*

```
EEEEEEE   M     M    CCCCC    U     U   RRRRRR
E         MM   MM   C     C   U     U   R     R
EEEEEE    M M M M   C         U     U   RRRRRR
E         M  M  M   C         U     U   R   R
E         M     M   C     C   U     U   R    R
EEEEEEE   M     M    CCCCC     UUUUU    R     R
```

U S E R ' S M A N U A L

V e r s i o n 1 R 3 K (r e v . 0 4)

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October 1989

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Overview

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Introduction

EMCUR--Ensemble Monte Carlo at the University of Rochester--is an ensemble Monte Carlo simulator for III-V compound semiconductor devices developed at the University of Rochester. This version (1R3K) is a one-dimensional (1D in r space) device simulation program, which is suitable for simulating non-steady-state transport processes in bulk materials, heterojunction bipolar transistors (HBT), heterostructure hot-electron diode/transistors (HHED/HHET), relaxation of photogenerated carriers, etc. It is not, however, suitable for modeling such device structures as MESFET where a 2D (in r space) structure is required, or quantum well heterostructures where a 2D (in k space) scattering formalism for the 2D electron gas (2DEG) needs to be implemented, or HEMT (High Electron Mobility Transistor) where a 2D structure in both r and k spaces is needed.

The band-structure model used in the program is a three-valley (G-L-X) conduction band with nonparabolicity for any III-V ternary compound material (default is AlGaAs). The scattering mechanisms included are ionized impurity scattering, polar optical phonon scattering, acoustic phonon scattering, intervalley and intravalley phonon scatterings, and electron-electron scattering. Statistics in each valley as well as each individual scattering mechanism can be enabled/disabled by the user.

A piece-wise constant GAMMA approach is employed with "fast self-scattering" technique for the selection of the scattering mechanisms. An "adaptive" maximum electron energy, Emax*, in each valley (*=1, 2, 3 for G, X, L valleys) is used to ensure that the electron energy in valley * will never exceed Emax* during the simulation. The program also automatically disables the use of piece-wise constant GAMMA approach when the scattering rate is not a monotonic increasing function of energy.

A self-consistent Poisson solver and a self-consistent screening model are built in the program which, if invoked, calculate the local potential, field, charge density, and the scattering rates (through the screening length) using the evolving distribution functions in a self-consistent way.

A variety of options can be chosen for specifying the initial states of the ensemble in terms of its r- and k-space as well as time domain properties. An ensemble representing the background electrons only, or photoinjected carriers only, or both, can be specified. In k space, the particles can be launched from one of the five user-specified distributions: Maxwellian, hemi-Maxwellian, velocity-weighted Maxwellian, Gaussian (in energy), or delta-function (in k space) distributions. In r space, the (background) electrons can assume a delta-function, a uniform, or a user-specified distribution, while the photoinjected carriers assume an exponentially decaying function distribution. In the time domain, the shape of the laser pulse can be a rectangular pulse, a Gaussian pulse, or an inverse hyperbolic cosine function shaped pulse. The state of the ensemble can also be input from the results of the previous run in the continuous-run mode.

In this manual, input card format is first described in detail, followed by examples of typical outputs produced by EMCUR. Input/output file formats are discussed in Appendices.

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General Input Card Format

EMCUR takes as input a user-specified file which contains cards written in the general format as described below. There are twelve types of cards plus comment lines (identified by a star '*' on the first column) and a special *END card (appearing on the first four columns). Each card consists of two parts: a card name (identifier) preceded by a period '.' on the first column, and a list of parameters (specifiers) that form the body of the card. The parameter list is identified by a plus sign '+' on the first column, followed by several parameter specifiers separated by a comma ',' and ended with a semicolon ';'. A parameter specifier is defined as the integral entity of a parameter name (not to exceed 6 characters) followed by an equal sign '=' followed by the parameter value (not to exceed 10 characters). The following illustrates the general format of an input card:

```
column 1
|
.CARDName
+       Param1=value1,  Param2=value2,  Param3=value3;
+       Param4=value4,  Param5=value5,  Param6=value6;
```

The values of the assignment can take real, integer, or logical form depending on the type of the variable. In this manual, <r>, <i>, or <l> are used to indicate the type of values of the above form, respectively.

The valid card names are listed below, only the first five characters are significant (a card name must appear on a single line), and valid parameter names associated with each card are listed in Appendix A. (Note that card and parameter names are case sensitive.)

GRID	MATERial	BANDS
DEVICe	MECHAnism	POISSon
BOUNDary	INITState	COMPUte
MODEL	PLOT	SAVEFile

Spaces and tabs between the parameter specifiers are insignificant. Comment lines may appear anywhere in the input cards, which are ignored by the parser routine. Any characters after the 'semicolon' on each parameter list line, or after the 75th column, are ignored. Any lines after the *END card, or after the 100th line, are also ignored. No blank lines are allowed in the input cards. Since parameter names and values are allowed only up to 6 and 10 characters respectively, it is recommended that no spaces appear around the 'equal sign' in the assignments.

The default input deck is shown in Appendix A. Examples of some commonly encountered invalid card format are shown below with explanations:

```
Invalid Card/Parameter  Explanation

column 1
|
DEVICE                  Card name must be preceded by a period.
=       Udpg=.true.;    Parameter list must be preceded by a plus sign.
.BANDS  Xval=.false;    Card name must appear on a single line (Xval is
                        ignored).
                        No blank line is allowed.
.INIT State             Spelling error in the card name (should be IN-
                        ITState).
+       TGauss=t;       Spelling error in the parameter name (should be
```

```
                          Tgauss).
    +       Wsigma = 0.1;   The number of characters (including the space
                            before '=’!) in the parameter name exceeds 6.
    +       Ksbg=2 Kspc=4;  No comma between the parameter specifiers.
    +       Zdepth=0.2,     The parameter list must be terminated by a
                            semicolon.
    * END                   No space between '*' and 'END' is allowed.
```

In summary, the following general rules should be applied in writing an input card file:

(1) The first column must be a character among a star '*' (for comment line), a period '.' (for card name), or a plus sign '+' (for parameter list).
(2) The input file must be ended with a line starting by '*END' (optional characters may follow '*END'). If this is the only (and the least) four characters appeared in an input file, then the program uses the default input deck (see Appendix A) as the input.
(3) Each line of the parameter list (body of a card) must be ended with a semicolon ';'.
(4) Parameter specifiers must be separated by comma ',' with no more than 6 characters in the parameter names and no more than 10 characters in the parameter values.
(5) Card and parameter names are case sensitive. They must appear exactly the same as provided in this manual.
(6) The valid region of the input file is defined by a region of 75 columns x 100 lines, without blank lines inside the body of the file.

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Input Card Description

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The GRID Card

SYNTAX

```
.GRID
+       Emax1=<r>,      Emax2=<r>,      Emax3=<r>;
+       DEmax1=<r>,     DEmax2=<r>,     DEmax3=<r>;
+       Nepts1=<n>,     Nepts2=<n>,     Nepts3=<n>;
+       Iepwi1=<n>,     Iepwi2=<n>,     Iepwi3=<n>;
+       Iepwd1=<n>,     Iepwd2=<n>,     Iepwd3=<n>;
+       Vdlow=<r>,      Vdupr=<r>,      Ndpts=<n>;
+       Nbpts=<n>,      Nzpts=<n>,      Ntpts=<n>;
+       Bmax=<r>,       Zmax=<r>,       Tmax=<r>;
```

DESCRIPTION

The GRID card specifies the number of bins in the simulation structure in r and k spaces as well as in the time domain. All the grids are set up uniformly.

In k space, a maximum energy (Emax*) is specified in each valley (*=1, 2, 3 for G, X, L valleys), and the number of energy bins is specified through Nepts*. When the "piece-wise constant GAMMA approach" is employed for the self-scattering approximation, the initial energy bin index corresponding to the maximum total scattering rate, GAMMA, is determined by Iepwi*. During the simulation, if an electron's energy E happens to exceed E(Iepwi*), the energy bin index Iepwi* is increment by Iepwd* until E exceeds Emax*. In this case (E>Emax*), Emax* is automatically updated to Emax*+DEmax*, and the energy grid is re-setup. The number of bins in the energy/velocity distribution histograms is specified by Ndpts. The upper bound for the energy histogram is determined dynamically by the program from the value max{Emax1,Emax2,Emax3}, while the lower/upper bounds for the velocity histogram are specified by Vdlow/Vdupr.

In r space, the simulation region (device length) is specified by Zmax, with Nzpts number of spatial bins. If the "tunneling boundary condition" (see Ltbc in the BOUNDARY card) is used, the barrier region is determined through Bmax and Nbpts.

In the time domain, the simulation time is specified by Tmax, and the sampling interval (number of time steps) is specified by Ntpts.

PARAMETERS

Emax* The (initial) maximum energy in each valley. (Default: 1.0, unit: eV)

DEmax* The increment energy in each valley which is used to expand energy grids in case of electron energy exceeding Emax*. (Default: 0.5, unit: eV)

Nepts* The number of energy bins in each valley. (Default: 40, 20, 20 for *=1, 2, 3)

Iepwi* The initial energy bin index corresponding to the maximum total scattering rate in each valley when the piece-wise constant GAMMA approach is used. (Default: 20, 10, 10 for

*=1, 2, 3)

Iepwd* The increment in the energy bin index in each valley. (Default: 5)

Vdlow The lower bound for the velocity distribution histogram. (Default: -15e7, unit: cm/s)

Vdupr The upper bound for the velocity distribution histogram. (Default: 15e7, unit: cm/s)

Ndpts The number of bins in the energy/velocity distribution histograms. (Default: 20)

Nbpts The number of spatial bins in the barrier region (valid only if Ltbc=.true). (Default: 20)

Nzpts The number of spatial bins in the simulation region. (Default: 20)

Ntpts The number of time steps in the simulation. (Default: 20)

Bmax The length of the barrier region (valid only if Ltbc=.true). (Default: 0.1, unit: um)

Zmax The length of the simulation region (device length). (Default: 0.1, unit: um)

Tmax The total simulation time. (Default: 1.0, unit: ps)

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The MATERIAL Card

SYNTAX

```
.MATERial
+       Ldef=<l>,       Lgaas=<l>,      Lalas=<l>;
+       Lgap=<l>,       Ltgap=<l>,      Gtemp=<l>;
+       ECoff1=<r>,     ECoff2=<r>,     ECoff3=<r>;
```

DESCRIPTION

The MATERIAL card specifies band and material parameters used in the simulation. The program provides its own default parameters for the AlGaAs system, which can be modified through Lgaas, Lalas, Ltgap, and/or Lgap by user-defined data files (see Appendix B for the format of the data files). The above specifiers are not in effect when Ldef is set to .true.

PARAMETERS

Ldef — Flag for defining band and material parameters used in the program. If Ldef=.true, the program uses its own default parameters. (Default: .true)

Lgaas — Flag for defining GaAs band and material parameters (valid only if Ldef=.false). If Lgaas=.true, then a file named 'GaAs', which contains GaAs parameters, must exist. (Default: .false)

Lalas — Flag for defining AlAs band and material parameters (valid only if Ldef=.false). If Lalas=.true, then a file named 'AlAs', which contains AlAs parameters, must exist. (Default: .false)

Lgap — Flag for defining AlGaAs band-gap parameters (valid only if Ldef=.false). If Lgap=.true, then a file named 'Gap', which contains AlGaAs band gap parameters, must exist . (Default: .false)

Ltgap — Flag for defining temperature coefficients of GaAs band gap parameters (valid only if Ldef=.false). If Ltgap=.true, then a file named 'Tgap', which contains GaAs band gap parameters, must exist. (Default: .false)

Gtemp — Flag, if .true, the temperature-dependent band gaps of GaAs is used (valid only for uniform GaAs samples, i.e., Ualx=.false and Xdev=0.0 in the DEVICE card). (Default: .true)

ECoff* — The conduction band off-sets (percentage of the band discontinuity) between the device material (e.g., GaAs) and the barrier material (e.g., AlAs) in each valley (*=1, 2, 3 for G, X, L valleys), (valid only if Ltbc=.true in the BOUNDARY card). (Default: 0.6)

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The BANDS Card

SYNTAX

```
.BANDS
+       Gval=<l>,       Xval=<l>,       Lval=<l>;
```

DESCRIPTION

The BANDS card specifies which valley (or band) is in effect during the simulation. The default band structure is a three-valley conduction band with nonparabolicity for the AlGaAs ternary system. When, for example, the X valley is disabled (Xval=.false), the intervalley scattering occurs only between G and L valleys.

PARAMETERS

Gval Flag specifying the presence of the G valley. (Default: .true)

Xval Flag specifying the presence of the X valley. (Default: .true)

Lval Flag specifying the presence of the L valley. (Default: .true)

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The DEVICE Card

SYNTAX

```
.DEVICe
+       Udpg=<l>,       Ufld=<l>,       Uvbs=<l>;
+       Ualx=<l>,       Doping=<r>,     Field=<r>;
+       Vbias=<r>,      Xdev=<r>,       Xbar=<r>;
+       Temp=<r>;
```

DESCRIPTION

The DEVICE card specifies the operating conditions of the device under investigation, such as temperature, doping, composition, and applied field/bias. The program first assumes uniform doping, field, bias, and composition profiles as specified by the specifiers Doping, Field, Vbias, and Xdev (Xbar for the barrier region if Ltbc=.true in the BOUNDARY card), respectively. User-specified non-uniform profiles for doping, field, bias, and/or composition can be supplied from data files by "turning on" the flags Udpg, Ufld, Uvbs, and/or Ualx, respectively (see Appendix C for the format of the data files).

