Validation Analysis and Test of Semiconductor Device Simulator GSRES

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Abstract— Basic drift-diffusion model (DDM) of carriers in semiconductor using in a numerical simulator: General Semiconductor Radiation Effect Simulator (GSRES), is studied in order to identify and reduce the numerical errors of this semiconductor simulator. Numerical approximations of the semiconductor device EMP effect simulator is analysed. Numerical errors caused by approximation of the field distribution of lattice temperature, and approximation the of the recombination rate and generation rate are studied. Application range of this simulator is analysed according to the numerical errors caused by these approximations. Terms of the simulator that should be improved and enhanced precision are given.

1. INTRODUCTION

Numerical simulation of semiconductor devices can reflect the physical phenomena and mechanisms of devices, and is important in effect study. This simulation method is proved to be efficient and accurate as many research papers showed [1–5]. A two-dimension semiconductor device Electromagnetic pulse effect simulator GSRES (General Semiconductor Radiation Effect Simulator) is using widely in numerical simulation radiated field (EMP, HPM) effect of semiconductor device, which is developed by our research group. This simulator contains modeling modularmeshing modulardata-base of material parameters and Graphical User Interface (GUI). The numerical simulation of carriers bases on Drift-Diffusion Model (DDM). Two-dimension semiconductor device and simple circuit can be simulation numerically by this simulator [6–9].

The demand of analysis of error sources rises up while manufacturer technic of device and precision of experiments are developing [10–12]. For another reason, Verification and validation (V&V) analysis is required for engineering implementation of GSRES. Bases on these requirement, physical models (DDM) in GSRES are analysed, possible error sources are evalueated, and contemplation. of capability of upgrade version GSRES is established.

1.1. Basic Drift-diffusion Model in GSRES

Response capability of device is determined by the movement of carriers in semiconductor material [8, 13, 14]. Drift-Diffusion model is used more and more widely in numerical simulation of semiconductor device since the first use by Gummel. Drift-Diffusion model is based on this equation

$$\begin{cases} \frac{\partial n}{\partial t} = \nabla \cdot \left(\mu_n n \overrightarrow{E_n} + \mu_n \frac{k_b T}{q} \nabla n \right) - (U - G) \\ \frac{\partial p}{\partial t} = -\nabla \cdot \left(\mu_p p \overrightarrow{E_p} - \mu_p \frac{k_b T}{q} \nabla p \right) - (U - G) \\ \nabla \cdot \varepsilon \nabla \psi = -q \left(p - n + N_D^+ - N_A^- \right) - \rho_s \end{cases} \tag{1}$$

where n is the concentration of carrier electron and p for hole; N_D^+ is the concentration of effective ionic donors and N_A^- for acceptor; μ_n is mobility of electron and μ_p for hole; $\overrightarrow{E_n}$ is the equivalent electric field intensity to electron and $\overrightarrow{E_p}$ for hole; ψ is electrostatic potential; ρ_s is the static charge and interphase charge; U is the recombination term of carrier. G is the generation term of carrier; T is temperature; q is charge of electron.

Equation (1) is the basic and mostly used calculation model in GSRES. Analysis of error sources is base on this model in this paper.

2. APPROXIMATION IN SIMULATION MODEL

The basic DDM in Equation (9) is educed by the solution of electromagnetic Poisson equation base on energy band and tight-banding theory. In the educe process of basic DDM, these assumptions are taken: (a) velocity of carriers much more less than light; (b) collisions of carriers in the semiconductor material are elastic; (c) collisions of carriers do not effect gap of energy band; (d) temperatures of carriers and lattice are equality. Approximations of calculation model in GSRES concenter in two: (1) the approximations induced by energy band and tight banding theory; (2) approximations induced by DDM. In this paper, our error analysis focuses on the approximations induced by DDM.

In DDM used in GSRES, approximations mostly in: (a) distribution and change of temperature; (b) recombination and generation rate of carrier; (c) mobility model.

