Model of Defect Evolution and Carrier Reactions in a Neutron Recoil Cascade and Comparison with Experiment

by S. M. Myers and W. R. Wampler

Motivation—Atomic displacements produced in Si by impinging MeV neutrons are not randomly dispersed, instead being localized in damage cascades caused by the primary Si recoils from the relatively infrequent neutron collisions. Such clustering can have substantial effects both on the time evolution of the defects and, as a result of local electrostatic fields, on the interactions of carriers with the defects. Quantitative modeling of transient neutron effects on transistor performance requires understanding of the nature and magnitude of these phenomena. For several decades prior to QASPR, there were debates and rough estimates but no detailed modeling.

Accomplishment—We previously developed the code Cluster to treat the transport and reactions of defects and carriers (39 species including multiple charge states) within a single, radially symmetric recoil cascade. In these calculations, the starting radial profiles of the primal vacancies and Si interstitials are obtained by correlation-function analysis of defect maps from binary-collision and molecular-dynamics simulations of the cascade-forming collisions. In 1st-generation modeling of transistors for QASPR, the device codes have assumed randomly dispersed defects and made only rudimentary use of the predictions of Cluster, e.g., reducing the starting concentrations of primal defects to account for rapid vacancy-interstitial recombination within the core of a cluster.

We progressed from this beginning in two stages. First, the fidelity of Cluster was assessed by comparing its predictions to experimental results. We restricted these comparisons to cases where the measured properties arise predominantly from a single local condition, allowing them to be predicted on the basis of one Cluster calculation. This requirement is not satisfied by the electrical properties of a bipolar transistor, whose behavior reflects the combined influences of multiple disparate regions. Instead, we employed published minority-carrier lifetimes in neutron- and electron-irradiated solar cells and bulk Si, along with defect densities and defect-charging kinetics observed by Robert Fleming in his Deep Level Transient Spectroscopy (DLTS) studies under QASPR. Generally good agreement was obtained without adjustment of model parameters. Figure 1 shows the time dependence of the annealing factor (AF), related to the minority-carrier lifetime τ by

$$\mathrm{AF} = \frac{\tau^{-1}(\mathrm{t}) - \tau^{-1}(\text{pre rad})}{\tau^{-1}(\text{long time}) - \tau^{-1}(\text{pre rad})} ,$$

for n- and p-type solar cells at various levels of carrier injection following pulsed neutron irradiation. The model calculations capture both the forms of the transients and their variations with doping and carrier injection.

In view of this success, we proceeded to develop the transistor model 1DC, which incorporates multiple (typically 40) instances of Cluster to treat the varying local concentrations of carriers, dopants, and impurities. Evaluation of the utility of 1DC for QASPR purposes is underway.

Significance—The code 1DC may provide the basis for more accurate, 2nd-generation modeling of transistors and other bipolar Si devices in the QASPR program.

Sponsors for various phases of this work include: Nuclear Weapons Program: Nuclear Survivability, Advanced Simulation & Computing, Enhanced Surety, and Enhanced Surveillance Campaigns

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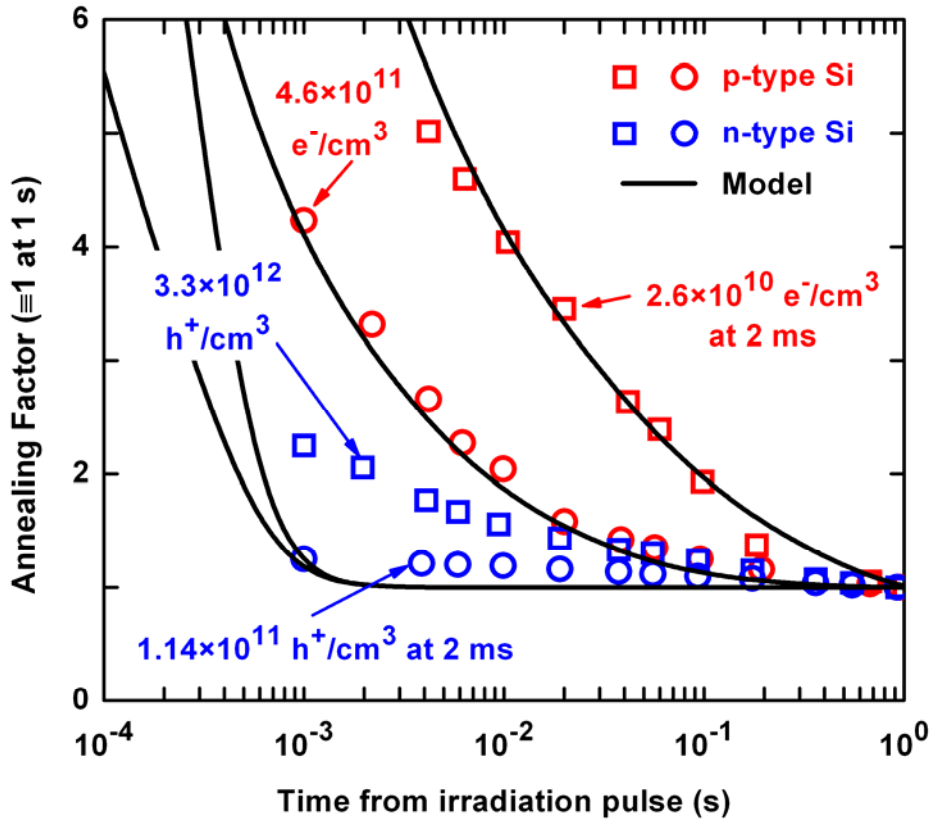

Figure 1. Time-dependent annealing factor for solar cells after pulsed-neutron irradiation in SPR, from the Cluster model [1] and from experiment [2]. The elevated minority-carrier concentrations resulting from constant injection are indicated for the specific time of 2 ms, since these concentrations vary with time as the damage responsible for recombination undergoes annealing.

[1] S. M. Myers, P. J. Cooper, and W. R. Wampler, J. Appl. Phys. **104**, 044507 (2008).

[2] B. L. Gregory and H. H. Sander, IEEE Trans. Nucl. Sci. **NS-14**, 116 (Dec. 1967).