Validation of nuclear reaction models relevant to cosmic-ray neutron induced single-event effects in microelectronics

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Abstract. The accuracy of nuclear reaction models used in the PHITS (Particle and Heavy Ion Transport code System) code, i.e., the INC model, the QMD model and the event generator mode (e-mode) with the evaluated nuclear data library JENDL-3.3 are validated to apply it to the simulations on single-event effects in advanced microelectronic devices. The model calculations are compared with available experimental data of light-ion production (i.e., proton and alpha particle) from neutron-induced reactions on natSi and 16O, which are the major constituent elements of silicon semiconductor devices over the wide energy range. Comparisons of calculated and measured data for light-ion production indicate that the e-mode calculation with JENDL-3.3 provides better agreement with the experimental data below 20 MeV, and the QMD model reproduces them reasonably well at energies larger than 20 MeV.

1. Introduction

In recent years, single-event effects (SEEs) induced by cosmic-ray neutrons have been recognized as a key reliability concern for modern microelectronic devices. As illustrated schematically in Fig. 1, secondary ions are generated primarily via the nuclear interaction of the cosmic-ray neutron with a constituent atomic nucleus in the device, then deposit the charge along their tracks. The deposited charge is collected to one of the nodes holding the memory information by drift and diffusion mechanisms. When the collected charge exceeds the critical charge, stored data are upset and a temporary malfunction called soft error is finally caused. The increase in the soft error rate (SER) will become a serious concern as the device size is scaled down. Since it is not easy to shield electronic equipments from cosmic-ray neutrons, it is required to take measures in the design stage of devices and circuits by means of modern SER simulations [1].

We have been developing a soft error simulator based on a particle transport code and a 3-D device simulator. The PHITS code [2] (Particle and Heavy Ion Transport code System) is used to simulate primary physical mechanisms, i.e., nuclear reactions and the subsequent charge deposition processes. To predict the SER precisely, it is necessary to employ highly reliable models describing each physical process leading to the soft errors. In the present work,
the accuracy of the nuclear reaction models used in the PHITS code is validated. The model calculations are compared with available experimental data, and finally it is recommended which nuclear reaction models are the most suitable to apply to simulations of the soft errors caused by cosmic-ray neutrons for modern devices.

2. Nuclear Reaction Models in PHITS

The PHITS code has some nuclear reaction models, such as the INC (intra-nuclear cascade) model [3] and the QMD (quantum molecular dynamic) model [4] to describe the dynamical processes and the GEM (generalized evaporation model) [5] to describe the subsequent evaporation process. The PHITS code has a unique option called "event generator mode (e-mode) [6]” with the evaluated nuclear data libraries, which can describe neutron-induced reactions at energies below 20 MeV by taking into account the conservation of energy and momentum.

3. Soft Error Simulation based on the Sensitive Volume Model

Cosmic-ray neutron induced soft errors for modern devices were simulated using the PHITS code and the sensitive volume (SV) model [7]. In the SV model, it is assumed that all the charge generated in the SV is collected to the nodes. The configuration of the test device used in the simulation is illustrated in Fig. 2 and the cosmic-ray neutron spectrum predicted by EXPACS [8] is presented in Fig. 3. A silicon oxide insulation layer 0.35 µm thick is placed on a 1.0 × 1.0
Figure 4. SER calculated by the INC model and the QMD model.

Figure 5. Influence of secondary ion species and incident neutron energy on soft errors.

× 0.5 mm³ silicon substrate. A 3.0 µm metal layer consisting of copper and silicon oxide is located on an insulation layer and a 0.5 mm silicon oxide package layer is placed on a metal layer. The size of the defined sensitive volume is 0.1 × 0.1 × 0.5 µm³, corresponding to that for SRAMs with modern 45nm technology [9]. The cosmic-ray neutrons are incident on the test device vertically.

Figure 4 shows the SER calculated by the INC model and the QMD model as a function of the critical charge. In each calculation, the e-mode option with JENDL-3.3 [10] was employed in the neutron energy range below 20 MeV. The INC calculation is about 20% smaller than the QMD calculation. This indicates that the difference in the reaction models has considerable impact on soft error simulations and it is necessary to validate nuclear reaction models by comparisons with experimental cross section data.

