Detector Model Parameter Simulation based on Monte Carlo and Fluka Software

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***Abstract* — One detector model parameter simulation method based on Monte Carlo and Fluka Software has been proposed in this paper to improve the response of detector for thermal neutron and attain detection sensitivity and detection efficiency of detector. First, α particle attained from neutron reacting with 6LiF at conversion layer and 3H particle angular distribution energy spectrum has been analyzed; second, analogue simulation has been made for 4H-SiC Schottky diode model parameters with adoption of Monte Carlo method and Fluka software; finally, simulation analysis has been made for the influence of 4H-SiC detector on relationship between current pulse characteristics of α particle with different energies and instantaneous current pulse of α particle under fixed voltage.**

Keywords - monte carlo; fluka software; detector; parameter simulation; sensitivity

I. INTRODUCTION

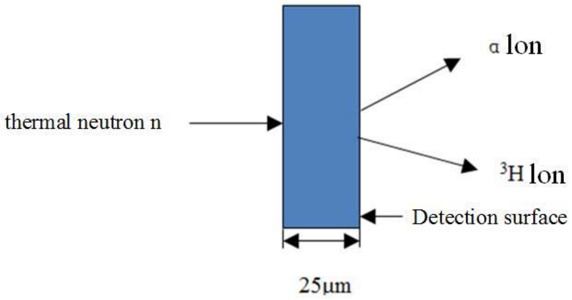
As an important and basic particle of composing material atomic nucleus, neutron presents electric neutrality. Neutron irradiation will damage instrument quality or human health. Neutron detection plays a significant role in safety monitoring of nuclear power plant, nuclear material monitoring, space physics and clinical medicine etc.

Detection efficiency is an important performance index of detector, which describes the detection ability of detector for the number of particle entering detector within the same unit time. It is the proportion between detected particle number and the total entered particle number. Factors affecting this index of the detector mainly include size of detector depletion region, detector structure as well as the sensitivity of detector for the detected particle, in which the influence of detection sensitivity is greater. Resolution ratio of detector for incident particle is another important performance index of detector, including energy and location of incident particles and resolution rate of time. Energy resolution requires that the detector is with the ability of identifying particles with similar energy; position resolution and time resolution determine the spatial and time values of particle entering into detector. Detector is adopted to measure the half width of line (FWHM) to describe the energy resolution of detector for particles entering detector. In addition, the performance indexes of detector also include linear response and particle identification ability. Linear response describes the linear relationship between detection information output by detector and entering position strength and energy of entered particles; while particle identification ability expresses the sensitivity of detector for the particles to be detected and other interfering impure particles.

Therefore, analyzing detector characteristics accurately is of great value for using detector reasonably. To improve the response degree of detector for thermal neutron, this paper has adopted Monte Carlo calculation method and Fluka software to realize detector model parameter simulation to attain accurate analysis of the detector performance.

II. REACTION MODEL DESCRIPTION

Monte Carlo calculation method is also called as random sampling technique, statistical test method or statistical simulation method, which is a numerical calculation method selecting random number repeatedly to calculate physical or mathematical problems and is applied to each research field extensively. Fluka software is a Monte Carlo program developed by Italy National Institute of Nuclear Physics and European Center for Nuclear Research jointly and is used for simulating and studying particle transportation process and interaction process between particle and matter. It is with wide application range and can simulate the problems of neutron, photon, electron and other particles in substance transportation. Picture 1 has listed the reaction model used by simulated angular distribution energy spectrum.



Picture 1. 6LiF(n,α)3H Reaction Model

In the reaction model as shown in picture 1, dimension design of 6LiF is 80μm×80μm and the thickness is 25μm. During simulation, thermal neutron n enters into 6LiF conversion layer directly. As described earlier, the dimension of reaction layer is suitable. For the low energy neutron with energy lower than 20MeV, when adopt Fluka statistical operation, software divide the neutron energy between 10e-11MeV and 20MeV into 260 energy groups; relatively, when neutron energy is bigger than 20MeV, software defines it as an energy box. When operate the reaction process of low energy neutron, Fluka adopts LOW-NEUT card and it defines the operation method of operating low energy neutron and physical process of matter interaction in Fluka. Attachment A lists the input document for simulation.

III. DETECTOR SIMULATION PHYSICAL MODEL

When simulating characteristics of semiconductor device, it needs to use drift diffusion model in semiconductor physics. The compositions of this model include three basic equations, including poisson equation, continuity equation of carrier and transport equation of carrier.