PARAMETERS

Udpg — Flag, if .true, a user-supplied data file named 'Udpg' is used to override the uniform doping profile. (Default: .false)

Ufld — Flag, if .true, a user-supplied data file named 'Ufld' is used to override the uniform field profile. This option is useful in imposing a user-defined, time- and space-dependent field distribution. (It is invalid if Lpois=.true in the POISSON card.) (Default: .false)

Uvbs — Flag, if .true, a user-supplied data file named 'Uvbs' is used to override the constant applied bias. This option is useful for specifying a time-dependent applied bias, and in conjunction with the specifiers Lpois=.true and Ibcr=1 (see the POISSON card), field distributions inside the device subject to the time-varying boundary condition can be calculated self-consistently, and high-frequency responses be eventually studied. (Default: .false)

Ualx — Flag, if .true, a user-supplied data file named 'Ualx' is used to override the uniform composition profile. In this case, the band and material parameters, such as band gaps, effective masses, etc., would be space dependent. (Default: .false)

Doping — The uniform (background) doping concentration in the device. (Default: 1e17, unit: 1/cm^3)

Field — The uniform field distribution in the device. (Default: 50e3, unit: V/cm)

Vbias — The constant applied bias on the right boundary with respect to the left boundary (zero reference). (Default: 0.5, unit: V)

Xdev The uniform Al composition, x, for the Al(x)Ga(1-x)As system in the device. (Default: 0.0)

Xbar The uniform Al composition, x, for the Al(x)Ga(1-x)As system in the barrier region (valid only if Ltbc=.true in the BOUNDARY card). (Default: 1.0)

Temp The lattice temperature. (Default: 300, unit: K)

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The MECHANISM Card

SYNTAX

```
.MECHAnism
+       Limpty=<l>,     Loptic=<l>,     Lacous=<l>;
+       Lintra=<l>,     Linter=<l>,     Leesct=<l>;
```

DESCRIPTION

The MECHANISM card enables/disables the indicated scattering mechanisms. By turning on or off the selected mechanisms, one can examine the effect of a particular scattering mechanism on the transport processes. (Note: when some scattering mechanisms are deliberately turned off, the functional form of the total scattering rate versus energy changes.)

PARAMETERS

Limpty Flag that, if .false, disables the ionized impurity scattering. (Default: .true)

Loptic Flag that, if .false, disables the polar optical phonon scattering. (Default: .true)

Lacous Flag that, if .false, disables the acoustic phonon scattering. (Default: .true)

Lintra Flag that, if .false, disables the intravalley scattering. (Default: .true)

Linter Flag that, if .false, disables the intervalley scattering. Note that if intervalley scattering is disabled, electrons would remain in the valley in which they initially reside. (Default: .true)

Leesct Flag that, if .false, disables the electron-electron scattering. When the e-e scattering is enabled, the total scattering rate in each valley is updated for each time step during the simulation. (Default: .false)

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The POISSON Card

SYNTAX

```
.POISSon
+       Lpois=<l>,      Ldepl=<l>,      Ibcl=<i>;
+       Ibcr=<i>,       Fldl=<r>,       Fldr=<r>;
```

DESCRIPTION

The POISSON card specifies whether the self-consistent Poisson solver is to be used or not. There are two types of boundary conditions (B.C.'s) for the Poisson solver: (1) fixed voltage and (2) fixed field at the boundaries. The specifiers Ibcl/Ibcr take the value 1 or 2 for the first (fixed voltage) or the second (fixed field) B.C.'s at the left/right boundaries, respectively. When Ibcl/Ibcr=1, the voltage is set to zero at the left boundary, and Vbias (or a user-specified value if Uvbs=.true in the DEVICE card) at the right boundary. If Ibcl/Ibcr=2, the field is set to Fldl/Fldr at the left/right boundary. (Note: the condition Ibcl=Ibcr=2 has no single solution and is therefore not allowed.) Possible combinations of the B.C.'s are: Ibcl=Ibcr=1; Ibcl=1, Ibcr=2; Ibcl=2, Ibcr=1. One can also impose a user-defined depletion charge inside the device by specifying Ldepl=.true This option is useful, for example, for simulating carrier transport in a surface field region in which a surface charge and depletion charge is present at the device boundary.

All the parameters are not in effect if Lpois=.false.

PARAMETERS

Lpois — Flag that, if .true, enables the self-consistent calculation of the Poisson equation, which updates the potential and field distributions inside the device at each time step using the current local charge densities. (Default: .false)

Ldepl — Flag, if .true, a user-supplied data file named 'Depl' (see Appendix C for the format) is used to provide depletion charges inside the device. (Default: .false)

Ibcl — Flag that takes the value 1 or 2 for specifying the B.C.'s (fixed voltage or fixed field) at the left boundary. (Default: 1)

Ibcr — Flag that takes the value 1 or 2 for specifying the B.C.'s (fixed voltage or fixed field) at the right boundary. (Default: 1)

Fldl — The field imposed at the left boundary (valid only if Ibcl=2). (Default: 0.0, unit: V/m)

Fldr — The field imposed at the right boundary (valid only if Ibcr=2). (Default: 0.0, unit: V/m)

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The BOUNDARY Card

SYNTAX

```
.BOUNDary
+       Lpbc=<l>,       Ltbc=<l>,       Inj=<n>;
+       Ksbc=<i>,       Telec=<r>,      Velec=<r>;
```

DESCRIPTION

The BOUNDARY card specifies what actions to take if an electron is out of the device from either boundary during the simulation. There are three types of boundary conditions which are mutually exclusive:

(1) Periodic boundary condition (if Lpbc=.true): this option can be used to simulate transport in infinite bulk materials. The electron out of one boundary is brought back to the other boundary with the same k, and simulation continues.

(2) Tunneling boundary condition (if Ltbc=.true): this occurs only at the right boundary (assuming an accelerating field is applied), and is useful for simulating heterostructure hot-electron diode/transistors. The electron out of the right boundary is first tested whether it has high enough energy to overcome the barrier. If it can, then "thermionic emission" occurs, and another electron with an independent k is injected from the left boundary; otherwise, the tunneling probability is calculated taking into account the current interface charge density, and a pseudorandom number is used to test whether this electron can tunnel through the barrier. If "tunneling" occurs, then the same procedure as for thermionic emission is carried out; otherwise, this electron is returned to the right boundary, and simulation continues. (The left boundary is assumed to be a "perfect absorbing boundary," see below.)

(3) Perfect absorbing boundary condition (if Lpbc=Ltbc=.false): this is for simulating ohmic contacts or other absorbing boundaries. The electron out of either boundary is assumed to be absorbed by that boundary, and another electron with an independent k from a user-specified distribution is injected from the left boundary.

There are three types of boundary conditions in k space, specified through the parameter Ksbc: 1--Maxwellian, 2--hemi-Maxwellian, 3--velocity-weighted Maxwellian. Each of them can be a "heated" (Telec>Temp) and/or a "drifted" (Velec>0 or Velec<0) distribution, where Temp (see the DEVICE card) is the lattice temperature.

In r space, the "injection plane" can be placed inside the device through the specifier Inj.

PARAMETERS

Lpbc Flag for specifying periodic boundary condition. (Default: .false)

Ltbc Flag for specifying tunneling boundary condition. (Default: .false)

Inj The spatial bin index for the injection plane which can be either at the left boundary (Inj=1) or inside the device (1<Inj<Nzpts, where Nzpts is the number of spatial bins specified in the GRID card). This parameter specifies the physical location of carrier injection rather than the physical device boundary, which is especially useful in connection with the Zdelta specifier (see the INITSTATE card).

Ksbc Flag that takes the value 1, 2, or 3 for specifying Maxwellian, hemi-Maxwellian, or velocity-weighted Maxwellian distributions in k space, respectively. (Default: 1)

Telec The electron temperature in the "drifted Maxwellian" distribution specified by Ksbc. (Default: 300, unit: K)

Velec The electron average drift velocity in the "drifted Maxwellian" distribution specified by Ksbc. (Default: 0.0, unit: cm/s)

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The INITSTATE Card

SYNTAX

```
.INITState
+       Voccu1=<r>,     Voccu2=<r>,     Voccu3=<r>;
+       Tdelta=<l>,     Trectg=<l>,     Tgauss=<l>;
+       Tinvch=<l>,     Ksbg=<i>,       Kspc=<i>;
+       Wpulse=<r>,     Wsigma=<r>,     Wfwhm=<r>;
+       Zdelta=<l>,     Zunif=<l>,      Zuser=<l>;
+       Lambda=<r>,     Efwhm=<r>,      Dinj=<r>;
+       Zdepth=<r>,     Einj=<r>,       DEinj=<r>;
```

DESCRIPTION

The INITSTATE card specifies the initial states of the ensemble in terms of r-space, k-space, and the time domain properties. When the continuous-run mode is in effect, specifically, when Rcont=.true and Rfirst=.false (see the COMPUTE card), the program takes the output from the previous run as the initial states instead, and therefore, all the specifiers in this card are not in effect.

In r space, four types of initial spatial distributions can be specified: (1) if Zdelta=.true: a delta-distribution at the position specified by the spatial bin index Inj in the BOUNDARY card. This option is useful for testing ideas and simulating transport processes in bulk materials; (2) if Zunif=.true: a uniform distribution. For this option, if Lpois=.true in the POISSON card, then Udpg in the DEVICE card must be set to .false, i.e., the doping profile is also uniform such that initially the (background) electrons cancel out the ionized impurity donors; (3) if Zuser=.true: a user-supplied, arbitrary distribution from a file named 'Zusr'. For this option, if Lpois=.true in the POISSON card, then Udpg in the DEVICE card must also be set to .true, and the file 'Zusr' must be identical to the file 'Udpg' for the same reason as stated above; and (4) if Laser=.true (see the MODEL card): an exponentially decaying function specified by the parameters Zdepth and Zmax. This option is for simulating photoinjected carriers. In this case, Zdelta specifier is always disabled. Whether Zunif or Zuser is valid or not depends on the specifier Lbkgrd in the MODEL card: if Lbkgrd=.true, i.e., the background electron sub-ensemble is present, one of them must be .true, otherwise they are not in effect. (See details in the MODEL card.)

In k space, there are five types of initial k distributions specified by the parameters Kspc and/or Ksbg for specifying photoinjected carriers and/or background electrons, respectively. The parameters Kspc/Ksbg take the value 1, 2, 3, 4, or 5 for Maxwellian, hemi-Maxwellian, velocity-weighted Maxwellian, Gaussian, and delta-function distributions, respectively. The first three options are identical to the specifier Ksbc in the BOUNDARY card, they can be a "heated" and/or a "drifted" Maxwellian distribution through the specifiers Telec and/or Velec in the BOUNDARY card. The fourth option (Gaussian in energy) can be specified by the parameters Lambda (Lambda) and Efwhm (DE). The Gaussian distribution is centered at the "excess energy" of {1.24/Lambda-Eg} (in eV) where Eg (in eV) is the band gap and Lambda (in um) is the wavelength of the laser source, and with an "energy width" of DE (in eV). The fifth option (delta-function in k space) can be specified by the parame-

ters Einj and DEinj. This is really a pulse distribution in energy centered at Einj with a width of DEinj, and a delta-function in k space with px=py=0 and pz=[2m*Einj/(1+a Einj)]^1/2, where m* is the effective mass and a is the nonparabolicity parameter. The initial valley occupancy can also be specified via Voccu* where *=1, 2, 3 for G, X, L valleys.

In the time domain, there are two classes of the initial shape of the ensemble: One is a delta-function distribution (Tdelta=.true) which implies that the entire ensemble is launched at t=0. This option must be used when Laser=.false (see: the MODEL card), i.e., no photoinjected carriers; and it is invalid when Rcont=.true and Rfirst=.false (see: the COMPUTE card), i.e., this is a continuous run. The other is the introduction of a time-varying ensemble which is only for photoinjected carriers for the first run (Laser=.true and Rfirst=.true in the COMPUTE card). There are three options to choose from for the shape of the time-varying ensemble: (1) if Tpulse=.true: a rectangular-shaped pulse of width Wpulse is injected; (2) if Tgauss=.true: a Gaussian-shaped pulse of width (2 x standard deviation) Wsigma is injected, which expands about 2.2 x Wsigma in time; and (3) if Tinvch=.true: an inverse hyperbolic cosine function shaped pulse of width (full width at half maximum) Wfwhm is injected, which expands about 1.2 x Wfwhm in time.

