```
#########################################################################
############
#
#    Master Script for an AlGaN/GaN HEMT for pH measurement (modified for device optimization testing
- variable drain bias)
#    made 7/24/2015
#    This script makes the grid for the structure, calls files describing the physics, runs the simulation, and
plots the simulation results
#
#########################################################################
############

#simulation parameters
pdbSetDouble Math iterLimit 1000            ;#sets the max number of Newton iterations to 1000
math device dim=2 col umf none scale
DevicePackage
#-------------------------------------------------------------------------------------------------------------------
----
#---------------------------------Include Source Files-----------------------------------------------------------
----------
# include files
source GaN_modelfile_mo.tcl            ;# this file add the materials in the structure and specifies their
material properties and specifies Ohmic contacts for S D B and Schottky for G
source Poisson.tcl
source Continuity.tcl
#-------------------------------------------------------------------------------------------------------------------
----
#---------------------------------Create Structure---------------------------------------------------------------
---------
#proc called Struct2D that defines grid (default unit is microns)

#gate Length increment
set gateLinc 0.0 ; #a 0.15 increment is a +0.30um growth with gate length of 1.3um.

proc Struct2D {} {
   if {1} {                          ;# the [if {1}] tcl statement allows one to comment out the text between the
brackets if {1} is set to {0}. This is nice to use if you want to make multiple structures and easily change
between them.

   line x loc=-0.3 spac=0.05 tag=NTop
   line x loc=-0.0005 spac=0.0001 tag=Oxtop
   line x loc=0.0 spac=0.0001 tag=AlGaNTop
   line x loc=0.015 spac=0.0008 tag=AlGaNBottom
   line x loc=1.8 spac=0.2 tag=GaNBottom
   line x loc=2.0 spac=0.02 tag=AlNBottom
   line x loc=3.0 spac=1.5 tag=BBottom
         }

         if {1} { ;# 1 um gate (no T gate)
   #gate Length increment
   set gateLinc 0.0
```

```
  line y loc=(-2.0-$gateLinc) spac=0.1 tag=Left
  line y loc=(-1.25-$gateLinc) spac=0.5
  line y loc=(-0.50-$gateLinc) spac=0.01 tag=Oxleft
  line y loc=(-0.15-$gateLinc) spac=0.1
  line y loc=0.0  spac=0.10
  line y loc=(0.15+$gateLinc) spac=0.1
  line y loc=(0.50+$gateLinc) spac=0.01 tag=Oxright
  line y loc=(1.25+$gateLinc) spac=0.5
  line y loc=(2.0+$gateLinc) spac=0.1 tag=Right
  }


#use the tags above to create the material regions
        #Bulk
  region SiC xlo=AlNBottom xhi=BBottom ylo=Left yhi=Right

  #thin AlN layer
  region AlN xlo=GaNBottom xhi=AlNBottom ylo=Left yhi=Right

  #Buffer
  region GaN xlo=AlGaNBottom xhi=GaNBottom ylo=Left yhi=Right

  #AlGaN under gate
  region AlGaN xlo=AlGaNTop xhi=AlGaNBottom ylo=Left yhi=Right

  #DL
  region GaO xlo=Oxtop xhi=AlGaNTop ylo=Oxleft yhi=Oxright

  #gate metal/electrolyte
  region Electrolyte xlo=NTop xhi=Oxtop ylo=Oxleft yhi=Oxright

  #passivation layers
  region Nitride xlo=NTop xhi=AlGaNTop ylo=Left yhi=Oxleft
  region Nitride xlo=NTop xhi=AlGaNTop ylo=Oxright yhi=Right

        #initialize the grid (this command creates the grid with the specified regions)
  init

  #Create the contacts
  contact name=G Electrolyte xlo=-0.40 xhi=-0.28 ylo=(-0.75-$gateLinc) yhi=(0.75+$gateLinc) add
depth=1.0
  contact name=B SiC xlo=2.9 xhi=7.0 add depth=1.0
  contact name=S AlGaN ylo=(-3.4-$gateLinc) yhi=(-1.99-$gateLinc) xlo=-1.5 xhi=0.0149 add depth=1.0
  contact name=D AlGaN ylo=(1.99+$gateLinc) yhi=(3.4+$gateLinc) xlo=-1.5 xhi=0.0149 add depth=1.0

  # the x and y pts need to be a little larger than the grid specifications to capture all of the grid points
  # you can specify the depth of the contact into the page by depth=X. With depth=1.0 the current units
are A/um. With the depth specified, the current unit will be in A.