A. Poisson Equation

$$\varepsilon_s \nabla^2 \phi = e(n - p + N_A^- - N_D^+) - \rho_s \qquad (1)$$

Poisson equation is used to calculate the electric potential distribution, in which *εs* is dielectric constant, *φ* is potential, *e* is electron charge, *n* and *p* are electron and hole density, *NA-* and *ND+* are ionized acceptor and donor impurity concentration respectively and *ρs* is surface charge density.

B. Continuity Equation of Carrier

$$\begin{aligned} \nabla \vec{J}_n - e\frac{\partial n}{\partial t} &= U \\ \nabla \vec{J}_p + e\frac{\partial p}{\partial t} &= U \end{aligned} \qquad (2)$$

Continuity equation of carrier is used to calculate each carrier concentration in semiconductor device, in which $\vec{J}_n$ and $\vec{J}_p$ are current densities of electron and hole, *n* and *p* are concentrations of electron and hole and *U* is compound rate.

C. Transport Equation of Carrier

$$\begin{aligned} \vec{J}_n &= en\mu_n\vec{E} + eD_n\nabla n \\ \vec{J}_p &= en\mu_p\vec{E} - eD_p\nabla p \end{aligned} \qquad (3)$$

Transport equation of carrier can be used to calculate electron and hole concentrations, in which $\vec{E}$ is electric field intensity, *μn* and *μp* are mobility rates of electron and hole respectively, *Dn* and *Dp* are diffusion coefficients of electron and hole:

$$\begin{aligned} D_n &= \mu_n k_0 T / e \\ D_p &= \mu_p k_0 T / e \end{aligned} \qquad (4)$$

In the formula, *k*0 is Boltzmann constant and *T* is absolute temperature. Mobility rate is an important parameter needs to be considered during semiconductor device simulation. Doping concentration, temperature and electric field affect the change of mobility rate. Under the situation with low electric field intensity, mobility rate can be described with Masetti model:

$$\mu_n = \frac{947 \times (T/300)^{-2.4}}{1 + \left[\left((N_A + N_D)/1.94\right) \times 10^{17}\right]^{0.61}} cm^2/V\cdot s \qquad (5)$$

$$\mu_n = 15.9 + \frac{124 \times (T/300)^{-2.4}}{1 + \left[(N_A + N_D)/1.76 \times 10^{17}\right]^{0.34}} cm^2/V\cdot s \qquad (6)$$

Under the situation with high electric field intensity, mobility rate is described with Canali Model [28]:

$$\mu(E) = \frac{\mu_{low}}{\left[1 + \left(\mu_{low}E/V_{sat}\right)^{\beta}\right]^{1/\beta}} \qquad (7)$$

In the above formula, μ_{low} is low field mobility, V_{sat} is saturated electron drift velocity and β is amount related to temperature:

$$\beta_n(T) = 1.1 \times \left(\frac{T}{300}\right)^{0.66} \qquad (8)$$

$$\beta_p(T) = 1.213 \times \left(\frac{T}{300}\right)^{0.17} \qquad (9)$$

The band width of SiC under room temperature is 3.26eV, band gap narrowing effect can be described with Slotboom model:

$$\Delta E_g(N) = 0.009\left[\ln(N/1\times10^{17}) + \sqrt{\left(\ln\left(N/1\times10^{17}\right)\right)^2 + 0.5}\right] eV \qquad (10)$$

In the formula, *N* is doping concentration, $\Delta E_g(N)$ is the decrease amount of E_g. Compound model requested by simulation, the mainly adopted compound model is based on doped SRH compound:

$$R_{net}^{SRH} = \frac{np - n_{i,eff}^2}{\tau_p(n + n_1) + \tau_n(p + p_1)} \qquad (11)$$

In which, τ_n and τ_p are the life of electron and hole and $n_{i,eff}$ is effective carrier concentration. Because the ionized impurity energy of SiC material is big, under high temperature, the impurities can't be ionized completely and the incomplete ionization models of impurity are as following:

$$N_D^+ = \frac{N_D}{1+2\exp\left(\frac{E_{Fn}-E_D}{kT}\right)} \tag{12}$$

$$N_A^- = \frac{N_A}{1+4\exp\left(\frac{E_{Fp}-E_A}{kT}\right)} \tag{13}$$

In the formula, *EFn* and *EFp* are quasi Fermi levels of electron and hole; *ND* and *NA* are doping concentrations of donor and acceptor. Under the high electric field, conduction band electrons attain adequate energy to collide with valence electron. The valence electron is excited to enter into conduction band and produces electron-hole pair, and then use impact ionization model:

$$G = \alpha_n n v_n + \alpha_p p v_p \tag{0-1}$$

αn and αp are impact ionization coefficients of electron and hole, as following:

$$\alpha_n = 3.25\times10^5\left(1-0.0329(T-300)\right)e^{-\left(\frac{1.71\times10^7}{E}\right)} \tag{0-2}$$

$$\alpha_p = 3.25\times10^6\left(1-0.0329(T-300)\right)e^{-\left(\frac{1.71\times10^7}{E}\right)} \tag{0-3}$$