PARAMETERS

Voccu* The initial valley occupancy in each valley (*=1, 2, 3 for G, X, L valleys). The sum of the three parameters must equal 1.0. (Default: 1.0, 0.0, 0.0 for *=1, 2, 3)

Tdelta Flag, if .true, all the electrons are in the device at t=0. (Default: .true)

Trectg Flag, if .true, the photoinjected electron sub-ensemble is introduced at each time step according to a rectangular-shaped function. (Default: .false)

Tgauss Flag, if .true, the photoinjected electron sub-ensemble is introduced at each time step according to a Gaussian-shaped function. (Default: .false)

Tinvch Flag, if .true, the photoinjected electron sub-ensemble is introduced at each time step according to an inverse hyperbolic cosine shaped function. (Default: .false)

Ksbg Flag that takes the value 1, 2, 3, 4, or 5 for specifying Maxwellian, hemi-Maxwellian, velocity-weighted Maxwellian, Gaussian (in energy), or delta-function (in k space) distributions, respectively, in k space for the background electron sub-ensemble (invalid if Laser=.true and Lbkgrd=.false in the MODEL card). (Default: 1)

Kspc Flag that takes the value 1, 2, 3, 4, or 5 for specifying Maxwellian, hemi-Maxwellian, velocity-weighted Maxwellian, Gaussian (in energy), or delta-function (in k space) distributions, respectively, in k space for the photoinjected electron sub-ensemble (invalid if Laser=.false in the MODEL card). (Default: 4)

Wpulse The pulse width for the rectangular pulse if Trectg=.true. (Default: 0.2, unit: ps)

Wsigma The pulse width (2 x standard deviation) for the Gaussian pulse if Tgauss=.true. (Default: 0.2, unit: ps)

Wfwhm The pulse width (full width at half maximum) for the inverse hyperbolic cosine function pulse if Tinvch=.true. (Default: 0.2, unit: ps)

Zdelta Flag, if .true, all the electrons are at the position specified by the spatial bin index Inj in the BOUNDARY card (invalid if Laser=.true in the MODEL card). (Default: .true)

Zunif Flag, if .true, all the (background) electrons are spatially distributed according to a uniform distribution. (Default: .false)

Zuser Flag, if .true, all the (background) electrons are spatially distributed according to a user-specified distribution from a data file named 'Zusr' (see Appendix C for the format). (Default: .false)

Lambda The wavelength of the laser pulse for the photocarrier injection (valid only if Laser=.true in the MODEL card and Kspc=4). (Default: 0.590, unit: um)

Efwhm The energy width of the laser pulse for the photocarrier injection (valid only if Laser=.true in the MODEL card and Kspc=4). (Default: 1e-3, unit: eV)

Dinj The injection level of the laser for the photocarrier injection (valid only if Laser=.true in the MODEL card). (Default: 1e12, unit: 1/cm^2)

Zdepth The optical penetration depth for the photocarrier injection (valid only if Laser=.true in the MODEL card). (Default: 0.1, unit: um)

Einj The energy at which a delta- or a pulse-like function in energy is centered for the injected carrier ensemble. (Default: 1.0, unit: eV)

DEinj The energy width of the injected carrier ensemble. (Default: 1e-3, unit: eV)

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The COMPUTE Card

SYNTAX

```
.COMPUte
+       Rcont=<l>,      Rfirst=<l>,     Naccu=<i>;
+       Lproc1=<l>,     Lproc2=<l>,     Iseed=<i>;
+       Ntotal=<i>,     Nbkgrd=<i>,     Nphoto=<i>;
+       Itobv1=<i>,     Itobv2=<i>,     Itobv3=<i>;
```

DESCRIPTION

The COMPUTE card specifies the computational control parameters, such as the mode of operation, the seed of the pseudorandom number (PRN) generator, the size of the ensemble, and the observation times.

There are two modes of operation: single run and continuous run, which are specified by the parameters Rcont and Rfirst. The continuous-run mode is useful for expanding time axis without losing temporal resolution. Since the number of time steps in a single run is limited (Ntpts<=100), tradeoffs must be made between a longer simulation time and a finer temporal resolution if this mode is unavailable. This presents especially a severe problem when simulating photogenerated carriers using very short laser pulses, where the requirement of a femtosecond temporal resolution and a steady-state statistics may require excessive simulation time. With the continuous-run mode, one can split a longer run into a sequence of shorter runs in which the subsequent runs take as input the output of the states of the ensemble from the previous run. It is noteworthy that, to preserve consistency, the sampling interval should be kept constant from run to run.

The program has its own PRN generator which produces machine-independent, uniformly distributed pseudorandom numbers in (0,1). There are two characteristics, among others, of the Monte Carlo (MC) technique using PRN generators: independence and reproducibility. The results of the average quantities of a MC simulation should be independent, within the statistical error, from run to run as long as the ensemble size is large enough, without regard to the seed of the PRN generator. On the other hand, a MC simulation should be exactly reproducible with the same seed of the PRN generator.

The total size of the ensemble is specified by the parameter Ntotal (not to exceed 30,000), and two other parameters (Nbkgrd and Nphoto) specifying the sub-ensembles for the background and photoinjected carriers, respectively. If there is no photocarrier injection (Laser=.false in the MODEL card), one must set Nphoto=0 and Nbkgrd=Ntotal. If Laser=.true, according to Lbkgrd in the MODEL card, one must set either Nbkgrd=0, Nphoto=Ntotal if Lbkgrd=.false (without background electrons) or Nbkgrd!=0, Nphoto!=0, Nbkgrd+Nphoto=Ntotal if Lbkgrd=.true (with background electrons).

The distribution histograms, such as energy/velocity distributions, spatial distributions, potential/field/concentration profiles, scattering-rate patterns, etc., can be sampled and output at three user-specified instances through the parameters Itobv1, 2, 3 in disk files for post-graphical processing.

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PARAMETERS

Rcont Flag, if .true, the continuous-run mode is enabled. The program outputs a data file named 'STATE.OUT', which contains the states of the ensemble {Iv, z, px, py, pz} as well as other relevant variables. This file is to be used as the input for the subsequent run as the initial conditions ('STATE.OUT' must be renamed to 'STATE.IN' before subsequent run). Whether the current run is a continuous run or not depends on the specifier Rfirst below. (Default: .false)

Rfirst Flag (valid only if Rcont=.true) that specifies the mode of the current run. If Rfirst=.true, the program performs the same as in the single-run mode except that a 'STATE.OUT' file is output upon normal termination for the subsequent run. If Rfirst=.false (and Rcont=.true), a file named 'STATE.IN' (renamed from 'STATE.OUT' of the previous run) must exist. It is recommended that one use the same input cards of the previous (first) run, and change Rfirst=.true to Rfirst=.false for the continuous run. (Default: .true)

Naccu Flag that takes the value 1 or 0 for specifying the format of data in the file 'STATE.OUT' (valid only if Rcont=.true). Since the file 'STATE.OUT' takes a large amount of disk space (more than 4 x Ntotal x b where Ntotal is the ensemble size and b is the number of bits for each record). Trade-offs can be made between the accuracy and the disk space by specifying Naccu=1 for the long format (D23.16--16-digits accuracy) or Naccu=0 for the short format (D15.8--8-digits accuracy). (Default: 0)

Lproc1 Flag that, if .true, enables monitoring the run-time process by printing out the "DO variable" of the outer-loop (time-loop) in the program to the standard I/O. (Default: .false)

Lproc2 Flag that, if .true, enables monitoring the number of times that the piece-wise constant GAMMA approach is employed in each valley during the program run. (Default: .false)

Iseed The seed of the built-in PRN generator. (Default: 1)

Ntotal The total number of "superparticles" (total ensemble size). (Default: 10)

Nbkgrd The number of "background particles" (background sub-ensemble size). Nbkgrd must be equal to Ntotal if Laser=.false, and Nbkgrd must be equal to zero if Laser=.true and Lbkgrd=.false. (Default: 10)

Nphoto The number of "photoinjected particles" (photocarrier sub-ensemble size). Nphoto must be equal to Ntotal if Laser=.true and Lbkgrd=.false, and Nphoto must be equal to zero if Laser=.false. (Default: 0)

Itobv* The user-defined, three different intermediate instances (0<Itobv*<Ntpts, where Ntpts is the number of time steps specified in the GRID card) for which distribution histo-

grams are sampled and output for post-graphical processing.
(Default: 5, 10, 15 for *=1, 2, 3)

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The MODEL Card

SYNTAX

```
.MODEL
+       Laser=<l>,      Lbkgrd=<l>,     Lscrng=<l>;
```

DESCRIPTION

The MODEL card specifies the physical models used in the program. There are two types of models that one can specify: One is the inclusion of photoinjected carriers (through Laser) with or without background electrons (through Lbkgrd). The other is the inclusion of a "self-consistent screening model" (through Lscrng).

When there is no photocarrier injection (Laser=.false), the total ensemble is only the background electrons which are present at t=0, and distributed spatially according to Zdelta, Zunif, or Zuser (see the INITSTATE card). With photocarrier injection (Laser=.true), there are two options to choose from: (1) without background electrons (Lbkgrd=.false), then the total ensemble is the photoinjected carriers with a pulse shape specified by Trectg, Tgauss, or Tinvch (see the INITSTATE card) and a spatial exponentially decaying function profile with a penetration depth of Zdepth (see the INITSTATE card); (2) with the background electrons (Lbkgrd=.true), then the total ensemble is split into two parts--the background electron sub-ensemble and the photoinjected carrier sub-ensemble. When the Poisson solver is invoked (Lpois=.true in the POISSON card), the two sub-ensembles are normalized separately to their "supercharges." In addition, holes are introduced into the simulation region as photocarriers are injected, with the same spatial distribution as that of the electrons. But the holes are assumed to be immobile during the simulation (infinitely large effective mass).

When the self-consistent screening model is employed (Lscrng=.true), the screening length, which affects the scattering rate/angle of the optical phonon and ionized impurity scatterings as well as electron-electron scattering rate, is updated at each time step during the simulation. In this case, the scattering table in each valley is also updated at the end of each time step if the above mentioned mechanisms are operative. If Lscrng=.false, however, the Debye-Huckel screening model is used instead.

This card should be specified in close connection with the cards INITSTATE and COMPUTE.

PARAMETERS

Laser — Flag, if .true, photogenerated carriers from a laser pulse is to be simulated, with or without the background electrons. (Default: .false)

Lbkgrd — Flag (valid only if Laser=.true), if .true, background electrons is also imposed on the photoinjected carriers. (Default: .false)

Lscrng — Flag that, if .true, enables the inclusion of the self-consistent screening model. (Default: .false)

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The PLOT Card

SYNTAX

```
.PLOT
+       Lplots=<l>,     Nstep=<i>;
```

DESCRIPTION

The PLOT card specifies the plots of simulation results to be output on a line printer. The information includes the valley occupancy and average energy/velocity versus time in each valley as well as in all valleys combined. Due to normalization concerns, it is recommended that, when this option is enabled, one specify the number of time steps (Ntpts in the GRID card) to be a multiple of 4, preferably 40 or 80. If Ntpts=80, one should set Nstep to 2 such that each plot would appear on a single page.

PARAMETERS

Lplots Flag that, if .true, enables the output of a data file (for the line printer) named 'Plots' which contains plots of the valley occupancy, average energy/velocity versus time in each valley as well as in all valleys combined. When both background and photoinjected sub-ensembles are present (Laser=.true and Lbkgrd=.true in the MODEL card), information on those two separate sub-ensembles is also available. (Default: .false)

Nstep An integer (normally taking the value 1 or 2) for specifying the steps on the time axis for the plots. If Nstep=2, for example, each plot would have Ntpts/2 number of points on the time axis, where Ntpts is the total number of time steps (see the GRID card). (Default: 1)

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The SAVEFILE Card

SYNTAX

```
.SAVEFile
+       Dhisto=<l>,     Dtevol=<l>,     Dsmech=<l>;
+       Dspdev=<l>,     Dgamma=<l>,     Dpfcsp=<l>;
```

DESCRIPTION

The SAVEFILE card specifies classes of simulation data to be saved on disk files for post-graphical processing. There are six classes of simulation results to be processed: (1) if Dhisto=.true: energy, velocity, and spatial distribution histograms; (2) if Dtevol=.true: time evolution of the ensemble averages, such as average energy/velocity, valley occupancy, ensemble means, scattering angles, mean free times/paths, etc.; (3) if Dsmech=.true: time and space dependence of the scattering patterns due to each operative mechanism, and scattering rates versus time; (4) if Dspdev=.true: space dependence of the average energy and velocity; (5) if Dgamma=.true: scattering rate tables as a function of energy, as well as maximum total scattering rate versus time used in the simulation; and (6) if Dpfcsp=.true: potential, field, electron concentration, and net charge density profiles. (See Appendix D for the format of the data files.)

In the above data files, the information contains values in each separate valley as well as in all valleys combined; for histograms or spatial dependencies, the information is sampled at the initial time, three user-specified intermediate instances (specified by Itobv* in the COMPUTE card), and the final time.