}
#end Struct 2D procedure (remember you still need to call the procedure)
```

```
Struct2D
#calls the procedure

        #plot the grid and contacts to make sure everything is correct
        plot.2d bound grid
   plot.2d contact=G !cle
   plot.2d contact=B !cle
   plot.2d contact=S !cle
   plot.2d contact=D !cle

#-------------------------------------------------------------------------------------------------------------------------------
---
#-----------------------------------------Specify Solution Variables-----------------------------------------------------------
----------
# we are solving for Qfn , Qfp, and DevPsi (device potential), temp is a constant and set to 300 K
solution add name=DevPsi solve negative damp continuous pde          ;# potential in semiconductor
solution add name=Qfp solve negative damp continuous pde
solution add name=Qfn solve negative damp continuous pde

solution add name=Cl solve !negative damp pde                        ;# Cl ion concentration
solution add name=H solve !negative damp pde                         ;# hydrogen ion concentration
solution add name=Na solve !negative damp pde                        ;# Na ion concentration
solution add name=A solve !negative damp pde                         ;# acid species concentration
solution add name=SOH2 solve !negative damp pde                                  ;#positive interface
charge

solution add name=Temp const val=300.0
#solution add name=Temp solve pde !negative continuous damp

# these are needed if donor or acceptor traps are included
solution add name=ETemp solve const val = 300.0 continuous
solution add name=HTemp solve const val = 300.0 continuous
solution add name=Donor solve const val = 10.0
solution add name=Acceptor solve const val = 10.0

#-------------------------------------------------------------------------------------------------------------------------------
---
#-----------------------------------------Specify the Doping (this includes static traps)--------------------------------------
--------------
        # the GaN doping is most important when fitting to an experimental IV curve; it is usually p-type
   #GaN Doping units are /cm3, negative sign is p-type,
   sel z= 2.0e14*Mater(GaN) name=GaN_Doping

   #AlGaN Doping
   sel z= 1.0e0*Mater(AlGaN) name=AlGaN_Doping

   #AlN doping
   sel z= 1.0e12*Mater(AlN) name=AlN_Doping

   #SiC doping
   sel z= 1.0e12*Mater(SiC) name=SiC_Doping
```

```
   #GaN2 doping, GaN cap layer (no physics included)
   sel z= 1.0e0*Mater(GaN2) name=GaN2_Doping

         #for new gate lengths
         set SDedge [expr (1.9+$gateLinc)]

   #Source and Drain contact doping-from contact to 2DEG to make contacts ohmic (Gaussian profile is
used in the expression)
   sel z=(1e19*(y>$SDedge)+(y<=$SDedge)*1.0e19*exp(-(y-$SDedge)*(y-
$SDedge)/($SDedge*0.02*0.02)))*(exp(-(x*x)/($SDedge*0.03*0.03))) name=Drain_Doping
   sel z=(1e19*(y<-$SDedge)+(y>=-$SDedge)*1.0e19*exp(-
(y+$SDedge)*(y+$SDedge)/($SDedge*0.02*0.02)))*(exp(-(x*x)/($SDedge*0.03*0.03)))
name=Source_Doping

   #Total doping
   sel
z=GaN_Doping+AlGaN_Doping+Drain_Doping+Source_Doping+SiC_Doping+AlN_Doping+GaN2_Doping
name=Doping

#-------------------------------------------------------------------------------------------------------------------------
---
#----------------------------------------Specify the AlN ratio in the AlGaN-----------------------------------------------
------------
         # this is used in the modelfile to calculate AlGaN material parameters
         sel z=0.25 name=AlN_Ratio

#-------------------------------------------------------------------------------------------------------------------------
---
#----------------------------------------Species Concentrations and Mobilities--------------------------------------------
---------------
#concentrations
         set Av 6.02e23                                                ;# Avogadro's number, ions/mol
