A NEW MODEL OF PRIMARY RADIATION DAMAGE IN MATERIALS

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Accurate quantification of radiation-induced damage is critical for advancing nuclear, ion implantation and semiconductor technologies [1]. The current international standard, the Norgett-Robinson-Torrens displacements per atom (NRT-dpa) model, exhibits significant limitations in physical accuracy [2]. Specifically, in metals, the NRT-dpa model overestimates the number of surviving point defects by a factor of three due to athermal recombination during the picosecond thermal spike phase. Conversely, it underestimates the extent of atomic mixing (replacements) by a factor of up to thirty [3]. To resolve these profound discrepancies, in 2015 the expert group of Nuclear Energy Agency OECD proposed two physically realistic models that complement the existing NRT-dpa standard: the athermal recombination-corrected dpa (arc-dpa) and replacements per atom (rpa) [4, 5]. Although these two models provide accurate predictions of surviving stable defects and reliably quantify the true extent of atomic mixing, they are fundamentally limited in their ability to describe the essential qualitative features of radiation damage. In particular these models yield no insight into the dynamic, spatial distribution of defects, the morphology of surviving clusters, or the influence of crystal lattice symmetry on the radiation damage.

In this work, we introduce a novel approach that overcomes these limitations. Our methodology relies on Voronoi tessellation analysis for identification and classification of defects and atomic mixing, followed by adaptive kernel density estimation to precisely map their distribution. Contrary to the conventional view that the distribution of defects in irradiated solids is random and unpredictable, our results demonstrate that while primary radiation damage is a highly stochastic and complex process, the final distribution of defects follows a specific pattern uniquely defined by crystal symmetry. This behavior persists until the accumulated radiation damage is large enough to break the underlying symmetry, ultimately leading to the radiation-induced amorphization of the material. Our findings provide new insights into the mechanisms of radiation damage in materials, which can be leveraged in the search for advanced radiation-resistant materials.

Keywords: *radiation damage, lattice and molecular dynamics of materials under extreme conditions*

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