PARAMETERS

Dhisto Flag that, if .true, enables the output of a data file named 'His.data' which contains energy/velocity/space distribution histograms in each valley as well as in all valleys combined at the initial, three intermediate, and the final times. (Default: .false)

Dtevol Flag that, if .true, enables the output of: (a) a data file named 'Tev.data' which contains time evolution of ensemble averages, such as average energy and velocity, valley occupancy, ensemble means, scattering angles, mean free times/paths, etc., in each valley as well as in all valleys combined; (b) a data file named 'Vvt.data' (if Lpois=.true in the POISSON card) which contains the time dependence of the potential at the right boundary; (c) a data file named 'Ivt.data' which contains the "current" versus time (actually the number of particles impinged on the right boundary during each time step), if Ltbc=.true in the BOUNDARY card, the "current" also includes "emission current" and "tunneling current;" and (d) a data file named 'Zve.data' which contains the trajectory in the time domain of the state {valley, position, velocity, and energy} of the first electron in the ensemble. When Laser=.true and Lbkgrd=.true (see the MODEL card), two data files named 'Pcev.data' and 'Bgev.data' are output which contains time evolution of the average energy and velocity as well as valley occupancy for the photocarrier and the background electron sub-ensembles,

respectively. (Default: .false)

Dsmech Flag that, if .true, enables the output of a data file named 'Mec.data' which contains time and space dependence of the scattering patterns due to each mechanism. Also, scattering rates (in 1/s) versus time (in ps) for each operative mechanism are output in the following files: 'Rtotal' for total scattering rate; 'Rself' for self-scattering rate; 'Rimpty' for impurity scattering rate; 'Racous' for acoustic phonon scattering rate;

Dspdev Flag that, if .true, enables the output of a data file named 'Sev.data' which contains space dependence of the average energy and velocity in each valley as well as in all valleys combined at the initial, three intermediate, and the final times; and (if Lscrng=.true in the MODEL card) a data file named 'Linv.data' which contains the space dependence of the inverse screening length sampled at the initial, three intermediate, and the final times. (Default: .false)

Dgamma Flag (valid only if Lscrng=.true in the MODEL card or if Leesct=.true in the MECHANISM card) that, if .true, enables the output of a data file named 'Gam.data' which contains the total scattering rate table in each valley sampled at the initial, three intermediate, and the final times, and a data file named 'Gmax.data' which contains the maximum total scattering rate in each valley at each time step. (Default: .false)

Dpfcsp Flag (valid only if Lpois=.true in the POISSON card) that, if .true, enables the output of a data file named 'PFC.data' which contains the potential, field, electron concentration, and net charge density profiles at the initial, three intermediate, and the final times. (Default: .false)

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The *END Card

SYNTAX

*END (Optional comments)

DESCRIPTION

This is a special card, which must appear on the first four columns of the last line of an input file. (Lines after the line with *END are ignored.) If this is the only (and the least) four characters (except for other comment lines) appeared in an input file, then the program assumes that all the parameters take their default values.

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*

Examples

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Example 1. Steady-State Transport Properties

PURPOSE

1. Demonstrate how to simulate steady-state transport properties in bulk GaAs;
2. Compare the simulation results with experiments to check the validity of the program.

DESCRIPTION

In order to simulate steady-state transport properties in bulk materials, a "long device" (2 um) is used, with a pulse of electrons injected inside the device (Inj=10) to eliminate the contact effect. An ensemble of Ntotal=5,000 electrons with an initial Maxwellian distribution (Ksbg=1) in equilibrium with the lattice (Te=Temp=300 K) is then followed under the influence of a uniform applied field (Ufld=.false) for 5 ps with 50-fs sampling interval (Tmax=5 ps, Ntpts=100). An intrinsic GaAs material is assumed (Doping=1e10 1/cm^3, Xdev=0.0), and thus the impurity scattering is disabled (Limpty=.false).

To eliminate the influence of the initial transients, a time average between 4 and 5 ps of a quantity (say, average velocity) is performed to obtain the steady-state value of that quantity. In this way, a steady-state velocity versus field curve, for example, can be obtained by simulating the transport process at different applied field strengths.

INPUT FILE(S)

Example 1:

```
*TITLE  Example 1 - Steady-state transport properties
*FILE   ex1.10: Field=10 kV/cm.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Ndpts=80,       Nzpts=80,       Ntpts=100;      !-, -, -
+       Zmax=2.0,       Tmax=5.0;                       !um, ps
.DEVICe
+       Field=10.0D3,   Vbias=1.0,      Doping=1.0D10;  !V/cm, V, 1/cm^3
.MECHAnism
+       Limpty=.FALSE.;                                 !-
.BOUNDary
+       Lpbc=.TRUE.,    Inj=10;                         !-, -
.COMPUte
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
+       Ntotal=5000,    Nbkgrd=5000;                    !-, -
+       Itobv1=10,      Itobv2=20,      Itobv3=40;      !-, -, -
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                        !-, -
.SAVEFile
+       Dtevol=.TRUE.;                                  !-
*
*END    End of Example ex1.10.
```

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OUTPUTS

EMCUR.out:

```
                        ********************************
                        * EMCUR: Version 1R3K (rev.04) *
                        ********************************


                         *** Simulation Parameters ***

 Simulation time:  Tmax =  5.000 (ps) with 100 number of time steps

 Device length:  Zmax =  2.000 (um) with 80 number of spatial bins

 Doping (uniform):  Doping =  0.100E+11 (1/cm^3)

 Lattice temperature:  Temp =   300.0 (K)

 Ensemble size:  Ntotal =  5000,  Nbkgrd =  5000,  Nphoto =     0


                           *** Output Parameters ***

 Number of reflections on the left/right boundary:
 Mlref =       0,  Mrref =       0

 Number of changes in the piece-wise constant GAMMA approach:
 G: Mechg1 =   3,  X: Mechg2 =   0,  L: Mechg3 =   0

 Final valley occupancies:
 G: Voccu1 =  0.412,  X: Voccu2 =  0.006,  L: Voccu3 =  0.581

 Final maximum energies:
 G: Emax1 =   1.00,  X: Emax2 =   1.00,  L: Emax3 =   1.00 (eV)

 Number of times to invoke the pseudo-random number generator:
 INIT:  Mran1 =     54046,      EMCS:  Mran2 =   2935762,
 SMEC:  Mran3 =   2435762,      FNLS:  Mran4 =    764670,
 TUNL:  Mran5 =         0,      EESR:  Mran6 =         0,
 Total: Mran0 =   6190240


                       *** Scattering Mechanism Summary ***

  Mtotal    Mself   Minter   Mintra   Moptic   Macous   Mimpty   Meesct
 -------- -------- -------- -------- -------- -------- -------- --------
  2435762  2053427    49850    88729   217645    26111        0        0
 100.000%  84.303%   2.047%   3.643%   8.935%   1.072%   0.000%   0.000%
 100.000%   0.000%  13.038%  23.207%  56.925%   6.829%   0.000%   0.000%


  Program started at: Fri Aug 11 12:35:21 1989
  Program stopped at: Fri Aug 11 19:21:08 1989
  CPU time:   2608.426     sec.,    2606.675     usr.,    1.750130     sys.
```

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Example 2. Non-Steady-State Transport Properties

PURPOSE

1. Illustrate time- and space-dependent phenomena and hot-electron effect in idealized high-field transport processes;
2. Show how to impose user-specified field distributions.

DESCRIPTION

Non-steady-state transport properties, such as time- and space-dependent phenomena, in GaAs are investigated. In example 2a, a time-pulse configuration of the field (spatially uniform) is applied to a "homogeneous" bulk GaAs. Distribution histograms are sampled at three intermediate instances: just before the onset of the high-field pulse (t=1 ps); during the ballistic motion (t=1.2 ps); and in the relaxation regime (t=1.5 ps). Both ballistic/overshoot motion and undershoot (Jones-Rees effect) [2] are observed. In example 2b, a space-pulse configuration of the field (time constant) is applied to simulate "inhomogeneous" systems. In this example, a uniform spatial distribution of the electrons is assumed (Zunif=.true), and spatial overshoot of both average energy and average velocity is observed.

In both cases, the periodic boundary condition is used (Lpbc=.true).

INPUT FILE(S)

Example 2a:

```
*TITLE  Example 2 - Non-steady-state transport properties
*FILE   ex2a: Time-pulse: 2 ps.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Ndpts=80,       Nzpts=80,       Ntpts=80;       !-, -, -
+       Zmax=2.0,       Tmax=4.0;                       !um, ps
.DEVICe
+       Ufld=.TRUE.;                                    !-
.BOUNDary
+       Lpbc=.TRUE.,    Inj=10;                         !-, -
.COMPUte
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
+       Ntotal=5000,    Nbkgrd=5000;                    !-, -
+       Itobv1=20,      Itobv2=24,      Itobv3=30;      !-, -, -
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                        !-, -
.SAVEFile
+       Dhisto=.TRUE.,  Dtevol=.TRUE.,  Dsmech=.TRUE.;  !-, -, -
*
*END    End of Example ex2a.
```

Example 2b:

```
*TITLE  Example 2 - Non-steady-state transport properties
*FILE   ex2b: Space-pulse: 0.1 um.
```

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```
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Ndpts=80,       Nzpts=80,       Ntpts=80;       !-, -, -
+       Zmax=0.4,       Tmax=4.0;                       !um, ps
.DEVICe
+       Ufld=.TRUE.;                                    !-
.BOUNDary
+       Lpbc=.TRUE.;                                    !-
.INITState
+       Zdelta=.FALSE., Zunif=.TRUE.;                   !-, -
.COMPUte
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
+       Ntotal=5000,    Nbkgrd=5000;                    !-, -
+       Itobv1=10,      Itobv2=20,      Itobv3=40;      !-, -, -
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                        !-, -
.SAVEFile
+       Dhisto=.TRUE.,  Dtevol=.TRUE.,  Dsmech=.TRUE.;  !-, -, -
+       Dspdev=.TRUE.;                                  !-
*
*END    End of Example ex2b.
```

File 'Ufld' for ex2a:

```
                                                Column 1
                                                |
Line 1 ..................... (It=0,Iz=0)        2.0D5
Line 2 ..................... (It=0,Iz=1)        2.0D5
                ...                             ...
Line 80+1 .................. (It=0,Iz=80)       2.0D5
Line (80+1)+1 .............. (It=1,Iz=0)        2.0D5
Line (80+1)+2 .............. (It=1,Iz=1)        2.0D5
                ...                             ...
Line 2(80+1) ............... (It=1,Iz=80)       2.0D5
         .                                      .
         .                                      .
         .                                      .
Line 20(80+1)+1 ............ (It=20,Iz=0)       2.0D5
Line 20(80+1)+2 ............ (It=20,Iz=1)       2.0D5
                ...                             ...
Line 21(80+1) .............. (It=20,Iz=80)      2.0D5
Line 21(80+1)+1 ............ (It=21,Iz=0)       20.0D5
Line 21(80+1)+2 ............ (It=21,Iz=1)       20.0D5
                ...                             ...
Line 22(80+1) .............. (It=21,Iz=80)      20.0D5
         .                                      .
         .                                      .
         .                                      .
Line 60(80+1)+1 ............ (It=60,Iz=0)       20.0D5
Line 60(80+1)+2 ............ (It=60,Iz=1)       20.0D5
                ...                             ...
Line 61(80+1) .............. (It=60,Iz=80)      20.0D5
Line 61(80+1)+1 ............ (It=61,Iz=0)       2.0D5
Line 61(80+1)+2 ............ (It=61,Iz=1)       2.0D5
                ...                             ...
Line 62(80+1) .............. (It=61,Iz=80)      2.0D5
```

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```
         .                                      .
         .                                      .
         .                                      .
Line 80(80+1)+1 ............ (It=80,Iz=0)       2.0D5
Line 80(80+1)+2 ............ (It=80,Iz=1)       2.0D5
               ...                              ...
Line (80+1)(80+1) .......... (It=80,Iz=80)      2.0D5
```

File 'Ufld' for ex2b:

```
                                                Column 1
                                                |
Line 1 ..................... (It=0,Iz=0)         2.0D5
Line 2 ..................... (It=0,Iz=1)         2.0D5
               ...                              ...
Line 21 .................... (It=0,Iz=20)        2.0D5
Line 22 .................... (It=0,Iz=21)        20.0D5
               ...                              ...
Line 41 .................... (It=0,Iz=40)        20.0D5
Line 42 .................... (It=0,Iz=41)        2.0D5
               ...                              ...
Line 80+1 .................. (It=0,Iz=80)        2.0D5
Line (80+1)+1 .............. (It=1,Iz=0)         2.0D5
Line (80+1)+2 .............. (It=1,Iz=1)         2.0D5
               ...                              ...
Line (80+1)+21 ............. (It=1,Iz=20)        2.0D5
Line (80+1)+22 ............. (It=1,Iz=21)        20.0D5
               ...                              ...
Line (80+1)+41 ............. (It=1,Iz=40)        20.0D5
Line (80+1)+42 ............. (It=1,Iz=41)        2.0D5
               ...                              ...
Line 2(80+1) ............... (It=1,Iz=80)        2.0D5
         .                                      .
         .                                      .
         .                                      .
Line 80(80+1)+1 .............. (It=80,Iz=0)      2.0D5
Line 80(80+1)+2 .............. (It=80,Iz=1)      2.0D5
               ...                              ...
Line 80(80+1)+21 ............. (It=80,Iz=20)     2.0D5
Line 80(80+1)+22 ............. (It=80,Iz=21)     20.0D5
               ...                              ...
Line 80(80+1)+41 ............. (It=80,Iz=40)     20.0D5
Line 80(80+1)+42 ............. (It=80,Iz=41)     2.0D5
               ...                              ...
Line (80+1)(80+1) ............ (It=80,Iz=80)     2.0D5
```

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Example 3. Non-Steady-State Transport in GaAs n-i-n Structures

PURPOSE

1. Calculate time- and space-dependent phenomena in GaAs n-i-n structures;
2. Demonstrate how to use "continuous run;"
3. Show the field and carrier distributions calculated by the self-consistent Poisson solver.

