Study of Charge Carrier Distribution in an OLWA Unit Cell using COMSOL

Summary of research activity carried out by Eric Mannarino during summer 2012
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1. Introduction

In the study of the optical leaky wave antenna (OLWA) that comprises silicon (Si) perturbations it is important to determine the carrier concentration within the silicon regions to retrieve the Si complex optical refractive index under electric or optical stimulation. Using COMSOL's built in continuity equations along with the Shockley-Read-Hall equation for recombination, a model was designed to look at carrier distribution within the three main subdomains (Fig. 1) and along boundaries. Three modules were used for the model: one electrostatics (to model band bending and internal voltage caused by differences in carrier concentrations), and two convection/diffusion modules (one each to model electron and hole distribution).

The model consists of three regions as shown in figure 1. The upper region is the silicon nitride waveguide, the lower region is the silicon dioxide substrate, and the middle region is the silicon perturbation (un-doped). These regions each have their own recombination terms based on their material properties.

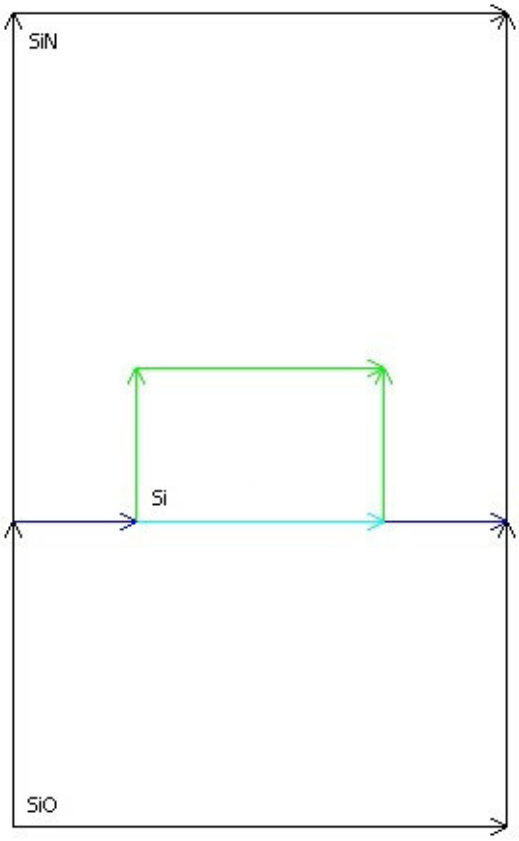


Figure 1. SiN is silicon nitride (Si_3N_4), Si is the silicon (Si) perturbation, and SiO is the silicon dioxide (SiO_2) substrate.

2. Problem Setup

The objective of this analysis is to determine the electron and hole carrier distributions inside the silicon (Si) region. Recombination at boundaries accounted for by assuming that all carriers from the silicon nitride or silicon oxide region annihilate carriers exiting the silicon perturbation. This is a relatively insignificant amount since there are few charge carriers in the insulators, and most of the recombination is expected to happen within the regions. The generation rate that is given as a constant for this model can be later used to create a parametric sweep of charge carrier distribution based on generation rates.

Most of the equations used to describe carrier distribution are built into the COMSOL modules. The Schottky Read Hall recombination model is not, and the iterations used are shown in Figure 3.
The continuity equation used to describe charge carrier density under time dependant phenomena (such as carrier generation and recombination) is given as Equation (1) and (2) where n pertains to the negative charge carriers (electrons) and p to the positive charge carriers (holes).

$$\frac{\partial n}{\partial t} = G_n + U_n + \frac{1}{q}\nabla \cdot J_n \quad (1)$$

(1)

$$\frac{\partial p}{\partial t} = G_p + U_p - \frac{1}{q}\nabla \cdot J_p \quad (2)$$

G is the given generation rate
U is the recombination rate
J is the charge carrier current density [Eqs. (3), (4)]

$$J_n = q\mu_n n\mathcal{E} + qD_n\nabla \mathrm{n} \quad (3)$$

$$J_p = q\mu_p p\mathcal{E} + qD_p\nabla \mathrm{p} \quad (4)$$

D is the diffusion coefficient
n and p are the electron and hole concentrations
μ is the charge carrier mobility

Surface recombination occurs between the Si-Si_3N_4 and Si-SiO_2 boundaries. This action is described for the minority carriers by equation (5), where x=0 is the boundary location.

$$qD_p \left.\frac{dp_n}{dx}\right|_{x=0} = qS_p[p_n(0) - p_{no}] \quad (5)$$

S is the surface recombination velocity
p_{no} is the hole concentration in thermal equilibrium

The COMSOL implementation is described next.