2.1. Approximation Caused by Distribution and Change of Temperature

In Equation (9), the basic DDM takes approximations in the distribution and change of temperature, the temperature of lattice is assumed to be uniformity and invariablenes and no temperature effect is taken into the model. If the gradient term of temperature is not 0, the DDM in (1) now is

$$\begin{cases} \frac{\partial n}{\partial t} = \nabla\cdot\left(\mu_n n\overrightarrow{E_n} + \mu_n \frac{k_b T}{q}\nabla n + \mu_n \frac{k_b n}{q}\nabla T\right) - (U-G) \\ \frac{\partial p}{\partial t} = -\nabla\cdot\left(\mu_p p\overrightarrow{E_p} - \mu_p \frac{k_b T}{q}\nabla p - \mu_p \frac{k_b p}{q}\nabla T\right) - (U-G) \\ \nabla\cdot\varepsilon\nabla\psi = -q\left(p - n + N_D^+ - N_A^-\right) - \rho_s \\ \rho c_p \frac{\partial T}{\partial t} = \nabla\cdot\kappa\nabla T + \vec{J}\cdot\vec{E} + (E_g + 3k_b T)\cdot(U-G) \end{cases} \tag{2}$$

The forth equation in (2) is equation of heat generation and diffusion. ρ is mass density. c_p is heat capacity. κ is heat diffusion coefficient. E_g is gap of energy band. This equation means: thermal energy which is absorbered or released in unit volume contains three parts: induced by heat diffusion as the first term; induced by current as the second term; induced by generation and recombination of carriers as the third term.

In Equation (2), the gradient term of temperature is not 0, but temperature of carriers is set to be same with the temperature of lattice, the difference between these two is ignored. When considered the difference, the forth term in Equation (2) must be changed, the equation current density of electron and hole and the equation of heat diffusion of lattice is

$$\begin{cases} \overrightarrow{J_n} = q\mu_n n\overrightarrow{E_n} + k_b\mu_n(n\nabla T_n + T_n\nabla n) \\ \overrightarrow{J_p} = q\mu_p p\overrightarrow{E_p} - k_b\mu_p(p\nabla T_p + T_p\nabla p) \\ \rho c_p \frac{\partial T}{\partial t} = \nabla\cdot\kappa\nabla T + (E_g + \omega_n + \omega_n)\cdot(U-G) + \frac{n(\omega_n - \omega_0)}{\tau_{\omega_n}} + \frac{p(\omega_p - \omega_0)}{\tau_{\omega_p}} \end{cases} \tag{3}$$

$\overrightarrow{J_n}$ is current density of electron. $\overrightarrow{J_p}$ is current density of hole. T_n is the temperature of electron. T_p is the temperature of hole. ϖ_0 is the balance energy of carriers (when temperature of carriers equivalent to lattice). τ_{ω_n} is the energy relaxation times of electrons and τ_{ω_p} is the energy relaxation times of holes.

The calculation model in (3) considered the energy exchange between carriers and lattice. Carriers exchange energy with lattice by collision, and can be characterized by energy relaxation times. This model is much more precise than models in (1) and (2), and cost much more computer memory resource and CPU time for numerical simulation.

2.2. Approximation Caused by Recombination and Generation Rate of Carrier

In GSRES, recombination of carriers are numerically simulated by three mechanism [8, 14]: Shockley-Read-Hall (SRH) recombination mechanism; Auger recombination mechanism; direct recombination mechanism. SRH recombination characterizes the recombination of carriers nearby impurity and defects. These impurity and defects which facilitate recombination are defined as recombination centers. Auger recombination characterizes the recombination of electron-hole pair with the help of another carrier which absorbs energy from the electron-hole pair. Direct recombination characterizes the recombination of electron-hole pair directly with the help of an electron's transition from conduction band to valence band. Commonly, SRH recombination is the mostly mechanism in semiconductor material. Auger recombination taking more and more rate as the density of carriers increasing. Direct recombination arises in high injection levels (for instance: power device) only.

In GSRES, these three recombination mechanisms are simulated separately for the difficulty form numerical simulation. Total recombination rate is the sum of these three.

$$U = U_n = U_p = U_{\mathrm{SRH}} + U_{\mathrm{dir}} + U_{\mathrm{Auger}} \tag{4}$$

The term in right side means SRH recombination rate, direct recombination rate and Auger recombination rate.

$$\begin{cases} U_{\text{SRH}} = \frac{pn - n_{ie}^2}{\tau_p\left[n + n_{ie}\exp\left(\frac{\text{ETRAP}}{kT_L}\right)\right] + \tau_n\left[p + n_{ie}\exp\left(\frac{-\text{ETRAP}}{kT_L}\right)\right]} \\ U_{\text{Auger}} = \text{AUGN}\left(pn^2 + nn_{ie}^2\right) + \text{AUGN}\left(np^2 - pn_{ie}^2\right) \\ U_{\text{dir}} = \text{DIRECT}\left(np^2 - n_{ie}^2\right) \end{cases} \tag{5}$$

τ_n and τ_p are lifetime of electron and hole, which rest with density of impurity.

$$\begin{cases} \tau_n = \frac{\text{TAUN0}}{1 + N_{total}/\text{NSRHN}} \\ \tau_n = \frac{\text{TAUP0}}{1 + N_{total}/\text{NSRHP}} \end{cases} \tag{6}$$

The implicit value in Equations (5) and (6) of parameters in GSRES can be found in Reference [8].