DESCRIPTION

This example is a follow-up of the previous one, but is put into a realistic device structure context. The device structure is defined by a lightly-doped GaAs (doped with 1x10^12 1/cm^3) sandwiched between two n+ regions doped with 1x10^16 1/cm^3. A time-dependent external bias is applied to the device to create a field similar to that in the example 2. The field profile inside the device is calculated self-consistently by the Poisson solver (Lpois=.true).

After the first 4-ps simulation (ex3a), the state of the ensemble is stored in a disk file, 'STATE.OUT', which is used as the input for the continuous run of another 4 ps. Rename this file to 'STATE.IN' and turn off the Rfirst flag in the COMPUTE card of the input file (ex3b) for the subsequent run.

INPUT FILE(S)

Example 3a:

```
*TITLE  Example 3 - Non-steady-state transport in GaAs n-i-n structure
*FILE   ex3a: First run: 4 ps.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Ndpts=80,       Nzpts=80,       Ntpts=80;       !-, -, -
+       Zmax=0.4,       Tmax=4.0;                       !um, ps
.DEVICe
+       Udpg=.TRUE.,    Uvbs=.TRUE.;                    !-, -
.POISSon
+       Lpois=.TRUE.;                                   !-
.BOUNDary
+       Lpbc=.TRUE.;                                    !-
.INITState
+       Zdelta=.FALSE., Zuser=.TRUE.;                   !-, -
.COMPUte
+       Rcont=.TRUE.;                                   !-
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
+       Ntotal=5000,    Nbkgrd=5000;                    !-, -
+       Itobv1=20,      Itobv2=24,      Itobv3=30;      !-, -, -
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                        !-, -
.SAVEFile
+       Dhisto=.TRUE.,  Dtevol=.TRUE.,  Dsmech=.TRUE.;  !-, -, -
+       Dspdev=.TRUE.,  Dpfcsp=.TRUE.;                  !-, -
*
```

```
*END    End of Example ex3a.
```

Example 3b:

```
*TITLE  Example 3 - Non-steady-state transport in GaAs n-i-n structure
*FILE   ex3b: Continuous run: 4 ps.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Ndpts=80,       Nzpts=80,       Ntpts=80;       !-, -, -
+       Zmax=0.4,       Tmax=4.0;                       !um, ps
.DEVICe
+       Udpg=.TRUE.,    Vbias=0.2D0;                    !-, V
.POISSon
+       Lpois=.TRUE.;                                   !-
.BOUNDary
+       Lpbc=.TRUE.;                                    !-
.INITState
+       Zdelta=.FALSE., Zuser=.TRUE.;                   !-, -
.COMPUte
+       Rcont=.TRUE.,   Rfirst=.FALSE;                  !-, -
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
+       Ntotal=5000,    Nbkgrd=5000;                    !-, -
+       Itobv1=20,      Itobv2=40,      Itobv3=60;      !-, -, -
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                        !-, -
.SAVEFile
+       Dhisto=.TRUE.,  Dtevol=.TRUE.,  Dsmech=.TRUE.;  !-, -, -
+       Dspdev=.TRUE.,  Dpfcsp=.TRUE.;                  !-, -
*
*END    End of Example ex3b.
```

File 'Udpg' and 'Zusr':

```
                                        Column 1
                                        |
Line 1 .......... (Iz=0)                1.0D22
Line 2 .......... (Iz=1)                1.0D22
        ...                             ...
Line 21 ......... (Iz=20)               1.0D22
Line 22 ......... (Iz=21)               1.0D18
        ...                             ...
Line 41 ......... (Iz=40)               1.0D18
Line 42 ......... (Iz=41)               1.0D22
        ...                             ...
Line 81 ......... (Iz=80)               1.0D22
```

File 'Uvbs':

```
                                        Column 1
                                        |
Line 1 .......... (It=0)                0.2D0
Line 2 .......... (It=1)                0.2D0
        ...                             ...
Line 21 ......... (It=20)               0.2D0
Line 22 ......... (It=21)               2.0D0
        ...                             ...
```

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```
Line 61 ......... (It=60)              2.0D0
Line 62 ......... (It=61)              0.2D0
        ...                            ...
Line 81 ......... (It=80)              0.2D0
```

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Example 4. Relaxation of Photoinjected Carriers

PURPOSE

1. Simulate relaxation process of photoinjected carriers in bulk GaAs;
2. Show the effect of the excitation energy on the relaxation dynamics by temperature- and composition-tuning of the band gaps.

DESCRIPTION

Photogenerated carriers from a 30-fs, Gaussian-shaped laser pulse is injected into a piece of "bulk" GaAs (Lpbc=.true). The injected electrons assume a spatial exponentially decaying function with a penetration depth of Ldepth=0.15 um. The Poisson solver is not employed; instead, a uniform field of 2 kV/cm is imposed to prevent the electrons from being stuck.

The effect of the excitation energy on the relaxation process is investigated by temperature-tuning the band gaps (Temp=300/77 K), or by composition-tuning the band gaps (Xdev=0.0/0.2). Results of the simulation in examples 4a/4b show the drastic difference between above and below X-valley/L-valley excitations, respectively.

INPUT FILE(S)

Example 4a1:

```
*TITLE  Example 4 - Relaxation of Photo-injected carriers
*File   ex4a1: Lambda=645 nm, T=300 K.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Emax1=2.0,      Emax2=2.0,      Emax3=2.0;      !eV, eV, eV
+       Ndpts=80,       Nzpts=80,       Ntpts=80;       !-, -, -
+       Zmax=0.4,       Tmax=0.4;                       !um, ps
.DEVICe
+       Vbias=0.08D0,   Field=2.0D3;                    !V, V/cm
.BOUNDary
+       Lpbc=.TRUE.;                                    !-
.INITState
+       Tdelta=.FALSE., Tgauss=.TRUE.,  Wsigma=0.03;    !-, -, ps
+       Zdelta=.FALSE., Zdepth=0.15;                    !-, um
+       Kspc=4,         Lambda=0.645,   Efwhm=22.0D-3;  !-, um, eV
.COMPUte
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
+       Ntotal=5000,    Nbkgrd=0,       Nphoto=5000;    !-, -, -
+       Itobv1=10,      Itobv2=20,      Itobv3=50;      !-, -, -
.MODEL
+       Laser=.TRUE.;                                   !-
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                        !-, -
.SAVEFile
+       Dhisto=.TRUE.,  Dtevol=.TRUE.,  Dsmech=.TRUE.;  !-, -, -
+       Dspdev=.TRUE.;                                  !-
```

```
*
*END    End of Example ex4a1.
```

Example 4a2:

```
*TITLE  Example 4 - Relaxation of Photo-injected carriers
*File   ex4a2: Lambda=645 nm, T=77 K.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Emax1=2.0,      Emax2=2.0,      Emax3=2.0;      !eV, eV, eV
+       Ndpts=80,       Nzpts=80,       Ntpts=80;       !-, -, -
+       Zmax=0.4,       Tmax=0.4;                       !um, ps
.DEVICe
+       Vbias=0.08D0,   Field=2.0D3,    Temp=77.0;      !V, V/cm, K
.BOUNDary
+       Lpbc=.TRUE.;                                    !-
.INITState
+       Tdelta=.FALSE., Tgauss=.TRUE.,  Wsigma=0.03;    !-, -, ps
+       Zdelta=.FALSE., Zdepth=0.15;                    !-, um
+       Kspc=4,         Lambda=0.645,   Efwhm=22.0D-3;  !-, um, eV
.COMPUte
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
+       Ntotal=5000,    Nbkgrd=0,       Nphoto=5000;    !-, -, -
+       Itobv1=10,      Itobv2=20,      Itobv3=50;      !-, -, -
.MODEL
+       Laser=.TRUE.;                                   !-
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                        !-, -
.SAVEFile
+       Dhisto=.TRUE.,  Dtevol=.TRUE.,  Dsmech=.TRUE.;  !-, -, -
+       Dspdev=.TRUE.;                                  !-
*
*END    End of Example ex4a2.
```

Example 4b1:

```
*TITLE  Example 4 - Relaxation of Photo-injected carriers
*File   ex4b1: Lambda=710 nm, Xdev=0.0.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Emax1=2.0,      Emax2=2.0,      Emax3=2.0;      !eV, eV, eV
+       Ndpts=80,       Nzpts=80,       Ntpts=80;       !-, -, -
+       Zmax=0.4,       Tmax=0.4;                       !um, ps
.DEVICe
+       Vbias=0.08D0,   Field=2.0D3;                    !V, V/cm
.BOUNDary
+       Lpbc=.TRUE.;                                    !-
.INITState
+       Tdelta=.FALSE., Tgauss=.TRUE.,  Wsigma=0.03;    !-, -, ps
+       Zdelta=.FALSE., Zdepth=0.15;                    !-, um
+       Kspc=4,         Lambda=0.710,   Efwhm=22.0D-3;  !-, um, eV
.COMPUte
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
```

```
+       Ntotal=5000,    Nbkgrd=0,       Nphoto=5000;    !-, -, -
+       Itobv1=10,      Itobv2=20,      Itobv3=50;      !-, -, -
.MODEL
+       Laser=.TRUE.;                                   !-
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                        !-, -
.SAVEFile
+       Dhisto=.TRUE.,  Dtevol=.TRUE.,  Dsmech=.TRUE.;  !-, -, -
+       Dspdev=.TRUE.;                                  !-
*
*END    End of Example ex4b1.
```

Example 4b2:

```
*TITLE  Example 4 - Relaxation of Photo-injected carriers
*File   ex4b2: Lambda=710 nm, Xdev=0.2.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Emax1=2.0,      Emax2=2.0,      Emax3=2.0;      !eV, eV, eV
+       Ndpts=80,       Nzpts=80,       Ntpts=80;       !-, -, -
+       Zmax=0.4,       Tmax=0.4;                       !um, ps
.MATERial
+       Gtemp=.FALSE.;                                  !-
.DEVICe
+       Vbias=0.08D0,   Field=2.0D3,    Xdev=0.2;       !V, V/cm, -
.BOUNDary
+       Lpbc=.TRUE.;                                    !-
.INITState
+       Tdelta=.FALSE., Tgauss=.TRUE.,  Wsigma=0.03;    !-, -, ps
+       Zdelta=.FALSE., Zdepth=0.15;                    !-, um
+       Kspc=4,         Lambda=0.710,   Efwhm=22.0D-3;  !-, um, eV
.COMPUte
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
+       Ntotal=5000,    Nbkgrd=0,       Nphoto=5000;    !-, -, -
+       Itobv1=10,      Itobv2=20,      Itobv3=50;      !-, -, -
.MODEL
+       Laser=.TRUE.;                                   !-
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                        !-, -
.SAVEFile
+       Dhisto=.TRUE.,  Dtevol=.TRUE.,  Dsmech=.TRUE.;  !-, -, -
+       Dspdev=.TRUE.;                                  !-
*
*END    End of Example ex4b2.
```

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Example 5. Photocarrier Transport in GaAs Surface Fields

PURPOSE

1. Simulate the transport and relaxation of photogenerated carriers at the GaAs/oxide interface;
2. Demonstrate the influence of the background electrons on the photoinjected carriers;
3. Illustrate the impact of the e-e scattering on the relaxation processes, as well as the total scattering rate.

DESCRIPTION

This is a simulation of a fairly realistic situation. The same laser source as in the previous example (ex4a1) is used. The surface charge is modeled by a sheet of charge at the boundary, together with the depletion charge induced by the surface charge specified through the file 'Depl' (Ldepl=.true). The Poisson solver is invoked, with boundary conditions of constant voltage (Ibcl=1) at the surface and constant field in the bulk (Ibcr=2). The potential at the right boundary is kept floating to monitor the potential drop across the sample. Perfect absorbing boundary is assumed (Lpbc=Ltbc=.false), and electrons impinged on the right boundary are brought back to the left boundary with a hemi-Maxwellian distribution (Ksbc=2).

In example 5a, photocarriers alone are simulated (Lbkgrd=.false). In example 5b, background electron sub-ensemble is imposed on the photoinjected electron sub-ensemble (Lbkgrd=.true). In example 5c, e-e scattering mechanism is turned on (Leesct=.true), and the scattering rate table is updated at each time step.

INPUT FILE(S)

Example 5a:

