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Time dependent modeling of single particle displacement damage in silicon devices

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ABSTRACT

An approach combining molecular dynamics simulations with Kinetic Monte Carlo simulations is proposed to model the temporal evolution of single particle displacement damage in silicon. The three dimensional distributions of primary defects induced by Si recoils within 10 ps are obtained by molecular dynamics simulations and subsequently the long-term evolution (over 10^5 s) of multiple types of defects is simulated with Kinetic Monte Carlo technique fed by molecular simulation results. Based on classical Shockley–Read–Hall theory, the annealing factors of radiation-induced dark current related to the evolution of defects are predicted for photodiodes of 0.18 μm CMOS image sensors under neutron irradiation. The calculation results are consistent with the experimental data.

1. Introduction

In harsh radiation environments, long time operation of CMOS active pixel image sensors is threatened by displacement damage [1–4]. Radiation-induced defects in depletion regions of photodiodes in the array of pixels could cause the increase of dark current due to the generation of electrons and holes on the defect energy levels [2]. In some extreme events, a large number of defects created in the depletion region could raise the dark current beyond a threshold, hence inducing a “hot pixel” [1,4]. The displacement damage is a multiscale phenomenon involving processes spanning a wide range of time and spatial scales. To better understand this complicated issue, an integration of multiple methods over the relevant length and timescales is therefore required [5].

Previous studies have treated the time-dependent behavior of radiation-induced defects for particular aspects, such as the chemical rate theory for defect reactions in electron-irradiated silicon solar cells [6], the phenomenological model for annealing of randomly distributed defects in silicon detectors [7–8], the one-dimensional continuum model for defect reactions in pulse-neutron-irradiated bipolar junction transistors (BJTs) [9], the Kinetic Monte Carlo (KMC) simulations for the annealing of defects and the recovery of base current of BJTs irradiated by electrons and neutrons [10]. In the above studies for neutron-irradiated devices, the binary collision approximation (BCA) was used to provide initial coordinates of primary defects. BCA codes can adequately describe the spatial distribution of energy deposition and the amount of doping profiles for a broad range of energies. However, multiple interactions, which are important in the low energy regime, are not taken into account in BCA calculations, and therefore detailed configurations of the displacement damage cannot be determined well by this technique [11]. Molecular dynamics (MD) technique is well known to provide accurate descriptions of the creation of defects during collision cascades at atomic level (~nanometers, ~picoseconds) [12–15]. When considering the thermal activation processes, the KMC technique becomes one of the most appropriate methods to track the evolution of defects on a timescale that permits comparisons with the experiments [10,16–17]. Consequently, the combination of MD and KMC simulations makes it possible to explore the annealing behavior of electric properties of silicon devices associated with the evolution of defects.

The primary aim of the current study is to develop a multiscale approach for assessing the temporal evolution of single particle displacement damage in silicon from the initial damage cascades created by primary knock-on atoms (PKAs) ($t \leq 10$ ps) to stable defects ($t > 10^5$ s) via coupling MD with KMC simulations, and consequently to investigate the annealing kinetics of single particle displacement damage (SPDD) events in neutron-irradiated photodiodes of CMOS image sensors (CISs, also called APSs). In Section 2, the expressions for calculating the defect-induced dark current are derived. In Section 3, a BCA code is used to estimate the energy of neutron-induced primary recoils. Based on the BCA results, MD and KMC simulations are performed to study the production

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and long-term evolution of defects. The simulation results are discussed in Section 4 and finally, some conclusions are drawn in Section 5.

2. Macroscopic characteristic of defect-induced dark current

The increase of dark current during and after irradiation is mainly due to the generation of electrons and holes on the defect energy levels, and could be assessed in the framework of classical Shockley–Read–Hall (SRH) theory [18–19]. In this study, only defects located in the depletion region lead to dark current generation because the relative contribution to total reverse current made by generation current in the depletion region dominates over the diffusion current [20]. Before irradiation, the minority carrier lifetime is calculated as $\tau_{n0,p0} = (v_{th}\sigma_{n,p}N_t)^{-1}$ [21] where v_{th} is the thermal velocity of electrons and holes, $\sigma_{n,p}$ is the capture cross sections for electrons and holes in cm^2, N_t is the number of defect density in cm^{-3} which is given by N/Ax_d, where N is the number of defects in the depletion region, and A and x_d are the area and depth of the depletion region, respectively. During and after irradiation, the density of defects is increased and the minority carrier lifetime is consequently decreased. Having summed up the contributions of multiple types of defects, we obtain

$$\tau_{n,p} = \frac{Ax_d}{v_{th}} \left\{ \sum_{j=1}^{k} \left[\sigma_{n,p,j}(N_{j0}+N_j)\right] \right\}^{-1} \tag{1}$$

where j denotes different kinds of defects, N_{j0} refers to the number of defects for pre-irradiation and N_j stands for the number of new defects.

The generation lifetime associated with a defect represents the relative frequency of carrier emission [20]. The expressions for the generation lifetime for pre- (τ_{g0}) and post-irradiation (τ_g) are given by Eqs. (2) and (3):

$$\tau_{g0} = \left\{ \sum_{j=1}^{k} \left[\tau_{n0}\exp\left(\frac{E_i - E_{t,j}}{k_BT}\right) + \tau_{p0}\exp\left(\frac{E_{t,j} - E_i}{k_BT}\right) \right]^{-1} \right\}^{-1} \tag{2}$$

$$\tau_{g} = \left\{ \sum_{j=1}^{k} \left[\tau_{n}\exp\left(\frac{E_i - E_{t,j}}{k_BT}\right) + \tau_{p}\exp\left(\frac{E_{t,j} - E_i}{k_BT}\right) \right]^{-1} \right\}^{-1} \tag{3}$$

where $E_{t,j}$ is the energy level of defect j, k_B is the Boltzmann's constant and T is the temperature in K.