3. Model Description and Simulation Setup

The settings for the constants and scalar expressions are given in figures 2 and 3.

Settings for boundary and subdomain conditions are given as follows:

For the electrostatics module:

External boundaries are set to ground and internal boundaries are set to continuity. Each subdomain's initial conditions are set to 0, the Constitutive relation is set as $D=\varepsilon_0\varepsilon_r E$; the layer thickness is set as d=970nm (to match the height of the Si_3N_4 region); space charge density is set as $\rho=q*(n_i-c_n+c_p)$ (where

n_i is replaced by the carrier concentration relevant to the particular subdomain and c_n and c_p are the charge carrier concentrations); and ε_r is set to the relevant value for the subdomain.

For the convection and diffusion (electron) module:

External boundaries are set as insulation/symmetry. The Si-Si_3N_4 and Si-SiO_2 boundaries are set as concentration with cn_0=ni_Si- ni_SiN and cn_0=ni_Si- ni_SiO respectively. The Si_3N_4-SiO_2 boundary is set as continuity.

The subdomain settings for Si_3N_4 are diffusion coefficient D (isotropic) = Dn_SiN; recombination R= -SRHR_SiN; x-velocity u=mun_SiN*psix; and y-velocity v= mun_SiN*psiy. The initial conditions are set as ni_SiN.

The subdomain settings for SiO_2 are diffusion coefficient D (isotropic) = Dn_SiO; recombination R= -SRHR_SiO; x-velocity u=mun_SiO*psix; and y-velocity v= mun_SiO*psiy. The initial conditions are set as ni_SiO.

The subdomain settings for Si are diffusion coefficient D (isotropic) = Dn_Si; recombination (with some generation rate G) R=-SRHR_Si+G; x-velocity u=mun_Si*psix; and y-velocity v= mun_Si*psiy. The initial conditions are set as ni_Si.