```
*TITLE  Example 5 - Photo-carrier Transport in GaAs Surface Fields
*File   ex5a: Photo-carrier only.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Emax1=2.0,      Emax2=2.0,      Emax3=2.0;      !eV, eV, eV
+       Ndpts=80,       Nzpts=80,       Ntpts=80;       !-, -, -
+       Zmax=0.4,       Tmax=0.4;                       !um, ps
.POISSon
+       Lpois=.TRUE.,   Ldepl=.TRUE.,   Ibcr=2;         !-, -, -
.BOUNDary
+       Ksbc=2;                                         !-
.INITState
+       Tdelta=.FALSE., Tgauss=.TRUE.,  Wsigma=0.03;    !-, -, ps
+       Zdelta=.FALSE., Zdepth=0.15;                    !-, um
+       Kspc=4,         Lambda=0.645,   Efwhm=22.0D-3;  !-, um, eV
.COMPUte
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
+       Ntotal=5000,    Nbkgrd=0,       Nphoto=5000;    !-, -, -
+       Itobv1=10,      Itobv2=20,      Itobv3=50;      !-, -, -
```

```
.MODEL
+       Laser=.TRUE.;                                       !-
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                            !-, -
.SAVEFile
+       Dhisto=.TRUE.,  Dtevol=.TRUE.,  Dsmech=.TRUE.;      !-, -, -
+       Dspdev=.TRUE.,  Dpfcsp=.TRUE.;                      !-, -
*
*END    End of Example ex5a.
```

Example 5b:

```
*TITLE  Example 5 - Photo-carrier Transport in GaAs Surface Fields
*File   ex5b: With background electrons.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Emax1=2.0,      Emax2=2.0,      Emax3=2.0;      !eV, eV, eV
+       Ndpts=80,       Nzpts=80,       Ntpts=80;       !-, -, -
+       Zmax=0.4,       Tmax=0.4;                       !um, ps
.POISSon
+       Lpois=.TRUE.,   Ldepl=.TRUE.,   Ibcr=2;         !-, -, -
+       Ksbc=2;                                         !-
.INITState
+       Tdelta=.FALSE., Tgauss=.TRUE.,  Wsigma=0.03;    !-, -, ps
+       Zdelta=.FALSE., Zunif=.TRUE.,   Zdepth=0.15;    !-, -, um
+       Kspc=4,         Lambda=0.645,   Efwhm=22.0D-3;  !-, um, eV
.COMPUte
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
+       Ntotal=10000,   Nbkgrd=5000,    Nphoto=5000;    !-, -, -
+       Itobv1=10,      Itobv2=20,      Itobv3=50;      !-, -, -
.MODEL
+       Laser=.TRUE.,   Lbkgrd=.TRUE.;                  !-, -
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                        !-, -
.SAVEFile
+       Dhisto=.TRUE.,  Dtevol=.TRUE.,  Dsmech=.TRUE.;  !-, -, -
+       Dspdev=.TRUE.,  Dpfcsp=.TRUE.;                  !-, -
*
*END    End of Example ex5b.
```

Example 5c:

```
*TITLE  Example 5 - Photo-carrier Transport in GaAs Surface Fields
*File   ex5c: With e-e scattering.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Emax1=2.0,      Emax2=2.0,      Emax3=2.0;      !eV, eV, eV
+       Ndpts=80,       Nzpts=80,       Ntpts=80;       !-, -, -
+       Zmax=0.4,       Tmax=0.4;                       !um, ps
.MECHAnism
+       Leesct=.TRUE.;                                  !-
.POISSon
+       Lpois=.TRUE.,   Ldepl=.TRUE.,   Ibcr=2;         !-, -, -
```

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```
.BOUNDary
+       Ksbc=2;                                             !-
.INITState
+       Tdelta=.FALSE., Tgauss=.TRUE.,  Wsigma=0.03;    !-, -, ps
+       Zdelta=.FALSE., Zunif=.TRUE.,   Zdepth=0.15;    !-, -, um
+       Kspc=4,         Lambda=0.645,   Efwhm=22.0D-3;  !-, um, eV
.COMPUte
+       Lproc1=.TRUE.,  Lproc2=.TRUE.;                  !-, -
+       Ntotal=10000,   Nbkgrd=5000,    Nphoto=5000;    !-, -, -
+       Itobv1=10,      Itobv2=20,      Itobv3=50;      !-, -, -
.MODEL
+       Laser=.TRUE.,   Lbkgrd=.TRUE.;                  !-, -
.PLOT
+       Lplots=.TRUE.,  Nstep=2;                        !-, -
.SAVEFile
+       Dhisto=.TRUE.,  Dtevol=.TRUE.,  Dsmech=.TRUE.;  !-, -, -
+       Dspdev=.TRUE.,  Dpfcsp=.TRUE.,  Dgamma=.TRUE.;  !-, -, -
*
*END    End of Example ex5c.
```

File 'Depl':

```
                                    Column 1
                                    |
Line 1 .......... (Iz=0)            -5.0D15
Line 2 .......... (Iz=1)            1.0D23
         ...                        ...
Line 11 ......... (Iz=10)           1.0D23
Line 12 ......... (Iz=11)           0.0D0
         ...                        ...
Line 81 ......... (Iz=80)           0.0D0
```

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*

Appendices

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Appendix A. Default Input Deck

```
*TITLE  EMCUR (Version 1R3K.04) Default Input Deck.
*       This file contains default values of all cards used in EMCUR.
*-------------------------------------------------------------------------*
*
*CARDName               Parameter List                  Units
*--------               --------------                  -----
.GRID
+       Emax1=1.0,      Emax2=1.0,      Emax3=1.0;      !eV, eV, eV
+       DEmax1=0.5,     DEmax2=0.5,     DEmax3=0.5;     !eV, eV, eV
+       Nepts1=40,      Nepts2=20,      Nepts3=20;      !-, -, -
+       Iepwi1=20,      Iepwi2=10,      Iepwi3=10;      !-, -, -
+       Iepwd1=5,       Iepwd2=5,       Iepwd3=5;       !-, -, -
+       Vdlow=-15.0D7,  Vdupr=15.0D7,   Ndpts=20;       !cm/s, cm/s, -
+       Nbpts=20,       Nzpts=20,       Ntpts=20;       !-, -, -
+       Bmax=0.1,       Zmax=0.1,       Tmax=1.0;       !um, um, ps
.MATERial
+       Ldef=.TRUE.,    Lgaas=.FALSE.,  Lalas=.FALSE.;  !-, -, -
+       Lgap=.FALSE.,   Ltgap=.FALSE.,  Gtemp=.TRUE.;   !-, -, -
+       ECoff1=0.6,     ECoff2=0.6,     ECoff3=0.6;     !-, -, -
.BANDS
+       Gval=.TRUE.,    Xval=.TRUE.,    Lval=.TRUE.;    !-, -, -
.DEVICe
+       Udpg=.FALSE.,   Ufld=.FALSE.,   Uvbs=.FALSE.;   !-, -, -
+       Ualx=.FALSE.,   Doping=1.0D17,  Field=50.0D3;   !-, /cm^3, V/cm
+       Vbias=0.5D0,    Xdev=0.0,       Xbar=1.0;       !V, -, -
+       Temp=300.0;                                     !K
.MECHAnism
+       Limpty=.TRUE.,  Loptic=.TRUE.,  Lacous=.TRUE.;  !-, -, -
+       Lintra=.TRUE.,  Linter=.TRUE.,  Leesct=.FALSE.; !-, -, -
.POISSon
+       Lpois=.FALSE.,  Ldepl=.FALSE.,  Ibcl=1;         !-, -, -
+       Ibcr=1,         Fldl=0.0,       Fldr=0.0;       !-, V/m, V/m
.BOUNDary
+       Lpbc=.FALSE.,   Ltbc=.FALSE.;   Inj=1           !-, -, -
+       Ksbc=1,         Telec=300.0,    Velec=0.0;      !-, K, cm/s
.INITState
+       Voccu1=1.0,     Voccu2=0.0,     Voccu3=0.0;     !-, -, -
+       Tdelta=.TRUE.,  Trectg=.FALSE., Tgauss=.FALSE.; !-, -, -
+       Tinvch=.FALSE., Ksbg=1,         Kspc=4;         !-, -, -
+       Wpulse=0.2,     Wsigma=0.2,     Wfwhm=0.2;      !ps, ps, ps
+       Zdelta=.TRUE.,  Zunif=.FALSE.,  Zuser=.FALSE.;  !-, -, -
+       Lambda=0.590,   Efwhm=1.0D-3,   Dinj=1.0D12;    !um, eV, /cm^2
+       Zdepth=0.1,     Einj=1.0;       DEinj=1.0D-3;   !um, eV, eV
.COMPUte
+       Rcont=.FALSE.,  Rfirst=.TRUE.,  Naccu=0;        !-, -, -
+       Lproc1=.FALSE., Lproc2=.FALSE., Iseed=1;        !-, -, -
+       Ntotal=10,      Nbkgrd=10,      Nphoto=0;       !-, -, -
+       Itobv1=5,       Itobv2=10,      Itobv3=15;      !-, -, -
.MODEL
+       Laser=.FALSE.,  Lbkgrd=.FALSE., Lscrng=.FALSE.; !-, -, -
.PLOT
+       Lplots=.FALSE., Nstep=1;                        !-, -
.SAVEFile
+       Dhisto=.FALSE., Dtevol=.FALSE., Dsmech=.FALSE.; !-, -, -
+       Dspdev=.FALSE., Dgamma=.FALSE., Dpfcsp=.FALSE.; !-, -, -
*
*END    End of Default Input Deck.
```

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EMCUR Input Cards With Defaults
(Version 1R3K.04)

Card #/Name	Param #/Name	Type	Range	Default	Units
01 / GRID					
	01.01 / Emax1	R*8	[0.0,-)	1.0D0	eV
	01.02 / Emax2	R*8	[0.0,-)	1.0D0	eV
	01.03 / Emax3	R*8	[0.0,-)	1.0D0	eV
	01.04 / DEmax1	R*8	[0.0,-)	0.5D0	eV
	01.05 / DEmax2	R*8	[0.0,-)	0.5D0	eV
	01.06 / DEmax3	R*8	[0.0,-)	0.5D0	eV
	01.07 / Nepts1	I*4	[1,Nemax]	40	-
	01.08 / Nepts2	I*4	[1,Nemax]	20	-
	01.09 / Nepts3	I*4	[1,Nemax]	20	-
	01.10 / Iepwi1	I*4	[1,Nepts1]	20	-
	01.11 / Iepwi2	I*4	[1,Nepts2]	10	-
	01.12 / Iepwi3	I*4	[1,Nepts3]	10	-
	01.13 / Iepwd1	I*4	[1,Nepts1]	5	-
	01.14 / Iepwd2	I*4	[1,Nepts2]	5	-
	01.15 / Iepwd3	I*4	[1,Nepts3]	5	-
	01.16 / Vdlow	R*8	(-,-)	-15.0D7	cm/s
	01.17 / Vdupr	R*8	(-,-)	15.0D7	cm/s
	01.18 / Ndpts	I*4	[1,Ndmax]	20	-
	01.19 / Nbpts	I*4	[1,Nbmax-1]	20	-
	01.20 / Nzpts	I*4	[1,Nzmax]	20	-
	01.21 / Ntpts	I*4	[1,Ntmax]	20	-
	01.22 / Bmax	I*4	(0.0,-)	0.1D0	um
	01.23 / Zmax	I*4	(0.0,-)	0.1D0	um
	01.24 / Tmax	I*4	(0.0,-)	1.0D0	ps
02 / MATERial					
	02.01 / Ldef	L*4	t,f	t	-
	02.02 / Lgaas	L*4	t,f	f	-
	02.03 / Lalas	L*4	t,f	f	-
	02.04 / Lgap	L*4	t,f	f	-
	02.05 / Ltgap	L*4	t,f	f	-
	02.06 / Gtemp	L*4	t,f	t	-
	02.07 / ECoff1	R*8	[0.0,1.0]	0.6D0	-
	02.08 / ECoff2	R*8	[0.0,1.0]	0.6D0	-
	02.09 / ECoff3	R*8	[0.0,1.0]	0.6D0	-
03 / BANDS					
	03.01 / Gval	L*4	t,f	t	-
	03.02 / Xval	L*4	t,f	t	-
	03.03 / Lval	L*4	t,f	t	-
04 / DEVICe					
	04.01 / Udpg	L*4	t,f	f	-
	04.02 / Ufld	L*4	t,f	f	-

```
*                04.03 / Uvbs      L*4    t,f            f        -       *
*                04.04 / Ualx      L*4    t,f            f        -       *
*                04.05 / Doping    R*8    (0.0,-)        1.0D17   1/cm^3  *
*                04.06 / Field     R*8    (-,-)          50.0D3   V/cm    *
*                04.07 / Vbias     R*8    (-,-)          0.5D0    V       *
*                04.08 / Xdev      R*8    [0.0,1.0]      0.0D0    -       *
*                04.09 / Xbar      R*8    [0.0,1.0]      1.0D0    -       *
*                04.10 / Temp      R*8    (0.0,-)        300.0D0  K       *
*                                                                          *
* 05 / MECHAnism                                                           *
*                                                                          *
*                05.01 / Limpty    L*4    t,f            t        -       *
*                05.02 / Loptic    L*4    t,f            t        -       *
*                05.03 / Lacous    L*4    t,f            t        -       *
*                05.04 / Lintra    L*4    t,f            t        -       *
*                05.05 / Linter    L*4    t,f            t        -       *
*                05.06 / Leesct    L*4    t,f            f        -       *
*                                                                          *
* 06 / POISSon                                                             *
*                                                                          *
*                06.01 / Lpois     L*4    t,f            f        -       *
*                06.02 / Ldepl     L*4    t,f            f        -       *
*                06.03 / Ibcl      I*4    1,2            1        -       *
*                06.04 / Ibcr      I*4    1,2            1        -       *
*                06.05 / Fldl      R*8    (-,-)          0.0D0    V/m     *
*                06.06 / Fldr      R*8    (-,-)          0.0D0    V/m     *
*                                                                          *
* 07 / BOUNDary                                                            *
*                                                                          *
*                07.01 / Lpbc      L*4    t,f            f        -       *
*                07.02 / Ltbc      L*4    t,f            f        -       *
*                07.03 / Inj       I*4    [1,Nzpts]      1        -       *
*                07.04 / Ksbc      I*4    1,2,3          1        -       *
*                07.05 / Telec     R*8    (0.0,-)        300.0D0  K       *
*                07.06 / Velec     R*8    (-,-)          0.0D0    cm/s    *
*                                                                          *
* 08 / INITState                                                           *
*                                                                          *
*                08.01 / Voccu1    R*8    [0.0,1.0]      1.0D0    -       *
*                08.02 / Voccu2    R*8    [0.0,1.0]      0.0D0    -       *
*                08.03 / Voccu3    R*8    [0.0,1.0]      0.0D0    -       *
*                08.04 / Tdelta    L*4    t,f            t        -       *
*                08.05 / Trectg    L*4    t,f            f        -       *
*                08.06 / Tgauss    L*4    t,f            f        -       *
*                08.07 / Tinvch    L*4    t,f            f        -       *
*                08.08 / Ksbg      I*4    1,2,3,4,5      1        -       *
*                08.09 / Kspc      I*4    1,2,3,4,5      4        -       *
*                08.10 / Wpulse    R*8    (0.0,Tmax)     0.2D0    ps      *
*                08.11 / Wsigma    R*8    (0.0,Tmax/2.2) 0.2D0    ps      *
*                08.12 / Wfwhm     R*8    (0.0,Tmax/1.2) 0.2D0    ps      *
*                08.13 / Zdelta    L*4    t,f            t        -       *
*                08.14 / Zunif     L*4    t,f            f        -       *
*                08.15 / Zuser     L*4    t,f            f        -       *
*                08.16 / Lambda    R*8    (0.0,-)        0.590D0  um      *
*                08.17 / Efwhm     R*8    (0.0,-)        1.0D-3   eV      *
*                08.18 / Dinj      R*8    (0.0,-)        1.0D12   1/cm^2  *
*                08.19 / Zdepth    R*8    (0.0,Zmax)     0.1D0    um      *
*                08.20 / Einj      R*8    (0.0,-)        1.0D0    eV      *
*                08.21 / DEinj     R*8    (0.0,-)        1.0D-3   eV      *
```

