Elemental Nuclear Data Application libraries for Materials Sciences

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Nuclear interactions can be the source of atomic displacement and post-short-term cascade annealing defects in irradiated structural materials. Such quantities are derived from, or can be correlated to, nuclear kinematic simulations of the energy spectra of primary atomic recoil distributions, and the quantification of the numbers of secondary defects produced per primary as a function of the available recoils, residuals and emitted particles. Recoil kinematics of neutral, residual, charged and multi-particle emissions are now more rigorously treated based on modern, complete and enhanced nuclear data parsed in state-of-the-art processing tools. Novel data forms for 83 naturally occurring element (assembled from their isotopic parts) that include total and partial neutron defect production, gas production cross section and kerma factors, have been systematically and uniquely derived from ENDF/B-VIII.0, JENDL-4.0, JEFF-3.3 and TENDL-2017 files using the most recent of NJOY2016's HEATR and GAPSR module protocols. Another module of NJOY2016, GROUPR, has also been used to process residual nucleus (A>4) and emitted particle (A<4) fine group recoil matrices, based on energy-angle distribution library files covering all 287 stable targets. The novel forms are being inputted to inventory and transport codes, to seamlessly simulate total dpa, gas production, prompt and decay kerma rates, but also now channel-based energy distribution spectra and dpa. Those well-established nuclear response functions and derived quantities form a better basis from which the multi-scale simulations (nuclear-atomic-molecular-material) can expand. With the computational power now available one may even contemplate the deployment of uncertainty propagation, if and when available within the nuclear data sources.