The generation mechanism of carrier in GSRES is simulated by using an experimental equation advised by Selberherr [8, 14].

2.3. Approximation Caused by Mobility Model

Using mobility model pertinently can efficiently reduce numerical error, and extend the application of DDM. Mobility model contains three types in the main [14]: weak field model; surface model; strong field model; A integrated mobility model ordinarily combines weak field model and surface model, with modification due to the intensity of electric field.

Various mobility models are modularized in GSRES. A weak field model mostly used is Analytic Mobility Model, which is numerically fitting by experimental results. It is accurate in the simulation of diodes. Another weak field model is Philips Mobility Model, which is exactitude in the simulation of silicon triode. Lombardi surface model mostly used in simulation of silicon MOS device. Lucent model combines the modification of saturation velocity bulk mobility and surface mobility in strong field. Hewlett-Packard model can get the same precision in the simulation of MOS device as Lucent model, but can reduce CPU time efficiently.

These mobility models contains physical mechanism that not in DDM, in order to be tally with test results. For instance, enhanced diffusion effect caused by heat carriers is taken into modification of strong field. Impair effect caused surface state and letdown of carriers density caused by quantum well on Si-SiO_2 interface are both taken into surface mobility model. In fact, mobility models are modifications and complements for DDM, which improve simulation precision, extend application area, at the same time, aggrandizement instability and complicacy of calculation.

3. ANALYSIS OF ERROR SOURCES

Approximation of temperature and approximation of mobility are found to be the main numerical sources of GSRES while using this simulator [10–12].

3.1. Errors Caused by Approximation of Temperature

Generation of heat happens in the same time with current. In the case when current is weak, Joule heat is small, so alteration of device's temperature is low. In that time, effect of temperature to performance of device can be ignored [10]. However, if the current is strong, the effect of the temperature to performance of device may be prominent.

In the case of strong field, insufficiency of energy exchange may happen because the velocity of carrier is too fast. Insufficiency of energy exchange may happen if the field last for a too short time. Avoidance of these case can improve simulation precision. Fig. 1 is the simulation result of 1.5KECA39 unidirectional TVS diode, which is a micron device. The numerical data is tally with test data [12].

3.2. Errors Caused by Approximation of Mobility

Mobility model is an modification and an complement for DDM. Numerical error will extremely be reduced by using pertinent mobility model contrapose to different structures and parameters. For instance, Lucent mobility model, which combines Philips Mobility Model and Lombardi surface Mobility Model, is not often used in simulation of simple device (like diode) for the reason of huge amount of calculation. But it can efficiently ameliorate numerical precision of the simulation of MOS device because the intense field in tunnel.

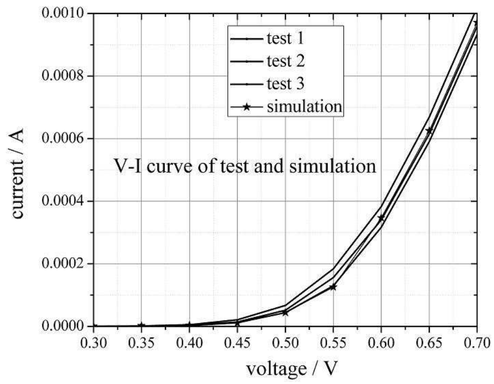

Figure 1: I-V curve of 1.5KECA39 unidirectional TVS diode.

As mentioned in part 3.1, if the scale of device on one direction is too small, simulation of thermal effect will be difficult For GSRES. Using surface Mobility model which considers quantum wall effect can extend the application of GSRES to these submicron device and nano scale device.

4. ANALYSIS OF APPLICATION SCOPE OF GSRES

In order to decide the application scope of GSRES, a validation test is taken. If the simulation error is less than that of the validation test, GSRES is indicated to be suitable. Otherwise, GSRES is indicated to be out of the application scope and inapplicable, modification should be taken in the calculation/physics model or the initial parameters.

In test, errors are mainly caused by two parts: the random error of samples and the errors of instrument. In the first, Character of TVS diodes are tested to find the random errors of these diode of same type. The errors are showed in Table 1.

