1 "(1.0+($Ghighalpha*($GEn2_1))+($GEn1_2))"
   #set testmob1 "($num1)/($denom1)"

   #set hole mobility as constant
   pdbSetDouble GaN2 Hole mob 100

   #pdbSetDouble GaN2 Elec mob 440
         #-------------------------------------------------------------------------------------------------


#--------------------AlGaN-------------------------------------------------------------------------
mater add name=AlGaN
   #define the parameters for AlGaN - all depend on a AlN_Ratio being set as a spatial variable
   pdbSetDouble AlGaN DevPsi RelEps 9.0

   #set AlGaN electron affinity
   pdbSetDouble AlGaN Affinity "((2.02275*(1-AlN_Ratio))+1.07725)"

   #set AlGaN bandgap-Don't know where the 1.3 value comes from
   pdbSetDouble AlGaN Eg "(6.13*AlN_Ratio+[pdbDelayDouble GaN Eg]*(1-AlN_Ratio)-1.0*AlN_Ratio*(1-
AlN_Ratio))"

   #Set Ev and Ec using AlGaN Ei as zero
   pdbSetDouble AlGaN Hole Ev "((-[pdbGetDouble AlGaN Affinity])-([pdbGetDouble AlGaN
Eg])+(DevPsi))"
   pdbSetDouble AlGaN Elec Ec "((-[pdbGetDouble AlGaN Affinity])+(DevPsi))"

   #copied from Full deck, don't know where the constants come from
   pdbSetDouble AlGaN Elec me "((0.4*AlN_Ratio+0.20*(1-AlN_Ratio)))"
```

```
   pdbSetDouble AlGaN Hole mh "((1.5*AlN_Ratio+3.53*(1-AlN_Ratio)))"

   set me ([pdbDelayDouble AlGaN Elec me])
   set mh ([pdbDelayDouble AlGaN Hole mh])
   pdbSetDouble AlGaN Elec Nc (2.50945e19*sqrt($me*$me*$me)*sqrt(Temp*Temp*Temp/2.7e7))
   pdbSetDouble AlGaN Hole Nv (2.50945e19*sqrt($mh*$mh*$mh)*sqrt(Temp*Temp*Temp/2.7e7))

   #-------------constant mobilities----------------------------------
   pdbSetDouble AlGaN Elec mob 1213.3

   pdbSetDouble AlGaN Hole mob 0.2

#-------------------------SiC-------------------------------------------------------------------------
mater add name=SiC

   #define the parameters for SiC
   pdbSetDouble SiC DevPsi RelEps 9.6

   #set SiC electron affinity
   pdbSetDouble SiC Affinity 3.7

   #set SiC bandgap
   pdbSetDouble SiC Eg "3.2-((3.3e-2*Temp*Temp)/(1.0e5+Temp))"


   #Set Ev and Ec using SiC Ei as zero
   pdbSetDouble SiC Hole Ev "((-[pdbGetDouble SiC Affinity])-([pdbGetDouble SiC Eg])+(DevPsi))"
   pdbSetDouble SiC Elec Ec "((-[pdbGetDouble SiC Affinity])+(DevPsi))"

   #copied from GaN need to look up constants for SiC
   pdbSetDouble SiC Hole Nv (4.6e19*sqrt(Temp*Temp*Temp/2.7e7))
   pdbSetDouble SiC Elec Nc (2.3e18*sqrt(Temp*Temp*Temp/2.7e7))


   pdbSetDouble SiC Elec mob 230

   pdbSetDouble SiC Hole mob 0.20



#---------------------------------------AlN-----------------------------------------
mater add name=AlN

   #Set Youngs Modulus and Poissons Ratio(google)
         pdbSetString AlN YoungsModulus 3.31e12
         pdbSetString AlN PoissonRatio 0.22


   #define the parameters for AlN
   pdbSetDouble AlN DevPsi RelEps 8.5
```

```
   #set AlN electron affinity
   pdbSetDouble AlN Affinity 1.2121

   #set AlN bandgap
   #pdbSetDouble AlN Eg 3.0
   pdbSetDouble AlN Eg "6.13+((1.80e-3*300*300)/(1.462e3+300))-((1.80e-
3*Temp*Temp)/(1.462e3+Temp))"

   #Set Ev and Ec using AlN Ei as zero
   pdbSetDouble AlN Hole Ev "((-[pdbGetDouble AlN Affinity])-([pdbGetDouble AlN Eg])+(DevPsi))"
   pdbSetDouble AlN Elec Ec "((-[pdbGetDouble AlN Affinity])+(DevPsi))"

   #Set AlN Nc and Nv
   pdbSetDouble AlN Hole Nv (4.6e19*sqrt(Temp*Temp*Temp/2.7e7))
   pdbSetDouble AlN Elec Nc (2.3e18*sqrt(Temp*Temp*Temp/2.7e7))


   pdbSetDouble AlN Elec mob 230

   pdbSetDouble AlN Hole mob 0.20
#-----------------------------------------------------------------------------------