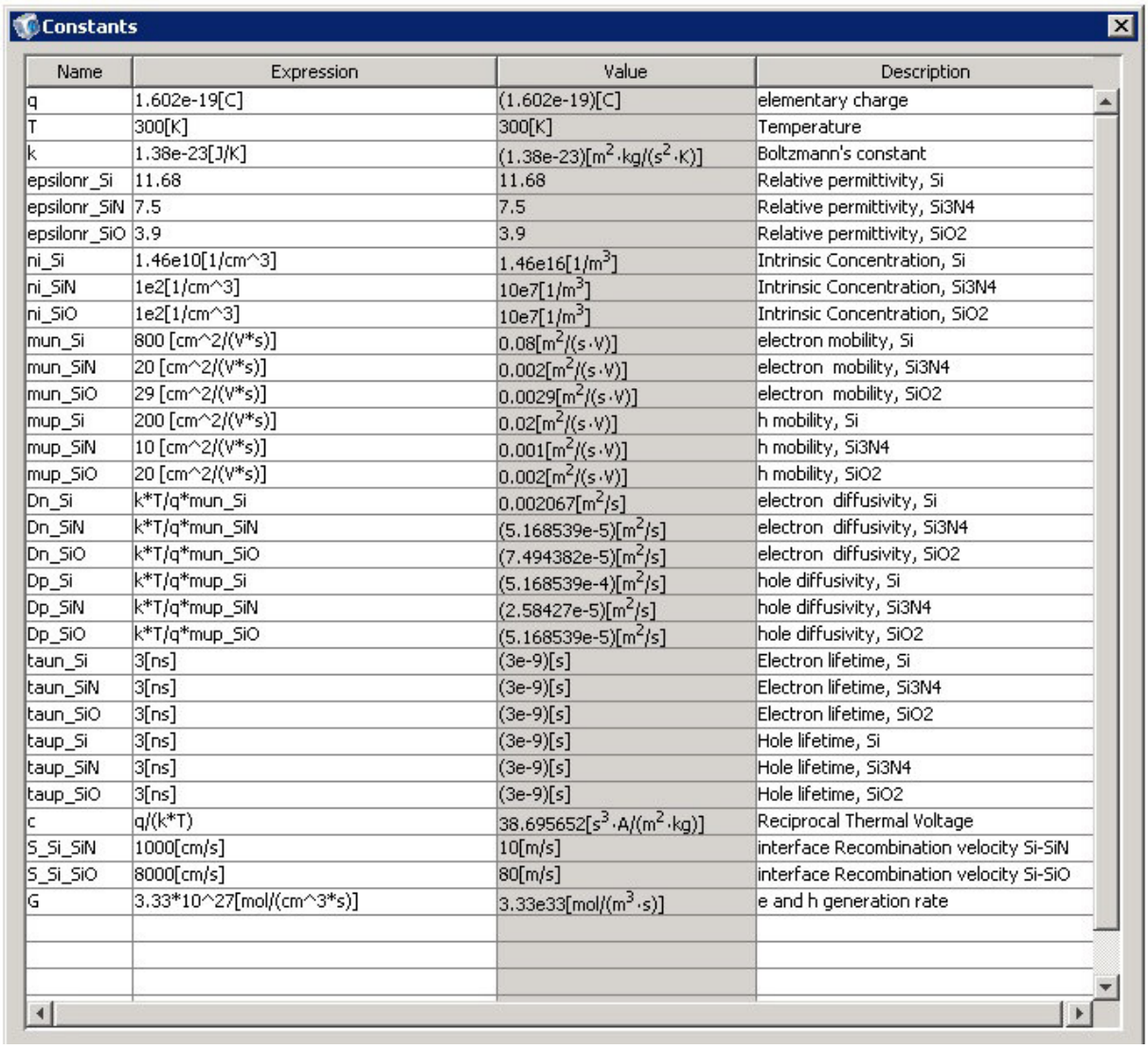
For the convection and diffusion (hole) module:

External boundaries are set as insulation/symmetry. The Si-Si_3N_4 and Si-SiO_2 boundaries are set as concentration with cp_0=ni_Si-ni_SiN and cp_0=ni_Si-ni_SiO. The Si_3N_4-SiO_2 boundary is set as continuity.

The subdomain settings for Si_3N_4 are diffusion coefficient D (isotropic) = Dp_SiN; recombination R= -SRHR_SiN; x-velocity u=mup_SiN*psix; and y-velocity v= mup_SiN*psiy. The initial conditions are set as ni_SiN.

The subdomain settings for SiO_2 are diffusion coefficient D (isotropic) = Dp_SiO; recombination R= -SRHR_SiO; x-velocity u=mup_SiO*psix; and y-velocity v= mup_SiO*psiy. The initial conditions are set as ni_SiO.

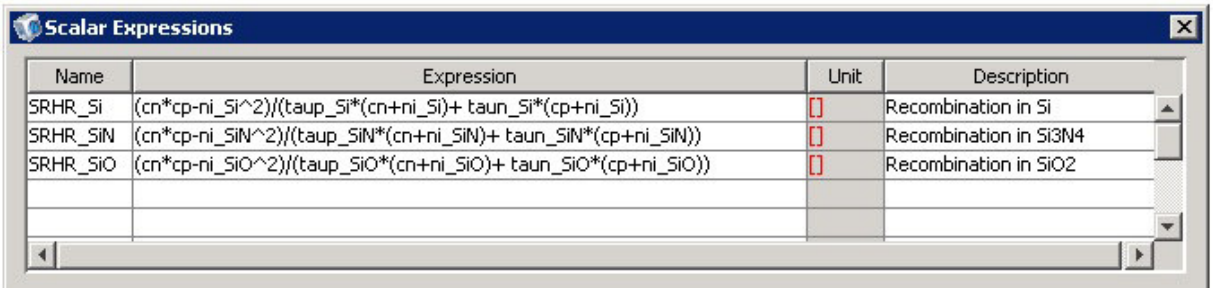
The subdomain settings for Si are diffusion coefficient D (isotropic) = Dp_Si; recombination (with some generation rate G) R=-SRHR_Si+G; x-velocity u=mup_Si*psix; and y-velocity v= mup_Si*psiy. The initial conditions are set as ni_Si.



