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NEUTRON DISPLACEMENT CROSS-SECTIONS FOR MATERIALS FROM BE TO U CALCULATED USING THE ARC-DPA CONCEPT

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ABSTRACT

The recently proposed athermal recombination-corrected dpa model enables, as compared to the standard NRT model, an estimation of the actual damage production in irradiated materials taking into account lattice defects surviving the thermal annealing. On this basis, advanced displacement damage cross-sections were prepared for a number of materials ranging from Be to U. For Fe, Ni, Cu, Pd, Ag, W, Pt, and Au the parameters included in the arc-dpa formalism were taken from literature and for other materials were estimated using a semi-empirical systematic approach. The approach is based on the use of investigated correlations between minimum, averaged, and effective threshold displacement energy and a number of quantities such as melting temperature, material density, cohesive energy, and others. The modified version of the NJOY-2016 processing code was applied to generate improved displacement cross-sections with the current versions of the nuclear data libraries JEFF, ENDF/B, JENDL, and TENDL. Displacement cross-sections, based on the data of JEFF, ENDF/B, and JENDL, were extended up to 200 MeV neutron energy using the TENDL data. Special efforts were made to evaluate the uncertainty of obtained displacement cross-sections. The evaluation takes into account the spread of the total reaction cross-section and parameters of the arc-dpa model.

KEYWORDS
Displacement cross-section, displacement energy, neutron irradiation, nuclear data library

1. INTRODUCTION

The recently proposed alternative to the standard NRT model [1] the athermal recombination-corrected dpa (arc-dpa) model [2,3] makes possible a more accurate estimate of the actual damage production in irradiated materials.

According to the arc-dpa concept [2,3] the number of stable defects produced under irradiation is parameterized in the following form

$$N_d(T_{dam}) = \begin{bmatrix} 0 & when \quad T_{dam} < E_d \\ 1 & when \quad E_d < T_{dam} < 2E_d / 0.8 \\ \frac{0.8}{2E_d}\xi_{arcdpa}(T_{dam})\, T_{dam} & when \quad 2E_d / 0.8 < T_{dam} \end{bmatrix}, \tag{1}$$

where T_{dam} is the “damage energy” [1], or the energy available for atom displacements in elastic collisions calculated using the Robinson formula [4].

The value of E_d in Eq.(1) is the displacement energy averaged over all lattice directions [5], which is often named as "the effective displacement threshold energy" [6]. Below it is called "the averaged displacement threshold energy", to distinguish it from the effective threshold energy E_{deff} used in the analyses of radiation damage in reactors [7].

The defect generation efficiency, equal to the ratio of calculated number of defects to one predicted by the NRT model, is calculated as follows [2,3]

$$\xi_{arcdpa}(T_{dam}) = \frac{1 - c_{arcdpa}}{\left(2E_d / 0.8\right)^{b_{arcdpa}}} T_{dam}^{b_{arcdpa}} + c_{arcdpa}, \quad (2)$$

where b_{arcdpa} and c_{arcdpa} are parameters.

The goal of this work is the calculation of atomic displacement cross-section using the arc-dpa equations Eq.(1),(2) for materials from Be to U irradiated with neutrons at energies up to 200 MeV. The arc-dpa parameters obtained in Ref.[2,3,8] for a number of materials and parameters estimated using semi-empirical approach [9] were applied for calculations. Recoil energy distributions were extracted from nuclear data libraries JEFF-3.3T3 [10], ENDF/B-VIII.beta4 [11], JENDL-4.0 [12], and TENDL-2015 [13] after processing with the NJOY code [14].

The method of calculation and results obtained are discussed below.

2. ESTIMATION OF PARAMETERS OF ARC-DPA EQUATIONS

The estimation of b_{arcdpa} and c_{arcdpa} parameters is briefly described below. Details can be found in Ref.[9].

The parameter c_{arcdpa} represents the asymptotic value of defect generation efficiency $\xi(T_{dam})$ and the b_{arcdpa} parameter describes the rate of its decrease with the growth of T_{dam}. For most materials the asymptotic value of defect generation efficiency can be calculated as following

$$c_{arcdpa} = E_d / E_{deff}, \quad (3)$$

where E_{deff} is the effective threshold displacement energy, defined from a condition that the averaged value of defect generation efficiency in experiments for neutron irradiation of materials $\langle\xi\rangle$ is equal to unity [6].