Table 1: Random errors of TVS diode.

	Sample 1	Sample 1	Sample 1	errors
breakdown voltage	39.9	38.7	38.8	3.1%
junction Capacitance, $1/C_D^2$-V curve (100 Hz)/10^{16} cm^2/CV	−6.676	−7.068	−6.685	5.9%
junction Capacitance, $1/C_D^2$-V curve (1 MHz)/10^{16} cm^2/CV	−6.641	−7.092	−6.644	6.8%
I-V curve (0.7 V)	0.00102	0.00096	0.00093	9.2%

Random error from samples (TVS diode) is from 3.1% to 9.2%, much greater than that of the instrument. In this case, error in test process is mainly caused by random error from samples, and the range of test process error is from 3.1% to 9.2%.

As a result, if the simulation error is less than 3.1% (as shown in Fig. 1), we may say that GSRES in the right application scope, because the numerical error is much less than random error in test. But, in the other hand if the simulation error is greater than 9.2%, GSRES may be out of the application scope, and modification of numerical method and physics model must be taken.

Figure 2 gives an example of that out of application scope. Change of temperature in TVS diode under an 1.8 V voltage lasts for 4 ns is 35.2 K and under an 1.5 V voltage lasts for 15 ns is 45.7 K, 11.7% and 15.1% equally. In high voltage or long time case, basic DDM is out of application scope, it must be modified and energy balance model should be used.

Figure 3 gives another example of that out of application scope. Basic DDM can not simulates deep submicron device quite precisely as analysed in part 3. Fig. 4 gives the output characteristics and transfer characteristics of deep submicron MOSFE. Parameters of MOSFET and experiment result are download form website [15]. As Fig. 4 shows, simulation error of basic DDM is over 20%, and out of application scope, while energy balance model shows and precisely simulation result.

As simulation result shows, GSRES with basic DDM can simulate low voltage, small temperature change and micron device precisely. But high voltage, great temperature change and deep submicron device is out of application scope.

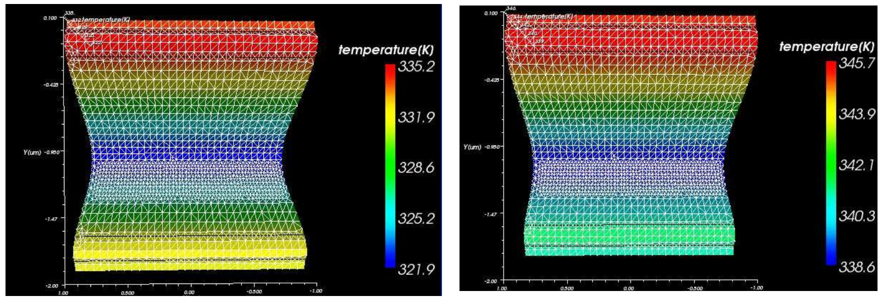

Figure 2: Change of temperature in TVS diode, parameter of diode model is same with tested sample.

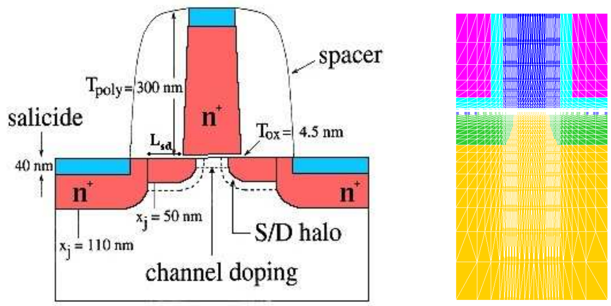

Figure 3: Deep submicron MOSFET model download from website.