In addition, heavy ion enters into device to accumulate energy and produce a lot of electron-hole pairs to form current pulse. It also needs to use heavy ion model to simulate calculation:

$$G(l,w,t) = G_{LET}R(w,l)T(t) \tag{0-4}$$

In the formula, *GLET* is carrier generation rate produced after heavy ion entering into material and its unit is pairs/cm3; *R*(*w,l*) and *T*(*t*) are the functions of generation rate in space and time. If *l<lmax* (the maximum range of particle incident)

$$G(l,w,t) = 0 \tag{0-5}$$

If l≥lmax, T(t) is defined as the form of Gaussian function,

$$T(t) = \frac{2\square\exp\left[-\left[\frac{t-t_0}{\sqrt{2}\square s_{hi}}\right]^2\right]}{\sqrt{2}\square s_{hi}\sqrt{\pi}\left[1+erf\left[\frac{t_0}{\sqrt{2}\square s_{hi}}\right]\right]} \tag{0-6}$$

In the formula, t0 is the time of particle incident; shi is the characteristics value of Gaussi function. For the distribution function R(w,l) in space, it is exponential function form by default:

$$R(w,l) = \exp\left(-\frac{w}{w_t(l)}\right) \tag{0-7}$$

Or the Gaussian function form,

$$R(w,l) = \exp\left(-\left(\frac{w}{w_t(t)}\right)^2\right) \tag{0-8}$$

In the formula, w is the radius of energy accumulation of particle at one position; wt is the characteristic radius of particle incident in material in heavy particle model and is the function of incident distance l. Generation rate of linear energy transfer (LET) carrier:

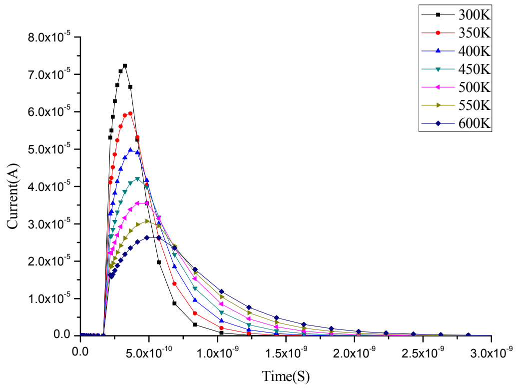
$$G_{LET}(l) = a_1 + a_2 l + a_3 e^{a_4 l} + k'\left[c_1(c_2+c_3 l)^{c_4} + LET\_f(l)\right] \tag{0-9}$$

In the formula, *LET_f*(*l*) is the function of incident distance *l*, the unit by default is pairs/cm3. If use key word PicoCoulomb in the model, its unit is pC/μm.

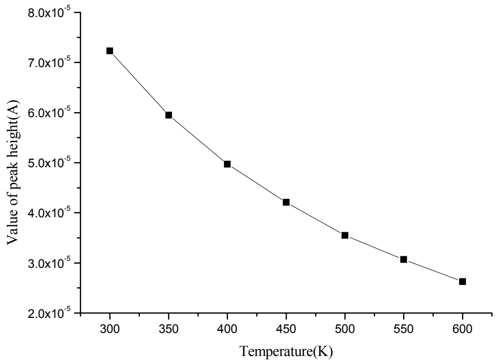
IV. SIMULATION RESULTS AND ANALYSIS

For easy simulation, this paper has set 0.2MeV unit energy interval when use Fluka software to extract angular distribution energy spectrum of α particle and 3H particle generated after 6LiF(α, n)3H reaction; Extracted 11 energy values of α particle with the energy between 0.15MeV and 2.05MeV and then adopted angular distribution energy spectrum data in the following work to simulate and study the influence of 4H-SiC detector on thermal neutron and α particle current pulse characteristics after nuclear reaction happens to 6LiF. α particle with certain energy enters into 4H-SiC detector and electron-hole is produced due to energy accumulation. In this process, the generation rate of electron-hole pair is assumed to meet the form of Gaussian function in time and space; one electron-hole pair consuming 7.8eV energy on average is produced; average energy consumption affects the generation ratio of α particle introducing electron-hole pair into SiC detector [34].

(1) The relationship between temperature and α for α particle instantaneous current pulse; picture 2 and picture 3 list pulse changes and pulse height changes of α particle with 2.05MeV energy within 300K and 600K under 150V reverse bias voltage and alignment conditions.