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```
*                                                                              *
* 09 / COMPUte                                                                 *
*                                                                              *
*                09.01 / Rcont     L*4    t,f            f        -          *
*                09.02 / Rfirst    L*4    t,f            t        -          *
*                09.03 / Naccu     I*4    0,1            0        -          *
*                09.04 / Lproc1    L*4    t,f            f        -          *
*                09.05 / Lproc2    L*4    t,f            f        -          *
*                09.06 / Iseed     I*4    -              1        -          *
*                09.07 / Ntotal    I*4    [1,Nens]       10       -          *
*                09.08 / Nbkgrd    I*4    [1,Nens]       10       -          *
*                09.09 / Nphoto    I*4    [1,Nens]       0        -          *
*                09.10 / Itobv1    I*4    [1,Ntpts]      5        -          *
*                09.11 / Itobv2    I*4    [1,Ntpts]      10       -          *
*                09.12 / Itobv3    I*4    [1,Ntpts]      15       -          *
*                                                                              *
* 10 / MODEL                                                                   *
*                                                                              *
*                10.01 / Laser     L*4    t,f            f        -          *
*                10.02 / Lbkgrd    L*4    t,f            f        -          *
*                10.03 / Lscrng    L*4    t,f            f        -          *
*                                                                              *
* 11 / PLOT                                                                    *
*                                                                              *
*                11.01 / Lplots    L*4    t,f            f        -          *
*                11.02 / Nstep     I*4    1,2            1        -          *
*                                                                              *
* 12 / SAVEFile                                                                *
*                                                                              *
*                12.01 / Dhisto    L*4    t,f            f        -          *
*                12.02 / Dtevol    L*4    t,f            f        -          *
*                12.03 / Dsmech    L*4    t,f            f        -          *
*                12.04 / Dspdev    L*4    t,f            f        -          *
*                12.05 / Dgamma    L*4    t,f            f        -          *
*                12.06 / Dpfcsp    L*4    t,f            f        -          *
*                                                                              *
*------------------------------------------------------------------------------*
* Notes:                                                                       *
*       L*4 = LOGICAL*4     Nemax = 40     Ndmax = 80      t = .TRUE.        *
*       I*4 = INTEGER*4     Nbmax = 81     Ntmax = 100     f = .FALSE.       *
*       R*8 = REAL*4        Nzmax = 80     Nens = 30000                      *
*                                                                              *
*------------------------------------------------------------------------------*


*------------------------------------------------------------------------------*
*                                                                              *
*                      EMCUR Input Card Logical Relations                      *
*                              (Version 1R3K.04)                               *
*                                                                              *
*------------------------------------------------------------------------------*
*                                                                              *
*        If                        Parameters Not In Effect                    *
* -----------------   ------------------------------------------------------ *
* Ldef=t              Lgaas, Lalas, Lgap, Ltgap                                *
* Ltbc=f              Nbpts, Bmax, Xbar, ECoff*                                *
* Lpois=f             Ldepl, Ibcl, Ibcr, Fldl, Fldr                            *
* Rcont=f             Rfirst, Naccu                                            *
* Laser=f             Lbkgrd, Zdepth, Dinj, Kspc                               *
```

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```
* Laser=t              Zdelta                                                *
* Laser=t, Lbkgrd=f    Zunif, Zuser, Ksbg                                    *
* Rcont=t, Rfirst=f    Emax*, Voccu*, Tdelta, Trectg, Tgauss, Tinvch,        *
*                      Ksbg, Kspc, Wpulse, Wsigma, Wfwhm, Zdelta, Zunif,     *
*                      Zuser, Lambda, Efwhm, Dinj, Zdepth, Einj, DEinj       *
*                                                                            *
* IF ( Lpois=t ) THEN                                                        *
*    ( ( Ibcl=1, Ibcr=1 ), Vbias=<r> ) |                                     *
*    ( ( Ibcl=1, Ibcr=2 ), Fldr=<r> ) |                                      *
*    ( ( Ibcl=2, Ibcr=1 ), Fldl=<r>, Vbias=<r> )                             *
*                                                                            *
* IF ( Laser=t ) THEN                                                        *
*    Tdelta=f, Zdepth=<r>, Dinj=<r>,                                         *
*    ( ( Trectg=t, Wpulse=<r> ) | ( Tgauss=t, Wsigma=<r> ) |                 *
*      ( Tinvch=t, Wfwhm=<r> )                                               *
*    ),                                                                      *
*    ( ( ( Kspc=1 | Kspc=2 | Kspc=3 ), Telec=<r>, Velec=<r> ) |              *
*      ( Kspc=4, Lambda=<r>, Efwhm=<r> ) |                                   *
*      ( Kspc=5, Einj=<r>, DEinj=<r> )                                       *
*    )                                                                       *
*                                                                            *
* IF ( Laser=t, Lbkgrd=t ) THEN                                              *
*    ( Nphoto=<i> (i>1), Nbkgrd=<i> (i>1), Nphoto+Nbkgrd=Ntotal ),           *
*    ( ( Zunif=t, Zuser=f ) | ( Zunif=f, Zuser=t )                           *
*    ),                                                                      *
*    ( ( Ksbg=1 | Ksbg=2 | Ksbg=3 ), Telec=<r>, Velec=<r> ) )               *
*                                                                            *
* IF ( Laser=t, Lbkgrd=f ) THEN                                              *
*    Nphoto=<i> (i>1), Nbkgrd=0, Nphoto=Ntotal                               *
*                                                                            *
*----------------------------------------------------------------------------*
* Notes:                                                                     *
*       <r> = REAL values  <i> = INTEGER values  t = .TRUE.  f = .FALSE.     *
*       Param* = Param1, Param2, Param3 (for G, X, L valleys)                 *
*       ( Param1, Param2 ) - BOTH Param1 AND Param2 must be specified         *
*       ( Param1 | Param2 ) - EITHER Param1 OR Param2 must be specified       *
*                                                                            *
*----------------------------------------------------------------------------*
```

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Appendix B. Format of Data Files for Band and Material Parameters

The band and material parameters used in EMCUR can be altered by supplying user-defined data files in the format described below. Data are read by "FORTRAN list-directed sequential READ statement," and therefore, the order of occurrence of each record is significant.

Parameters for GaAs and AlAs binary systems are specified in the files 'GaAs' and 'AlAs', respectively, with the following notations: Param1 for GaAs, Param2 for AlAs, and Param(1,2,3) for values in the G, X, L valleys, respectively. For ternary materials (e.g., Al(x)Ga(1-x)As), the ternary alloy parameter, T-AlGaAs(x), is approximated by linear interpolation of the properties of the two binary compounds, A-AlAs and B-GaAs:

T-AlGaAs(x) = x A-AlAs + (1 - x)B-GaAs

where x is the Al mole fraction. In files 'GaAs' and 'AlAs', Mass is the effective mass ratio, a is the nonparabolicity parameter, s is the acoustic wave velocity, g is the material density, El and Eh are the low- and high-frequency dielectric constants respectively, DEFei is the intravalley (or equivalent intervalley) deformation potential, DEFni is the (non-equivalent) intervalley deformation potential, HWei is the intravalley phonon energy, HWni is the intervalley phonon energy, and HWop is the longitudinal optical phonon energy.

The band-gap parameters in each valley are specified using quadratic approximation [file 'Gap']:

EgG(x) = Eg1(1) + Eg2(1)x + Eg3(1)x^2
EgX(x) = Eg1(2) + Eg2(2)x + Eg3(2)x^2
EgL(x) = Eg1(3) + Eg2(3)x + Eg3(3)x^2

for the ternary system.

The temperature-dependent band gaps for GaAs is determined from [file 'Tgap']

Eg(*) = Ego(*) - Tcoef(*)To^2/(To + 204)

where *=1, 2, 3 for G, X, L valleys, and To (see the DEVICE card) is the lattice temperature (in K).

The format of the data files, 'GaAs', 'AlAs', 'Gap', and 'Tgap', is shown below, with the same values as the defaults used in the program.

'GaAs' FILE FORMAT [3]

```
0.063D0, 0.58D0, 0.222D0                !Mass1(1,2,3) (Mo)
0.0610D0, 0.204D0, 0.461D0              !a1(1,2,3) (1/eV)
5.240D3, 5.360D3, 10.92D0, 12.90D0      !s1(m/s), g1(kg/m^3), Eh1, El1
0.0D0, 0.7D0, 1.0D0                     !DEFei1(1,2,3) (eV/cm)
1.0D0, 1.0D0, 0.5D0                     !DEFni1(1,2,3) (eV/cm)
7.0D0, 9.27D0, 9.20D0                   !DEFac1(1,2,3) (eV)
0.0D0, 0.0299D0, 0.0290D0               !HWei1(1,2,3) (eV)
0.0299D0, 0.0278D0, 0.0293D0, 0.03536D0 !HWni1(1,2,3), HWop1 (eV)
```

'AlAs' FILE FORMAT [4]

```
0.140D0, 0.37D0, 0.240D0                !Mass2(1,2,3) (Mo)
```

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```
0.2510D0, 0.251D0, 0.570D0                !a2(1,2,3) (1/eV)
5.820D3, 3.698D3, 8.5D0, 10.9D0           !s2(m/s), g2(kg/m^3), Eh2, El2
0.0D0, 1.0D0, 0.5D0                       !DEFei2(1,2,3) (eV/cm)
1.0D0, 0.5D0, 0.5D0                       !DEFni2(1,2,3) (eV/cm)
12.2D0, 9.5D0, 12.5D0                     !DEFac2(1,2,3) (eV)
0.0D0, 0.0473D0, 0.0400D0                 !HWei2(1,2,3) (eV)
0.0473D0, 0.0413D0, 0.0473D0, 0.03536D0 !HWni2(1,2,3), HWop2 (eV)

'Gap' FILE FORMAT [5]

1.42D0, 1.905D0, 1.7D0                    !Eg1(1,2,3) (eV)
1.087D0, 0.1D0, 0.695D0                   !Eg2(1,2,3) (eV)
0.438D0, 0.16D0, 0.0D0                    !Eg3(1,2,3) (eV)

'Tgap' FILE FORMAT [6]