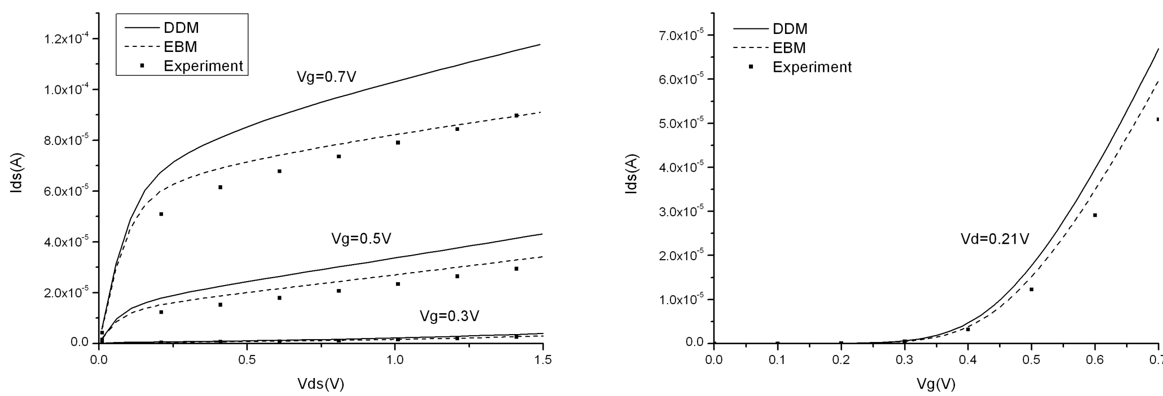

Figure 4: Output characteristics and transfer characteristics of deep submicron MOSFET.

5. CONCLUSION

In this paper, DDM in semiconductor effect simulator GSRES is analysed theoretically. For normal devices, current inside device increases as load voltage increase, which resulting in an augment of Joule heat. As a result, the temperature of device is not uniformity and invariablenes, gradient term of temperature is not 0. Equation (1) is not suitability, so modification of lattice temperature and carrier temperature must be introduced into DDM. Carriers exchange energy with lattice by collision, and can be characterized by energy relaxation times or mean free path. The numerical errors will increase because the insufficiency of energy exchange in the case when the scale of device is too small, or the electric field is too strong, or the period of load voltage pulse is too short. In order to reduce error, simulations of deep submicron device and strong field should be avoided.

Mobility model is an modification and an complement for DDM. Pertinently use of mobility model can efficiently reduce numerical error. Appropriate mobility model considers strong field effect and quantum well effect can efficient reduce the error and extend the application area such as deep submicron device and nano scale device. This is the next target for our development and improvement of GSRES.

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REFERENCES

1. Gummel, H. K., "A self-consistent iterative scheme for one-dimensional steady state transistor calculations," *IEEE Trans. Electron Devices*, Vol. 9, No. 11, 455–465, 1964.
2. Yee, J. H., "Modeling of current and thermal mode second breakdown phenomenon," *Electrical Overstress/Electrostatic Discharge Symposiums Proceedings*, 76–81, 1982.
3. Orvis, W. J., "Modeling and testing for second breakdown phenomena," *Electrical Overstress/Electrostatic Discharge Symposiums Proceedings*, 108–117, 1983.
4. Zhou, H., Z. Du, and K. Gong, "Overshoot phenomena in PIN diode under EMP with fast rise time," *High Power Laser and Particle Beams*, Vol. 17, No. 5, 783–787, 2005.
5. Wang, B. and K. Huang, "Response of high power PIN diode limiter to electromagnetic pulse descending edge," *High Power Laser and Particle Beams*, Vol. 20, No. 7, 1177–1181, 2008.
6. Ding, G., F. Han, and J. Wang, "2D hydrodynamic simulation of GaAs metal-semiconductor-field-effect-transistor," *High Power Laser and Particle Beams*, Vol. 18, No. 7, 1144–1148, 2006.
7. Ding, G., J. Wang, D. Zhang, et al., "A general purpose two-dimensional semiconductor simulator," *Chinese Journal of Computational Physics*, Vol. 24, No. 2, 247–252, 2007.
8. Ding, G. and X. Zhang, *GSS User's Manual*, Northwest Institute of Nuclear Technology, Xi'an, 2008.
9. Xuan, C., D. Gong, H. Xie, et al., "Semiconductor device/circuit mixed-type simulation and its application in HPM effects," *Microelectronics*, Vol. 39, No. 3, 424–428, 2009.
10. Li, Y., C. Xuan, and J. Wang, "Study of response to electromagnetic pulse of PIN diode," *Proceedings of EME*, 280–283, 2012.
11. Li, Y., C. Xuan, H. Xie, et al., "Response of PIN diode to electromagnetic pulse," *High Power Laser and Particle Beams*, Vol. 25, No. 8, 2061–2066, 2013.
12. Li, Y., Y. Liu, C. Xuan, et al., "Study of modeling and validation of TVS diode," Submitted.
13. Sze, M., *Physics of Semiconductor Device Solid*, Suzhou University Press, Suzhou, 2002.
14. Ye, L., *Semiconductor Physics*, High Education Press, Beijing, 2007.
15. http://www-mtl.mit.edu/researchgroups/Well/.