

DeOSt Simulation

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Introduction

This program simulates several characterization techniques that can be applied to photoconductive semiconductors : the Modulated PhotoCurrent (MPC) experiment, the steady-state dark and photoconductivity (SSPC) experiment, the Constant Photocurrent Method (CPM) in AC and DC, the Dual Beam Photoconductivity (DBP), the Transient PhotoCurrent (TPC), the Steady-State Photocarrier Grating (SSPG), the Moving Grating Techniques (MGT), the Oscillating Photocarrier Grating technique (OPG) and the Photo-Induced Transient Spectroscopy (PITS). It calculates also the absorption of a user-defined material.

The material is defined via a density of localized states in the gap. This density of states (DOS) can include :

- Four monovalent acceptor states (0 if empty, - if occupied)
- Four monovalent donor states (0 if occupied, + if empty)
- One conduction band tail equivalent to a monovalent acceptor state
- One valence band tail equivalent to a monovalent donor state
- Three densities of amphoteric states (-/0/+)
- Three densities of multivalent states (0/+ /++)
- One defect pool of amphoteric states (-/0/+)

The other material parameters (energy gap, conduction and valence band density of states, carrier mobilities, etc...) can be adjusted.

‘Experimental’ parameters (flux, temperatures, frequency etc...) can be chosen by the user.

All the calculated results (MPC, SSPC, absorption, CPM, DBP, TPC, SSPG, MGT, OPG, PITS) are saved in **files**, can be **plotted** and compared to experimental results afterward.

Main Window

On opening the Main window is blank and the only menus available are **Files** and **Plots**. The **Files** menu allows opening of a data file for further calculation and the **Plots** menu allows plot of the results of a previous calculation. The choice of a data file with the **Files** menu opens the Data window.

Once a data file has been chosen another menu can be opened : **Definition**.

A click on **Definition** followed by a click on **Data** opens the Fermi level window and a Concentration window. These two windows can be opened also by a click on **Display** in the Data window. A click on **Display** plots the density of states (DOS) and opens also a window with a plot of the density of states.

Once a data file has been chosen and opened all the menus are available including **Calculations** and **Format**.

The Data window contains all the parameters concerning the density of states and experimental parameters used during calculations. These parameters can be modified, adjusted and then saved into a data file (extension **.dat**). For more details see **Definition**.

To modify a parameter in the Data window, you have to follow the procedure detailed below.

Click on the down arrow of the data box you want to modify. The various labels and values of the parameters appear in a box.

Select the parameter you want to modify and click on it. Use the scroll bar if necessary.

Type the new value of the parameter directly on the highlighted characters and press ENTER.

You can check that the parameter value has been modified by repeating the first step and/or by clicking on **Display**.

Note that a check box is located on top of the data boxes corresponding to the definition of states distributions. If the box is checked, the contribution of these states to the MPC calculation is taken into account. Otherwise the contribution of the corresponding states to MPC is ignored. It allows to investigate on the individual contribution of each state to MPC signal but BE CAREFUL the global contribution is NOT the sum of each individual contribution. So these check boxes are just a help in the adjustment of the parameters of a particular distribution to determine its influence on the global MPC spectrum.

In this Main window will also be displayed, the density of states as defined by the user, the evolution of the states occupancy during a calculation and all the plots resulting from previous calculations.

The Fermi level window displays the energy position of the Fermi level E_F of the introduced density of states at $T = 300\text{K}$ at the opening of a data file and at the temperature of the calculation during all the calculations. The energy reference is the top of the valence band.

The Concentration window displays the concentrations (cm^{-3}) of the different densities of states distributions available in the Data window. For the multivalent states the concentrations are given by type of charge as well as the total concentration.

A Calculation window appears also while the program is running.

It displays the DC flux (F_{dc}) and the temperature at which the calculation is made, the generation rate (Gener.), the recombination rate (Recomb.) and the step number while the calculation is performed to match these two values as well as the electrical neutrality. The maximum number of steps is 500. This value can be reached if the differences between dark and illuminated values are small so that the program cannot converge toward the exact values. A message appears then asking if the user wants to proceed to the next temperature, if there is, or ends the calculation.

Values of n and p (cm^{-3}), concentrations of electrons and holes respectively, are given as well as the dark values of these quantities (n_0 and p_0). The lifetimes τ_{ae} for electrons and τ_{ah} for holes are also displayed.

Some other quantities can also appear like the gamma coefficient (g) of the photoconductivity, the frequencies (in Hz) at which the light is modulated for MPC simulations, the photon energy (in eV) for CPM and DBP calculations, the matrix dimension in TPC, the time evolution in PITS, etc depending on the type of calculation asked by the user.

Files

All the files saved by the program are ASCII files that can be read with the Notepad of Windows®.

The data files are saved in the directory \simulati\resultpc\ with the extension **.dat**.

- To open a file, click on **Files** then on **Open**. Go to the folder \simulati\resultpc\ if needed. A window opens showing all the data files save on the disk. Choose one and click **OK** or double click on the name. The Data window, containing all the parameters opens. A click on **Display** in this window plots the density of states associated to the data file and opens the Concentration window as well as the Fermi level window All the headings of the Menu are highlighted and one can proceed to any option.
- To save a file, click on **Files** then on **Save**. Go to the folder \simulati\resultpc\ if needed. A window opens showing the saved files and the path to the directory where the file will be saved. Give a name to your file (Myfile) and click **OK**. It is not necessary to give the extension **.dat** that will be added automatically. If the file already exists a warning is displayed. Click **Yes** to proceed and **No** to abort. If the DOS is plotted (e.g. after a click on **Display** of the Data window) a new window opens asking "Do you want to save the DOS?". If one answers **Yes** then the density of states as defined is saved in \simulati\resultpc\ the following way : Myfile_***.txt where *** is :
CBT for the conduction band tail, VBT for the valence band tail, Acci or Doni for the monovalent states ($1 \leq i \leq 4$)
DBn for the multivalent states ($1 \leq n \leq 6$), DnP, Dn0, DnM for the positive (or ++), neutral (or +) and negative (or 0) charged states respectively
POOL for the pool, POOLP, POOL0, POOLM for the positive, neutral and negative states of the Pool respectively
- Since files are rapidly accumulating on the disk, it is possible to delete some of them. Choose the **Delete** option in the **Files** menu. A window opens in which you can then select the name of the file to be deleted. A click on **OK** opens a message window. **ALL**

the files related to the chosen name will be deleted (i.e. all the files resulting from calculations based on the data file you have chosen). A click on **NO** abort the deleting session.

- To exit the program, click on **Files** then on **Exit**. A window opens asking "Are you sure?". A click on **Yes** ends the program.

The calculated files are saved on different directories with different extensions depending on their origin.

- The modulated photocurrent files resulting from the calculation of the **Modulated photocurrent** are saved in the directory \simulati\resulpcm\ under the following form : Myfile_**temp.txt**, 'temp' being the temperature (in K) at which the calculation was done. There are as many files as there were temperatures.
- The photoconductivity files resulting from the calculation of the **photoconductivity** are saved in \simulati\resultpc\ with a **.np** extension (Myfile.**np**). The results of the calculations on the gamma coefficient are saved in \simulati\resultpc\ with a **.gam** extension (Myfile.**gam**).
- The absorption files resulting from the calculation of the **absorption** are saved in \simulati\resulabs\ with a **.abs** extension (Myfile.**abs**). The DC **CPM** is saved in the same directory with an extension **.cpm**. The AC **CPM** and **DBP** files are saved in the same directory with an extension **.apm** and **.dbp** respectively. Finally, in this directory are saved files containing information on the tangent of the phase shift measured in AC CPM (extension **.atg**) or in DBP (extension **.tgt**).
- The Transient photocurrent files resulting from the calculation of the **TPC** are saved in \simulati\resultpc\ with a **.idt** extension (Myfile.**idt**) for the 'current' files and **.qdt** (Myfile.**qdt**) for the charge files.
- The SSPG and MGT files resulting from the calculation of the **SSPG** and **MGT** are saved in \simulati\resultsspg\Myfile\ with a **.spg** extension (Myfile_**temp.spg**) for the SSPG files and **.mgt** (Myfile_**temp.mgt**) for the **MGT** files, where 'temp' is the temperature (K) at which the simulation was done. A file containing an estimate of the density of states (NC/μ) from the **SSPG** calculation (Myfile.**bet**) is saved in \simulati\resultpc\.
- The OPG files calculated with the **OPG** option are saved in \simulati\resultopg\Myfile\ with an extension **.opg**. The files containing data calculated for the positive part of the wave are saved with a plus (Myfile_**+temp.opg**) and the files containing data calculated for the negative part of the wave are saved with a minus (Myfile_**-temp.opg**).
- The PITS files resulting from the calculation of the **PITS** are saved in \simulati\resultpit\Myfile\ with a **.pit** extension (Myfile_**pulsewidth_temp.pit**). Plotting the PITS files with DeOSt will create new files in a dedicated folder called PITS.
- The TFT files resulting from calculations on a **TFT** are saved in \simulati\resulttft\ . The potential distributions for each voltage are saved in files the names of which are built from the data file name, i.e. Myfile#**number.tft**, the number being that of the order in which the calculation was done. The variations of the conductivity vs the applied voltage are saved in the same resulttft folder under a file named Myfile.**ivg**.

The modulated photocurrent files can be formatted by the **Format** menu to be treated in a new way or as if they were experimental data. Once formatted, new files appear in

\simulati\resulpcm\ labeled Myfile_**temperature****TRAIT.txt**, in \simulati\resultpc\ labeled Myfile_**TRAIT.txt** and in \simulati\ labeled Myfile.**rou**. A file with the extension **.gac** is created resulting from the calculation of *gamma* (from the well known relation $I_{ph} \sim F^{\gamma}$) using the AC data of the modulated photocurrent calculation. This file is saved in \simulati\resultpc\.

Definition

This menu allows display of the data of a **.dat** file, to modify this data, to plot the density of states or the NC/μ quantity as function of energy, and to print these data and the graphs.

To display the data of a **.dat** file click on **Definition** then on **Data** : a Data window opens in the Main Window containing all the parameters that can be modified. If some modifications have been done on the data but this new data was not saved it is possible to come back to the original data by a click on **Definition** then on **Data**. This action resets all the data to the original values. It also opens a window, on the right hand side of the main window, in which the concentrations (cm^{-3}) of all the defined distributions are displayed.

To define a DOS one can use any of the proposed state distributions. So, a DOS can be made of :

- Four monovalent acceptor states (Acceptor 1-4)
- Four monovalent donor states (Donor 1-4)
- Six multivalent correlated states (Multi 1-6)
- One defect-pool
- Two band tails (CBT & VBT)

In a box labeled Exp. Data one can change some of the parameters of the simulated material but also some "experimental" parameters such as flux, frequency, temperature, temperature step, etc...

To modify a parameter, you have to follow the procedure detailed below.

Click on the down arrow of the data box you want to modify. The various labels and values of the parameters appear in a box.

Select the parameter you want to modify and click on it. Use the scroll bar if necessary.

Type the new value of the parameter directly in place of the highlighted characters and press ENTER.

You can check that the parameter value has been modified by repeating the first step and/or by clicking on **Display**.

Note that a check box is located on top of the data boxes corresponding to the definition of states distributions. If the box is checked, the contribution of these states to the MPC calculation is taken into account. Otherwise the contribution of the corresponding states to MPC is ignored. It allows investigations on the individual contribution of each defect to the MPC signal but BE CAREFUL the global contribution is NOT the sum of each individual contribution. These check boxes are just a help in the adjustment of the parameters of a particular distribution to determine its influence on the global MPC spectrum.

The position of the Fermi level at $T = 300$ K is calculated and displayed in the box labeled 'Ef0 – Ev'. This position is calculated by checking the electrical neutrality taking account of the state of charge of the defects and of the free carrier densities.

A click on **Display** plots the defined density of states at $T = 300$ K. Another way to plot the density of states is to click on **Definition** then on **pLots** and finally on **Density**. The band tails are displayed in blue, the acceptors in cyan, the donors in red, the correlated states in green with, for instance, the (-) in brown, the (0) in blue and the (+) in violet.

It is possible to plot also NC/μ for a given material. For this plot the gap is folded in two and the origin is both at the bottom of the conduction band and top of the valence band. Each defect is plotted with its appropriate N , C and μ . So each defect is plotted twice : first for the electrons (NC_n/μ_n) in blue and second for the holes (NC_p/μ_p) in green. Since the MPC technique always probes the lowest NC/μ , one can have an idea of what defects will be probed, by which type of carriers and how it will look like by looking at the lowest profile of the NC/μ plot.

Finally, one can have a print out of the parameters, or of the density of states or of NC/μ by a click on **Print** and then on **Parameters**, **dOs** or **NC/ μ** respectively. The print out uses the default printer connected to the computer.