#----------------Polarization Charge at AlGaN/GaN interface--------------------------------
#This is very important: it creates the 2DEG
#This value can be tuned to fit experimental data.


pdbSetString AlGaN_GaN DevPsi Equation  "1.06e13"
#-----------------------------------------------------------------------------------

#----------------------Schottky Contact at metal/AlGaN interface---------------------------
#set phiB
#per Ambacher et al, 1.3x+0.84, with x=0.25
set phiB 0.7   ;#tuned to fit experimental IV
#pdbSetString G DevPsi Equation "([pdbDelayDouble AlGaN Elec Ec])+G-$phiB"
#pdbSetBoolean G DevPsi Fixed 1
#-----------------------------------------------------------------------------------

#----------------------Ohmic Contact-------------------------------------------------------
#Electrical Boundary Conditions
#procedure for ohmic contacts (turn on in master file)
proc Ohmic {Mat Contact} {
   global Vt

   pdbSetDouble $Contact Qfp Rel.Error 1.0e-2
   pdbSetDouble $Contact Qfp Abs.Error 1.0e-2
   pdbSetDouble $Contact Qfp DampValue 0.025
   pdbSetDouble $Contact Qfn Rel.Error 1.0e-2
   pdbSetDouble $Contact Qfn Abs.Error 1.0e-2
   pdbSetDouble $Contact Qfn DampValue 0.025
   pdbSetDouble $Contact DevPsi Rel.Error 1.0e-2
```

```
   pdbSetDouble $Contact DevPsi Abs.Error 1.0e-2
   pdbSetDouble $Contact DevPsi DampValue 0.025

   #fixed boundary conditions = 1 = Dirchlet
   pdbSetBoolean $Contact Qfn Fixed 1
   pdbSetBoolean $Contact Qfp Fixed 1
   pdbSetBoolean $Contact DevPsi Fixed 1

   #Flux set to 1 means the particle fluxes will be calculated so that current can be calculated
   pdbSetBoolean $Contact Qfn Flux 1
   pdbSetBoolean $Contact Qfp Flux 1
   pdbSetBoolean $Contact DevPsi Flux 1

   pdbSetDouble $Contact Qfn Flux.Scale 1.602e-19
   pdbSetDouble $Contact Qfp Flux.Scale 1.602e-19
   pdbSetDouble $Contact DevPsi Flux.Scale 1.602e-19

   #
   set e "([pdbDelayDouble $Mat Elec Nc]) * exp(-([pdbDelayDouble $Mat Elec Ec] - Qfn) / ($Vt) )"
   set h "([pdbDelayDouble $Mat Hole Nv]) * exp(-(Qfp - [pdbDelayDouble $Mat Hole Ev]) / ($Vt) )"

   pdbSetString $Contact DevPsi Equation "Doping-$e+$h"          ;# use charge neutrality to define DevPsi
   pdbSetString $Contact Qfn Equation "Qfn+$Contact"             ;# Dirchlet BC, Qfn=contact potential
   pdbSetString $Contact Qfp Equation "Qfp+$Contact"             ;# Dirchlet BC, Qfp=contact potential
}
#-----------------------------------------------------------------------------------------------
#call procedure for source, drain, and body contacts
Ohmic AlGaN S
Ohmic AlGaN D
Ohmic SiC B
#-----------------------------------------------------------------------------------------------

#-----------------------Contact Resistance-----------------------------------------------------
if {1} { ;#can turn on and off, also tuned to fit to experimental data
pdbSetDouble S Qfn Resistance -100.0 ;#units will be Ohms-cm if width=1 at contact and Ohms if
width=(real contact depth)
pdbSetDouble D Qfn Resistance -100.0
}
#-----------------------------------------------------------------------------------------------

#-------------------------Fix for nonconvergence at high gate bias-------------------------------
#fix for hole spike at gate contact
#pdbSetString G Qfp Equation "Qfp+G"
#pdbSetBoolean G Qfp Fixed 1
#pdbSetDouble G Qfp Flux.Scale 1.602e-19
#-----------------------------------------------------------------------------------------------

#----------------------------- thermal transport parameters ----------------------------

pdbSetDouble GaN Thermalk "2.6725+(-4.25e-3*Temp)+(3.0e-6*Temp*Temp)"
pdbSetDouble GaN Heatcap "1.395+(5.14e-3*Temp)+(-3.67e-6*Temp*Temp)"
```

pdbSetDouble AlGaN Thermalk 0.33
pdbSetDouble AlGaN Heatcap 2.0

pdbSetDouble SiC Thermalk 1.20
pdbSetDouble SiC Heatcap 2.40

pdbSetDouble AlN Thermalk 2.85
pdbSetDouble AlN Heatcap 2.584