Interface Trap in QCAD

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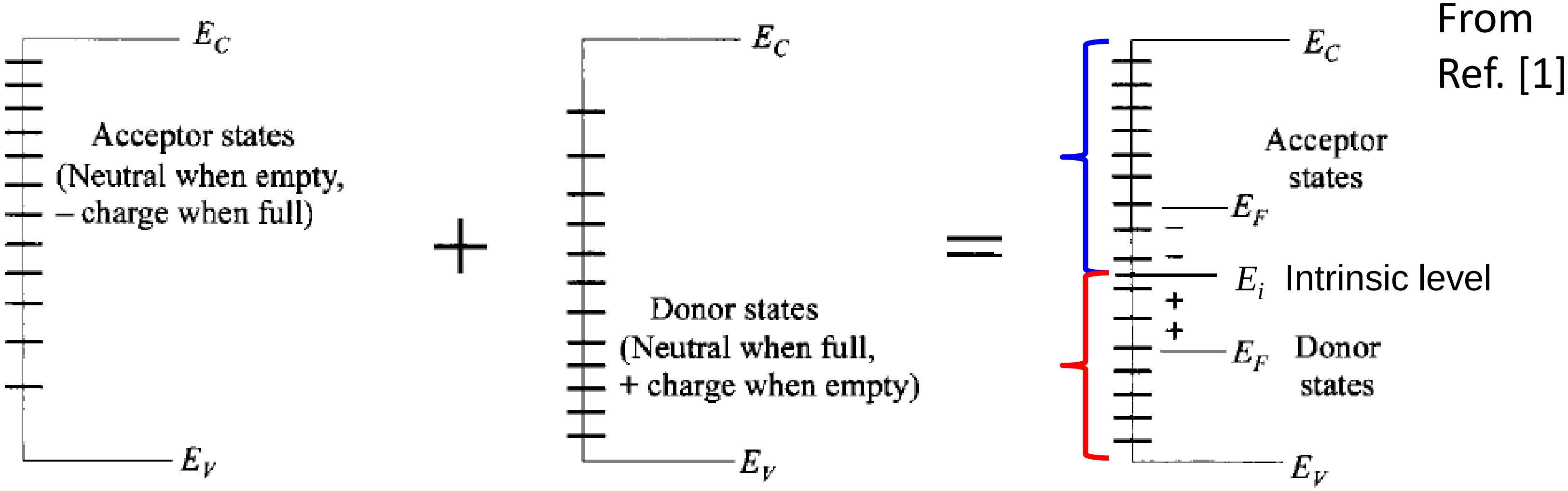
Interface Trap Basics - I

Two types of interface traps [1-4]:

- Acceptor type (or called eNeutral), which is neutral when empty of an electron, and negative charge when occupied by an electron
- Donor type (or called hNeutral), which is neutral when occupied by an electron, and positive charge when empty of an electron. (In another word, neutral when empty of a hole, and positive charge when occupied by a hole.)



[1] S. M. Sze and Kwok K. Ng, Chapter 4 in *Physics of Semiconductor Devices,* Third Edition (2007).
[2] Pascal Masson et al., Appl. Phys. Lett. **81** (18), 3392 (2002).
[3] Md Mahbub Satter and Anisul Haque, Solid-State Electronics **54**, 621 (2010).
[4] Zuhui Chen et al., Interface-trap modeling for silicon- nanowire MOSFETs, IEEE IRPS10 (2010).

Interface Trap Basics - II

Assuming acceptor traps above intrinsic Fermi level (Ei) and donor traps below Ei, the total charge contribution from interface traps is given by

$$Q_{it}(\boldsymbol{r}) = qN_{it}(\boldsymbol{r}) = q\left[-\int_{E_i}^{E_c} D_{it}(E_t,\boldsymbol{r}) f_{at}(E_t)\, dE_t + \int_{E_v}^{E_i} D_{it}(E_t,\boldsymbol{r}) f_{dt}(E_t)\, dE_t\right]$$

[C/cm^2] [#/cm^2] [#/(eV.cm^2)]