         set cCl  [expr (100.0e-3*$Av)*1e-3]          ;# M*ions/mol*l/cm3 = ions/cm3
         set cNa  [expr (100.0e-3*$Av)*1e-3]          ;# M*ions/mol*m3/cm3 = ions/cm3
         set cH   [expr (1.0e-1*$Av)*1e-3]            ;# ions/cm3
         set cA   [expr (1.0e-1*$Av)*1e-3]            ;# ions/cm3
         set Ns   1.0e15                                                ;# surface interface site density
/cm2

#mobilities and diffusivity constants
         set D_Na 1.96e-5              ;# cm2/s from Lopreore
         set D_Cl 2.03e-5              ;# cm2/s from Lopreore
         set D_H  8.24e-5              ;# cm2/s from Lopreore
         set D_A  2.00e-5              ;# cm2/s from Lopreore
         set Namob [expr {$D_Na/$Vt}]
         set Clmob [expr {$D_Cl/$Vt}]
         set Hmob [expr {$D_H/$Vt}]
         set Amob [expr {$D_A/$Vt}]

#assign mobility variable for each ion species
```

```
        pdbSetDouble Electrolyte Cl mob $Clmob
        pdbSetDouble Electrolyte Na mob $Namob
        pdbSetDouble Electrolyte H mob $Hmob
        pdbSetDouble Electrolyte A mob $Amob

#-------------------------------------------------------------------------------------------------------------------------------
----
#----------------------------------------Poisson in Electrolyte-------------------------------------------------------------
----------
proc Poisson_Electro {Mat} {
   global k q eps0 Vt

        pdbSetDouble $Mat DevPsi DampValue 0.025
   pdbSetDouble $Mat DevPsi Abs.Error 0.001
   pdbSetDouble $Mat DevPsi Rel.Error 0.01

   set eqn " ($eps0 * [pdbDelayDouble $Mat DevPsi RelEps] * grad(DevPsi) / $q) + (- Cl + H - A + Na)"
   pdbSetString $Mat DevPsi Equation $eqn
} ;#end Poisson proc
#-------------------------------------------------------------------------------------------------------------------------------
----
#----------------------------------------Continuity in Electrolyte----------------------------------------------------------
----------
proc Continuity2 {Mat} {
        global Vt Namob Clmob Hmob Amob

        #set eqn "ddt($species) - (([pdbDelayDouble $Mat $species mob]) * sgrad($species, -DevPsi /
$Vt))"

        set eqnNa "ddt(Na) - ($Namob) * sgrad(Na, -DevPsi/$Vt)"
        set eqnCl "ddt(Cl) - ($Clmob) * sgrad(Cl, DevPsi/$Vt)"
        set eqnH "ddt(H) - ($Hmob) * sgrad(H, -DevPsi/$Vt)"
        set eqnA "ddt(A) - ($Amob) * sgrad(A, DevPsi/$Vt)"


        pdbSetString $Mat Na Equation $eqnNa
        pdbSetDouble $Mat Na Abs.Error 1.0e-5
        pdbSetDouble $Mat Na Rel.Error 1.0e-3
        pdbSetString $Mat Cl Equation $eqnCl
        pdbSetDouble $Mat Cl Abs.Error 1.0e-5
        pdbSetDouble $Mat Cl Rel.Error 1.0e-3
        pdbSetString $Mat H Equation $eqnH
        pdbSetDouble $Mat H Abs.Error 1.0e-5
        pdbSetDouble $Mat H Rel.Error 1.0e-3
        pdbSetString $Mat A Equation $eqnA
        pdbSetDouble $Mat A Abs.Error 1.0e-5
        pdbSetDouble $Mat A Rel.Error 1.0e-3

}       ;#end Continuity proc
#-------------------------------------------------------------------------------------------------------------------------------
----
```

```
#----------------------------------------Call procedures describing Physics----------------------------------------
--------------
	#Poisson equation and trap ionization
	Poisson GaN2
	Poisson AlGaN
	Poisson_Ins Nitride
	Poisson_Ins GaO
	Poisson SiC
	Poisson AlN
	Poisson GaN
	Poisson_Electro Electrolyte

	#Continuity equations for electron, hole and transient trap simulation
	ElecContinuity GaN
	ElecContinuity AlGaN
	ElecContinuity SiC
	ElecContinuity AlN

	HoleContinuity GaN
	HoleContinuity AlGaN
	HoleContinuity SiC
	HoleContinuity AlN

	Continuity2 Electrolyte				;#call proc for electrolyte continuity
#----------------------------------------------------------------------------------------------------------------
----

#----------------------------------------Change in Ion Concentrations at Contact Proc----------------------------