An approximate evaluation of E_{deff} and E_d for solids can be made using their systematic dependence on values concerning the physical properties of materials [9]. The first systematic for E_{deff} was obtained in Ref.[7,15]: $E_{deff} = C_1 E_{dmin}$ and for the averaged displacement energy in Ref.[16]: $E_d = C_2 T_{melt}$, where E_{dmin} is the "displacement energy" [5,17] or minimum displacement threshold energy and T_{melt} is the melting temperature, C_i are parameters.

The systematic dependence of displacement energies was investigated in Ref.[9]. As a result, the evaluated values of E_d, E_{dmin}, and E_{deff} were obtained for materials from Li to U. To get new systematics of displacement threshold energies in Ref.[9], the correlations were examined between investigated values and different physical quantities, which values are known for many materials.

Table I shows examples of correlation coefficients calculated for E_d and different quantities: E_{dmin}, the atomic number (Z), the material density (ρ), the melting temperature (T_{melt}), and the cohesive energy (E_{coh}) and some of their combinations. The correlation with the atomic number is the weakest and with E_{dmin} , T_{melt}, and others is rather strong.

The cases of strong correlations were used to obtain different systematics of threshold displacement energies. The final values were calculated by a weighted summation of predictions of various systematics obtained [9]. Fig.1 shows example of estimated E_d values for materials from Li to U. The numerical data are given in Ref.[9].

Table I. Example of correlation coefficients $cov(E_d,x)/\sigma_{Ed}\sigma_x$ calculated for experimental E_d values [9] and various quantities. See details in the text

Quantity	Correlation coefficient
E_{dmin}	0.77
Z	0.38
ρ	0.54
T_{melt}	0.89
$T_{melt}^{3/2}$	0.90
E_{coh}	0.86
E_{coh}^{2}	0.90
$E_{coh}\ T_{melt}$	0.91

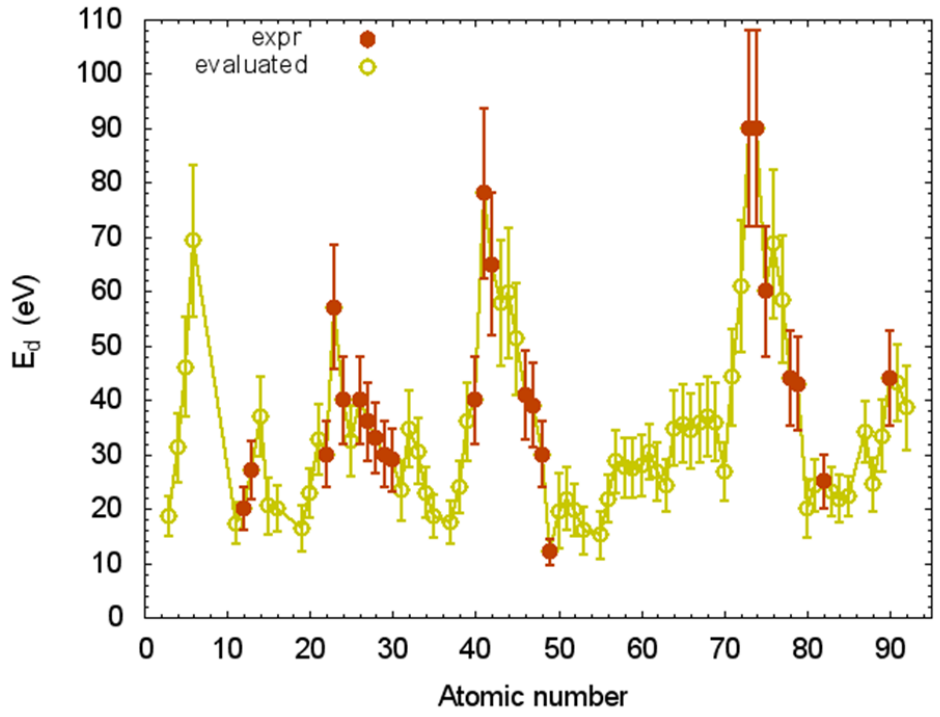

Figure 1. Estimated values of averaged displacement threshold energy E_d for different materials.

The c_{arcdpa} parameteres, calculated with Eq.(3) using evaluated E_d and E_{deff} values, are shown in Fig.2.