Definition of the distributions of monovalent states (Acceptor & Donor states)

The acceptor or donor states are made of Gaussian distributions. The state of charge is 0 when full (empty) or positive (negative) when empty (full) for the donors (acceptors). The data of these states is presented as follows :

- N_{max} = maximum value of the state in $\text{cm}^{-3}\text{eV}^{-1}$.
- E_{max} = energy position of N_{max} in eV, the zero of energy being taken at the top of the valence band ($E_v = 0$).
- $Sigma$ = the standard deviation of the gaussian distribution in eV.
The gaussian distribution is then $N(E) = N_{max} \exp[-(E_{max} - E)^2 / 2 / Sigma^2]$
- C_n = the electron capture coefficient in cm^3/s at $T = 300$ K.
- C_p = the hole capture coefficient in cm^3/s at $T = 300$ K.
- $Eactn$ = the power of $T/300$ if one wants to vary C_n as function of T :
 $C_n = C_n(300)(T/300)^{Eactn}$.
- $Eactp$ = the power of $T/300$ if one wants to vary C_p as function of T :
 $C_p = C_p(300)(T/300)^{Eactp}$.
- C_{opt} = optical matrix element in $\text{cm}^{5/2}\text{eV}$. This quantity is used to calculate the coefficient of the convolution product when one calculates optical transitions from (toward) deeper (higher) states toward (from) these states :
 $Coefficient = C_{opt}(\text{first type of states}) * C_{opt}(\text{second type of states}) / h\nu$.

Definition of the band tail states

The band tails can have rather complicated shapes. They can be made of two exponential distributions plus a Gaussian distribution. The valence band tail (VBT) is of donor type and the

conduction band tail (CBT) is of acceptor type. The parameters that can be adjusted for the conduction band tail are :

- T_c = the characteristic temperature of the deepest exponential distribution (K).
 - N_{ext} = the extrapolation of the deepest exponential distribution toward the conduction band edge ($\text{cm}^{-3}\text{eV}^{-1}$).
- Therefore the deepest exponential distribution can be written :
 $N(E) = N_{ext} \exp[-(E_c - E)/kT_c]$, k being the boltzmann constant.
- E_{coup} = the energy position of the intersection of the deepest and the shallowest exponential distribution (eV).

The energy reference of E_{coup} is the valence band edge ($E_v = 0$). The characteristic temperature of the shallowest exponential distribution is calculated and labeled T_{cu} . The extrapolation of this exponential distribution at the conduction band edge is $N(E_c)$ density of states at E_c ($\text{cm}^{-3}\text{eV}^{-1}$).

If one enter 0 or a value lower than 10 for T_c , the program fixes the T_c value at 10 K for calculation considerations but the conduction band tail is then ignored.... Nevertheless, the "conduction band tail" can be used as an acceptor state by means of the gaussian distribution that can be positioned anywhere in the gap.

- N_{max} = the value of the maximum of the Gaussian distribution ($\text{cm}^{-3} \text{eV}^{-1}$).
- E_{max} = the energy position of N_{max} referred from E_v (eV).
- $Sigma$ = the standard deviation of the Gaussian distribution (eV).

The gaussian distribution is then $N(E) = N_{max} \exp[-(E_{max} - E)^2/2/Sigma^2]$

- C_n = capture coefficient for electrons of the CBT states at 300 K (cm^3s^{-1})
- C_p = capture coefficient for holes of the CBT states at 300 K (cm^3s^{-1})
- $Eactn$ = the power of $(T/300)$ if one wants to activate the electron capture cross section:
 $C_n = C_n(300)[T/300]^{Eactn}$
- $Eactp$ = the power of $(T/300)$ if one wants to activate the hole capture cross section:
 $C_p = C_p(300)[T/300]^{Eactp}$
- C_{opt} = optical matrix element in $\text{cm}^{5/2}\text{eV}$. This quantity is used to calculate the coefficient of the convolution product when one calculates optical transitions from (toward) deeper (higher) states toward (from) these states :

$Coefficient = C_{opt}(\text{first type of states}) * C_{opt}(\text{second type of states}) / h\nu$.

The same value is used for the conduction band.

The same type of parameters holds for the valence band tail (changing c into v !) assuming that the valence band tail is made of donor states.

The above parameters as well as some of the 'experimental parameters' (e.g. NEc , NEv , see below) are used to define the DOS at and above or below the band edges.

A parabolic band of states is defined, corresponding to the well known distribution of extended states in a crystalline semiconductor. In the case of the conduction band one has

$$N_{cpara}(E) = NEc * \text{Sqrt}(E - E_{c0})$$

and for the valence band one has

$$N_{vpara}(E) = NE_v * \text{Sqrt}(E_{v0} - E)$$

Note that E_{v0} and E_{c0} are not the energies at the band edges defined by E_v and E_c . In hydrogenated amorphous silicon $E_{c0} - E_{v0}$ would correspond to a Tauc gap.

In case of band tails, at the band edges, I assume that the exponential and the parabolic distributions are equal. In the case of the conduction band it gives

$$N(E) = N(E_c) * \exp[-(E_c - E)/kT_{cu}] = N_{cpara}(E) = NE_c * \text{Sqrt}(E - E_{c0})$$

that is $N(E_c) = NE_c * \text{Sqrt}(E_c - E_{c0})$

I also assume that the derivatives of these two quantities at E_c are the same, leading to

$$N(E_c)/kT_{cu} = 0.5 * NE_c / \text{Sqrt}(E_c - E_{c0})$$

From these equations one finds

$$E_c - E_{c0} = kT_{cu}/2 \quad N(E_c) = NE_c * \text{Sqrt}(kT_{cu}/2)$$

For the valence band it leads to

$$E_{v0} - E_v = kT_{vu}/2 \quad N(E_v) = NE_v * \text{Sqrt}(kT_{vu}/2)$$

Note that since $N_c = NE_c * 0.89 * (kT)^{3/2}$, with a 'raisonnable' value of T_{cu} , one has roughly $N_c \approx kT * N(E_c)$.

Note also that it is this definition of the DOS above or below the edges that is used in the calculation of the absorption for transitions from extended states toward extended states.

To summarize, when the band tails are made of two exponentials, the DOS can be written:

$$\begin{aligned} N(E) &= N_{ext} * \exp[-(E_c - E)/kT_c] & \text{for } E_v < E < E_{coup} \\ N(E) &= N(E_c) * \exp[-(E_c - E)/kT_{cu}] & \text{for } E_{coup} < E < E_c \\ N(E) &= NE_c * \text{Sqrt}(E - E_{c0}) & \text{for } E > E_c \end{aligned}$$

for the conduction band tail, and

$$\begin{aligned} N(E) &= N_{ext} * \exp[-(E - E_v)/kT_v] & \text{for } E_c > E > E_{coup} \\ N(E) &= N(E_v) * \exp[-(E - E_v)/kT_{vu}] & \text{for } E_{coup} > E > E_v \\ N(E) &= NE_v * \text{Sqrt}(E_{v0} - E) & \text{for } E < E_v \end{aligned}$$

for the valence band tail, the N_{ext} and E_{coup} being those defined for each band tail respectively.

Definition of the distributions of multivalent defect states

Multivalent states can have three states of charge. Two types of multivalent states are available. One for which the states of charge are -/0/+ and one for which the states of charge are 0/+/. The data of these states is presented as follows :

- N_{max} = maximum value of the state in $\text{cm}^{-3}\text{eV}^{-1}$.
- E_{max} = energy position of N_{max} in eV, the zero of energy being taken at the top of the valence band ($E_v = 0$).
- $Sigma$ = the standard deviation of the gaussian distribution in eV.
The Gaussian distribution is then $N(E) = N_{max} \exp[-(E_{max} - E)^2 / 2 / Sigma^2]$
- E_u = the correlation energy (eV)

- C_{n0} = the electron capture coefficient in cm^3/s at $T = 300$ K for the neutral (-/0/+) or positive (0/+ /++) state of charge.
- C_{p0} = the hole capture coefficient in cm^3/s at $T = 300$ K for the neutral (-/0/+) or positive (0/+ /++) state of charge.
- R_n = the ratio of the electron capture coefficients of (0/+) or (+ /++) : i.e. $C_{n+} = R_n C_{n0}$.
- R_p = the ratio of the hole capture coefficients of (-/0) or (0/+) : i.e. $C_{p-} = R_p C_{p0}$.
- E_{actn} = the power of $T/300$ if one wants to vary C_n as function of T : $C_n = C_{n0}(T/300)^{E_{actn}}$.
- E_{actp} = the power of $T/300$ if one wants to vary C_p as function of T : $C_p = C_{p0}(T/300)^{E_{actp}}$.
- C_{opt} = optical matrix element in $\text{cm}^{5/2}\text{eV}$. This quantity is used to calculate the coefficient of the convolution product when one calculates optical transitions from (toward) deeper (higher) states toward (from) these states :

$$\text{Coefficient} = C_{opt}(\text{first type of states}) * C_{opt}(\text{second type of states}) / h\nu.$$

Definition of the defect pool

The defect pool is calculated according to the work of Powell and Deane (see Ref. [8]). This pool is made of amphoteric correlated states (-/0/+). The calculation of the pool is done with $I=2$. It is the characteristic temperature of the upper part of the valence band tail (T_{vu}) which is used to calculate to pool shape if the valence band tail is made of two exponential distributions.

- $[H]$ = concentration of hydrogen in the material in cm^{-3} .
- E_{max} = energy position of the pool in eV, the zero of energy being taken at the top of the valence band ($E_v = 0$).
- σ = the standard deviation of the Gaussian distribution in eV.
- E_u = the correlation energy in eV
- T_{equi} = the equilibrium temperature of the material (K). Above this temperature the pool is calculated for each temperature, below it is left as it was defined with T_{pool} .
- T_{pool} = temperature at which the pool was frozen in the material (K).
- C_{n0} = the electron capture coefficient in cm^3/s at $T = 300$ K for the neutral state of charge.
- C_{p0} = the hole capture coefficient in cm^3/s at $T = 300$ K for the neutral state of charge.
- R_n = the ratio of the electron capture coefficients of (0/+) : i.e. $C_{n+} = R_n C_{n0}$.
- R_p = the ratio of the hole capture coefficients of (-/0) : i.e. $C_{p-} = R_p C_{p0}$.
- E_{actn} = the power of $T/300$ if one wants to vary C_n as function of T : $C_n = C_{n0}(T/300)^{E_{actn}}$.
- E_{actp} = the power of $T/300$ if one wants to vary C_p as function of T : $C_p = C_{p0}(T/300)^{E_{actp}}$.

- C_{opt} = optical matrix element in $\text{cm}^{5/2}\text{eV}$. This quantity is used to calculate the coefficient of the convolution product when one calculates optical transitions from (toward) deeper (higher) states toward (from) these states :

$$\text{Coefficient} = C_{opt}(\text{first type of states}) * C_{opt}(\text{second type of states}) / h\nu.$$

Definition of the experimental parameters

The "experimental" parameters are material and experiment dependent. One can choose :

- F_{dc} = the "experimental" flux (in $\text{cm}^{-2}\text{s}^{-1}$)
- μ_{n} = the extended states electronic mobility ($\text{cm}^2/\text{V/s}$)
- μ_{p} = the extended states hole mobility ($\text{cm}^2/\text{V/s}$)
- $NE_c = 4\pi(2m^*/h^2)^{3/2} (\text{cm}^{-3}\text{eV}^{-1.5})$, h being the Planck constant and m^* the electron mass, from which one obtains the equivalent density of states at the bottom of the conduction band $N_c = NE_c * 0.89 * (kT)^{3/2} (\text{cm}^{-3})$.
- $NE_v = 4\pi(2m^*/h^2)^{3/2} (\text{cm}^{-3}\text{eV}^{-1.5})$, h being the Planck constant and m^* the hole mass, from which one obtains the equivalent density of states at the top of the valence band $N_v = NE_v * 0.89 * (kT)^{3/2} (\text{cm}^{-3})$.
- E_{gap} = the band gap at 300 K (eV)
- dE_g = the variation of the gap with temperature (eV/K). When the band gap is varied the defect maximum energy positions are also varied proportionally to their positions in the gap at $T = 300$ K.
- T_{dep} = the lowest "experimental" temperature (K)
- T_{fin} = the highest "experimental" temperature (K)
- ΔT = the step of temperature between each experimental temperature (K)
- f_{min} = the minimum experimental frequency (Hz)
- N_{bf} = the number of frequencies for a given temperature. The frequencies are such that $f(i+1) = 1.5 * f(i)$.
- N_{pas} = the number of energy steps in the gap of the material.
- ν_{hop} = the attempt to hop frequency (s^{-1}).
- R_0 = the decay length of the wave function of a given states (cm).
- $Field$ = the field applied in between the 'electrodes' (V/cm).
- α = absorption coefficient (cm^{-1}). This value fixes the penetration depth of the 'light' used to perform the simulation. After calculation of the absorption curve one can deduce to which wavelength it corresponds.
- ϵ_{psr} = Relative permittivity of the material. $\epsilon = \epsilon_{psr} * 8.854 \times 10^{-14} \text{ F/cm}$.

