Preprint for the publication in IEEE transactions on device and materials reliability.. 18, 3, p. 481-483 3 p.

Molecular dynamics simulations of heavy ion induced defects in SiC Schottky diodes

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***Abstract* – Heavy ion irradiation increases the leakage current in reverse-biased SiC Schottky diodes. This work demonstrates, via molecular dynamics simulations, that a combination of bias and ion-deposited energy is required to produce the degradation.**

***Index Terms* – Ion radiation effects, Modeling, Power semiconductor devices, Schottky diodes, Silicon carbide**

I. Introduction

SILICON CARBIDE (SiC) power devices are of great interest for their possible use in power applications in spaceborne electronics. However, SiC power devices (MOSFETs and diodes) are sensitive to heavy-ion particle radiation such as that found in space. Javanainen *et al.* [1] previously discussed the leakage current in SiC Schottky diodes resulting from heavy-ion exposure. This paper examines the physical processes that result in that leakage current.

SiC Schottky diodes may exhibit Single Event Burnout (SEB) similar to that observed in silicon-based power devices; at bias voltages below the SEB threshold, however, SiC Schottky diodes also exhibit ion-induced increases of reverse leakage current, as illustrated in Figure 1. The leakage current may begin to increase during irradiation at operating biases significantly lower than the rated breakdown voltage [1]–[8]. For the 650 V devices in this work, semi-permanent increases in ion-induced leakage occur at a bias as low as 150 V. Device simulations have been used to attribute this to a highly localized temperature rise that goes above the phase transition temperature of SiC [4], [5]. Even though the temperature recovers after the ion strike, physical modifications of the crystal occur, as evidenced by the changes in the current-voltage characteristics. Simulated temperature effects due to ion and bias also have been reported by Abbate *et al.* [7], [8] and by Witulski *et al*. [6].

In order to study the permanent defects generated by the heavy-ion and bias-induced Joule heating, we use molecular dynamics (MD) to simulate the effect of ion impact on the SiC crystal structure. The ion energy deposition in these simulations

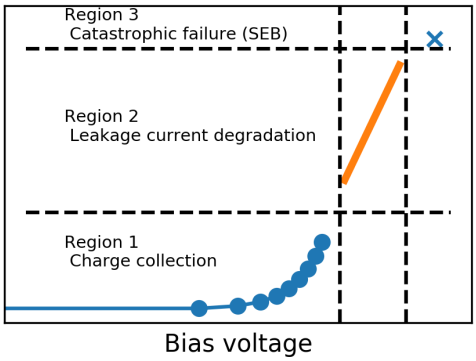

Figure 1. Three response regions observed in SiC diodes exposed to heavy-ion irradiation. After Kuboyama *et al.* [2].

is defined by the average Linear Energy Transfer (LET) (also known as electronic stopping force, S_e) value for 1217-MeV Xe ions, that is 62.4 MeV/(mg/cm^2). This corresponds to experimental values used earlier [1], [4], [5].

Because MD simulations cannot include the electric field or current transport, technology computer-aided design (TCAD) simulations are used to obtain the temporal and spatial temperature and carrier distributions in biased devices. These data are used as input for MD simulations that describe the response of the SiC lattice structure to the energy dissipation due to the Joule heating.

II. Experimental and TCAD Results

The experimental results used to inform the simulations presented in this paper have been published previously [1], [4], [5].

The SiC Schottky diodes exhibit strong dependence on the ion species (or LET) and reverse bias applied during the irradiation. The current work concentrates only on Xe-ions.

TCAD simulations have indicated that the synergetic effects between the heavy-ion induced ionization and the applied bias lead to SiC lattice temperatures that exceed the phase transition point of the material. This is illustrated in Figure 2, where the

This work was supported by the European Space Agency (ESA/ESTEC Contract 4000111630/14/NL/PA), and the Academy of Finland under the Finnish Centre of Excellence Programme 2012-2017 (Project No 2513553, Nuclear and Accelerator Based Physics). It was also funded in part, by an Early State Innovations grant (NNX17AD09G) from NASA's Space Technology Research Grants Program, and the MATRENA doctoral programme and the Academy of Finland (Grant No 1269 696).

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TCAD-simulated time evolution of the lattice temperature is presented for four different bias conditions.

However, TCAD simulations are not capable of giving information on material changes that may occur at these high temperatures. Hence, for ion-induced damage formation we used molecular dynamics simulations that are discussed below.