-----------------
proc Dir.contact2 {Contact} {

global cCl cNa cH cA

pdbSetBoolean $Contact Cl Flux 0
pdbSetBoolean $Contact Cl Fixed 1
pdbSetBoolean $Contact Na Flux 0
pdbSetBoolean $Contact Na Fixed 1
pdbSetBoolean $Contact H Flux 0
pdbSetBoolean $Contact H Fixed 1
pdbSetBoolean $Contact A Flux 0
pdbSetBoolean $Contact A Fixed 1

pdbSetString $Contact Cl Equation "Cl-$cCl"
pdbSetString $Contact Na Equation "Na-$cNa"
pdbSetString $Contact H Equation "H-$cH"
pdbSetString $Contact A Equation "A-$cA"
}	;#end electrolyte ion conc proc

#----------------------------------------------------------------------------------------------------------------
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```
#-----------------------------------------Initialize all contacts to 0V-----------------------------------------------------
---------

        #contact name=G Electrolyte voltage supply=3.0
   contact name=B SiC voltage supply=0.0
   contact name=S AlGaN voltage supply=0.0
   contact name=D AlGaN voltage supply=0.0

   pdbSetBoolean B Temp Fixed 0
        pdbSetString B Temp Equation "(2.7*(Temp-300.0))/0.00125"

#-----------------------------------------------------------------------------------------------------------------------
----
#-----------------------------------------Run the Initial Guess Procedure-----------------------------------------------
-------------
#Initial guess procedure, call for all materials

proc Init {Mat} {

newton $Mat eqn=Doping+Donor-Acceptor+Hole-Elec var=DevPsi damp=0.025
}

Init GaN
Init AlGaN
Init AlN
Init SiC

sel z=$cH*Mater(Electrolyte) name=H1
sel z=0 name=H2
sel z=H1+H2 name=H
sel z=$cNa*Mater(Electrolyte) name=Na
sel z=$cCl*Mater(Electrolyte) name=Cl
sel z=$cA*Mater(Electrolyte) name=A
sel z=6.1 name=DevPsi

Dir.contact2 G                          ;#call for ion concentration change at contact (electrolyte) proc
#-----------------------------------------------------------------------------------------------------------------------
----
#-----------------------------------------Run and Plot------------------------------------------------------------------
--------

set WinA [CreateGraphWindow]    ;# absorbed charge v. pH (H+, A- and total)
set WinB [CreateGraphWindow]    ;# semiconductor potential v. pH
set WinC [CreateGraphWindow]    ;# Id-Vds curve (point measurement)
set WinD [CreateGraphWindow]    ;# net adsorbed charge v. position (y-direction) across pH range


device                                                                          ;# multiple
device commands to help with convergence
device
device
```

```
device

pdbSetString AlGaN_GaO DevPsi Equation " -3.26e12"     ;# polarization charge for AlGaN-DL
pdbSetString AlN_GaN DevPsi Equation "2.2e13"                  ;# polarization charge for AlN-GaN
pdbSetString AlGaN_Nitride DevPsi Equation " -3.26e13"  ;# polarization charge for AlGaN-Nitride
pdbSetString AlGaN_GaN DevPsi Equation  "1.06e13"              ;# polarization charge for AlGaN-GaN

device init
device
device
device

#-----------------------------------------Energy Band Diagram v. Position (X-Direction, DL/AlGaN)----------
-----------------------------------------------------------
sel z=Econd
plot.1d y.v=0.0 plot_name=Band label=Ec !cle
sel z=Eval
plot.1d y.v=0.0 plot_name=Band label=Ev !cle
sel z=Qfp
plot.1d y.v=0.0 plot_name=Band label=Qfp !cle
sel z=Qfn
plot.1d y.v=0.0 plot_name=Band label=Qfn !cle
sel z=DevPsi
plot.1d y.v=0.0 plot_name=Band label=DevPsi !cle

sel z=Doping
plot.1d x.v=0.0 plot_name=DopingX label=Doping !cle
sel z=Doping
plot.1d y.v=0.0 plot_name=DopingY label=Doping !cle


#specify solution variable for negative oxide surface site SO
solution add name=SO solve !negative damp pde

#-----------------------------------------pH increment and adsorbed charge derivation----------------------
---------------------
if {1} {
#Kfa is a the forward reaction rate coefficient for the SO equation.