When the temperature is varied, calculations using a constant T step can be performed or calculations using a constant $1000/T$ step. In the first case, the user has simply to give the temperature step ΔT and the program will calculate at different temperatures linearly increasing with the temperature step provided this step is larger than one. If $\Delta T < 1$ the programs works with a constant $1000/T$ step ($\Delta(1/T)$) equal to the value provided by the user.

In this case, the temperature step to the next temperature is calculated according to $\Delta T = (\Delta 1/T) * T / (1000/T - (\Delta 1/T))$, starting from the lowest temperature. It is likely that the final temperature fixed by the user will not be exactly reached.

Calculations

The **Calculations** menu is available only if a data file has been loaded with the **Files** menu and the data displayed by means of the **Definition + Data** menu or after a click on the **Display** button of the Data window. Many types of calculations are available : Modulated photocurrent, photoconductivity, Absorption, CPM (In DC and AC), DBP, TPC, SSPG, MGT, PITS and TFT. During calculations a window opens displaying the progression of the calculation.

Except for the TFT calculation, for all the calculations the "sample" is supposed to be in coplanar geometry, the two parallel electrodes being 1 cm long. The applied field applied between them can be fixed in the Data window (*Field*). The thickness of the sample is chosen equal to $1/\alpha$, α being the absorption coefficient that can be also chosen in the Data window.

If multivalent states are included in the DOS it is also possible to display their occupation functions except for the PITS and TFT calculations. Answer **Yes** to the prompt. The occupation function distributions under dark and under illumination will be displayed during 2 s. Under dark the D- (0), D0 (+) and D+(++) occupation functions are displayed in dark yellow, dark mauve and brown, respectively. Under illumination they are displayed in yellow, magenta and red, respectively. The positions of the quasi Fermi levels for holes and electrons are displayed by green and red vertical lines respectively.

All these calculations are made in the framework of a trapping/release model, except when hopping is taken into account. During a calculation a window opens displaying its progression.

It displays the DC flux (*Fdc*) and the temperature at which the calculation is made, the generation rate (Gener.), the recombination rate (Recomb.) and the step number while the calculation is performed to match these two values (Gener. = Recomb.) as well as the electrical neutrality. The maximum number of steps is 500. This value can be reached if the differences between dark and illuminated values are small so that the program cannot converge toward the exact values. A message appears then asking if the user wants to proceed to the next temperature, if there is, or ends the calculation.

Values of n and p (cm^{-3}), concentrations of electrons and holes respectively, are given as well as the dark values of these quantities (n_0 and p_0). The lifetimes τ_{ae} for electrons and τ_{ah} for holes are also displayed.

Some other quantities can also appear like the gamma coefficient (g) of the photoconductivity, the frequencies (in Hz) at which the light is modulated for MPC simulations, the photon energy (in eV) for CPM and DBP calculations, the matrix dimension in TPC, the time evolution in PITS, etc... depending on the type of calculation asked by the user (see the Annexe)..

When the temperature is varied, calculations using a constant temperature step (ΔT) can be performed or calculations using a constant $1000/T$ step. In the first case, the user has simply to give the temperature step in the Exp. Data box of the Data window and the program will calculate at different temperatures linearly increasing with the temperature step provided this step is larger than one. If this step is smaller than one, the program works with a constant $1000/T$ step equal to the value provided by the user. In this case, the temperature step to the next temperature is

calculated according to $\Delta T = \Delta 1/T * T / (1000/T - \Delta 1/T)$, starting from the beginning temperature. It is likely that the final temperature will not be exactly reached.

Modulated photocurrent

This part of the program calculates the response of the "sample" to the application of a DC light with a flux F_{dc} plus a light modulated at different frequencies for different temperatures as fixed in the Exp. Data box of the Data window. Obviously a first part of this calculation aims at the determination of the photoconductivity, that is the determination of the occupation of states under light at the chosen temperature. The gamma (g) coefficient is also calculated and displayed. Then, the influence of the modulation is calculated for the different frequencies. One can fix in the Data window the minimum frequency (f_{min}) to begin with and the total number of frequencies to be used (nbf). Frequencies are deduced from one another by $f(i+1)=f(i)*1.5$. The F_{ac} flux is chosen a hundred times lower than the steady flux F_{dc} . During calculation the occupancy of the density of states is displayed. The empty monovalent states are in red and the full ones are in green. For the multivalent states, the D- (or 0) are in brown, the D0(+)/D-(0) for holes are in green, the D0(+)/D-(0) for electrons are in blue and the D+(++) are in mauve. The pseudo Fermi levels for holes and electrons are displayed by green and red vertical lines respectively. Moreover, the bands of the probed states either by holes and electrons are displayed (e.g. light blue for the conduction band tail).

It is possible to introduce a pause for printing the density of states and its occupancy at each temperature during the calculation. For that answer **YES** to the prompt. During calculation a box appears during 2 seconds with different choices : **Next**, **Print** and **End**. A click on **Next** resume the program to the next step, a click on **Print** prints the curves displayed on the screen on the default printer, a click on **End** ends the program. If none of these options are chosen the program resumes its progression to the next step after 2 seconds.

If the option to display the multivalent states occupation function has been chosen as well as a pause for printing it is possible to print this graph on the default printer by a click on **Print**.

The program offers also the possibility to calculate the MPC data taking account of the hopping of carriers from one localized state to another in addition to the 'traditional' multiple trapping. This calculation is based on matrix resolution. To limit the size of these matrices this calculation is possible only if the DOS is made of monovalent states with the same capture coefficients. The size of the matrix can also be limited by the user by choosing the number of energy steps (N_{pas}) to define the DOS in the Exp. Data box of the Data window. It is also possible to fix the value of the attempt-to-hop frequency (ν_{hop} in s^{-1}) and the extent of the wave function of the state (R_0 in cm).

The results, with or without hopping, are saved in `simulati\resulpcm` in different files corresponding to the different temperatures such as `Myfile_temp.txt` where 'temp' is the temperature (K) at which the calculation was performed. In each file the first column corresponds to the frequency (Hz), the second column to the modulus (A) and the third to the phase shift (°). Calculation results with and without hopping are saved under the same file name so to compare with and without hopping you have to perform two calculations with different 'Myfile' names.

Photoconductivity

This part of the program calculates the dark and photo conductivity of a given "sample" from the minimum to the maximum temperature with the chosen temperature step and flux in the Exp.

Data box of the Data window. The dark Fermi level position is calculated by solving electrical neutrality at each temperature.

For the photogeneration the absorption is supposed to be uniform and the generation rate is $G_{dc} = \alpha \times F_{dc}$. The densities of electrons and holes are calculated at each temperature by solving the continuity equations and checking that generation = recombination and the electrical neutrality. The calculation is made twice : first for G_{dc} and second for $G_{dc} \times 1.1$. A value of the gamma (g) coefficient (photoconductivity = $K \times G_{dc} \times g$) is then calculated and displayed ($g = ***$) in the Calculation window. During calculation the occupancy of the density of states is displayed. The empty monovalent states are in red and the full ones are in green. For the multivalent states, the D- (or 0) are in brown, the D0(+)/D-(0) for holes are in green, the D0(+)/D-(0) for electrons are in blue and the D+(++) are in mauve. The pseudo Fermi levels for holes and electrons are in green and red respectively.

Two files are created and saved in \simulati\resultpc\ :

- Myfile.**np** in which the first column is the temperature (K), the second and third column the values of n and p (cm^{-3}) respectively and the last column the position of the dark Fermi level referred to the valence band (eV).
- Myfile.**gam** in which the first column is the position of the pseudo Fermi level for electrons ($E_{fn} - E_v$ (eV)), the second column the position of the pseudo Fermi level for holes ($E_{fp} - E_v$ (eV)), the third column the values of NC/μ corresponding to the gamma 'density of states', and the last column the values of gamma.

The program offers also the possibility to calculate the conductivity and photoconductivity taking account of the hopping of carriers from one localized state to another in addition to the 'traditional' multiple trapping. This calculation is based on matrix resolution. To limit the size of these matrices, this calculation is possible only if the DOS is made of monovalent states with the same capture coefficients. The size of the matrix can also be limited by the user by choosing the number of energy steps (N_{pas}) to define the DOS in the Data window (Exp. Data). It is also possible to fix the value of the attempt-to-hop frequency (nu_{hop} in s^{-1}) and the decay length of the wave function of the states (R_0 in cm). The program calculates the contribution of the hopping alone under illumination and under dark, and of the multiple trapping alone also under illumination and under dark. The results are saved in a file Myfile.**hop** in simulati\resultpc. This file is build the following: the first column corresponds to the temperature, the second column to the conductivity due to hopping alone, the third column to the conductivity due to hopping and multiple trapping (MT) contributions, the fourth column to the conductivity linked to multiple trapping alone and the last column to the dark conductivity due to hopping alone.

Some other files containing the occupation function distributions taking or not account of the hopping are also recorded in simulati\resultpc\Myfile_hop\ under the name Myfile_**temp_occup.txt** where 'temp' is the temperature at which the calculation was done. In these files the first column is the energy position referred to the top of the valence band, the second column the occupation function without hopping and the third column the occupation function taking account of the hopping contribution.

Note that hopping is not taken into account in the calculation of the gamma coefficient.

Absorption

This part of the program calculates the "absorption" of the sample at 300 K, that is all the possible optical transitions between full states and empty states. The photon energy is varied between an energy slightly lower than $E_{gap} - E_F$ to an energy slightly larger than the energy gap. Note that the final result may be very different from experimental results for two reasons. First the "sample" is supposed to be under dark, the occupation functions being those of dark equilibrium. Second, the optical capture cross sections can be adjusted for each type of states by choosing a C_{opt} value for each of them. These optical capture cross sections are supposed to be independent of energy. The coefficient of the convolution integral between empty and full states for transitions between two types of states is the product of their corresponding C_{opt} divided by $h\nu$. If no values for the C_{opt} are given they are chosen so that the coefficient of the convolution product is equal to $1.8E-38/h\nu$ to match the results of the hydrogenated amorphous silicon but it will certainly not fit with another type of material.

However, this part of the program can give a rather good overview of the available optical transitions that would occur on a real sample.

CPM

This part of the program simulates a CPM experiment performed at 300 K with a steady, but not constant, flux of light. The energy scale of the photon energy is automatically determined taking account of the gap width and of the Fermi level position. At the lowest photon energy the photoconductivity is calculated as follows:

- Determination of all the possible optical transitions and calculation of the occupation functions of the defects introduced in the gap.
- Determination of electron and hole generations
- Resolution of the continuity equations for electrons and holes
- Verification of the electrical neutrality.

As in the experiment, one has to choose a rather high value for the flux. $F_{dc} = 10^{+15} \text{ cm}^{-2}\text{s}^{-1}$ is a good order of magnitude. Indeed, even though the program works under double precision the resolution of all these equations is rather difficult if the free carrier densities under light are not very far from the values under dark. The calculation results in a somewhat noisy curve if the flux is chosen too low.

For the next photon energies the same calculation is done but the DC flux is adjusted until the obtained photoconductivity is the same as the one calculated with the lowest photon energy. The DC flux (F_{dc}), the light energy ($h\nu$), the generation of holes and electrons ($Gener.n$, $Gener.p$), and the concentration of free electrons (n) and free holes (p) as well as the concentrations under dark (n_0 , p_0) are displayed in the Calculation window.

At each photon energy the following quantities are also calculated:

- Absorption coefficient linked to the generation of electrons: Alpha n (G_n/F_{dc})
- Absorption coefficient linked to the generation of holes : Alpha p (G_p/F_{dc})
- Global absorption coefficient taking account of the states occupancy: Alpha Fdc
- The $\mu\tau$ products for electrons and holes.

Finally, for comparison, another absorption coefficient is calculated assuming, as in the "absorption" part, that the material is under dark equilibrium.

All these data are saved in `simulati\resulabs\Myfile.cpm`.

I have added a calculation of AC CPM which is not exactly the AC CPM experiment. At each photon energy, once the DC flux has been adjusted so that to obtain a constant DC photocurrent, the program calculates, with the occupation functions defined by the below gap DC flux, what would be the answer of the "sample" (σ and phase shift) to an AC excitation at the same photon energy and at a frequency fixed by the value introduced in the data box (f_{min}). It is not precisely the experimental AC CPM in which the flux is adjusted so as to obtain a constant AC current at each photon energies but it is not far from it.

The calculation proceeds exactly as the calculation done for DBP (See below).

All the data ($h\nu$, $\sigma/q/F_{ac}$, Alpha n, Alpha p, Alpha Fdc, Alpha dark, ϕ) are saved in `simulati\resulabs\Myfile.apm`.

Another file is created containing the evolution of the real (r) and imaginary (i) part of the AC electron (n) and hole (p) concentrations in cm^{-3} . The first column corresponds to the photon energy in eV, the second column to n_r , the third column to n_i , the fourth column to p_r , the fifth column to p_i and the last column to the values of the tangent of the phase shift between the excitation and the response of the sample. This file is saved in the directory `simulati\resulabs` under the file `Myfile.atg`.

