Multiscale Modeling of Radiation Effects in Semiconductor Devices

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Understanding micro-mechanisms of displacement and ionization damage is the key to conquer the degradation in optoelectronic properties of semiconductor devices under irradiation. In view of the difficulties in experimental irradiation and detection, the relevant theoretical modeling is critical but always challenging. Therefore, a sequential multiscale modelling framework is developed to simulate defect and carrier generation, evolution and interactions in semiconductors under irradiation (Figure 1). The model combines the density functional theory for defect property calculations [1], the Monte Carlo software (IM3D) for primary defect generation [2], the object kinetic Monte Carlo software (RAM-KMC) for charged defect evolution [3] and the improved continuity rate model (IRadMat-CMoS) based on the SRH theory for defect charging [4]. Two key issues in Si/SiC-based devices under irradiation are thus studied: 1) Total ionizing dose (TID) effect in Si-based MOS devices under γ-ray irradiation [5, 6]. It shows that, with increasing TID, the oxide charged defects increase to saturation and the electric field increases following the universal 2/3 power law. The radiation-hardening performance of devices can be improved by choosing a thin oxide layer with high permittivity and low hydrogen concentration as well as under high gate voltages (Figure 2). 2) Defect identification of neutron-irradiated Si and SiC [7, 8]. The annealed defect concentration is first taken into account for multidimensional simulations of deep-level transient spectroscopy (DLTS). Strict defect-identification is thus achieved by comparing the simulated DLTS with the experimental ones (Figure 3). It provides new theoretical methods and guidance for exploring failure mechanisms, identifying deep-level defects and radiation hardening of semiconductor devices under irradiation.

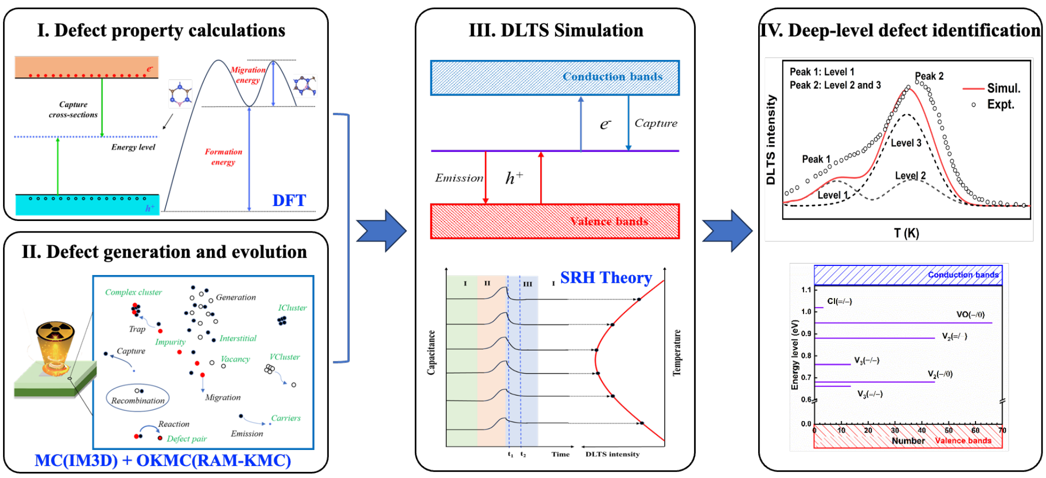

Figure 1. A sequential multiscale model for radiation effects in semiconductors.

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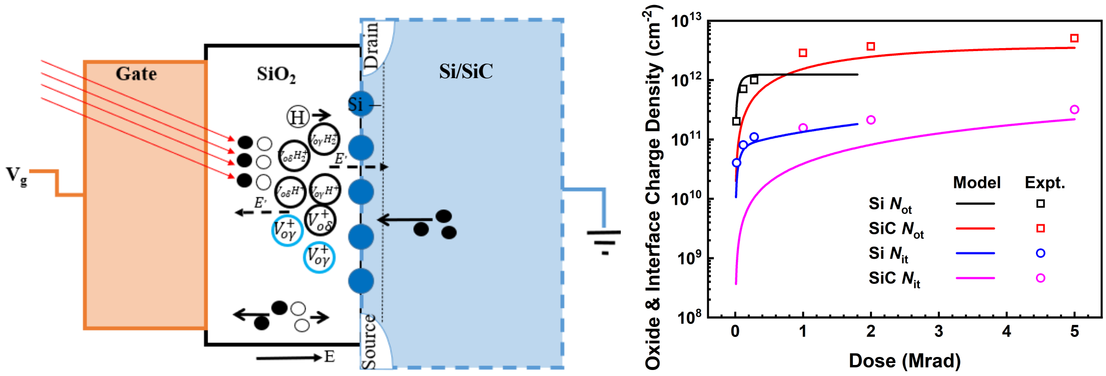

Figure 2. Dynamic mechanism and experimental verification of the TID effect in Si and SiC-based MOS devices under γ-ray irradiation.

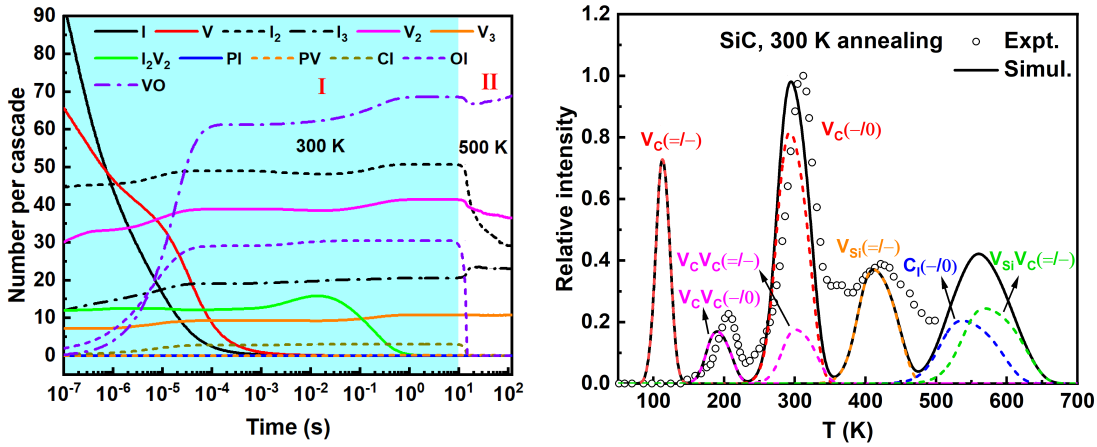

Figure 3. Multiscale modeling of defect/carrier co-evolution in Si under neutron irradiation and thermal annealing; and deep-level defect identification of 4H-SiC devices based on a multidimensional modeling of DLTS spectroscopy.

Keywords： multiscale modeling; radiation effects, displacement/ionization, radiation hardening, semiconductor devices

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BIOGRAPHY

Prof. Yonggang Li has completed his PhD from Physics Department, University of Science and Technology of China in 2009 and was a visiting scholar at the Massachusetts Institute of Technology from 2012 to 2014. He is now the deputy Director of the Department of Computational Physics and Quantum Materials, Institute of Solid State Physics, Chinese Academy of Sciences. He was awarded as an outstanding member of the Youth Innovation Promotion Association of Chinese Academy of Sciences. He is a committee member of the Computational Materials Science Branch, Chinese Materials Research Society, and a council member of the Computational Physics Branch, Chinese Nuclear Society. He has published more than 65 papers in reputed journals, and been authorized 3 Chinese patents, 9 software copyrights and 1 open-source copyright.