Raw PKA data files

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July 24, 2015

This document explains the content and format of the raw primary knock-on atom (PKA) data associated with the curves and tables presented in the nuclear physics handbook [1] and its supplement [2].

The data files – one for each element considered in the main report – contained in the downloadable (@ `http://www.ccfe.ac.uk/easyii_handbooks.aspx`) tar-ball are the direct output from the `SPECTRA-PKA` code, which collapses the recoil cross section matrices from NJOY [3] with a neutron irradiation spectra (in this case a typical first wall fusion DEMO spectrum) – both of which are in a high resolution (660 energy bins below 30 MeV) energy-group structure. It also performs the important merging of PKA spectra from different target nuclides, which is almost always necessary for real materials including most elements that usually have more than one isotope in their naturally occurring composition. Furthermore, it produces total PKA spectra and spectra summed as a function of recoiling nuclide and element, which are likely to be most useful for atomistic modelling of radiation damage formation and evolution. The nuclide and elemental sums, in particular, are the distributions plotted in the main report, and the elemental sums are also given in tabular form in the supplement [2]. Note, however, that in those graphs and tables the PKAs s^{-1} per target from the raw files described below are converted to PKAs s^{-1} cm^{-3} using standard density values for each element.

In each data file, data-blocks are separated by pairs of blank lines and each block starts and ends with one or more comment lines – each beginning with a #.

The different data-blocks are as follows:

- The first block (denoted as "index 0") contains the input neutron spectrum in energy group format. Each line of the block corresponds to a given energy group and gives the lower and upper energy boundaries of the group (in MeV) and the total flux in that group.

- `SPECTRA-PKA` processes each input target nuclide in turn and in the data file there are a set of PKA distributions associated with each one. The section for a given target includes every reaction channel processed (some may appear twice if they produce both a heavy residual and a light particle such as a proton), and a few relevant summed distributions (e.g. total (n,α) recoils where the raw nuclear data is split into energy-level partials).

- For each reaction channel the PKA distribution is given in one block (where the target and recoil species is also given in the header comments) in four columns (low & high energy bounds, PKAs s^{-1} per target in energy group, and normalised-to-one PKAs in group). There then follows a second block that contains the results of an alternative normalisation procedure, where, instead of the simple division by the total in the previous block, the data is first converted to group-average PKAs (rather than total PKAs in group).

- Note that in the set for each target (say ^{54}Fe or ^{56}Fe in Fe), the PKAs rates assume 100% of that target. In other words, the relative fractions of different targets in the composition are not taken into account. These fractions are, however, considered when generating the global nuclide and elemental sum distributions given at the end of each file (see below).

- After all individual target results, the remainder of the file contains summed distributions (over all targets and all channels with appropriate target-fraction weights) for both individual nuclides (e.g. alphas, ^{55}Fe, ^{56}Fe, ^{55}Mn, ^{53}Cr, etc, recoiling in Fe), and for elements (e.g. He, Fe, Mn, Cr, etc, recoiling in Fe). After all of these, there is then a total distribution (with light gas particles emitted), which might perhaps be useful for a basic approximation (for example, in atomistic simulations where the interatomic potential only considers one species) to sample as a total PKA distribution.

  – the sum distributions are all given in five column format: low & high energy group bounds, total PKAs in group, normalised-to-one PKAs in group, and cumulative PKAs.

References

[1] M. R. Gilbert and J.-Ch. Sublet, "Handbook of activation, transmutation, and radiation damage properties of the elements simulated using FISPACT-II & TENDL-2014; Magnetic Fusion Plants," Tech. Rep. CCFE-R(15)26, CCFE, 2015. available to download from http://www.ccfe.ac.uk/easyii_handbooks.aspx.

[2] M. R. Gilbert and J.-Ch. Sublet, "PKA distributions of the elements simulated using TENDL-2014," Tech. Rep. CCFE-R(15)26-supplement, CCFE, 2015. available to download from http://www.ccfe.ac.uk/easyii_handbooks.aspx.

[3] R. E. MacFarlane, D. W. Muir, R. M. Boicourt, and A. C. Kahler, "The NJOY Nuclear data processing system – LA-UR-12-27079," Version 2012-032. http://t2.lanl.gov/nis/publications/NJOY2012.pdf.