DBP

This part of the program simulates a DBP experiment performed at 300 K with a continuous, constant and adjustable (in the Exp. Data box of the Data window) flux of light whose photon energy is higher than the gap, and an alternating flux of light with variable photon energy. The energy scale of the photon energy of the alternating flux is automatically determined taking account of the gap width and of the Fermi level position. At the lowest photon energy the AC flux is fixed at $10^{+12} \text{ cm}^{-2}\text{s}^{-1}$. The frequency of the AC flux is chosen equal to the minimum frequency (f_{min}) given in the Data window. The DC flux must not be chosen too low because the calculation of the DBP has been made assuming that the AC contribution is only a small perturbation of the DC contribution. The 'current' is calculated as follows:

First, the influence of the DC flux is calculated with the

- Calculation of the occupation functions under a DC flux of the defects introduced in the gap.
- Determination of electron and hole generations due to the DC flux
- Resolution of the continuity equations for electrons and holes
- Verification of the electrical neutrality.

Once this calculation finished it is possible to save the energy distribution of the occupation functions of the states involved in it. These files are saved in `simulati\resultpc` under the form `Myfile_FD.dbi` or `.poo` for the occupations functions under dark of the multivalent states i or for the pool respectively. For the occupation functions under illumination the files are named `Myfile_FL.dbi` or `.poo`. In these files the first column corresponds to the energy, the second column to f_{d0} (or +), the third to f_{d+} (or ++) and the fourth one to f_{d-} (or 0). For the monovalent states a single file is saved for the occupation under dark : `Myfile.fd`. For the occupation under illumination the files are saved as `Myfile_FL.type of state+number`. For instance for the

conduction band tail the extension is **cbt** whereas for the acceptor 1 the extension is **ac1**. In these files the first column corresponds to the energy referred to the valence band (eV), the second one to f_{occup} and the third one to $1 - f_{occup}$. It is also possible to have a print of the occupied states in the gap by clicking on **Print** appearing on the box following the message for recording the occupation functions. If one waits 2 s the calculation proceeds to the **Next** step.

Then the AC contribution is taken into account via the

- Determination of all the possible optical transitions and calculation of the occupation functions due to the AC flux of the defects introduced in the gap.
- Determination of electron and hole generations due to the AC flux
- The AC concentrations of electrons and holes are then calculated by solving a system similar to that of a standard MPC calculation. The modulus of the AC photoconductivity (σ) and its phase shift referred to the excitation are deduced from the solution of this system.

For the other photon energies the same calculation for the AC contribution is done but the AC flux is adjusted until the modulus of the photoconductivity obtained is the same as the one calculated with the lowest photon energy.

At each energy the following quantities are also calculated:

- Absorption coefficient linked to the AC generation of electrons: $\alpha_n (G_n/F_{ac})$
- Absorption coefficient linked to the AC generation of holes : $\alpha_p (G_p/F_{ac})$
- Global absorption coefficient taking account of the states occupancy under dark: α_{dark}
- Global absorption coefficient taking account of the states occupancy under light: α_{Fdc}

At the end of the calculation the ratios $\sigma/q/F_{ac}$ are normalized to the value of α_{Fdc} obtained at the highest energy. This procedure is similar to the one experimentally used where one normalizes σ/F_{ac} to optical measurements.

All these data ($h\nu$, $\sigma/q/F_{ac}$, $phase\ shift$, α_n , α_p , α_{dark} , α_{Fdc}) are saved in `simulati\resulabs\Myfile.dbp`.

Another file is created containing the evolution of the real (r) and imaginary (i) part of the ac electron (n) and hole (p) concentrations in cm^{-3} . The first column corresponds to the photon energy in eV, the second column to n_r , the third column to n_i , the fourth column to p_r , the fifth column to p_i and the last column to the values of the tangent of the phase shift between the excitation and the response of the sample. This file is saved in the directory `simulati\resulabs` under the form `Myfile.tgt`.

TPC

This part of the program simulates a TPC experiment performed with a continuous, constant and adjustable (in the Exp. Data box of the Data window) flux of light whose photon energy is higher than the gap, to which is added a pulse of light generating 10^{+6} carriers (holes and electrons, cm^{-3}). The DC flux can be chosen as low as $10^{+5} cm^{-2}s^{-1}$. The calculation of the TPC is therefore performed including contributions of both holes and electrons and the recombination

due to the applied DC flux. The calculation is made at the lowest temperature (T_{dep}) given in the Data window. The current density is calculated as follows:

First, the influence of the DC flux is calculated with the:

- Calculation of the occupation functions under a DC flux of the defects introduced in the gap.
- Determination of electron and hole generations due to the DC flux
- Resolution of the continuity equations for electrons and holes
- Verification of the electrical neutrality.

Then the pulse contribution is taken into account via the

- Determination of smallest increment of time dt .
- Determination of a matrix, taking account of dt and of the occupancy of the states, that assures the transition from one increment of time to the other.

The smallest increment of time is calculated according to the capture coefficients of the introduced defects. The calculation proceeds to the next step of time by multiplying the matrix by itself. The increment of time are therefore dt , $2*dt$, ..., 2^n*dt , up to a value either larger than 2 seconds or to a value fixed by the recombination.

Two files are created in `simulati\resultpc`: one containing the variations of the photocurrent density versus time (Myfile.**idt**), and a second one containing the variations of "charge" versus time [actually the integral of the photocurrent density] (Myfile.**qdt**).

SSPG

This part of the program simulates the SSPG experiment for all the temperatures fixed by T_{dep} , T_{fin} and $DltaT$.

BE CAREFUL : if you want this calculation at a single temperature you have to fix the temperature values identical ($T_{dep} = T_{fin}$) in the Exp. Data box of the Data windows. Otherwise the calculation will be made at all the temperatures.

First, the influence of the DC flux, fixed in the Data window, is calculated with the:

- Calculation of the occupation functions under a DC flux of the defects introduced in the gap.
- Determination of electron and hole generations due to the DC flux
- Resolution of the continuity equations for electrons and holes
- Verification of the electrical neutrality.

Then, the program calculates the excess density of current ΔJ resulting from the superimposition to the DC flux of another DC flux 20 times smaller. Finally it calculates the excess density of current resulting of the same superimposition of a small DC flux but taking account of the creation of a grating at the surface of the "sample" with different grating periods. The grating periods are fixed the following : the smaller one is 0.15 μm and the following ones are calculated as 0.15×1.6^i , i varying between 0 and 14. Thus, there are 15 different periods ranging from 0.15 to 108 μm . The different grating periods as well as the corresponding ratios of the current with interferences to the current without interferences (β) are saved in

simulati\resultsspg\Myfile\ in Myfile_**temp.spg** where 'temp' is the temperature at which the simulation was performed.

This calculation is based on the complete resolution of a system taking account of small spatial modulation of the flux impinging the "sample". The dielectric constant introduced in the calculation is $\varepsilon = Epsr * 8.854 \times 10^{-14}$ F/cm.

To match the theoretical developments the calculation must be made at low field (e.g. 100 V/cm), but it is possible to study the influence of the field on *Beta* vs grating period.

The simulation uses the *Beta* value calculated at the largest grating period (*Betalim*) to calculate the *NC/μ* values. If the SSPG calculation has been made at different temperatures, a 'DOS' (actually *NC/μ*) spectroscopy can be achieved. The data is saved in Myfile.**bet** in \simulati\resultpc\. The first column corresponds to $E_{fn} - E_v$ (eV), the second column to $E_{fp} - E_v$ (eV), the third column to *NC/μ* and the fourth column to *Betalim*.

MGT

This part of the program simulates the MGT experiment. This calculation is done in the same run as for SSPG.

BE CAREFUL : The calculation is made for all the temperatures defined by *Tdep*, *Tfin* and *DeltaT*. If you want this calculation at a single temperature you have to fix the temperature values identical ($T_{dep} = T_{fin}$) in the Exp. Data box of the Data window.

First, the influence of the DC flux, fixed in the Data window, is calculated with the:

- Calculation of the occupation functions under a DC flux of the defects introduced in the gap.
- Determination of electron and hole generations due to the DC flux
- Resolution of the continuity equations for electrons and holes
- Verification of the electrical neutrality.

Then, the program calculates the excess density of current *DeltaJ* resulting from the superimposition to the DC flux of a moving grating coming from the interferences between the high DC flux and of another DC flux twenty times smaller. The speed at which the grating is moving is determined by the product of the grating period and the delta frequency of the two beams. The grating periods are fixed and the same as for the SSPG. The deltas in frequency can be fixed in the Exp. Data box of the Data window by choosing the *deltaf* minimum (f_{min}) and the number of frequency (*nbf*). The *deltaf* are calculated as in the MPC calculation : $deltaf(i+1) = deltaf(i) * 1.5$. This calculation is based on the complete resolution of a system taking account both of a small spatial and time modulation of the flux impinging the "sample".

The applied field can be set to zero but in this case the SSPG is not calculated. The dielectric constant is set to $\varepsilon = Epsr * 8.854 \times 10^{-14}$ F/cm.

The results are saved in simulati\resultsspg\Myfile\ in Myfile_**temp.mgt** where 'temp' is the temperature at which the simulation was done. This file contains 16 columns. The first one is the *deltaf* (Hz) and the following ones the *deltaJ* (A/cm²) calculated for the different grating periods starting from the lowest (0.15 μm, second column) up to the largest one (108.8 μm, last column).

OPG

This part of the program simulates the OPG experiment.

BE CAREFUL : The calculation is made for all the temperatures defined by T_{dep} , T_{fin} and ΔT . If you want this calculation at a single temperature you have to fix the temperature values identical ($T_{dep} = T_{fin}$) in the Exp. Data box of the Data window.

First, the influence of the DC flux, fixed in the data window, is calculated with the:

- Calculation of the occupation functions under a DC flux of the defects introduced in the gap.
- Determination of electron and hole generations due to the DC flux
- Resolution of the continuity equations for electrons and holes
- Verification of the electrical neutrality.

Then, the program calculates the excess density of current ΔJ resulting from the superimposition to the DC flux of an oscillating grating coming from the interferences between the high DC flux and of another DC flux twenty times smaller. The grating periods are fixed and the same as for the MGT and SSPG. The increment of the grating period (Inc) is displayed in the Calculation window. The frequencies of the oscillating grating can be fixed in the Data window by choosing the minimum frequency (f_{min}) and the number of grating frequency (nbf). The increase of the frequency is calculated as in the MPC calculation : $f(i+1)=f(i)*1.5$. This calculation is based on the complete resolution of a system taking account both of a small spatial and time modulation of the flux impinging the “sample”.

The applied field is set to the value chosen by the user and the dielectric constant is set to $\epsilon = \epsilon_{psr} * 8.854 \times 10^{-14}$ F/cm.

The results are saved in `simulati\resultopg\Myfile\` in `Myfile_+_temp.opg` for the first half of a period and in `Myfile_-_temp.opg` where ‘temp’ is the temperature at which the simulation was done. This file contains 16 columns. The first one is the *Frequency* (Hz) and the following ones the ΔJ (A/cm²) calculated for the different grating periods starting from the lowest (0.15 μ m, second column) up to the largest one (108.8 μ m, last column). Theoretically some approximations can be done for large grating periods or for an n-type material. Two columns are added where the results of the calculations made with these approximations are recorded for the first grating period where they apply (approxn+ & approx+, and approxn- & approx-). For more details see Ref. [25].

In addition, the program performs a calculation of the DOS that one could extract knowing the small signal lifetime τ_n . This lifetime, and the DOS going with it, are calculated when one performs a simulation of either the photoconductivity, the MGT or the OPG techniques. The data is saved in `Myfile.opg` in the directory `\simulati\resultpc`. The first column corresponds to $E_{fn} - E_v$ (eV), the second column to $E_{fp} - E_v$ (eV) the third column to the OPG DOS (cm⁻³eV⁻¹), the fourth column to τ_n (s), the fifth one to the dielectric relaxation time (s), and the last one to the value of $1/\omega_{max}$ (s), ω_{max} corresponding to the angular frequency of the maximum of the ΔJ vs frequency curve calculated for a grating period of 26 μ m.

PITS

This part of the program simulates the PITS experiment. The calculation is made from the lowest temperature (T_{dep}) up to the highest (T_{fin}) with the temperature step (ΔT) fixed by the user. The user can choose before the calculation the duration of the pulse of light applied to the ‘sample’ from 1 ps up to 10 s.

The program calculates by means of an Euler implicit method how the states are filled during the pulse of light and how they empty after the end of it. As a consequence, this part of the program can simulate either the TPC experiment provided the pulse width is taken rather short (say 1-10 ps), the PITS experiment with a larger pulse (e.g. 100 μ s – 1 ms) or the photoconductivity if the pulse is long enough to reach steady-state conditions. With this part of the program, some other calculations like TPC and photoconductivity can be crossed-checked. For instance one can verify that the calculation of the steady-state conditions (i.e. values of n and p , quasi Fermi level positions, obtained with the **photoconductivity** menu in the same conditions of temperature and flux) gives results in agreement with those of the Euler implicit method. The calculation implies the definition of a matrix. It is recommended to choose a small value for the number of energy steps (N_{pas}) in the data window to avoid a quite long time of calculation.