Electron occupation of an acceptor trap at E_t level

Hole occupation of a donor trap at E_t level

It can be shown that, in the stationary and quasi-thermal equilibrium case, the occupation function follows the Fermi-Dirac distribution, i.e.,

$$f_{at} = \frac{1}{1 + g_a exp\left(\frac{E_t - E_F}{k_B T}\right)} \qquad f_{dt} = \frac{1}{1 + g_d exp\left(\frac{E_F - E_t}{k_B T}\right)}$$

g_a, g_d = Degeneracy factor, e.g., 4 for g_a, and 2 g_d for in Ref. [1]

Interface Trap Basics - III

For simplicity, assuming $D_{it}(E_t,\mathbf{r})$ = constant = D_{it}, the integration over energy can be carried out analytically, i.e.,

$$N_{at} = -\int_{E_i}^{E_c} \frac{D_{it}}{1 + g_a exp\left(\frac{E_t - E_F}{k_B T}\right)} dE_t = k_B T D_{it} ln \left| \frac{g_{a+\exp(x_u)}}{g_{a+\exp(x_l)}} \right|$$

$$x_u = \frac{E_F - E_c}{k_B T} \qquad x_l = \frac{E_F - E_i}{k_B T}$$

$$N_{dt} = \int_{E_v}^{E_i} \frac{D_{it}}{1 + g_d exp\left(\frac{E_F - E_t}{k_B T}\right)} dE_t = k_B T D_{it} ln \left| \frac{g_{d+\exp(y_u)}}{g_{d+\exp(y_l)}} \right|$$

$$y_u = \frac{E_i - E_F}{k_B T} \qquad y_l = \frac{E_v - E_F}{k_B T}$$

$$N_{it} = N_{at} + N_{dt} = k_B T D_{it} ln \left| \frac{g_{a+\exp(x_u)}}{g_{a+\exp(x_l)}} \right| + k_B T D_{it} ln \left| \frac{g_{d+\exp(y_u)}}{g_{d+\exp(y_l)}} \right|$$

Interface Trap Implementation in QCAD

Given the Poisson equation (in physical units),

$$-\nabla \cdot (\varepsilon_0 \varepsilon_r \nabla \phi) - q(p - n + C) = 0 \qquad \text{C} = {N_d}^{+} - {N_a}^{-}$$

QCAD solves the finite element weak form of the partially scaled equation,

$$\int \varepsilon_r \nabla \phi \cdot \nabla w d\Omega - \frac{q{x_0}^2}{\varepsilon_0} \int (p - n + C) w d\Omega = 0$$

Finite element volume basis function

Spatial scaling parameter

Interface trap charge is included as an additional term in the weak form,

$$\int \varepsilon_r \nabla \phi \cdot \nabla w d\Omega - \frac{q{x_0}^2}{\varepsilon_0} \int (p - n + C) w d\Omega - \frac{q x_0}{\varepsilon_0} \int N_{it} w_s dA = 0$$

Finite element surface basis function

Must integrate over an area

Interface Trap Implementation in QCAD

Suzey checked the code changes to the github repository on January 4, 2016

1. examples/QCAD/Poisson/materials.xml - add "sioxideinterface"
2. src/PHAL_FactoryTraits.hpp
- add id_qcad_poissonsource_interface to NeumannFactoryTraits struct
3. src/QCAD/CMakeLists.txt - add QCAD::PoissonSourceInterface to the list of evaluators
4. src/QCAD/evaluators/QCAD_PoissonSourceNeumann_Def.hpp no real change
5. src/QCAD/problems/QCAD_PoissonProblem.cpp
- Add "interface trap" to condNames
- Use "RCP<std::vector<string> > bcs" instead of "vector<string> bcs" to avoid compiling errors
- Add "bcs->push_back(NeuPoissonSrc);" when building the PoissonSourceNeumann evaluator
- Add "Schottky Barrier" and "Interface Traps" as a valid ParameterList in an input xml
- Add appropriate code to build the PoissonSourceInterface evaluator, similar to building PoissonSourceNeumann evaluator
6. src/QCAD/problems/QCAD_PoissonProblem.hpp
- add getPoissonSourceInterfaceEvaluatorParams(.) member function
7. src/problems/Albany_AbstractProblem.cpp
- add "Interface Traps" as a valid ParameterList in an input xml
8. create QCAD::PoissonSourceInterface evaluator to add voltage-dependent interface trap charge to the finite element weak form of the Poisson equation; it is modified from QCAD::PoissonSourceNeumann evaluator.