Constants

Name	Expression	Value	Description
q	1.602e-19[C]	(1.602e-19)[C]	elementary charge
T	300[K]	300[K]	Temperature
k	1.38e-23[J/K]	(1.38e-23)[$m^2 \cdot kg/(s^2 \cdot K)$]	Boltzmann's constant
epsilonr_Si	11.68	11.68	Relative permittivity, Si
epsilonr_SiN	7.5	7.5	Relative permittivity, Si3N4
epsilonr_SiO	3.9	3.9	Relative permittivity, SiO2
ni_Si	1.46e10[1/cm^3]	1.46e16[$1/m^3$]	Intrinsic Concentration, Si
ni_SiN	1e2[1/cm^3]	10e7[$1/m^3$]	Intrinsic Concentration, Si3N4
ni_SiO	1e2[1/cm^3]	10e7[$1/m^3$]	Intrinsic Concentration, SiO2
mun_Si	800 [cm^2/(V*s)]	0.08[$m^2/(s \cdot V)$]	electron mobility, Si
mun_SiN	20 [cm^2/(V*s)]	0.002[$m^2/(s \cdot V)$]	electron mobility, Si3N4
mun_SiO	29 [cm^2/(V*s)]	0.0029[$m^2/(s \cdot V)$]	electron mobility, SiO2
mup_Si	200 [cm^2/(V*s)]	0.02[$m^2/(s \cdot V)$]	h mobility, Si
mup_SiN	10 [cm^2/(V*s)]	0.001[$m^2/(s \cdot V)$]	h mobility, Si3N4
mup_SiO	20 [cm^2/(V*s)]	0.002[$m^2/(s \cdot V)$]	h mobility, SiO2
Dn_Si	k*T/q*mun_Si	0.002067[m^2/s]	electron diffusivity, Si
Dn_SiN	k*T/q*mun_SiN	(5.168539e-5)[m^2/s]	electron diffusivity, Si3N4
Dn_SiO	k*T/q*mun_SiO	(7.494382e-5)[m^2/s]	electron diffusivity, SiO2
Dp_Si	k*T/q*mup_Si	(5.168539e-4)[m^2/s]	hole diffusivity, Si
Dp_SiN	k*T/q*mup_SiN	(2.58427e-5)[m^2/s]	hole diffusivity, Si3N4
Dp_SiO	k*T/q*mup_SiO	(5.168539e-5)[m^2/s]	hole diffusivity, SiO2
taun_Si	3[ns]	(3e-9)[s]	Electron lifetime, Si
taun_SiN	3[ns]	(3e-9)[s]	Electron lifetime, Si3N4
taun_SiO	3[ns]	(3e-9)[s]	Electron lifetime, SiO2
taup_Si	3[ns]	(3e-9)[s]	Hole lifetime, Si
taup_SiN	3[ns]	(3e-9)[s]	Hole lifetime, Si3N4
taup_SiO	3[ns]	(3e-9)[s]	Hole lifetime, SiO2
c	q/(k*T)	38.695652[$s^3 \cdot A/(m^2 \cdot kg)$]	Reciprocal Thermal Voltage
S_Si_SiN	1000[cm/s]	10[m/s]	interface Recombination velocity Si-SiN
S_Si_SiO	8000[cm/s]	80[m/s]	interface Recombination velocity Si-SiO
G	3.33*10^27[mol/(cm^3*s)]	3.33e33[$mol/(m^3 \cdot s)$]	e and h generation rate

Figure 2. The values for constants used in this model



Scalar Expressions

Name	Expression	Unit	Description
SRHR_Si	(cn*cp-ni_Si^2)/(taup_Si*(cn+ni_Si)+ taun_Si*(cp+ni_Si))	[]	Recombination in Si
SRHR_SiN	(cn*cp-ni_SiN^2)/(taup_SiN*(cn+ni_SiN)+ taun_SiN*(cp+ni_SiN))	[]	Recombination in Si3N4
SRHR_SiO	(cn*cp-ni_SiO^2)/(taup_SiO*(cn+ni_SiO)+ taun_SiO*(cp+ni_SiO))	[]	Recombination in SiO2