During ‘illumination’ the minimum time step is 0.1 ps and the time is increased with multiplication by 1.2 at each step. When the time is larger than the pulse width, the ‘light’ is turned off. Hence, the pulse width chosen by the user is only an order of magnitude. The next time step is 10^6 times shorter than the pulse width to improve the time accuracy after the end of the pulse. As an example, with a chosen pulse width of 1 ms the actual pulse duration will be 1.03 ms. The next step will be $1.03 \times (1 + 10^{-6})$ ms and the time will be geometrically incremented with multiplication by 1.2 [$1.03 \times (1 + 1.2 \times 10^{-6})$; $1.03 \times (1 + 1.2 \times 1.2 \times 10^{-6})$; etc] up to around 10 s.

The evolution during calculation of the density of states occupancy is displayed. The empty monovalent states are in red and the full ones are in green. For the multivalent states, the D-(0) are in brown, the D0(+)/D-(0) for holes are in green, the D0(+)/D-(0) for electrons are in blue and the D(+++) are in mauve. The pseudo Fermi levels for holes and electrons are displayed by green and red vertical lines respectively. In addition, a window opens displaying the free electron and hole concentrations (n , p) the dt used for the calculation and the time t elapsed since the beginning of the ‘experiment’.

The files are saved in `simulati\resultpits\Myfile\`. In this folder the names of the files are organized according to the name of the data file to which some additional information is appended. First, an order of magnitude of the pulse width is appended (i.e. 1 ps, 10 ps, 100 ps, 1 ns, ... 100 ms, 1 s, 10 s) and second the temperature at which the calculation has been made. This finally gives something like `Myfile_1ms_200` if the calculation was made with a pulse width of 1 ms at a temperature of 200 K. The extension of the file is **.pit**.

In this file the first column corresponds to the time, the second to the photoconductivity, the third to the concentration of electrons n , and the fourth to the concentration of holes p .

The special folder `simulati\resultpits\Myfile\` is created because an extensive study of PITS implies simulations over a large range of temperature with a small temperature step, hence a rather large number of files are recorded.

TFT

This part of the program calculates the potential distribution and the variations of the conductivity of the material defined by the user with a voltage applied across the sample thickness as if it was included in a TFT device. The insulator is assumed to be 300 nm thick with a relative permittivity of 6. The relative permittivity of the material is E_{psr} fixed in the Exp. Data box of the Data window. A click on the **TFT** option of the calculation menu opens a window to define the sample thickness. On the same window an estimate of the Debye length is given. This estimate is based on the value of the density of states around the dark Fermi level. For calculation

reasons it is **HIGHLY** recommended to choose a sample thickness smaller than 5 times the Debye length. A click on **OK** starts the calculation.

The maximum voltage drop across the film is taken equal to 0.9 times the smallest distance of the Fermi level (in volts) from one of the bands. Different voltage values between this 'maximum' value and a 'minimum' value, the absolute value of which being equal to 1 mV, are chosen and the potential distribution through the sample thickness is calculated for each of them. The sign of the voltage drop between the insulator and the back side of the sample is chosen according to the position of the dark Fermi level (+ for n-type materials and – for p-type materials) but it is the absolute values that are recorded and displayed during the calculation. This latter assumes that close to the insulator ($x = 0$) the absolute value of the potential is maximum and equal to zero on the back side of the sample ($x = \text{sample thickness}$). The program determines the potential slope at $x = 0$ and the potential distribution accordingly for each of the possible voltages. It determines also the value of the bias that should be applied in between the top of the insulator and the back side of the sample. Finally, once the potential distribution is calculated the program calculates the mean value of the conductivity of the sample.

The calculation starts from the lowest voltage and, of course, ends with the highest. During the calculation a window opens displaying a plot of the distribution of the absolute values of the potential across the sample for each of the pre determined voltages. This allows following the progress of the calculation. If the DOS is high and/or the thickness too large the calculation can be rather long. A press on the 'escape' key stops it and the user can redefine either the thickness or the DOS. If the calculation is left to itself and the step becomes too small for the same reasons the program may stop by itself but after a rather large amount of time.

All the calculated data are saved in files in a folder named `simulati\resultTFT\`. The potential distributions for each voltage are saved in files the names of which are built from the data file name, i.e. `Myfile#number.tft`, the number being that of the order in which the calculation was done. In these files the first column is the position, the second the potential, the third its first derivative and the fourth its second derivative.

The variations of the conductivity vs the applied voltage are saved in the same `resultTFT` folder under a file named `Myfile.ivg`. The first column is the voltage drop across the insulator + the sample, the second column the voltage drop across the sample alone, and the third column the conductivity. The sample thickness is recalled on top of the recorded data.

Plots

This menu is designed to plot the results of the simulation after calculation. On a click many possibilities are offered :

MPC results, Photoconductivity results, Absorption results, CPM results, DBP results, TPC results, SSPG results, MGT results, g_{NC}/μ , OPG results, PITS results.

All the plots once displayed can be printed on the default printer by clicking on **Print**.

All the plots can be saved as an image by a double click on the corresponding page. After a double click a windows open that proposes to save an image of the display under a given name. A click on **YES** saves the image in the current folder under a **.bmp** format. This format can be quite large (more than 1 Mo) but can be reduced by opening the image with Paint® and saving it under a bitmap file with a reduced number of colors (16) or with a **.png** extension, for instance.

For all the calculations the "sample" is supposed to be in coplanar geometry, the two parallel electrodes being 1 cm long, the value of the field applied between them can be fixed in the Exp. Data box of the Data window. The thickness of the sample is chosen equal to $1/\alpha$, α being the absorption coefficient that can also be fixed in the Data window. The area through which the current is flowing and used for the calculation of the current is thus $1/\alpha$ (cm²).

MPC

Three types of plots are possible : Density of states (DOS), Phase shift versus frequency (pHi vs freq) and versus energy (phi vs E). The files are saved in simulati\resulpcm under Myfile_ **temp.txt** where 'temp' is the temperature at which the calculation was done which is also saved at the second line of the file. Then the first column corresponds to the frequency (Hz), the second column to the modulus (A) and the third column to the phase shift (°). For the three types of plots available, choose an option (DOS, pHi vs freq, phi vs E) and then select the data file with which the calculation was done : **Myfile.dat**.

● DOS

To plot the DOS, successive windows open to select various items :

The plots can be displayed with the (S)ame color (type s or S) for all the curves calculated at different temperatures or with (D)ifferent colors (default option) for each temperature.

Two types of plots can be displayed : either the DOS (N) (default option) in cm⁻³eV⁻¹ or $N(C)/\mu$ (type C or c), where C is the capture coefficient (in cm³/s) and μ the mobility of the carriers (in cm²/V/s), both as functions of the energy (in eV).

The carrier mobility can be chosen, either (H)ole (type h or H) or (E)lectron (default option).

The value of the capture coefficient used to calculate the energy scale can be fixed. The default value is 4E-8 cm³s⁻¹. To enter another value use this format (i.e. ###E-##). For electrons the energy scale is calculated according to the equation : $E_c - E = kT \ln(CN_c/\omega)$ where $N_c = NEc * 0.89 * (k*T)^{1.5}$ is the equivalent density of states at the bottom of the conduction band and k is the Boltzmann constant. (See the definition of experimental parameters for details).

The capture coefficient can be activated in power of temperature. For that answer **YES** to the prompt.

If the answer is **YES** then give the value of the power. The default value is 0.

Once the DOS calculated from the simulation results is plotted (option N or n), the DOS defined in the simulation can be plotted for comparison. For this last plot the energy origin can be chosen either at the (V)alence band (type v or V) or at the (C)onduction band (default option)

On the plot appears the name of the file, the minimum and maximum temperature used for the calculation as well as the temperature step. A click on the right button of the mouse displays the coordinates of the cursor position.

A message appears once a plot is achieved asking for a new plot. If one answers **YES** then it is possible to plot another MPC result and thus to compare the results of different calculations.

● Phi vs freq

With this option the evolution of the phase shift (in radian) of the alternating current with the frequency (in Hz) of the modulation for each temperature at which the simulation has been performed can be plotted either (O)ne by one or (A)ll together (default option). BE CAREFUL : the plotted phase shift is the opposite of the calculated phase shift (Phi plot= - Phi calc). When the option (O)ne by one is chosen a window opens with the different files available: choose the file Myfile_**temp.txt** for the wanted temperature.

On the plot appear the name of the file and the temperature at which the phase shift has been calculated.

A click on the right button of the mouse displays the coordinates of the cursor position.

● Phi vs E

This option allows plotting the variation of the phase shift (in radian) of the alternating current versus the same energy scale as the energy scale (in eV) used to plot the DOS. It can be used to put peaks of DOS into evidence. The calculated spectra for each temperature can be plotted either (O)ne by one or (A)ll together (default option). BE CAREFUL : the plotted phase shift is the opposite of the calculated phase shift (Phi plot= - Phi calc). When the option (O)ne by one is chosen a window opens with the different files available: choose the file Myfile_**temp.txt** for the wanted temperature.

The value of the capture coefficient C used to calculate the energy scale can be fixed. The default value is $4E-8 \text{ cm}^3\text{s}^{-1}$. To enter another value use this format (i.e. $\#.##E-##$). For electrons the energy scale is calculated according to the equation : $E_c - E = kT \ln(CN_c/\omega)$ where $N_c = N_{Ec} * 0.89 * (k*T)^{1.5}$ is the equivalent density of states at the bottom of the conduction band and k is the Boltzmann constant. (See the definition of experimental parameters for details).

On the plot appear the name of the file and the temperature(s) at which the phase shift has been calculated.

A click on the right button of the mouse displays the coordinates of the cursor position.

Photoconductivity

The dark conductivity and photoconductivity data calculated during the simulation can be plotted. Two calculations are available : one taking account only of the multiple trapping (MT) and another one taking account of the hopping. In the first case, the data is saved during calculation in Myfile.**np** in simulati\resultpc. The first column of this file corresponds to the temperature (K), the second column to the electron density (cm^{-3}), the third to the hole density (cm^{-3}) and the fourth to the Fermi level position under dark (eV). The dark conductivity is plotted with blue dots, the photoconductivity with green dots. The ordinates axis represents the conductivity (in S/cm) and the abscissa $1000/T$ (in K^{-1}).

If the hopping was taken into account during the calculation the data is saved in Myfile.**hop** in simulati\resultpc. The first column corresponds to the temperature, the second column to the photoconductivity (S/cm) due to hopping alone, the third column to the photoconductivity due multiple trapping (MT) contribution taking hopping into account, the fourth column to the photoconductivity linked to multiple trapping alone (without hopping!) and the last column to the dark conductivity due to hopping and MT. In this case the graph displays the variations with the reciprocal of temperature of the dark MT contribution (in blue), the hopping photoconductivity (Light blue), the photoconductivity due to MT contribution taking account of the hopping (brown), the photoconductivity due to MT alone (without hopping) (violet) and the sum of dark MT and hopping contributions (dark yellow).

On both plots (with or without hopping) the name of the file, the minimum and maximum temperatures as well as an estimate of the activation energy are displayed.

A click on the right button of the mouse displays the coordinates of the cursor position.

Absorption

The absorption curves calculated by the simulation can be displayed. The data is saved during calculation in Myfile.**abs** in simulati\resulabs. The first column of this file corresponds to the photon energies (eV) and the second one to the alpha values (cm^{-1}). The absorption coefficient (in cm^{-1}) is plotted versus the photon energy (in eV). The name of the file is shown on the plot with the same colour as the curve. At the end of the plot a window opens asking for another plot. If the answer is **NO** the program exits the absorption plot session, if the answer is **YES** a window opens in which one can choose another file to be plotted. It is then possible to compare different absorption curves one another. It is also possible to plot **experimental** absorption curves to be compared with the calculated ones. The experimental data file must be saved in ASCII format with an extension **.abs** and have two columns separated by a space: the first one the photon energy in eV and the second one the alpha values in cm^{-1} . The first line of the file must be a headline, for instance “hnu(eV) alfa(cm-1)”. This experimental file must be placed in the directory simulati\resulabs.

A click on the right button of the mouse displays the coordinates of the cursor position.

It is possible to have an estimate of the Urbach energy E_u in the region where $\ln(\alpha)$ varies linearly with $h\nu$ by clicking on a point of the curve with the left button of the mouse, move the pointer to another point of the linear part of the curve and release the mouse button. The Urbach energy is then displayed on the plot.