Interface Trap Specification in QCAD

Create a sideset in Cubit called sioxideinterface

```
<ParameterList name="Neumann BCs">
    <Parameter name="NBC on SS sioxideinterface for DOF Phi set interface trap"
type="Array(double)" value="{0}" />
</ParameterList>
```

Currently supports Uniform only

g_a

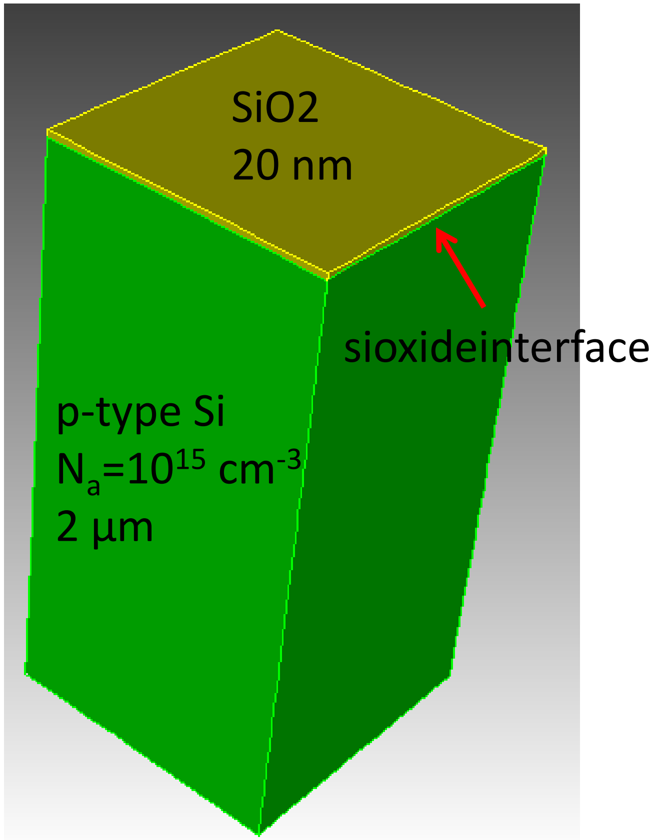
```
<ParameterList name="Interface Traps">
   <ParameterList name="Interface Trap for SS sioxideinterface">
     <Parameter name="Energy Spectrum" type="string" value="Uniform" />
     <Parameter name="Acceptor Degeneracy Factor" type="double" value="1" />
     <Parameter name="Donor Degeneracy Factor" type="double" value="1" />
     <Parameter name="Trap Density" type="double" value="1e12" />
     <Parameter name="Trap Type" type="string" value="Both" />
   </ParameterList>
</ParameterList>
```

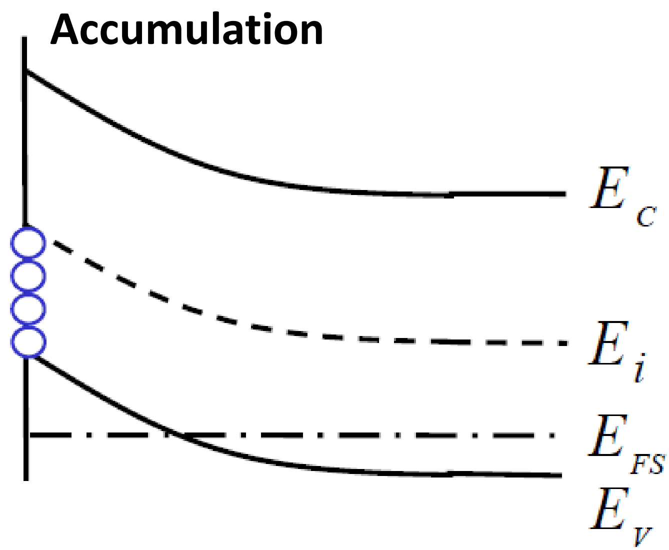
g_d

In units of [#/(eV.cm^2)]