Figure 3. The recombination equations used for this model

4. Simulation Results

In this initial simulation, the linear system solver used was Direct (PARDISO out of core), with stationary analysis for both electron and hole convection and diffusion. The solver used was also stationary. It should be noted that, once the values are refined (more on that in conclusion), a parametric sweep for generation rates could be made. In the stationary tab, relative tolerance was set at 1.0×10^{-6}, with a maximum of 50 iterations. The problem was solved as a highly nonlinear problem, with the check box for "Damped Newton" selected (automatic damping parameters).

Figure 4 a and b show two views of the logarithmic graph for electron carrier concentration [$\log_{10}(cn)$].

Figure 5 a and b show two views of the logarithmic graph for hole carrier concentration [$\log_{10}(cp)$].

5. Conclusion

The plots found for carrier concentration represent what the expected distribution should be. Although the model is accurate, some of the values used for the constants may not be. This will affect the shape of the graphs slightly, as well as the numbers given by the graphs. The constants in question are the following:

mun_SiN and mup_SiN - electron and hole charge carrier mobilities for silicon nitride (Si_3N_4) (estimated based on values found for the mobilities in SiO_2)

ni_SiN and ni_SiO - charge carrier concentrations for silicon dioxide (SiO_2) and silicon nitride (Si_3N_4) (given arbitrarily low values since the materials are insulators)

taun and taup for SiO_2 and Si_3N_4 - electron and hole lifetimes (generalized from carrier lifetime in silicon perturbation, 2.93ns)

G - general value for carrier generation rate in the silicon perturbation

Overall, this model is very close to being usable, as it only require minor refining of the aforementioned values. Also, surface recombination could be refined to be more accurate.