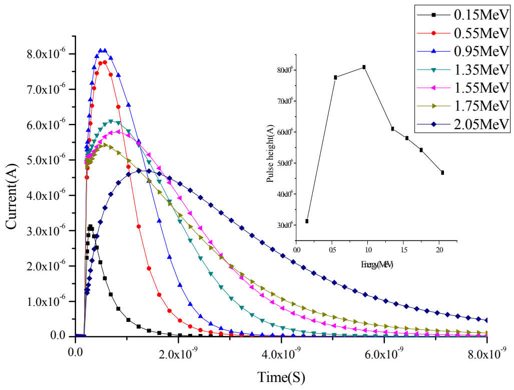
Picture 2. Changes of pulse of 2.05 MeV α particle with temperature from 300K to 600K under reverse bias voltage 150V



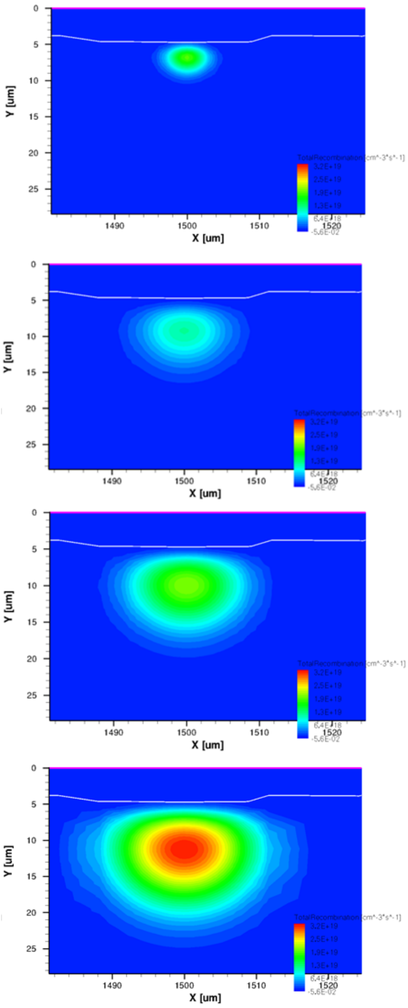
Picture 3. Changes of pulse height of 2.05 MeV α particle with temperature from 300K to 600K under reverse bias voltage 150V

It can be learnt from the experiment results in picture 2 and picture 3 that with the increase of temperature, the pulse height decreases gradually; the rising time and falling time of current pulse increase gradually. In fact, the mobility rate of carrier in diode increases rapidly with the increasing of temperature. In α particle incident trajectory, the collection of applied electric field for electron-hole pair introduced by α particle is slower than compound rate of electron-hole pair. The compound acceleration of electron-hole pair decreases the electron-hole number collected by electric field, and then the pulse height value decreases accordingly; it takes more time for the collection of less electron-hole pair by schottky electrode, which is presented as the rise of current pulse and increase of falling time.

(2) Analyze the influence of 4H-SiC detector on current pulse characteristics of α particle with different energies under fixed voltage. Picture 4 and picture 5 have listed that under alignment conditions, the influence of detector on instantaneous current pulse change and pulse height change of 7 α particles with different energies under 4V reverse bias voltage.



Picture 4. of Influence of Detector on Instantaneous Current Pulse Changes of α Particle under 4V Reverse Bias Voltage



Picture 5. Complex Situations of α Particle at 1.35MeV, 1.55MeV, 1.75MeV and 2.05MeV in Detector under 4V Bias

It can be learnt from the experimental results of picture 4 and picture 5 that under fixed bias voltage, the greater of the incident α particle energy, the higher instantaneous current pulse height; but when the energy is bigger than 0.95M, the current pulse height start to decrease. The greater of the incident α particle energy, the more electron-hole pair number produced by detector; under certain reverse bias voltage, the higher of the current pulse height output by detector. However, under fixed bias voltage, if the incident α particle energy keeps on increasing, it will produce electron-hole pair clouds with high concentration in 4H-SiC detector.

V. CONCLUSIONS

One detector model parameter simulation method based on Monte Carlo Fluka Software has been proposed in this paper; Monte Carlo method and Fluka software have been introduced to make analogue simulation for 4H-SiC Schottky diode model parameters to attain the relationship data between current pulse characteristics of α particle with different energies and instantaneous current pulse of α particle and then realize accurate analysis of detector characteristics. In the following, it will focus on making module development in Monte Carlo Fluka software, realizing generality and batch processing for detector characteristics analysis and then realizing the practical development of theoretical research.

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