CPM

The CPM curves calculated by the simulation can be displayed. During calculation the data for the DC CPM is saved in Myfile.**cpm** and for AC CPM in Myfile.**apm**, both being in simulati\resulabs. In the DC CPM file :

- the first column corresponds to the photon energies (eV),
- the second column is the CPM, that is the ratio of $(n \cdot \mu_n + p \cdot \mu_p)$ divided by the flux,
- the third column is Alpha n (cm^{-1}), that is the absorption coefficient linked to the generation of electrons (G_n/F_{dc}),
- the fourth column is Alpha p (cm^{-1}), that is the absorption coefficient linked to the generation of holes (G_p/F_{dc}),
- the fifth column displays Alpha Fdc (cm^{-1}) calculated taking account of the occupancy of the states under DC illumination,
- the sixth column represents Alpha dark (cm^{-1}) calculated taking the occupancy of the states under dark equilibrium into account,
- finally, the last two columns represent $\mu_{tau n}$ and $\mu_{tau p}$ respectively (cm^2/V).

All these quantities, except the μ_{tau} 's, are plotted as function of the photon energy. For the plot of the CPM, the values of $(n \cdot \mu_n + p \cdot \mu_p)/F_{dc}$ are normalized to the absorption coefficient. The colors of the curves are displayed in a caption. The name of the file appears on the plot.

A click on the right button of the mouse displays the coordinates of the cursor position.

In the AC CPM file :

- the first column corresponds to the photon energies (eV),
- the second column corresponds to the ratio Modulus(AC photoconductivity)/ q/F_{ac} ,
- the third column is Alpha n (cm^{-1}), that is the absorption coefficient linked to the generation of electrons (G_n/F_{ac}),
- the fourth column gives Alpha p (cm^{-1}), that is the absorption coefficient linked to the generation of holes (G_p/F_{ac}),
- The fifth column displays Alpha Fdc (cm^{-1}) calculated taking the occupancy of the states under DC light into account,
- The sixth column displays Alpha dark (cm^{-1}) calculated taking the occupancy of the states under dark equilibrium into account,
- the seventh column is the phase shift of the AC photoconductivity referred to the excitation in degrees.

Two types of plots can be done:

● DOS

All the above quantities, except the phase shift, are plotted as function of the photon energy. For the plot the ratio Modulus(AC photoconductivity)/ q/F_{ac} is normalized to the absorption coefficient. The colors of the curves are displayed in a caption. The name of the file appears on the plot.

● pHi vs E

The evolution of the phase shift of the alternating current with the photon energy can be displayed. The name of the data file appears on the plot.

For both plots, a click on the right button of the mouse displays the coordinates of the cursor position.

DBP

The DBP curves calculated by the simulation can be displayed. During calculation the data is saved in Myfile.**dbp** in the directory simulati\resulabs. In this file :

- the first column corresponds to the photon energies (eV),
- the second column corresponds to the ratio $\text{Modulus(AC photoconductivity)}/q/F_{ac}$
- the third column is the phase shift of the AC photoconductivity referred to the excitation in degrees,
- the fourth column is $\text{Alpha n (cm}^{-1}\text{)}$, that is the absorption coefficient linked to the generation of electrons (G_n/F_{ac}),
- the fifth column gives $\text{Alpha p (cm}^{-1}\text{)}$, that is the absorption coefficient linked to the generation of holes (G_p/F_{ac}),
- The sixth column displays $\text{Alpha dark (cm}^{-1}\text{)}$ calculated taking the occupancy of the states under dark equilibrium into account.
- The seventh column displays $\text{Alpha Fdc (cm}^{-1}\text{)}$ calculated taking the occupancy of the states under dc light into account.

Two types of plots can be done:

● DOS

All the above quantities, except the phase shift, are plotted as function of the photon energy. For the plot the ratio $\text{Modulus(AC photoconductivity)}/q/F_{ac}$ is normalized to the absorption coefficient. The colors of the curves are displayed in a caption. The name of the file appears on the plot.

● Phi vs E

The evolution of the phase shift of the alternating current with the photon energy can be displayed. The name of the data file appears on the plot.

For both plots, a click on the right button of the mouse displays the coordinates of the cursor position.

TPC

The TPC curves calculated by the simulation can be displayed. During calculation the photocurrent density vs time is saved in Myfile.**idt** and the charge vs time is saved in Myfile.**qdt** in the directory simulati\resultpc. In these files :

- The first column corresponds to the time in seconds

- The second column corresponds to the photocurrent density or to the charge

Actually, it is not exactly the charge that is saved but rather the integral over time of the photocurrent density $q*[\mu_n*n(t)+\mu_p*p(t)]*Field$. For each plot it is possible to zoom on a particular part of the curve. A click on the left button of the mouse defines a corner of a rectangle the dimension of which can be adjusted by moving the mouse keeping the left button pressed. The release of the button plots a zoom of the selected part of the curve. It is possible to come back to the original curve by clicking on the appropriate button on the plot.

For both plots $[I(t)$ and $q(t)]$ a click on the right button displays the coordinates of the cursor position.

SSPG

The SSPG curves calculated by the simulation (*Beta* vs grating period *Lambda*) can be displayed for grating periods up to 26 μm though the calculations are performed for grating periods up to 108 μm . During calculation the *Beta* vs *Lambda* is saved in Myfile_ **temp.spg**, where 'temp' is the temperature (in K) at which the calculation was made, in the directory simulati\resultsspg\Myfile\ . In these files :

- The first column corresponds to the grating period in μm
- The second column corresponds to the *Beta* values

For this plot, a click on the right button of the mouse displays the coordinates of the cursor position.

It is also possible to display the variations of $\beta NC/\mu$ versus energy. The β used in the calculation of the $\beta NC/\mu$ values is the one obtained with a grating of 108 μm . The $\beta NC/\mu$ values are saved in a file (Myfile.**bet**) in simulati\resultpc\ under the following form:

- The first column corresponds to $E_{fn} - E_v$ (eV)
- The second column corresponds to $E_{fp} - E_v$ (eV)
- The third column corresponds to NC/μ ($\text{cm}^{-2}\text{V}\text{eV}^{-1}$)
- The fourth column gives the *Beta* values @ 108 μm obtained during the calculation

The plot can be done with the origin taken at E_c (default position) or E_v (option v) and with E_{fn} (option n) or E_{fp} (option p) as the energy position (default is E_{fn}). It is possible to display the introduced NC/μ to compare with the results. For that the user is asked if he wants to use the extended states mobility and the capture coefficient of (E)lectrons or (H)oles (default option is E).

A click on the graph with the right button of the mouse display the coordinates of the cursor position.

MGT

The MGT curves calculated by the simulation can be displayed. During calculation the excess current densities *DeltaJ* vs the delta frequency *Deltaf* are saved in Myfile_ **temp.mgt**, where 'temp' is the temperature at which the simulation was done, in the directory simulati\resultsspg\Myfile\ . In these files :

- The first column corresponds to the delta frequency *Deltaf* (Hz)

- The following columns correspond to the ΔJ (A/cm²) calculated with different grating periods, the same as those used for the calculation of the SSPG.

Two types of plots can be chosen. Either ΔJ vs Δf or ΔJ vs *Grating speed*. The grating speed is calculated as (*grating period*)* Δf .

For both plots a click on the right button displays the coordinates of the cursor position.

gNC/μ

The gNC/μ distribution calculated from the gamma values during the MPC or photoconductivity calculations can be plotted. The gNC/μ values are saved in a file (**Myfile.gam**) such that:

- The first column corresponds to $E_{fn} - E_v$ (eV)
- The second column corresponds to $E_{fp} - E_v$ (eV)
- The third column corresponds to NC/μ (cm⁻²VeV⁻¹)
- The fourth column gives the gamma values obtained during the calculation

The plot can be done with the origin taken at E_c (default position) or E_v (option v) and with E_{fn} (option n) or E_{fp} (option p) as the energy position (default is E_{fn}). It is possible to display the introduced NC/μ to compare with the results. For that the user is asked if he wants to use the extended states mobility and the capture coefficient of (E)lectrons or (H)oles (default option is E).

A click on the graph with the right button of the mouse displays the coordinates of the cursor position.

OPG

The OPG curves calculated by the simulation can be displayed. During calculation the excess current densities vs the frequency are saved in **Myfile_+_temp.opg** and **Myfile_-_temp.opg**, where the signs (+ or -) corresponds to each half period of oscillation of the oscillating grating and 'temp' is the temperature at which the simulation was done. These files are saved in the directory `simulati\resultopg\Myfile\`. In these files :

- The first column corresponds to the frequency f (Hz)
- The following columns correspond to the ΔJ (A/cm²) calculated with different grating periods, the same as those used for the calculation of the MGT and SSPG.

Three types of plots can be chosen. The first two correspond to a plot of the excess OPG currents vs *frequency*, either J vs *frequency* (option **J vs Freq**) or ΔJ vs *frequency* (option **Jac vs Freq**). The first plot displays the variations of $J+$ and $J-$ as function of frequency, the second plot displays the variations of $[J- - J+]$ as function of frequency. In the case of a plot of $J+$ and $J-$, the $J+$ are in full symbols and the $J-$ in open symbols. The difference between each plot is particularly visible if the calculation has been achieved taking account of an applied DC field. For each plot, the corresponding grating period is displayed with the same color as that of the curve. For these first two plots a click on any of the data files (i.e. **Myfile_+_temp.opg** or **Myfile_-_temp.opg**) leads to the same final plot. In addition to the plot of the currents, the program displays with lines the results obtained with some approximations, in the case of a large grating period (approx- or approx+) or in the case of a predominance of the electrons (approx-

or approxn+), to be compared with the calculation without approximations. The approximate calculations are displayed for the first grating period for which they apply. For more details see Ref. [25].

The third plot (option **DOS opg**) corresponds to the DOS that one could extract knowing the small signal lifetime τ_n . This lifetime, and the DOS going with it, are calculated when one performs a simulation of either the photoconductivity, the MGT or the OPG techniques. The data is saved in Myfile.**opg** in the directory simulati\resultpc. The first column corresponds to $E_{fn} - E_v$ (eV), the second column to $E_{fp} - E_v$ (eV) the third column to the OPG DOS ($\text{cm}^{-3}\text{eV}^{-1}$), the fourth column to τ_n (s) the fifth column to the dielectric relaxation time (s) and the last one to $1/\omega_{\text{max}}$ (s), ω_{max} corresponding to the angular frequency of the maximum of the ΔJ vs frequency curve calculated for a grating period of 26 μm . A plot of the DOS introduced in the simulation can be superimposed for comparison.

For each plot a click on the right button displays the coordinates of the cursor position.

PITS

● The choice of **sigma(t)** plots the evolution with time of the transient photoconductivity calculated at given temperature and flux. The data are saved in a file (Myfile_**tpulse_temp.pit**), where 'tpulse' is the pulse duration and 'temp' is the temperature at which the simulation was performed, in the directory simulati\resultpit\Myfile\ . The files are built as the following:

- The first column corresponds to the time in (s)
- The second column corresponds to the photoconductivity $q*[\mu_n*n(t)+\mu_p*p(t)]$.
- The third column corresponds to the values of $n(t)$ (cm^{-3}).
- The fourth column corresponds to the values of $p(t)$ (cm^{-3}).

The two first lines of the file give the temperature (T), the flux (F_{dc}) at which the calculation was made, the corresponding values of the dark conductivity (labeled I_{dark}), the electron (τ_{ae}) and hole (τ_{ap}) lifetimes (in s), the width of the pulse of light (p_w in s) and the ratio of the progression of time ($step$).

The whole curve (i. e. $t = 0$ at the beginning of the light pulse) is first displayed. It is possible to zoom on a particular part of the curve. A click on the left button of the mouse defines a corner of a rectangle the dimension of which can be adjusted by moving the mouse keeping the left button pressed. The release of the button plots a zoom of the selected part of the curve. It is possible to come back to the original curve by clicking on the appropriate button on the plot.

It is also possible to plot only the PITS curve (i.e. $t = 0$ at the end of the light pulse) by clicking on the button located at the top left corner of the form. Several curves can be displayed at the same time on the plot for comparison but only the last plotted offers the possibility to switch from the whole curve to the PITS curve.

A click on the right button displays the coordinates of the cursor position.

● The choice of **n(t)+p(t)** plots the evolution with time of the transient free carrier concentrations (p in brown, n in green) calculated at given temperature and flux.