Alternative c_{arcdpa} values obtained for Fe, W [2,3], Ni, Cu, Pd, Ag, Pt, and Au [8] using the method of molecular dynamics are listed in Table II together with b_{arcdpa} parameters and E_d values used in the analysis [2,3,8].

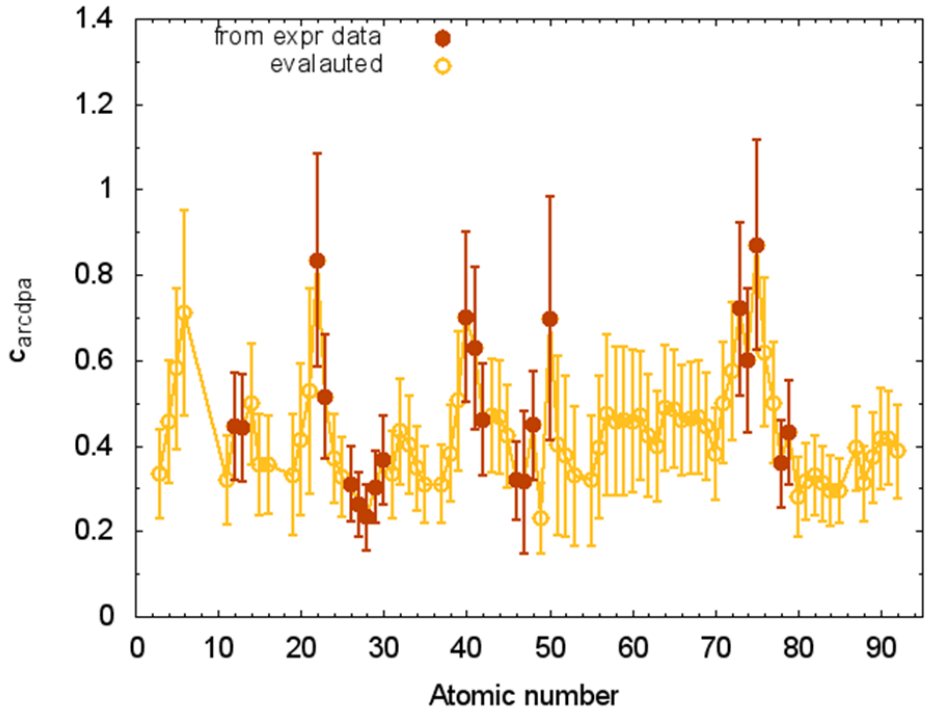

Figure 2. The c_{arcdpa} values evaluated for different materials.

Table II. Data obtained using the method of molecular dynamics in Refs.[2,3,8]

Material	E_d (eV)	b_{arcdpa}	c_{arcdpa}
Fe	40	-0.568	0.286
Ni	39	-1.006722	0.2268273
Cu	30	-0.54799	0.1177
Pd	41	-0.877387	0.1515293
Ag	39	-1.063006	0.257325
W	70	-0.564	0.119
Pt	42	-1.1216135	0.1115884
Au	43	-0.788966	0.1304146

As follows from the physical meaning of the b_{arcdpa} parameter, its exact value cannot be obtained using an approximate approach, similar to that discussed above. However, the analysis shows [9], that for most materials and types of neutron irradiation [9] the impact of the b_{arcdpa} parameter on the calculated averaged defect generation efficiency $<\xi>$ is relatively small. The illustration is given below. The averaged value of defect generation efficiency is calculated as follows

$$<\xi>=\int \sigma_d(E)\ \varphi(E)\,dE \Big/ \int \sigma_{d,NRT}(E)\ \varphi(E)\,dE\,, \qquad (4)$$

where σ_d is the displacement cross-section calculated according Eq.(1),(2), $\sigma_{d,NRT}$ is the cross-section obtained using the NRT model [1], $\varphi(E)$ is a neutron irradiation spectrum.

Fig.3 shows the typical dependence of $<\xi>$ on the b_{arcdpa} parameter.

