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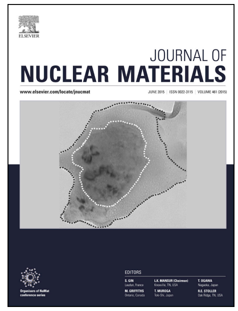

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Differential dpa calculations with SPECTRA-PKA

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Abstract

The processing code SPECTRA-PKA produces energy spectra of primary atomic recoil events (or primary knock-on atoms, PKAs) for any material composition exposed to an irradiation spectrum. Such evaluations are vital inputs for simulations aimed at understanding the evolution of damage in irradiated material, which is generated in cascade displacement events initiated by PKAs. These PKA spectra present the full complexity of the input (to SPECTRA-PKA) nuclear data-library evaluations of recoil events. However, the commonly used displacements per atom (dpa) measure, which is an integral measure over all possible recoil events of the displacement damage dose, is still widely used and has many useful applications – as both a comparative and correlative quantity. This paper describes the methodology employed that allows the SPECTRA-PKA code to evaluate dpa rates using the energy-dependent recoil (PKA) cross section data used for the PKA distributions. This avoids the need for integral displacement kerma cross sections and also provides new insight into the relative importance of different reaction channels (and associated different daughter residual and emitted particles) to the total integrated dpa damage dose. Results are presented for Fe, Ni, W, and SS316. Fusion dpa rates are compared to those in fission, highlighting the increased contribution to damage creation in the former from high-energy threshold reactions.

Keywords: displacements per atom (dpa), nuclear data processing, neutron irradiation, nuclear reaction channels

1. Introduction

The displacement per atom (dpa) measure of damage dose due to particle bombardment (irradiation) of materials is commonly (ubiquitously) used to estimate the atomic-level structural damage in irradiated materials. The so-called Norgett-Robinson-Torrens dpa or NRT-dpa [1] has been the standard evaluation method for several decades. While such an integral measure has obvious limitations [2, 3], and should be viewed as a "atomic damage dose" rather than a quantitative measure of damage creation [4], it has nonetheless shown to correlate with certain damage phenomena (see, for example, [5]). Furthermore, it provides a useful standard comparison between different irradiation experiments reported in the literature (provided the dpa model remains unchanged), and so there is continued interest in stable calculation of NRT-dpa values. For neutron irradiation, dpa rates are often obtained by folding the energy-dependent irradiation spectrum, usually measured/evaluated in units of neutrons cm^{-2} s^{-1}, with (neutron) energy-dependent displacement kerma (kinetic energy released per unit mass) cross sections σ_d (expressed in eV barns units in this context, where 1 barn is 10^{-24} cm^2). A modified Kinchin-Pease [6] formula, which has subsequently become known as the NRT model, is then applied to the scalar product result to obtain a dpa contribution from a particular target nuclide. A sum over all target nuclides in a material or element (weighted according to their fractional concentrations) produces the total NRT-dpa per second [4] for that composition.

However, the σ_d cross section vectors, which are es-

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