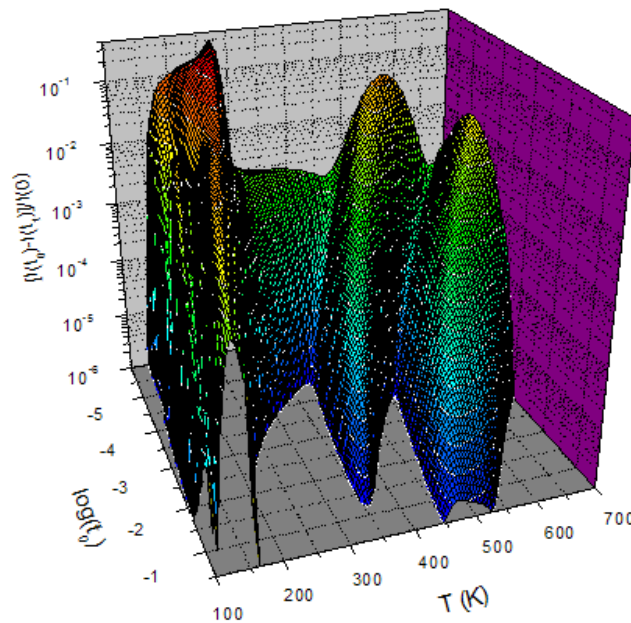
The whole curves (i. e. $t = 0$ at the beginning of the light pulse) are first displayed. It is possible to zoom on a particular part of the curve following the same procedure as for $\sigma(t)$.

It is also possible to plot the n and p evolutions with an origin of time taken at the end of the light pulse by clicking on the top left button. Several curves can be displayed at the same time on

the plot for comparison but only the last plotted offers the possibility to switch from the whole curve to the PITS curve.

A click on the right button displays the coordinates of the cursor position.

● The choice of **slopes(t0,T)** opens a window in which a time interval can be fixed and the type of slopes, linear (LIN) or logarithmic (LOG), can be chosen. The time interval fixes the limits of time between which the slopes are calculated. These limits of time take their origin at the END of the light pulse. In between these limits two sliding times are chosen, t_0 and t_1 , such as t_1 is just superior to $3xt_0$. This window of time is sliding from one time step used during the calculation to the other from the beginning time limit to the end time limit defined by the user and the following are calculated:



With a choice of **LIN** the absolute value of the quantity $S = [I(t_0) - I(t_1)]/I(t = 0)$ is calculated at each time step. These results are saved in a folder **PITS** created in the folder where the results of the pits calculation have been saved. They are saved in a file **Myfile+'pulsewidth'+napLIN+'-the power of ten of the lower time limit - the power of ten of the higher time limit'**. The first column contains all the t_0 values, the first line all the temperature values and at each intersection a value of $S(t_0, T)$. These data can be transformed into a matrix and plotted in a 3D system as shown above.

In this plot, each ridge corresponds to a maximum of emission of carrier by a defect level. For each t_0 , i. e. for each couple $\{t_0, t_1\}$ the corresponding emission rate e_n is calculated (see the PITS references for the way it is calculated), and the program searches for the temperature at which a maximum of S occurs. For a given t_0 the program investigates for up to four maxima. The results of this investigation are saved in the folder **PITS** under the name **Myfile+'pulsewidth'+maxLIN+'# of the max'+'-the power of ten of the lower time limit-the power of ten of the higher time limit'**. The first column is e_n , the second column the temperature, the third column $1000/T$, the fourth $(T/300)^{1.5}/e_n$ and the fifth t_0 . Normally if a level is predominantly emitting, a plot of the fourth column as function of the third should give a

straight line whose slope is the energy position of the defect level. If the capture coefficients have been varied with T^i then one should plot $(T/300)^{(1.5+i)}/e_n$ instead.

To avoid this last plot a file is made exactly as `Myfile+'pulsewidth'+napLIN+'-the power of ten of the lower time limit-the power of ten of the higher time limit'` described above except that the first line contains all the $1000/T$ values. It is saved under the name `Myfile+'pulsewidth'+nap1000T+'-the power of ten of the lower time limit-the power of ten of the higher time limit'`. A 3D plot can be achieved and the 'ridges' are the signature of a maximum of emission. These ridges should be straight as in an Arrhenius plot.

With a choice of **LOG** the $[\text{dlog}(I)/\text{d}T]/(T/300)^{1.5}$ quantity is calculated at each time step. The results of this calculation are saved under the same name as for the LIN choice: `Myfile+'pulsewidth'+napLOG+'-the power of ten of the lower time limit-the power of ten of the higher time limit'`. However, the main interest of this plot is to show that, when a level is predominantly emitting carriers, all the curve maxima gather on a single line the slope of which corresponds to the energy position of the level. The slope can be estimated by clicking with the left button on one point of the curve. Keeping the left button pressed move the cursor to another point. After releasing the button the activation energy E_a of the trap is automatically given. These results can be compared with those of the linear method afterward.

A research of the maximum is also performed as in the linear study and the maxima are saved under the name `Myfile+'pulsewidth'+maxLIN+'# of the max'-the power of ten of the lower time limit-the power of ten of the higher time limit'`.

Finally, a file `Myfile+'pulsewidth'+napITME+'-the power of ten of the lower time limit-the power of ten of the higher time limit'` is recorded in which the first column represents the times starting from the lower limit, the zero being taken at the end of the pulse, the first line displays the temperatures and each column contains the currents calculated at the temperature of the first line and at the times indicated in the first column.

To plot any of the above options open the directory where the **.pit** files are saved and click on any of the **.pit** files.

Format

The format menu can be used to create some new files that can bring more insight on the DOS of the studied material.

- This part of the program opens all the MPC files associated with one data file. The data file that will be treated is the one displayed in the Data window and its density of states must be plotted. For instance if the data file is **Myfile.dat** it will open all the files **Myfile_temp.txt**, where 'temp' is the temperature at which the calculation of the modulated photocurrent was done. In **Myfile_temp.txt** the data is saved in columns : *frequency* (Hz), *modulus* (A), *phase shift* (°). A new file is created **Myfile_tempTRAIT.txt** where the data is saved as follows :
frequency (Hz), *modulus* (A), *ABS(phase shift (°))*, *Omega* (s⁻¹), *tan(phase)*, *cos(phase)/modulus* (A⁻¹).

These files can then be used to plot the evolution of *tan(phase)* or *cos(Phase)/modulus* as functions of omega with a graphing and data analysis software. For instance it can be checked that if the MPC calculation was done in the recombination regime (e.g. High flux) *tan(phase)* → 0 and *cos(phase)/modulus* is constant.

- The slope of *tan(phase)* vs *omega*, at low *omega* is calculated from the first four points and used to determine a point of the density of states. For the plot of this density of states one has to choose the energy origin [(C)onduction band (default) or (V)alence band]. The energy is calculated from the photoconductivity (estimation of the position of the quasi Fermi level) assuming that the electrons [choice (C)] or the holes [choice (V)] are the majority carriers. A new file is created (**Myfile_trait.txt** in *simulati\resultpc*) in which are saved in columns :

Temperature (K), *n* (cm⁻³), *p* (cm⁻³), *Energy* (eV), DOS calculated from *tan(phase)* (cm⁻³eV⁻¹)

To check how this calculated DOS fits with the actual one, a plot of both is done and can be printed on the default printer (option **Print** of the **Plots** menu).

- The *gamma* values from the AC current are calculated. An estimate of *NC/μ* is derived from this calculation. A file **Myfile.gac** is recorded in *simulati\resultpc* in which the first column is the energy as calculated above, the second column *AC g-NC/μ*, and the third AC gamma
- Finally, a file containing all **Myfile_temp.txt** files is created (**Myfile.rou**) that can be used with a software that we have defined to analyze our experimental data. Thus, it is possible to compare instantaneously our experimental data with simulated one.

Examples

* a-Si:H simple density of states

The same density of states (DOS) and parameters were used to simulate several techniques. The basic data file is **a-Si:H_standard.dat**. The density of states is made of two exponential band tails and two Gaussian distributions of deep states (one acceptor, one donor). The capture cross-sections were taken the same for all the states. With these data the following 'experiments' were simulated:

- MPC in the high frequency (HF) regime (low flux, high modulation) from the file **aSiH_Standard_MPC-HF.dat**.
- MPC in the low frequency (LF) regime (high flux, low modulation) from the file **aSiH_Standard_MPC-LF.dat**.
- MPC in the high frequency regime taking account of the hopping from the file **aSiH_hopping.dat**.

In these files the DOS and its parameters were the same, only the 'experimental' parameters (e.g. the flux) were changed from one file to the other.

The results can be plotted on the same graph to see what are the respective influences of hopping or high or low flux on the final MPC results. These results can be compared to the introduced DOS.

The photoconductivity taking account of the hopping was calculated, saved in **aSiH_hopping.hop**, and can be displayed to be compared with the transport of carriers when only the trapping/release process is taken into account.

An example of the CPM calculation was created starting from the file **aSiH_Standard_MPC-LF.dat**. A plot of *mutaun* as function of the photon energy shows that the mobility×lifetime product is not constant on the range of explored photon energies though its variations are small (a factor 1.6 between the maximum value and the minimum one).

Examples of the DBP calculation were created starting from the files **aSiH_Standard_MPC-LF.dat** and **aSiH_Standard_MPC-HF.dat**. The influence of the DC flux can be compared on the final results.

SSPG, MGT and OPG techniques were also simulated starting from the **aSiH_standard.dat** file. For the MGT two calculations are proposed either with 0 V/cm or with 100 V/cm applied (**aSiH_standard_MGT_0V.dat** or **aSiH_standard_MGT_100V.dat**). In the first case the SSPG is not calculated since the field is null. For the MGT the plot of the excess current δI vs frequency calculated at 300 K shows that at low frequency the current is equal to zero. Then, with increasing frequency (which means a rising speed of the grating), $|\delta I|$ increases, reaches a maximum, to decrease toward 0 at even higher frequencies. δI is always negative because it is created by the movement of carriers in the internal field. When the frequency is low the internal field array and the electron array are in quadrature and the current is null. With increasing frequency the electron array moves faster than the internal field array which needs some time to reorganize via trapping and release. Both arrays are no longer in quadrature and a current appears

that increases with frequency until the speed of the grating is such that the carrier generation blurs the internal field array, the movement of carriers being too fast for the internal field array to reorganize properly. Eventually, the current reaches 0 at very high frequencies when the internal field array is completely erased.

In the case where 100 V/cm are applied the plot of dI/dJ vs frequency at 300 K shows that dI/dJ at low frequency is not equal to zero because the applied field breaks the quadrature between the carrier array and the internal field array. However, dI/dJ is negative which means that the essential of the current comes from the movement of carriers in the internal field. Again at high frequency the internal field array is blurred and the excess of current tends toward 0 (See Ref. [25] for more details).

* a-Si:H with defect-pool states

The illustration of a defect-pool is given in the file **aSiH_pool.dat**. It also shows how to define band tails with two exponential distributions each. The MPC in the HF regime and in the LF regime were simulated starting from **aSi:H_pool_HF.dat** and from **aSiH_pool_LF.dat**, respectively. In these files the DOS and its parameters were the same, only the 'experimental' parameters (e.g. the flux) were changed from one file to the other.

* GeTe phase change material

GeTe is a material that has been studied for years because it can be reversibly switched from amorphous to crystalline state. This phase transformation is accompanied by a change over decades of its conductivity. It is therefore foreseen as a possible candidate for data storage applications. The file **GeTe.dat** proposes a density of states of the amorphous phase. In this material holes are assumed to be the majority carriers. Hence, to plot the DOS calculated from MPC one has to choose the option (H)ole mobility to obtain a proper plot with a value of $C_p = 5 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$. It can be seen when comparing the introduced DOS and the MPC-DOS that the valence band tail is well reproduced but not the deep states. This is due to the much lower values chosen for their capture coefficients. For more details on the parameters introduced in the simulation see Ref. [6].

Note also that the optical capture coefficients C_{opt} have been adjusted to match the experimental results of the absorption vs $h\nu$ experimentally measured by Photothermal Deflection Spectroscopy (PDS).

* Crystalline materials

To illustrate the possibilities of this simulation to 'work' with crystalline materials, two data files are proposed.

- An **AsGa.dat** file, that uses a DOS that could be encountered in GaAs crystalline material, is proposed to illustrate the possibility to simulate the TPC experiment (**AsGa_TPC.dat**). This experiment was simulated at $T = 300 \text{ K}$. A plot of the calculated variations of $I(t)$ displays a curve with steps corresponding to the carriers generated by the short light pulse cascading down with time in the different trap levels introduced in the simulation. At a single temperature of 300 K all the trap contributions cannot be seen. The

simulation must be performed at lower temperatures to observe the contribution of the shallowest traps.

Simulations of the MPC experiment on the same 'material' (**AsGa_MPC.dat**) show one of the limits of this experiment. When one plot the MPC-DOS obtained from the simulation and compare it to the introduced DOS, it can be seen that the peak maxima are at the correct energy, provided the correct C_n has been chosen, but the maxima are always lower than expected. This is due to the limit of the approximations made to derive the expression of NC/μ . In the integrals from which one derives $N(E)$ is included a function peaked at E and decreasing as $\exp(1/kT)$ on each side. If the peaks of states are sharper than the function peaked at E , the final MPC-DOS is the correlation between the peak of states and the peaked function (see REF. [3] for more details). It can be seen on the plot of the MPC-DOS that the width of the peaks increases with energy (hence with T) along with the differences between the MPC-DOS and the true DOS maxima: the wider the MPC-DOS peak, the lower its maximum. This behavior reflects the enlargement of the function peaked at E with increasing temperature.