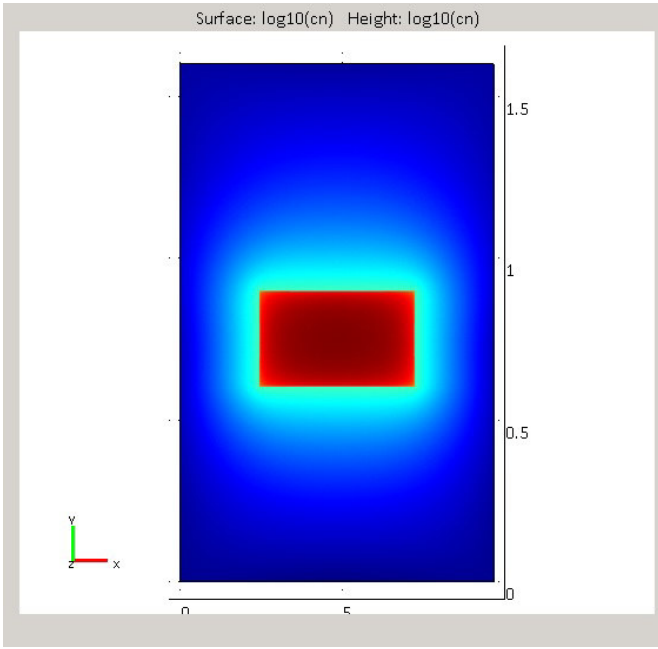


Figure 4a. Surface plot of $\log_{10}(cn)$

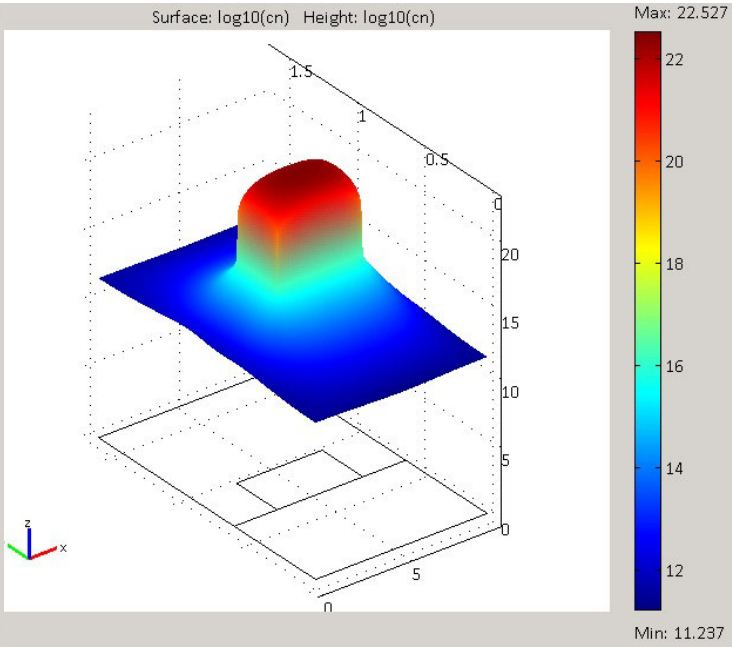


Figure 4b. Surface and height plot of $\log_{10}(cn)$

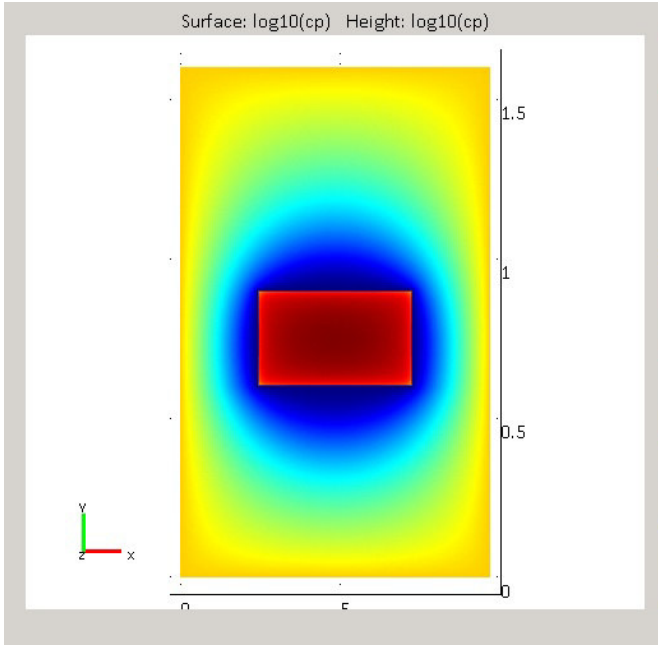


Figure 5a. Surface plot of $\log_{10}(cp)$

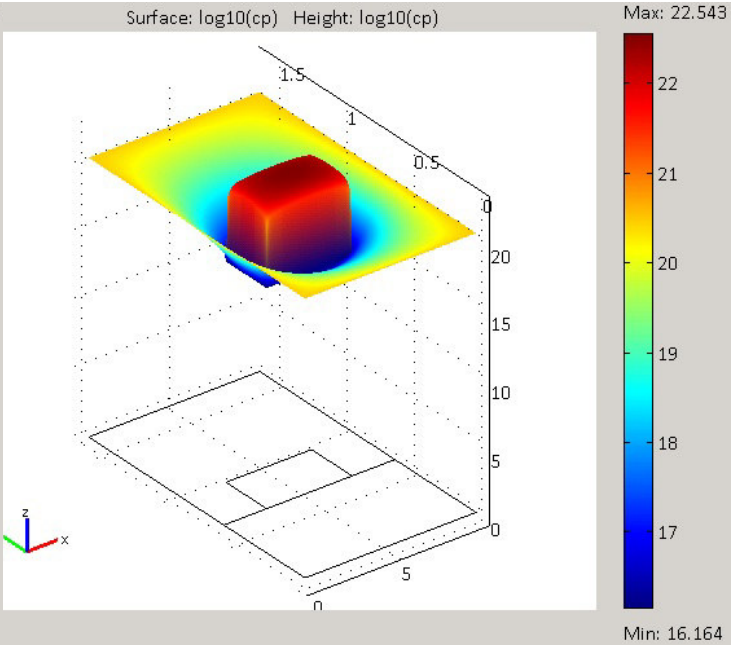


Figure 5b. Surface and height plot of $\log_{10}(cp)$

References

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