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Iron NRT- and arc-displacement cross sections and their covariances

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ABSTRACT

Displacement damage cross sections have been calculated for natural iron and its constituent individual isotopes based on the latest versions of the evaluated neutron data libraries ENDF/B-VIII.0 and TENDL-2017 using the conventional *NRT* and recently introduced athermal recombination-corrected (*arc)* displacement concepts. Their covariance matrices, which quantify the uncertainties and the associated energy-energy correlations, were assessed for the first time based on TENDL-2017 random data files representing the covariances of the underlying nuclear data. In addition to the nuclear data, the covariances due to the ion energy partition, the primary defect survival efficiency and the lattice threshold energy were also propagated to the damage quantities. The *arc*-dpa was computed employing all available results from molecular dynamics and binary collision simulations. The comparison of the spectrum-averaged *arc*-dpa with the few available measurements at fission reactors has demonstrated a reasonable agreement within the experimental and calculation uncertainties. The comparison with the current *NRT*-dpa standard, provided by ASTM up to 20 MeV but without uncertainty, has indicated differences up to 8% above 0.5 keV and 60% below.

1. Introduction

The *NRT* concept of displacement damage cross section (dpa – displacements per atom), proposed by Norgett et al. [1], provides a basis for the quantification of neutron and ion induced radiation effects in materials. It is also can be used as a scaling factor for the comparison and extrapolation of radiation databases accumulated at existing nuclear facilities to projected ones. Recently a new damage concept based on “athermal recombination-corrected (*arc*) dpa”, has been proposed by the OECD Primary Radiation Group [2] and has been adopted for the calculation of damage cross section data by the IAEA Coordinate Research Project on Radiation Damage [3]. *Arc*-dpa quantify the total number of primary lattice defects (i.e., the vacancy-interstitial pairs denoted as Frenkel pairs) which survive after annealing of the hot recoil cascade during the first 10–100 ps after initiation of the nuclear reaction.

The present work provides evaluations of *NRT*- and *arc*-dpa cross sections for the naturally occurring isotopes of iron and elemental iron based on the latest evaluated neutron cross section data files up to 200 MeV. Initial comparative studies of the *NRT*- and *arc*-dpa cross sections and spectrally averaged values for fission, fusion and material testing facilities were carried out but involved only lower energies and used the neutron data available at that time [4–5]. Furthermore, estimates of the dpa covariance matrices (i.e. the uncertainties and associated energy-energy correlations) are provided for the first time as resulting from the involved nuclear data and material physics modelling. This work is an extension of our previous study on the iron main isotope ^{56}Fe [6], covering now the covariance determination for the displacement damage in natural iron.

2. Methods used to compute *NRT*- and *arc*-dpa and their covariances

2.1. Definitions and computing of the damage energy and displacement cross sections

The damage energy *DE* at neutron energy *E* which will be transferred to atoms displaced from their lattice sites in metal can be computed either in the frame of the conventional *NRT* or the new *arc* concepts according to the formulations given, e.g. in [1,2,7]. Since we used the NJOY code to compute *DE*, only a simplified formula is given here to show the variables which we derived or sampled but omitting others such as integration over scattering angle etc.:

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$$DE_{NRT} = \sum_{j,i} \int_{E_d}^{\infty} \frac{d\sigma_j(E,\ T_i)}{dT_i} \hat{T}_i \ dT_i \quad DE_{arc} = \sum_{j,i} \int_{E_d}^{\infty} \nu(T_i) \frac{d\sigma_j(E,\ T_i)}{dT_i} \hat{T}_i \ dT_i \quad where \quad \hat{T}_i = \begin{cases} 0, & 0 < P(T_i)T_i < E_d \\ \frac{2\,E_d}{0.8}, & E_d < P(T_i)T_i < 2E_d/0.8 \\ P(T_i)T_i, & \frac{2\,E_d}{0.8} < P(T_i)T_i < \infty \end{cases} \tag{1}$$

In Eq. (1), $d\sigma_j(E,T_i)/dT_i$ is the energy differential cross section for the production of primary knock-on atoms (PKA) or charged particles i with kinetic energy T_i for the neutron-induced reaction channel j; $P(T_i)$ - the ion energy partition function (i.e., the fraction of recoil energy that becomes available for damage) [1,7]; $\nu(T_i)$ – primary defects survival efficiency or fraction of Frenkel pairs (FP) left after athermal cascade annealing phase; E_d – lattice threshold energy or averaged minimum energy needed to create one FP.

The latest official version 99 of the nuclear data processing code NJOY-2012 [7], was used to compute the damage energy for each stable iron isotope $^{54,56.57,58}$Fe from the latest versions of the modern nuclear data evaluations ENDF/B-VIII.0 [8] and TENDL-2017 [9].

The NJOY code implements a model for the damage energy that is not consistent with the NRT damage energy definition in Eq. (1) in the interval E_d $E_d < \hat{T}_i < 2$ $E_d/0.8$. In the case of iron this results in an underestimation of the *NRT*- and *dpa*-cross sections by factor of 2.0/0.8 = 2.5 at neutron energy E ≈ E_d*A/4 = 0.65 keV, where A is atomic mass number. For a rigorous implementation of the *NRT* definition we modified the HEATR module of NJOY as documented in [10].

The corresponding *NRT*- and *arc*-dpa cross sections are then derived according to:

$$\sigma_{NRT-dpa}(E) = \frac{0.8}{2\ E_d} DE_{NRT}(E) \text{ or } \sigma_{arc-dpa}(E) = \frac{0.8}{2\ E_d} DE_{arc}(E) \tag{2}$$

The *DE*- and *dpa*-cross sections for natural iron were produced from isotopic cross sections by the MIXR module of NJOY taking into account the isotope abundances a_n: ^{54}Fe – 5.9%, ^{56}Fe – 91.72%, ^{57}Fe – 2.1%, ^{58}Fe – 0.28%.