In previous studies, electric field enhancement (EFE) of the thermal emission of electrons and holes was evidenced to influence the dark current in some photodiodes [2]. However, Virmontois et al. [2] have reported that no EFE effect was observed in 0.18 μm CISs under proton and neutron irradiation, and they concluded that EFE does not seem to contribute significantly to the dark current in these devices. Consequently, the EFE is not taken into account in this study.

It is noteworthy that the irradiation flux was cautiously chosen in the experiments of interest to make sure only one interaction occurred at a time in a single pixel. In this low-dose regime, the overlap between different particle tracks is suppressed. The increased dark current is therefore called single particle displacement damage (SPDD) current, which can be calculated based on the difference of τ_g^{-1} and τ_{g0}^{-1} with the expression [20]:

$$I_{SPDD}(t) = \Delta I_{dark}(t) = I_{dark}(t) - I_{dark}(0) = qn_iAx_d\left[\frac{1}{\tau_g(t)} - \frac{1}{\tau_{g0}}\right] \tag{4}$$

where t stands for the time after the SPDD occurrence, I_{dark} and I_{dark0} refer to the dark current of the photodiode for post- and pre-irradiation, respectively. q is the basic charge, n_i is the intrinsic carrier concentration. Although the minority carrier lifetime is inversely proportional to the density of defects ($N_t = N/Ax_d$), the term Ax_d in Eq. (4) is canceled with Ax_d in Eq. (1), which means that the SPDD current is associated to N rather than N_t. SPDD current was calculated with different values of N_{j0}, and it turned out that the SPDD current is weakly dependent on this parameter. It was therefore assumed that N_{j0} ($j = 1, 2,\ldots, k$) has an identical value of 10^{10} cm^{-3} for simplicity.

The defect energy levels and cross sections for carrier capture are taken from Ref. [9], in which the parameters were selected based on previous experimental and theoretical results. Since different cross sections were reported for the same kind of defects [22–24], three representative cross sections were chosen depending on the electrostatic interaction, as was done in Ref. [9]. The cross section was set to be 3×10^{-14} cm^2 for attraction, 3×10^{-15} cm^2 when the defect is neutral, and 3×10^{-16} cm^2 for repulsion [9].

3. Modeling the defect production and evolution

From Eq. (1) to Eq. (4) one can see that it is essential to investigate the long-term evolution of defects to better understand the annealing kinetics of electrical properties given in irradiation experiments. This issue will be addressed below. The production and evolution of defects were simulated by three different codes. First, a BCA code was used to estimate the energies of Si recoils (also called primary knock-on atoms, PKAs) produced under neutron irradiation. Then an MD code was employed to determine the three dimensional distributions of primary defects induced by PKAs and finally, the KMC simulations were carried out to study the migration and interactions of various defects.

3.1. Aspects associated with primary knock-on atoms

In this study, we simulated the SPDD events induced by neutron mono-energetic beams in the photodiodes in 0.18 μm commercially available CIS processes from two different Asian manufacturers [4]. Since the displacement damage produced in Si devices starts with an incident neutron dislodging a Si atom, it is of importance to determine the energy of Si recoils (E_{PKA}) induced by neutrons. The BCA code—GEANT4 [25] (version GEANT4.9.6 was used in this study)—was used to simulate the production of PKAs induced by mono-energetic neutrons of 6 MeV, 15.52 MeV, 16.26 MeV, 18.04 MeV, and 20.07 MeV. The surface areas of the photodiodes are 74 μm^2 (Sensor 1) and 5 μm^2 (Sensor 2), with the pixel array 128 × 128 and 256 × 256, respectively. Neutron interactions were generated by direct sampling from ENDF/B-VII.1 cross section libraries [26]. Both elastic and inelastic processes were considered in the GEANT4 simulations using the G4NeutronHP (high precision) models. The elastic scattering cross section (σ_{el}) of silicon changes from 0.76 b to 1.08 b with respect to neutrons with energies stated above. Accordingly the elastic scattering mean free path (MFP_{el}) varies from 0.09 m to 0.13 m. Considering that the MFP_{el} is significantly larger than the size of the photodiodes, enlarged surface areas 100 μm^2 for Sensor 1 and 38 μm^2 for Sensor 2 and a relatively greater value for the depth 300 μm were used. This treatment could improve the simulation efficiency with minimum influence on the results of PKA energy distributions. The fluences (Φ) of neutrons were calculated by dividing the total number of incident neutrons by the surface area of the photodiodes, namely 6.1×10^9 cm^{-2} and 7.5×10^9 cm^{-2} for Sensor 1 and Sensor 2, respectively. They are on the same order-of-magnitude as those in the experiments. The GEANT4 simulation details are listed in Table 1.

Table 1
Parameters used in GEANT4 simulations.

Device type	Box size (μm^3)	E_n (MeV)	σ_{el} (barn)	MFP_{el} (m)	Φ (cm^{-2})
1	1280 × 1280 × 300	15.52	0.76	0.13	6.1×10^9
		16.26	0.79	0.13	
		18.04	0.89	0.11	
		20.07	0.91	0.11	
2	1152 × 1152 × 300	6	1.08	0.09	7.5×10^9