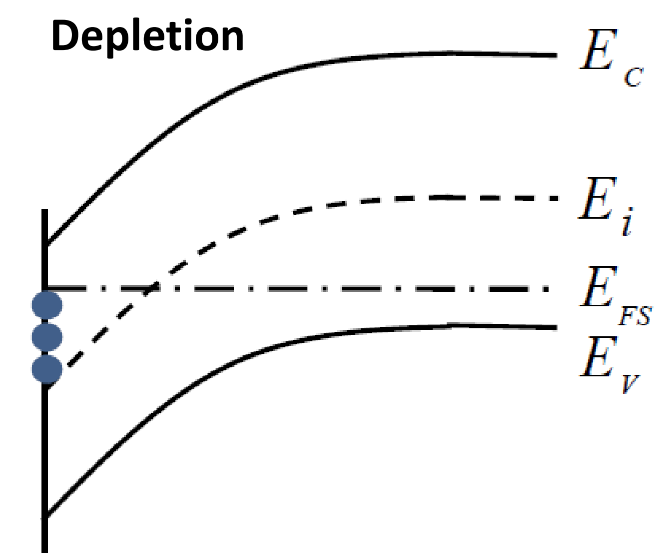
Trap Type can be either Donor, Acceptor, or Both
(For Both, acceptor trap above Ei and donor trap below Ei)