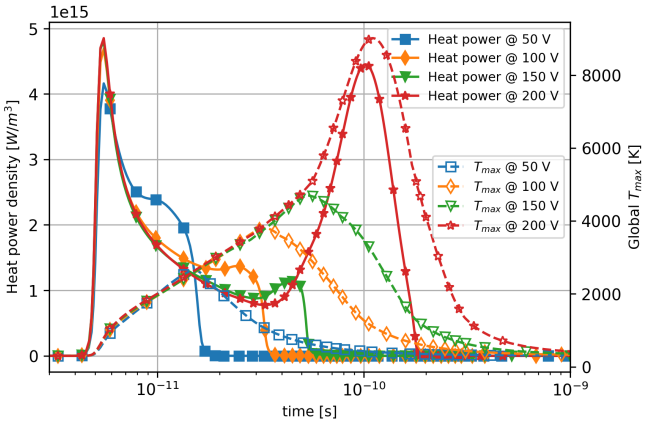


Figure 2. TCAD simulated temporal evolution of the heat power densities (solid) and the maximum lattice temperature (dashed) in SiC Schottky diode structure after Xe ion strike. The average LET value of 62.4 MeV/(mg/cm^2) is used for estimating the energy deposition by the ion. Different curves represent different reverse bias voltages applied on the Schottky diode.

III. MD Simulations

The molecular dynamics (MD) code PARCAS [9] is used to simulate the effects of heavy-ion impacts on different model damage states in 4H-SiC at room temperature. The Erhart-Albe SiC potential [10] is used to describe the Si-C interactions. This potential predicts a melting point between 3500-4000 K [11], compared to the experimental value of 3000 K [12]. In order to simulate the effect of energetic heavy ions in classical MD simulations (where electrons are not present explicitly), the heat added to the lattice due to the electronic excitations is estimated utilizing the inelastic thermal spike model [13]. In this model, two heat equations for electronic and atomic lattice subsystems, coupled through the electron–phonon coupling constant, are solved concurrently.

The energy deposited initially by the heavy-ion into the electronic subsystem is estimated from the electronic stopping power function of the ion in SiC as given by SRIM [14]. Solving these equations, one can estimate the evolution of the temperature in the lattice as a function of time and radial distance from the ion trajectory.

In order to see the effect of bias and find the correlation with the experimental results, we simulate the impact of a 1217-MeV Xe ion with an LET of 62.4 MeV/(mg/cm^2) in the SiC lattice with and without applied bias. In the heavy-ion experiments the unbiased case means that all the device pins are grounded.

$$C_e \frac{\partial T_e}{\partial t} = \nabla[K_e(\mathrm{T_e}) \cdot \nabla \mathrm{T_e}\,] - g(T_e - T_l) + A(r,t) \qquad (1)$$

$$C_l \frac{\partial T_l}{\partial t} = \nabla[K_l(\mathrm{T_l}) \cdot \nabla \mathrm{T}_l\,] + g(T_e - T_l) \qquad (2)$$

For the case without bias, we calculate the evolution of the electronic and lattice subsystems according to the thermal spike model (see eqns. 1 and 2), and use the same electronic parameters as in previous work [15]. The parameters employed are: electronic specific heat capacity $C_e = 1\,Jcm^{-3}K^{-1}$ [16], electronic heat conductivity $K_e = C_e D_e$ with diffusivity $D_e = 2\,cm^2s^{-1}$ [16], and electron-phonon coupling constant $g = K_e/\lambda$ [16]. In the latter, we estimate the electron-phonon mean free path to be $\lambda = 5.6\,nm$ as in [15]. Furthermore, we obtain the lattice parameters used in the calculation from [17], [18]. We give the initial energy deposition to the electron subsystem $A(r,t)$ according to the distribution from Waligorski et al. [19]; this distribution was obtained as a fit to Monte Carlo simulations of ion-induced electronic cascades. We calculate analytically the temperature evolution in the electron and lattice coupled subsystems until 100 fs, when the electrons have transmitted most of their energy to the lattice. We extract the lattice temperature profile at this moment and deposit the corresponding kinetic energy to the atoms in the MD cell. The MD simulations are used to obtain the structure of the track created by the passing ion after the first 100 ps when the energy has already dissipated into the bulk and the atoms in the core of the track have cooled down. The dimensions of the simulation cell used were 30x30x5 nm^3.

For the case when bias is applied, we use the results from previous TCAD work [5], where the evolution of the heat power density with time was calculated for the same ion as above with 200V applied. The evolution of the system is simulated with MD, while adding the time-dependent heat power distributions from the TCAD calculations. The dimensions of the simulation cell used were 92x105x5 nm^3.

The TCAD simulations show large spatial spread (around 40 nm) of the Joule heating, however due to limited computational resources we use a spatial Gaussian distribution of 23 nm FWHM. Therefore, these results correspond to a lower bound estimate of the damage produced by the irradiation with bias. The displacements of the atoms and the appearance of structural deformations due to the Joule heating are obtained from MD.

The results are indicative, as the phase transition point of the MD potential used here might not reproduce correctly the phase transition point of the SiC, underestimating the appearance of defects in the material.

IV. Results and Discussion

Figure 3 shows the radial distributions of the maximum temperature after Xe-ion strikes at different biases, obtained from the MD simulations. Without an applied bias, the lattice temperature rises slightly, but remains below the SiC melting temperature (3500-4000K)[11]. Also at 50V bias, the lattice temperatures obtained from both TCAD and MD simulations are relatively low. However, when higher bias is applied, the simulated lattice temperatures reach much higher values. Combining this with the fact that the thermal runaway temperature within SiC diode structures has been shown [20] to decrease with increasing reverse bias voltage, the simulation results support the idea that ion strikes at higher bias voltages are more

capable of generating lattice damage. Figure 4 illustrates the lattice structure after an ion strike with 0 and 200 V bias.

