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Understanding the Fundamental Driver of Semiconductor Radiation Tolerance with Experiment and Theory

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Abstract : Semiconductors, as the base of critical electronic systems, are exposed to damaging radiation while operating in space, nuclear reactors, and particle accelerator environments. What innate property allows some semiconductors to sustain little damage while others accumulate defects rapidly with dose is, at present, poorly understood. This limits the extent to which radiation tolerance can be implemented as a design criterion. To address this problem of determining the driver of semiconductor radiation tolerance, the first step is to generate a dataset of the relative radiation tolerance of a large range of semiconductors (exposed to the same radiation damage and characterized in the same way). To accomplish this, Rutherford backscatter channeling experiments are used to compare the displaced lattice atom buildup in InAs, InP, GaP, GaN, ZnO, MgO, and Si as a function of step-wise alpha particle dose. With this experimental information on radiation-induced incorporation of interstitial defects in hand, hybrid density functional theory electron densities (and their derived quantities) are calculated, and their gradient and Laplacian are evaluated to obtain key fundamental information about the interactions in each material. It is shown that simple, undifferentiated values (which are typically used to describe bond strength) are insufficient to predict radiation tolerance. Instead, the curvature of the electron density at bond critical points provides a measure of radiation tolerance consistent with the experimental results obtained. This curvature and associated forces surrounding bond critical points disfavors localization of displaced lattice atoms at these points, favoring their diffusion toward perfect lattice positions. With this criterion to predict radiation tolerance, simple density functional theory simulations can be conducted on potential new materials to gain insight into how they may operate in demanding high radiation environments.

Keywords : density functional theory, GaN, GaP, InAs, InP, MgO, radiation tolerance, rutherford backscatter channeling
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