set Kfa 2.58867e-11
#Kra is a the reverse reaction rate coefficient for the SO equation.
set Kra 1.0e5
#Kfb is a the forward reaction rate coefficient for the SOH2 equation.
set Kfb 2.58867e-11
#Krb is a the reverse reaction rate coefficient for the SOH2 equation.
set Krb 1.0e2
#Ns is the number of available surface sites
set Ns 1.0e15

# H interface equations for Electrolyte-DL
pdbSetString Electrolyte_GaO SO Equation "ddt(SO) - $Kra*($Ns-SO-SOH2) + $Kfa*(H(Electrolyte))*(SO)"
```

```
pdbSetString Electrolyte_GaO SOH2 Equation "ddt(SOH2) - $Krb*(SOH2) + $Kfb*(H(Electrolyte))*($Ns-SOH2-SO)"
pdbSetString Electrolyte_GaO H Electrolyte Equation "+ $Krb*(SOH2) - $Kfb*(H(Electrolyte))*($Ns-SOH2-SO) + $Kra*($Ns-SO-SOH2) - $Kfa*(H(Electrolyte))*(SO)"
pdbSetString Electrolyte_GaO DevPsi Equation "SOH2 - SO"

#ph increment
for {set inc 0} {$inc<10.5} {set inc [expr $inc+1.0]} {
        set mult [expr pow(10,$inc)]    ;# need to put in expr to evaluate right away to avoid syntax error in pdb equation
        pdbSetString G H Equation "H-($cH/$mult)"
        pdbSetString G A Equation "A-($cA/$mult)"

#drain bias ramp
for {set Vds 0.05} {$Vds<1.1} {set Vds [expr $Vds+0.1]} {
        contact name=D supply=$Vds
        device init
        device
        device
        set cur [expr (1.0e6*(-[contact name=D sol=Qfn flux] + [contact name=D sol=Qfp flux]))]  ;# plots the current versus time (mA/mm)
                        AddtoLine $WinC IdVd.$inc $Vds $cur
}

# ion distribution (X-direction, electrolyte/DL/AlGaN), p[ion] = -log10[ion conc]
sel z=log10(Na+1.0)
plot.1d y.v=0.0 !cle plot_name=electrolyte label=Na
sel z=log10(Cl+1.0)
plot.1d y.v=0.0 !cle plot_name=electrolyte label=Cl
sel z=log10(H+1.0)
plot.1d y.v=0.0 !cle plot_name=electrolyte label=H
sel z=log10(A+1.0)
plot.1d y.v=0.0 !cle plot_name=electrolyte label=A

#adsorbed charge derivation for electrolyte-DL
sel z=SOH2
set nit_plus [interface Electrolyte /GaO y.v=0.0 val]
puts $nit_plus
sel z=SO
set nit_minus [interface Electrolyte /GaO y.v=0.0 val]
puts $nit_minus

set int_chrg [expr ($nit_plus-$nit_minus)]
set pH 1+$inc
AddtoLine $WinA Int_chrg $pH $int_chrg
AddtoLine $WinA SOH2 $pH $nit_plus
AddtoLine $WinA SO $pH $nit_minus
#----------Electrostatic Potential and pH (Y-Direction)----------
sel z=DevPsi
set potential [interface Electrolyte /GaO y.v=0.0 val]
```

```
AddtoLine $WinB Potential $pH $potential
set potential [interface Electrolyte /GaO y.v=-0.25 val]
AddtoLine $WinB Potential2 $pH $potential
set potential [interface Electrolyte /GaO y.v=0.25 val]
AddtoLine $WinB Potential3 $pH $potential

#----------------------------------------Net Adsorbed Charge v Position (Y-Direction)----------------------------------
#these points are defined for 1 um gate length. For any other gate length, the y.v values must be changed.