1.519D0, 1.981D0, 1.815D0                 !Ego(1,2,3) (eV)
5.405D-4, 4.60D-4, 6.05D-4                !Tcoef(1,2,3) (eV/K)
```

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Appendix C. Format of Data Files for Doping, Field, Bias, and Composition Profiles

The assumed uniform doping, field, bias, and composition profiles for the simulated device structure can be overridden by user-defined data files 'Udpg', 'Ufld', 'Uvbs', and 'Ualx', respectively. A depletion charge can be imposed by specifying a data file 'Depl'. Arbitrary initial spatial distribution for the ensemble can also be supplied from file 'Zusr'. The format of these files are described below.

'Udpg' FILE FORMAT

```
                                  Column 1
                                  |
Line 1 .......... (Iz=0)                x.xxxDxx
Line 2 .......... (Iz=1)                x.xxxDxx
         ...                      ...
Line Nzpts+1 .... (Iz=Nzpts)     x.xxxDxx
```

where x.xxxDxx are the values of the doping concentration (in 1/m^3), and Nzpts is the number of spatial bins specified in the GRID card. (Note: total of Nzpts+1 lines.)

'Ufld' FILE FORMAT

```
                                                    Column 1
                                                    |
Line 1 ..................... (It=0,Iz=0)                   x.xxxDxx
Line 2 ..................... (It=0,Iz=1)                   x.xxxDxx
                ...                                 ...
Line Nzpts+1 ............... (It=0,Iz=Nzpts)      x.xxxDxx
Line (Nzpts+1)+1 ........... (It=1,Iz=0)                  x.xxxDxx
Line (Nzpts+1)+2 ........... (It=1,Iz=1)                  x.xxxDxx
                ...                                 ...
Line 2(Nzpts+1) ............ (It=1,Iz=Nzpts)      x.xxxDxx
          .                                         .
          .                                         .
          .                                         .
Line Ntpts(Nzpts+1)+1 ...... (It=Ntpts,Iz=0)      x.xxxDxx
Line Ntpts(Nzpts+1)+2 ...... (It=Ntpts,Iz=1)      x.xxxDxx
                ...                                 ...
Line (Ntpts+1)(Nzpts+1) .... (It=Ntpts,Iz=Nzpts)          x.xxxDxx
```

where x.xxxDxx are the values of the field (in V/m), Ntpts/Nzpts are the number of time steps/spatial bins specified in the GRID card. [Note: total of (Ntpts+1)(Nzpts+1) lines.]

'Uvbs' FILE FORMAT

```
                                  Column 1
                                  |
Line 1 .......... (It=0)                x.xxx
Line 2 .......... (It=1)                x.xxx
         ...                      ...
Line Ntpts+1 .... (It=Ntpts)     x.xxx
```

where x.xxx are the values of the bias voltage (in V), and Ntpts is the number of time steps specified in the GRID card. (Note: total of Ntpts+1 lines.)

'Ualx' FILE FORMAT

```
                                Column 1
                                |
Line 1 .......... (Iz=1)               x.xxx
Line 2 .......... (Iz=2)               x.xxx
       ...                     ...
Line Nzpts ...... (Iz=Nzpts)   x.xxx
```

where x.xxx are the values of the Al mole fraction, and Nzpts is the number of spatial bins specified in the GRID card. (Note: only Nzpts lines.)

'Depl' FILE FORMAT

The same as in the file 'Udpg'. [Surface charge can be placed at the first line (Iz=0).]

'Zusr' FILE FORMAT

The same as in the file 'Udpg'.

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Appendix D. Format of Output Data Files for Post-Graphical Processing

Numerical-oriented data files are output for post-graphical processing. These files can be converted to data files suitable for drivers of graphical software. The format of each data file is described below. Most of the contents of these files are pretty much self-explanatory. In general, data in each separate valley are designated as Param*, where *=0, 1, 2, 3 for C, G, X, and L valleys, respectively ("C" stands for all valleys "combined").

'His.data' FILE FORMAT

In this file, Edav*, Vdav*, and Cav* represent the ensemble averages of the energy, velocity, and spatial distribution histograms (arbitrary unit), respectively, in each valley. Data are collected at the initial (t=0), three intermediate (t=Itobv1,2,3), and final (t=Tmax) times. The five values on the last line are the maximum electron energies (in eV) for the energy histogram at the above mentioned five instances.

'Tev.data' FILE FORMAT

In this file, all the data are the ensemble averages versus time (It) in each valley. Emean*, Vmean*, and Zmean* are the ensemble means of the energy, velocity, and spatial distributions (in eV, cm/s, and um), respectively. Neav* is the ensemble average of the time the electron ensemble spent during each sampling interval, and hence, Neav1,2,3/Neav0 gives the valley occupancy for G, X, L valleys, respectively. Eeav* and Veav* are the ensemble averages of the electron energy and velocity (in eV and cm/s), respectively. Aimpav*, Aoptav*, and Aacsav* are the ensemble averages of scattering angles (in degree) for impurity, optical phonon, and acoustic phonon scatterings, respectively. Tmfav* and Lmfav* are the ensemble averages of mean free times and mean free paths (in ps and um), respectively.

'Bgev.data' and 'Pcev.data' FILE FORMAT

These two files contain ensemble averages for the background electron and photocarrier sub-ensembles, respectively. Contents of these two files are identical to the data Neav*, Eeav*, and Veav* described in the above 'Tev.data' file.

'Vvt.data' FILE FORMAT

This file contains boundary voltage (in V), Vright, as calculated by the Poisson solver as a function of time (It).

'Ivt.data' FILE FORMAT

In this file, "current density" versus time is collected at each time step. The total current density, J, (in A/cm^2) is interpreted as the number of superparticles impinged on the right boundary, normalized by their "supercharges." When the tunneling boundary condition is enabled (Ltbc=.true. in the BOUNDARY card), emission (Je) and tunneling (Jt) current densities (in A/cm^2) follow the total current density (J), and followed by the number of particles impinged on the right boundary during each sampling interval: Mrref for total, Memis due to emission, and Mtunl due to tunneling.

'Zve.data' FILE FORMAT

This file contains data for the trajectory in time (It) of the first electron in the ensemble: valley index Iv1, position Z(1) (in um), velocity V(1) (in 10^7 cm/s), and energy E(1) (in eV).

'Mec.data' FILE FORMAT

In this file, Tself, Tinter, Tintra, Toptic, Tacous, Timpty, and Teesct represent the number of scatterings due to each mechanism indicated during each sampling interval, respectively, as a function of time (It); Zself, Zinter, Zintra, Zoptic, Zacous, Zimpty, and Zeesct represent the number of scatterings due to each mechanism indicated as a function of distance (Iz) in each spatial bin sampled at the observation times (t=Itobv1,2,3) and the final time (t=Tmax), respectively.

'Rxxx' FILE FORMAT

In this series of data files where Rxxx represents Rtotal, Rself, etc. (see details in the SAVEFILE card), they have the same format: the first column is the time axis (in ps) and the second column is the corresponding scattering rate (in 1/s).

'Sev.data' FILE FORMAT

This file contains space dependence (Iz) of the average energy Eav* (in eV) and average velocity Vav* (in cm/s) in each valley, sampled at the initial (t=0), three intermediate (t=Itobv1,2,3) and final (t=Tmax) times.

'Linv.data' FILE FORMAT

This file contains inverse screening lengths (in 1/cm) as calculated using the self-consistent screening model, sampled at the initial (Linvdb0), three intermediate (Linvdb1, Linvdb2, Linvdb3), and final (LinvdbN) times, as a function of distance (Iz).

'Gam.data' FILE FORMAT

In this file, GAM* represents the total scattering rate (in 1/s) in valley *=1, 2, 3 as a function of energy (Ie). Data are sampled at the initial, three intermediate, and final times.

'Gmax.data' FILE FORMAT

This file contains maximum total scattering rate (in 1/s), GAMMA*, in each valley as a function of time (It).

'PFC.data' FILE FORMAT

In this file, potential Poten (in V), field Field (in V/cm), electron concentration Conc (in 1/cm^3), and net charge density Nele (in 1/cm^3) profiles are collected at the initial, three intermediate, and final times as a function of distance (Iz).

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Appendix E. EMCUR Error Messages

Run-Time Error Messages (File: 'EMCUR.err')

```
 IERR= 4: error in INIT: wrong value of Voccu1, Voccu2, or Vocc3 from input
          cards.
 IERR= 5: error in MAIN: wrong value of Tdelta, Trectg, Tgauss, or Tinvch
          from input cards.
 IERR= 6: error in INIT: wrong value of Lgauss, Lvwted, Lgauss, or
          Ldelta from input cards. Check input cards: Ksbg/Kspc/Ksbc.
 IERR= 7: error in FNLS: wrong value of Mscat from SMEC.
 IERR= 8: error in FNLS: wrong value of Eta from FNLS.
 IERR= 9: error in FNLS: wrong value of cosB from FNLS.
 IERR=10: error in EMCS: negative value of DSQRT.
 IERR=11: error in MAIN: wrong value of Ibcl/Ibcr from input cards.
 IERR=12: error in INIT: wrong value of Z(n). Check in MAIN. (n=*****)
 IERR=13: error in MAIN: wrong value of Ntupr. Check input  cards:  Wpulse/
          Wsigma/Wfwhm and Tmax.
```

Input File Syntax Error Messages (File: 'PARS.err')

```
 *** Kerr=71 *** Invalid parameter found:
 Input card     Valid card
 ----------     ----------
 xxxxx          CardName

 *** Kerr=72 *** Invalid parameter found:
 Input param     Valid param
 -----------     -----------
 xxxxxx          ParamName

 *** Kerr=81 *** Error in Nepts(*)/Nbpts/Nzpts/Ndpts/Ntpts:
 Input values   Valid values
 ------------   ------------
 Nepts1 = xx    [1,Nemax]
 Nepts2 = xx    [1,Nemax]
 Nepts3 = xx    [1,Nemax]
 Nbpts  = xx    [1,Nbmax-1]
 Nzpts  = xx    [1,Nzmax]
 Ndpts  = xx    [1,Ndmax]
 Ntpts  =xxx    [1,Ntmax]

 *** Kerr=82 *** Error in Itobv*/Iepwi(*)/Iepwd(*)/ECoff(*)/Xdev/Xbar:
 Input values   Valid values
 ------------   ------------
 Itobv1 = xx    [1,Ntpts]
 Itobv2 = xx    [1,Ntpts]
 Itobv3 = xx    [1,Ntpts]
 Iepwi1 =xx     [1,Nepts(1)]
 Iepwi2 =xx     [1,Nepts(2)]
 Iepwi3 =xx     [1,Nepts(3)]
 Iepwd1 =xx     [1,Nepts(1)]
 Iepwd2 =xx     [1,Nepts(2)]
 Iepwd3 =xx     [1,Nepts(3)]
 ECoff1 = x.x   [0.0,1.0]
 ECoff2 = x.x   [0.0,1.0]
 ECoff3 = x.x   [0.0,1.0]
 Xdev   = x.x   [0.0,1.0]
 Xbar   = x.x   [0.0,1.0]
```

```
 *** Kerr=83 *** Error in Ibcl/Ibcr/Ksbc/Ksbg/Kspc/Naccu:
 Input values   Valid values
 ------------   ------------
 Ibcl  = x      = 1,2
 Ibcr  = x      = 1,2
 Ksbc  = x      = 1,2,3,4,5
 Ksbg  = x      = 1,2,3,4,5
 Kspc  = x      = 1,2,3,4,5
 Naccu = x      = 0,1

 *** Kerr=84 *** Error in Ntotal/Nbkgrd/Nphoto:
 Input values   Valid values
 ------------   ------------
 Ntotal=xxxxx   [1,Ntotal]
 Nbkgrd=xxxxx   [1,Nbkgrd]
 Nphoto=xxxxx   [1,Nphoto]
 And Nbkgrd + Nphoto = Ntotal

 *** Kerr=85 *** Error in Ntotal/Nbkgrd/Nphoto:
 Input values   Valid values
 ------------   ------------
 Ntotal=xxxxx   [1,Ntotal]
 Nbkgrd=xxxxx   = 0
 Nphoto=xxxxx   [1,Nphoto]
 And Nphoto = Ntotal

 *** Kerr=86 *** Error in Ntotal/Nbkgrd/Nphoto:
 Input values   Valid values
 ------------   ------------
 Ntotal=xxxxx   [1,Ntotal]
 Nbkgrd=xxxxx   [1,Nphoto]
 Nphoto=xxxxx   = 0
 And Nbkgrd = Ntotal

 *** Kerr=91 *** Error in the last line:
 *END not found after 100 lines or by the EOF from the input file.

 *** Kerr=92 *** Error in line # xx:
 The first column in the input file must be "*", or ".", or "+".

 *** Kerr=93 *** Error in line # xx:
 EOL indicator (;) not found, or number of characters in this line  exceeds
75.

 *** Kerr=94 *** Error in line # xx:
 Number of characters in this parameter exceeds 6.

 *** Kerr=95 *** Error in line # xx:
 Number of characters in this parameter value exceeds 10.
```

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Notes

The following notations are used for special symbols:

<=	less than or equal to
!=	not equal to
n^m	n to the mth power
um	micro-meter