- An **SiC-Al&N&V&D1&B&O-10K.dat** file in which the DOS of the crystalline SiC is made of different defect levels (Al, N, V, UD1, B, O), some of them being linked to impurities. This file was made to illustrate the PITS experiments performed on such a material (see Ref. [30]). For the calculation the temperature range was 40 - 700 K and it was made each 10 K. When the simulation is performed one can see the filling, when the light pulse is ON, followed by the emptying, when the light pulse is OFF, of the defect states present in the gap by the carriers generated by the light.

The choice of the plot option **slopes(t0,T)** with the **Log** option displays a set of curves whose shape defines some 'ridges'. These 'ridges' correspond to the maximum of emission of carriers from a defect level after the end of the illumination. An order of magnitude of the activation energy of this maximum emission, corresponding to the energy position of the trap, can be obtained by setting the mouse pointer on one point of the 'ridge', clicking the left button of the mouse and moving the pointer along the ridge. When the button is released the energy activation, ΔE , is displayed on the graph.

This can only give an estimate of the activation energy. To have a better estimate one can use the files **SiC-Al&N&V&D1&B&O-10K-1ms-maxLIN+'# of the max'-7-0'** and plot the data as described in PITS plot. However, if the ΔT used to perform the PITS calculation is too large it is likely that the maxima will not be well defined and the activation energy impossible to calculate. That is why another simulation performed with temperatures in the range 250 - 700 K with a calculation each 2 K was done (**SiC-Al&N&V&D1&B&O-2K.dat** file). From the results of this calculation it is possible to define easily activation energies giving the position of some of the trap levels by plotting the data saved in **SiC-Al&N&V&D1&B&O-2K-1ms-+maxLIN+'# of the max'-7-0'**.

Note that the UD1 level was chosen as a multivalent state (-/0/+) fixed at an energy of 1.32 eV above E_v with a correlation energy of 0.91 eV that sets the emission of electrons from the (-) states at 2.23 eV above E_v that should give an activation energy $E_a = E_{gap} - 1.32 - 0.91 = 0.77$ eV.

In both cases (10 K or 2 K) a complete simulation is rather long as is also a complete PITS experiment.

A file has been created (**SiC-Al&N&V&D1&B&O-MPC.dat**) to illustrate the results of the MPC experiment on materials presenting amphoteric states. It shows a behavior expected for these peculiar states, in this example the UD1 state. For amphoteric states trapping and emission of an electron is slightly more complicated than with monovalent states. The + state has no electron, the 0 state has one electron at the energy of the defect E_d and the – state has two electrons, one at E_d and another one at the defect energy plus the correlation energy E_u . If the correlation energy is positive it means that the second electron is emitted from an energy $E_d + E_u$ closer to E_c than E_d . If one plots the MPC-DOS calculated with the **SiC-Al&N&V&D1&B&O-MPC.dat** file, using the UD1 C_{n0} to scale the energy, a peak of states appears around 0.75 eV in an energy region where there is no defect states. This peak corresponds to the contribution of the –/0 transition of the UD1 to the MPC response. Note that the energy position of this ‘peak’ (~ 0.75 eV) is in agreement with the results from the PITS simulation (~ 0.77 eV). For more details on the MPC response of a material with multivalent states see Ref. [4].

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It is impossible to quote all the references on which this software is based. The main ones are the following and, of course, the references in these references.

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How to modify the data in the Data window

Click on the down arrow of the data box you want to modify. The various labels and values of the parameters appear in a box.

Select the parameter you want to modify and click on it. Use the scroll bar if necessary.

Type the new value of the parameter directly on the highlighted characters and press ENTER.

You can check that the parameter value has been modified by repeating the first step and/or by clicking on **Display**.

Note that a check box is located on top of the data boxes corresponding to the definition of states distributions. If the box is checked, the contribution of these states to the MPC calculation is taken into account. Otherwise the contribution of the corresponding states to MPC is ignored. It allows to investigate on the individual contribution of each defect to the MPC signal but BE CAREFUL the global contribution is NOT the sum of each individual contribution. These check boxes are just a help in the adjustment of the parameters of a particular distribution to determine its influence on the global MPC spectrum.

How to install DeOSt

To use DeOSt create a folder 'Deost' in C: [C:\Deost] and copy the following documents in it:

- DEOSTV2.EXE, the main software
- The folder 'DLL Windows' containing some Windows files : Comdlg32.ocx, Sysinfo.ocx, MSVBVM60.dll, VB6FR.dll
- Some examples that are gathered in a folder 'Examples\simulati\resultpc'.
- Multmat.DLL, Syslin.DLL
- An help file (Helpdeost.chm)

The folder 'simulati' contains already some example files and can be dragged anywhere on the disk or you may create anywhere on the disk another folder 'simulati', and in this directory create at least another directory

resultpc in which the data files ***.dat are saved

 In which the photoconductivity files and some others will be saved.

The following directories may be created but if not the program will create them automatically if needed:

- resulpcm in which the modulated photocurrent results files will be saved,
- resulabs in which the absorption, CPM and DBP results files will be saved,
- resultpit in which the PITS files will be saved,
- resultsspg in which the SSPG and MGT files will be saved,
- resultopg in which the OPG results will be saved,
- resultTFT in which the TFT results will be saved.

Copy the examples ****.dat in the new \simulati\resultpc\ . The program may then use the data of this new 'simulati' folder to perform some new calculations.

In some languages the decimal symbol is a comma (,). DeOSt works with both decimal symbols, comma (,) or dot (.). However, the data and results of the calculations will be saved with the system symbol and some softwares do not work with comma (,) (e.g. Origin®). This symbol can be replaced by a dot (.) in the configuration panel. See for instance:

<http://resrequest.helpspot.com/index.php?pg=kb.page&id=279>

The simulation should run with several Windows® systems (from 95 up to Windows 10). For that copy the 'Windows DLL' files in 'C:\Windows\System32', if the system runs in 32 bits, or in 'C:\Windows\SysWOW64', if the system runs in 64 bits. In this last case the file Comdlg32.ocx must be installed in both 'C:\Windows\System32' and 'C:\Windows\SysWOW64'. If one or several of the 'Windows DLL' files are already in these folders **do not copy** them.

It is highly probable that at the first run of DeOSt you may face a problem with the Comdlg32.ocx file. To fix this problem follow the procedures exposed below.

Under Windows10 :

a/ click on 'Start' (the icon at the bottom left of the screen) and go to 'System Windows',

b/ right click on 'Command prompt' and choose 'Run as administrator'. A window must open with a line C:\Windows\System32> ,

c/type : regsvr32 %Systemroot%\System32\comdlg32.ocx.

Under Windows7 :

a/ click on '*Start*', then '*All programs*', then '*Accessories*',
b/ right click on '*Command prompt*' and choose '*Run as administrator*'. In the new window and after C:\Windows\System32>,
c/ type : regsvr32 %Systemroot%\System32\comdlg32.ocx

You may proceed by copying and paste the above command. If it is not possible, Be Careful, there is a space between 'regsvr32' and the end of the command !

The system should answer : "DllRegisterServer in C:\WINDOWS\System32\comdlg32.ocx succeeded".

You have to have administrator rights to follow the above procedures.

You may visit the following web sites that also explain how to fix this problem with the comdlg32.ocx.

<https://windowsfish.com/fix-comdlg32-ocx-missing-error/>

This program is huge and complicated therefore, though it was carefully tested, it would be surprising that no bugs are involved in it. If you find some bugs in this program or if you have any suggestions that could improve it, do not hesitate to contact :

christophe.longeaud@geeps.centralesupelec.fr

Annexe

This annexe gives some more details on the data displayed in the Calculation window during calculation.

MPC

During the MPC calculation the quantities n_r , n_i , p_r and p_i are displayed in the calculation window. They correspond to the in-phase (r) and out of phase (i) contributions of the free electrons (n) and free holes (p) to the alternating photocurrent.

Photoconductivity

During the calculation of the photoconductivity some data are displayed in the calculation window. One can find $Taue$, the electron lifetime, $Tauh$, the hole lifetime, g the gamma coefficient, and T_d the dielectric lifetime. The definition of these parameters is rather well-known and will not be recalled here.

Some other parameters are displayed which are less usual $Tau'n$, X_n , X_p , $Rtaue$, and $Rtauh$.

Under steady-state conditions the electrical neutrality is checked as well as the equality between recombination and generation $R = G$. Electrical neutrality implies that the negative charge $Q^- = Q^+$ the positive charge. $Tau'n$ is defined as

$$Tau'n = dQ^-/dG$$

and one has $Tau'n = Tau'p$, since $Q^- = Q^+$. It was shown in Ref. [25] that the knowledge of $Tau'n$ opens possibility of a DOS spectroscopy. In the program we use two different ways to calculate $Tau'n$ and the ratio of the results is displayed in the box with a '/'. This ratio must be close to one.

The other quantities come from the following integrals. If, for simplicity, we assume that the capture coefficients are the same for all the monovalent states we define:

$$\begin{aligned} I_1^n &= C_n \int_{E_V}^{E_C} (1-f) \tau N dE \\ I_2^n &= C_n \int_{E_V}^{E_C} (C_p p + e_p) (1-f) \tau N dE \\ I_3^n &= C_n C_p p \int_{E_V}^{E_C} \tau^2 N dE \end{aligned}$$

where

$$\frac{1}{\tau} = C_n n + C_p p + e_n + e_p \quad .$$

C_n (C_p) is the capture coefficient of electrons (holes), e_n (e_p) the emission rate of electrons (holes) from the states N at the energy E , n (p) the free electron (hole) concentration, and f the occupation function of the states. The same integrals can be calculated for holes replacing n by p and $1-f$ by f , giving I_1^p , I_2^p , and I_3^p , respectively. These integrals appear in all the calculations linked to several experiments like MPC, SSPG, MGT and OPG.

X_n and X_p are defined by

$$X_n = \frac{I_1^n}{I_3^n} - 1 \qquad X_p = \frac{I_1^p}{I_3^p} - 1 \quad .$$

It was shown in Ref. [18] that the expression of X_n could be simplified and that a DOS spectroscopy could be achieved from the knowledge of this quantity provided that the material was n-type. It was also shown that we must have $X_n < 1$ and $X_p < 1$. This can be verified during a calculation provided the quasi Fermi level is a few kT away from the dark Fermi level position.

Finally, one can define two lifetimes as

$$\frac{1}{\tau_n^R} = \frac{\partial R}{\partial n} \qquad \frac{1}{\tau_p^R} = \frac{\partial R}{\partial p} \quad .$$

It can be shown that $\frac{1}{\tau_n^R} = I_2^n$ and $\frac{1}{\tau_p^R} = I_2^p$ (see Eq. (8) of Ref. [22]). $Rtaue$ and $Rtauh$ are defined as the ratios

$$Rtaue = \frac{\tau_n}{\tau_n^R} \qquad Rtauh = \frac{\tau_p}{\tau_p^R} \quad .$$

It can be demonstrated that for an n-type material $\tau_p \approx \tau_p^R$. In this case $Rtauh \approx 1$. This can be verified during calculations performed on a material representative of a-Si:H for instance.

BE CAREFUL : In the program these parameters are only defined for monovalent states. In the case of multivalent states these parameters (X_n , X_p , $Rtaue$, $Rtauh$) have no signification.

CPM

During the AC CPM calculation the quantities n_r , n_i , p_r and p_i are displayed in the calculation window. They correspond to the in-phase (r) and out of phase (i) contributions of the free electrons (n) and free holes (p) to the alternating photocurrent generated by the AC flux. The modulus of the current density (Mod) and its phase shift (Phi) referred to the alternating flux are also displayed.

DBP

During the DBP calculation the quantities n_r , n_i , p_r and p_i are displayed in the calculation window. They correspond to the in-phase (r) and out of phase (i) contributions of the free electrons (n) and free holes (p) to the alternating photocurrent generated by the AC flux.

TPC

During calculation the calculation windows displays the increment of time (Inc), the time, the integral of the current density ($Q(t)$) and the dimension (Dim. Mat.) of the matrix defined to perform the calculation. It displays also the excess of carriers in each band as function of time, $deltan$ and $deltap$, and the number of time increments (Nbinc). It may happen that during calculation $deltan$ or $deltap$ become negative because of a too large trapping or recombination. It is always by a very small amount so, in this case, they are set to 0 and the calculation goes on but a warning is displayed ($dn < 0$ or $dp < 0$).

SSPG & MGT

In the MGT calculation the frequencies at which the calculation is performed are the differences of the light frequencies. These differences induce a movement of the grating at a speed $v_{gr} = \Lambda \delta f$ where Λ is the grating period. When the grating is moving a part of the free carriers is in phase with this movement and another part is out of phase depending on the trapping and release processes. It is these quantities that are displayed in the calculation window with an index r for the in-phase (n_r, p_r) and an index i for the out of phase (n_i, p_i) components of the free carrier distributions.

Software DEOST © CNRS 2002, herein after DEOST.

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