if {1} {
#positive oxide surface sites
sel z=SOH2

set t1 [interface Electrolyte /GaO y.v=-0.5 val]
set t2 [interface Electrolyte /GaO y.v=-0.375 val]
set t3 [interface Electrolyte /GaO y.v=-0.25 val]
set t4 [interface Electrolyte /GaO y.v=-0.125 val]
set t5 [interface Electrolyte /GaO y.v=0.0 val]
set t6 [interface Electrolyte /GaO y.v=0.125 val]
set t7 [interface Electrolyte /GaO y.v=0.25 val]
set t8 [interface Electrolyte /GaO y.v=0.375 val]
set t9 [interface Electrolyte /GaO y.v=0.4 val]
set t10 [interface Electrolyte /GaO y.v=0.5 val]
set t11 [interface Electrolyte /GaO y.v=0.48 val]
set t12 [interface Electrolyte /GaO y.v=0.5 val]

sel z=SO
        ;#negative oxide surface site

set m1 [interface Electrolyte /GaO y.v=-0.5 val]
set m2 [interface Electrolyte /GaO y.v=-0.375 val]
set m3 [interface Electrolyte /GaO y.v=-0.25 val]
set m4 [interface Electrolyte /GaO y.v=-0.125 val]
set m5 [interface Electrolyte /GaO y.v=0.0 val]
set m6 [interface Electrolyte /GaO y.v=0.125 val]
set m7 [interface Electrolyte /GaO y.v=0.25 val]
set m8 [interface Electrolyte /GaO y.v=0.375 val]
set m9 [interface Electrolyte /GaO y.v=0.40 val]
set m10 [interface Electrolyte /GaO y.v=0.45 val]
set m11 [interface Electrolyte /GaO y.v=0.48 val]
set m12 [interface Electrolyte /GaO y.v=0.5 val]

set T1 [expr $t1-$m1]
set T2 [expr $t2-$m2]
set T3 [expr $t3-$m3]
set T4 [expr $t4-$m4]
set T5 [expr $t5-$m5]
set T6 [expr $t6-$m6]
set T7 [expr $t7-$m7]
set T8 [expr $t8-$m8]
set T9 [expr $t9-$m9]
```

```
set T10 [expr $t10-$m10]
set T11 [expr $t11-$m11]
set T12 [expr $t12-$m12]

AddtoLine $WinD Intchrg.$inc -0.5 $T1
AddtoLine $WinD Intchrg.$inc -0.375 $T2
AddtoLine $WinD Intchrg.$inc -0.25 $T3
AddtoLine $WinD Intchrg.$inc -0.125 $T4
AddtoLine $WinD Intchrg.$inc 0.0 $T5
AddtoLine $WinD Intchrg.$inc 0.125 $T6
AddtoLine $WinD Intchrg.$inc 0.25 $T7
AddtoLine $WinD Intchrg.$inc 0.375 $T8
AddtoLine $WinD Intchrg.$inc 0.4 $T9
AddtoLine $WinD Intchrg.$inc 0.45 $T10
AddtoLine $WinD Intchrg.$inc 0.48 $T11
AddtoLine $WinD Intchrg.$inc 0.5 $T12
}
#-----------------------------------------SO/DevPsi v. Position Across pH Range-----------------------------------------
------
# SO v position (y-direction)

sel z=SO
plot.1d x.v=0.0005 plot_name=Intchrg label=SO.$inc !cle
set nitT_minus [interface Electrolyte /GaO x.v=0.0005 val]

                        puts $nitT_minus
                        sel z=Econd
                        plot.1d y.v=0.0 plot_name=Band2 label=Ec.$inc !cle
                        sel z=Eval
                        plot.1d y.v=0.0 plot_name=Band2 label=Ev.$inc !cle
                        sel z=Qfp
                        plot.1d y.v=0.0 plot_name=Band2 label=Qfp.$inc !cle
                        sel z=Qfn
                        plot.1d y.v=0.0 plot_name=Band2 label=Qn.$inc !cle

#DevPsi v position (x-direction, DL/AlGaN)
sel z=DevPsi
plot.1d y.v=0.0 plot_name=Band2 label=DevPsi.$inc !cle

#-----------------------------------------Current v. time and Carrier (E) Conc v. Position (X-Direction,
DL/AlGaN)-------------------------------------------------------------------------
plot.1d y.v=0.0 plot_name=elec_conc label=elec.$inc !cle

        }       ;#end for loop, increment pH

}       ;#end if{1}
```