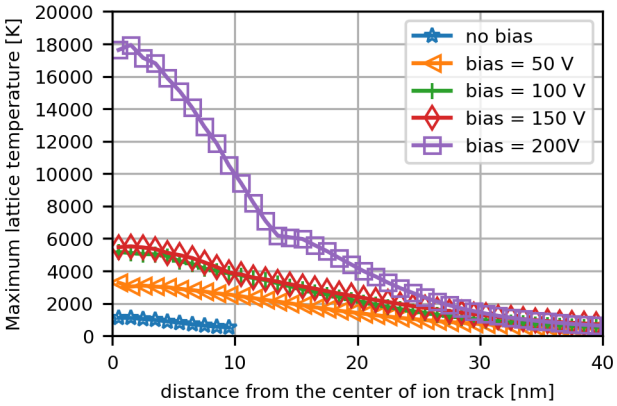
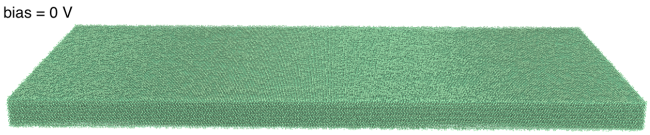


Figure 3. Radial distribution of the maximum temperature within the 4H-SiC lattice after the ion strike at different bias configurations.

At biases of 50 V and below the simulations do not show any permanent damage in the lattice. Figure 5 presents the radius of the ion-induced damage site within the SiC lattice as a function of applied bias as obtained from the MD simulations. In the experimental results reported earlier [4], the onset for permanent damage induced by Xe-ions was at about 130V. The difference in the damage onset between simulations (50 V) and experiments (130 V) can be explained by the limited size of the volume considered in the simulations. In real devices, the Joule heat can dissipate in much larger volume compared to the simulated structure. Also, the top metal layers, that can affect the heat transport, are not taken into account in the simulations.

All in all, the results agree with previous experimental results that have not shown any heavy-ion induced permanent damage in SiC at sufficiently low biases [4], or without any external electric fields [21]. The results with the higher applied bias suggest, however, that heavy-ion exposure can result in amorphous regions in the material about 10 nm in size. In the simulations, the energy deposited by Joule heating is very high, and sufficient to cause a phase transition in the material despite the high thermal conductivity of SiC. Even though the recrystallization rate of SiC is high, based on previous experience [15], it is unlikely that the material is able to recrystallize back completely to eliminate such a large defect, leaving permanent structural modifications in the material.



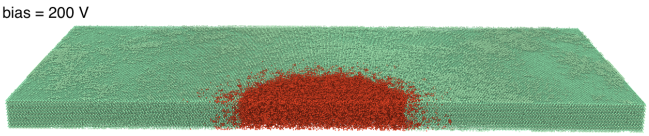


Figure 4. Simulation cell used in the MD simulations showing no damage (top) for 0V bias and damage (bottom) for 200V bias. The size is 92x105x5 nm^3. Material is 4H-SiC. The atoms are colored blue or red depending on if their local surrounding is crystalline or amorphous respectively.

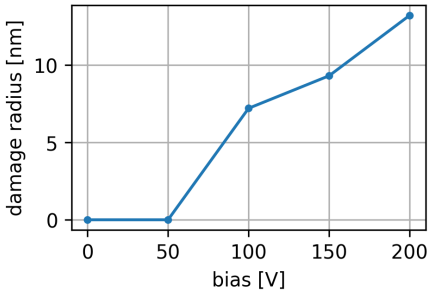


Figure 5. The MD simulated radius of ion-induced damage site in SiC as a function of applied bias voltage.

These simulations suggest that the Joule heating induced by the interplay of the ionization by the impinging ion, and the applied bias, is capable of producing permanent defects in SiC lattice. However, an ion, impinging on the material with sufficiently low or zero electric field, is not. The nanoscale defects observed in this work could potentially explain the source of the leakage current observed in the experiments under heavy-ion irradiation with applied bias.

V. Conclusions

Molecular dynamics simulations are used to examine heavy-ion induced material modifications in biased SiC Schottky diodes. The high power dissipation along the ion track in the biased structure results in violent lattice vibrations that can lead to permanent lattice damage if the bias voltage is sufficient.

The MD simulations suggest that there is a threshold voltage for the lattice damage, supporting recent experimental findings.

VI. Acknowledgments

The authors would like to thank Jean-Marie Lauenstein at NASA GSFC and Robert Weller, Robert Reed, Art Witulski and Dennis Ball at Vanderbilt University for discussions of heavy-ion radiation effects in SiC Schottky diodes. Some of these results were presented at the 2017 RADECS Conference in Geneva, October 2017.

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