Test Structure – PMOS Capacitor



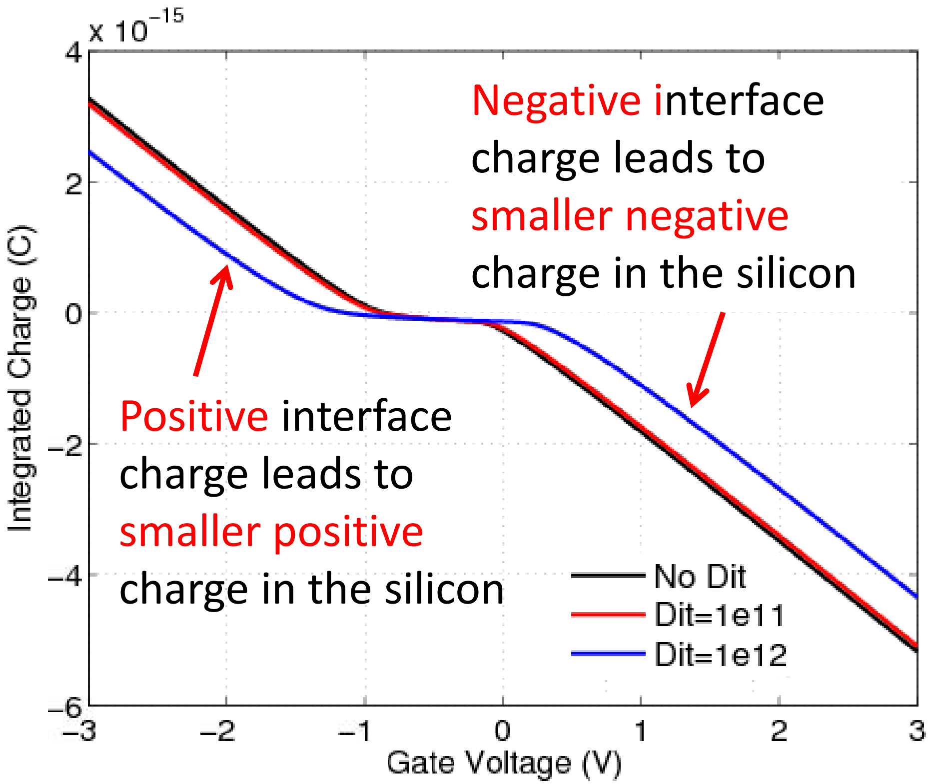


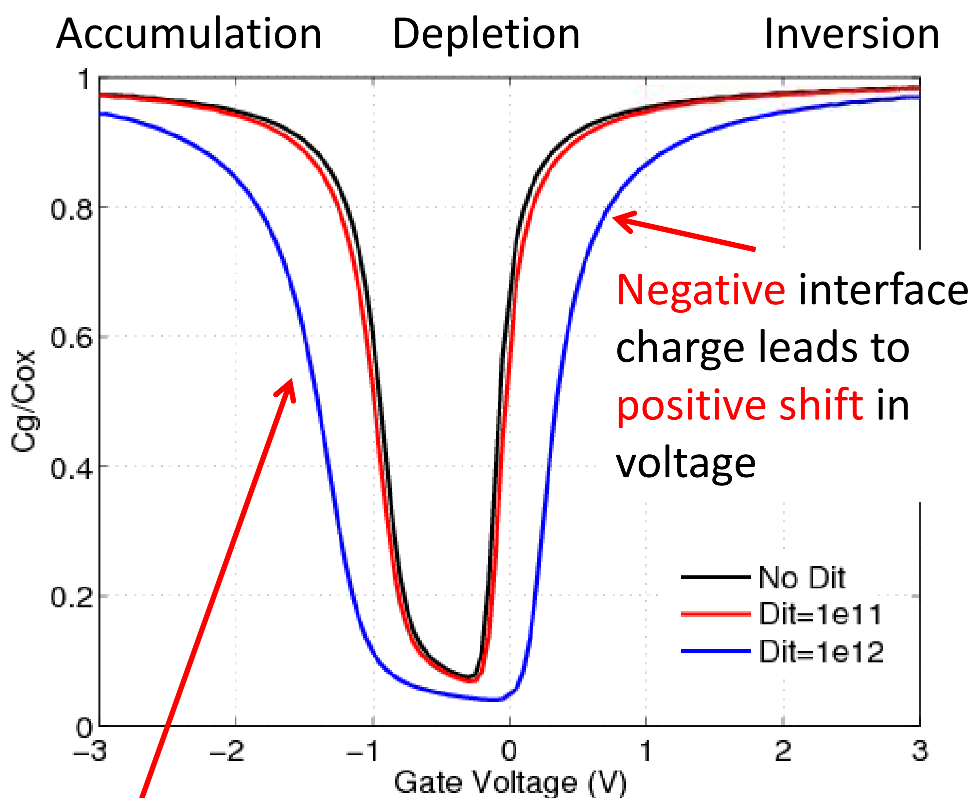
The excess positive interface charge leads to negative shift in voltage