In addition, the influence of secondary ion species and incident neutron energy on soft errors were examined to explore the soft error mechanism from a microscopic point of view. The results are shown in Fig. 5. It is clarified that light ions produced by the nuclear reaction are the major source of soft errors in the devices with the critical charge less than 1 fC. A similar tendency is also reported in ref. [11]. It is found that the neutron energy range mainly involved in terrestrial soft errors is from 1 MeV to 1 GeV.

4. Results and Discussion
The nuclear reaction models in the PHITS code were validated for light-ion production from neutron-induced reactions at energies ranging from MeV to GeV, based on the results given in the preceding section. Available experimental data of proton and alpha particle production from neutron-induced reactions on nat Si and 16O were applied to the validation.
Figure 6. Production cross sections of proton and alpha particle from neutron-induced reaction on natSi. The experimental data are taken from refs. [12, 13, 14, 15, 16]

First of all, the model calculations are compared with the experimental production cross sections of proton and alpha particle from neutron-induced reactions on natSi at incident energies up to 100 MeV in Fig. 6. As for proton production, the QMD model and the INC model calculations are in good agreement with the measured data over the whole energy range. Meanwhile, the QMD model reproduces the measured alpha production better than the INC model in the energy range above 20 MeV, and the e-mode calculation with JENDL-3.3 for alpha production provides better agreement with the measurement below 20 MeV than the QMD and INC models. The e-mode calculation for proton production overestimates proton production below 10 MeV. Since the effect of proton production for neutron energies below 10 MeV on soft error is considerably small as shown in Fig. 5, however, this overestimation does not prevent us from using the e-mode option in soft error simulations with PHITS.

Figure 7 shows the differential cross sections of proton and alpha particle from neutron-induced reactions on natSi and 16O. The agreement with proton production is good for either results of the INC model, the QMD model and the e-mode with JENDL-3.3. For alpha particle emission by the neutron-induced reaction at 15 MeV, the e-mode calculation with JENDL-3.3 reproduces measured data fairly well. The QMD model describes the emission of alpha particles at low emission energies well, whereas the INC model and the QMD model calculations underestimate the alpha particle emission at high emission energies. However, this underestimation might be weakly influenced on soft error simulations because the fraction of high-energy alpha emission was found to be less than 10 % of the total production.

In Fig. 8, double-differential cross sections of natSi (n,xp) and 16O(n,xp) reaction at 96 MeV are represented. The QMD calculation shows satisfactory agreement with the experimental data over the whole angular range. In contrast, the INC model underestimates the backward proton emission. These results indicate that the QMD model is more suitable for soft error simulations than the INC model.

Finally, double-differential production yield of proton and alpha particle from Si bombarded by 175 MeV quasi mono-energetic neutrons are shown in Fig. 9. The QMD model calculation reproduces the proton production well, but underestimate the alpha particle production largely, which is the same tendency as in the case of 96 MeV seen in Fig. 7.

5. Conclusions
The nuclear reaction models implemented in the PHITS code (i.e., the INC model, the QMD model and the e-mode with JENDL-3.3) was validated for simulations of the soft errors caused by cosmic-ray neutrons. Since light-ion production is expected to be the major source of soft errors in advanced microelectronic devices, the model calculations were compared with the
Figure 7. Differential cross sections of proton and alpha particle from neutron-induced reaction on natSi and 16O. The experimental data are taken from refs. [12, 14, 17, 18].

Figure 8. Double differential cross sections of proton and alpha particle from neutron-induced reaction on natSi and 16O. The experimental data are taken from refs. [14, 18].

The validation results indicate that the combined use of the e-mode with JENDL-3.3 and the QMD model lead to better prediction in the soft error simulation with PHITS. Further
Figure 9. Double-differential production yield of proton and alpha particle form $^{nat}$Si bombarded by 175 MeV quasi mono-energetic neutrons [21].

Improvement will be necessary for light-ion production near the reaction threshold energy and the emission of high-energy alpha particles toward more accurate soft error simulation.

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