In the present work the uncertainties and energy-energy correlations of *DE(E)* or *σ-dpa(E)* were computed independently from the different underling data or models, namely from: nuclear data, PKA energy partition function, FP survival efficiency and Ed. It means when one component was randomized, the others were used unperturbed.

2.2. Computation of the damage cross section covariances from TENDL-2017 evaluated neutron data files

The covariance matrix for *DE*- and *dpa*-cross sections were computed from five hundred TENDL-2017 random files which were generated by the Bayesian Monte Carlo method (i.e. by sampling and assigning the proper weights for the input parameters of the underlying nuclear reaction models) [9]. Each of these 500 random files were also processed by the NJOY code and additionally grouped into 228 energy bins to reduce the rank of covariance matrices but still retaining a rather detailed energy representation of cross sections. The energy group structure of VITAMIN-J 175 was chosen, which covers the energies from 10^{-5} eV to 19.64 MeV, plus 1 – 2 MeV wide bins up to 200 MeV.

The first order covariance matrix for values y_i (i.e., either $DE(E_i)$ or σ-$dpa(E_i)$) in every bin i was calculated from the N_{random} ensemble following the general definitions [11]:

$$cov(y_i, y_j) = \sum_{k=1}^{Nrandom} \frac{(y_i^k - \bar{y}_i)\left(y_j^k - \bar{y}_j\right)}{N_{random}}, \tag{3}$$

where indices i or j refer to the k random value of quantity y_i^k in the specific energy groups and $\bar{y}_i$ is an averaged value. The diagonal elements ($i = j$) of the covariance matrix provide the variance or square of the standard deviation σ_i:

$$\sigma_i^2 = cov(y_i,\ y_i) \tag{4}$$

The energy-energy correlation matrix was then calculated as:

$$cor(y_i,\ y_j) = \frac{cov(y_i,\ y_j)}{\sigma_i \sigma_j}, \quad cor(y_i,\ y_i) = 1 \tag{5}$$

The covariances matrices were firstly computed for each isotope ^{54,56,57,58}Fe from the corresponding isotopic TENDL-2017 random files. Then the covariance matrix for natural iron was obtained by summing up the variances of the individual isotopes taking into account the iron isotope abundances a_n and absence of the cross isotope correlations in the TENDL-2017 random evaluation:

$$cov_{nat}(E_i,\ E_j) = \sum_{n=1}^{4} a_n^2 * cov_n(E_i,\ E_j) \tag{6}$$

For illustration, the results of the calculation of the *NRT* damage energy and its uncertainties resulting from the nuclear data for natural iron and two isotopes ^{54,56}Fe are shown in Fig. 1. It is interesting to note that ^{56}Fe gives a dominant contribution to the *DE* cross section and the uncertainty at all energies except in the vicinity of 8 keV where the n - ^{54}Fe resonance prevails over ^{56}Fe. The energy-energy correlation matrix derived from TENDL-2017 neutron random files shows two energy

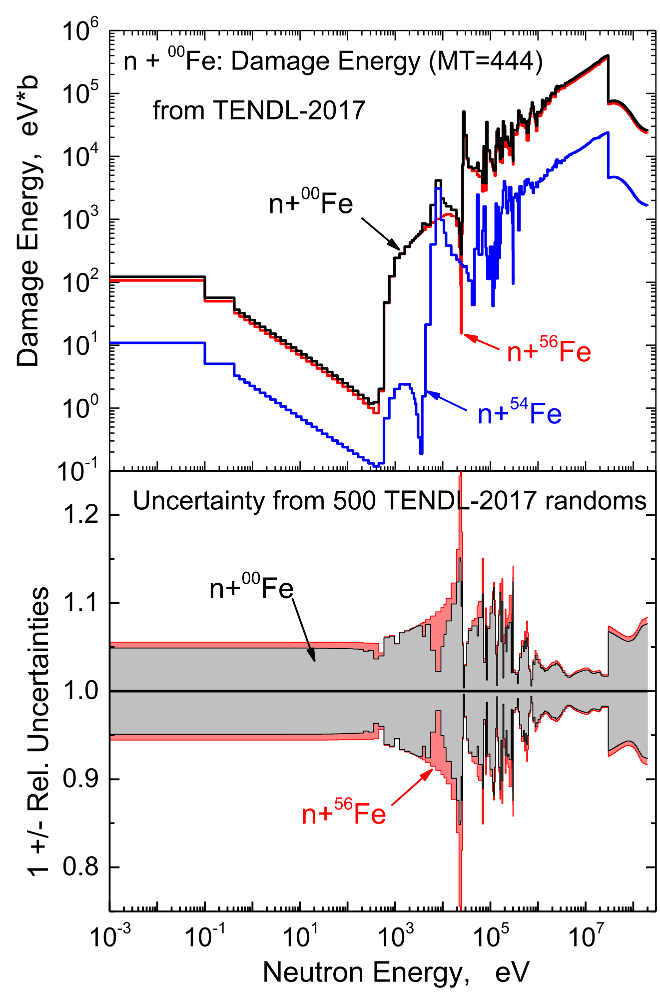

Fig. 1. The NRT damage energy (top) and uncertainty (bottom) derived from TENDL-2017 random files for natural iron. The contributions from ^{56}Fe and ^{54}Fe are depicted by colour curves.

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