The excess negative interface charge leads to positive shift in voltage

Effect of Interface Trap Density

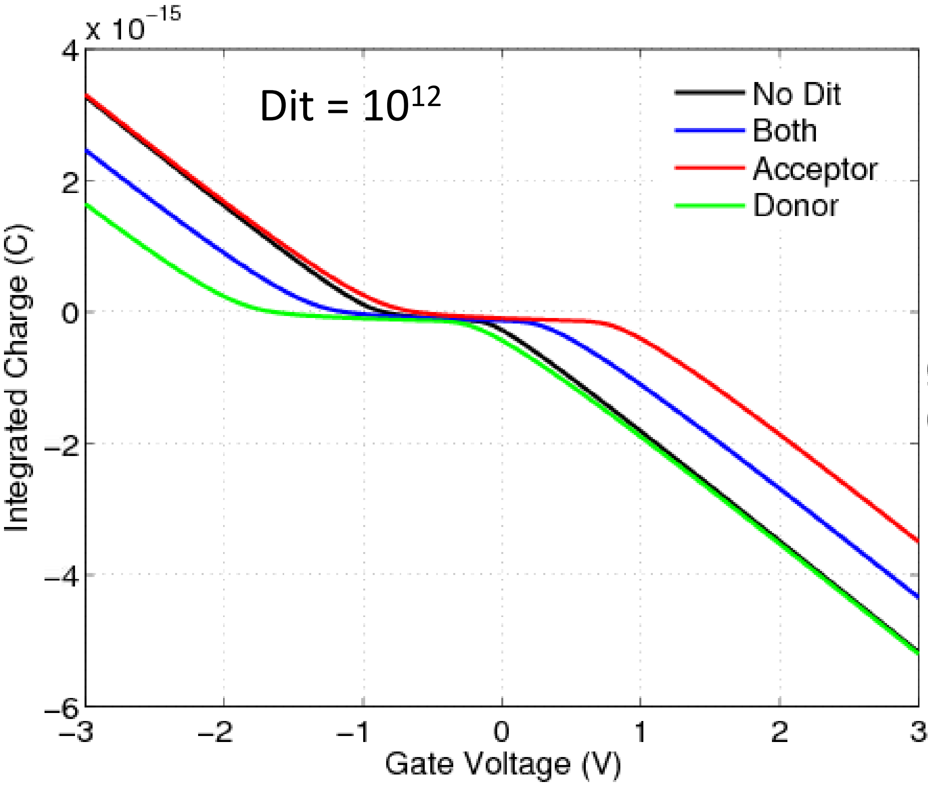


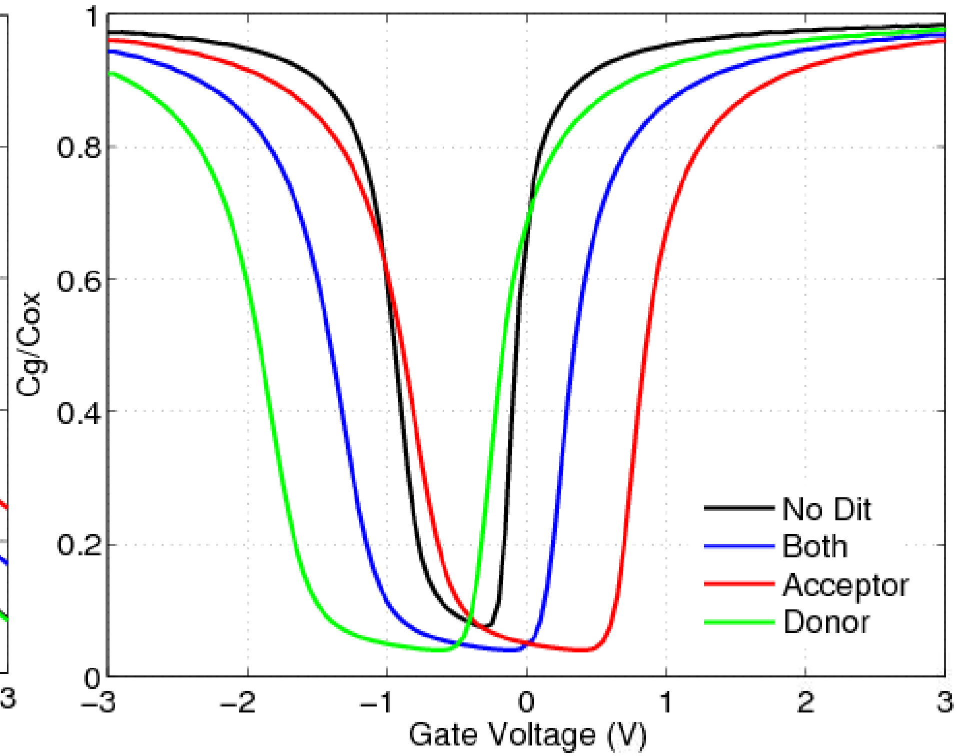


Positive interface charge leads to negative shift in voltage

$$C_g = \frac{-dQ_s}{dV_g}$$ DC capacitance

Effect of Interface Trap Type





- Different types of interface traps show quite different effects on the integrated charge in silicon, and on the gate capacitance.

Summary

- ❑ Interface traps have been implemented in the QCAD Poisson solver, which supports acceptor, donor, or both types of traps, and uniform trap density
- ❑ Test results on a PMOS capacitor indicate that interface traps show expected effects on the integrated charge and on the gate capacitance

Possible future work:

- ❑ Further testing and comparison with a known example is desired
- ❑ Implementation of a more realistic energy spectrum (e.g., a U-shaped spectrum, Gaussian decay from Ec and Ev) for interface traps
- ❑ Introduce spatial dependence in the trap space distribution
- ❑ Etc.