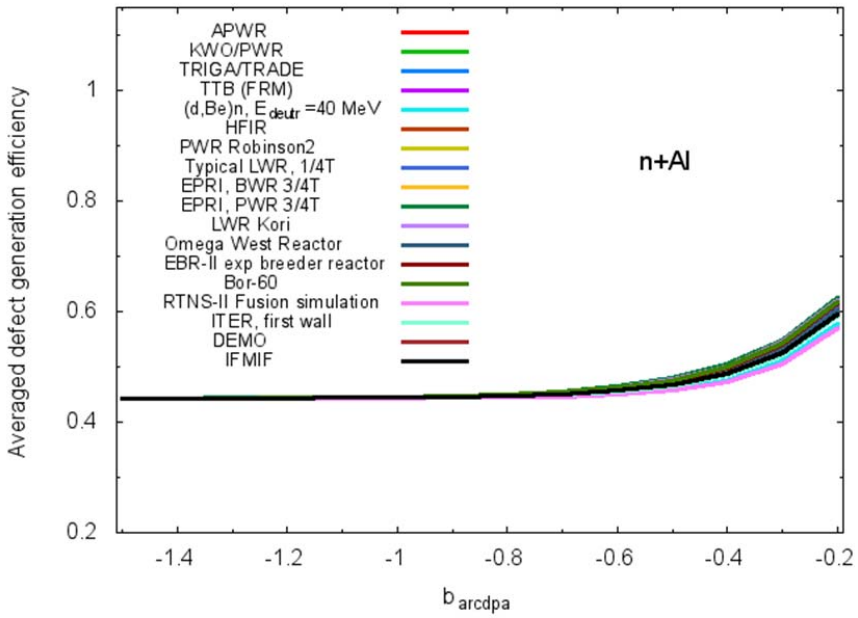

Figure 3. The $<\xi>$ values calculated for aluminum with different b_{arcdpa} values and for different irradiation conditions [9]. Nuclear data were taken from TENDL-2015

Based on the analysis of Ref.[9], the b_{arcdpa} value for most materials can be taken equal to the average of the values in Table II: $b_{arcdpa} = -0.8 \pm 0.3$.

For a number of materials, such as Co, Cd, In, Sm, Eu, Gd, Dy, and Hg [9], the use of this approximate value seems questionable.

Fig.4 illustrates the use of obtained b_{arcdpa} and c_{arcdpa} parameters for the calculation of the number of stable defects produced in beryllium. The result of molecular dynamics simulation, performed in Ref.[18] was not included in the analysis of arc-dpa parameters in Ref.[9].

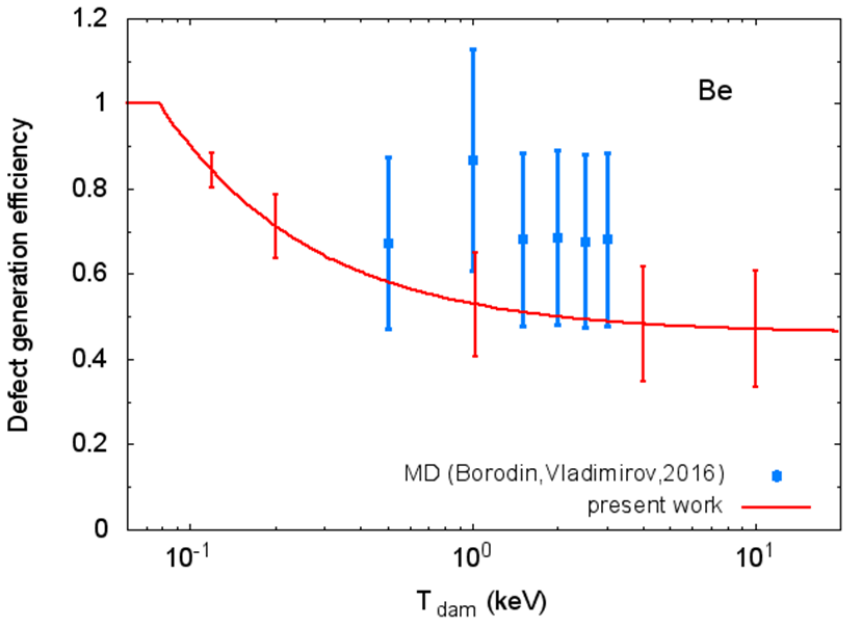

Figure 4. The defect generation efficiency estimated in the present work and calculated in Ref.[18] using the method of molecular dynamics (MD). The E_d value is equal to 31.2 eV.

3. CALCULATION OF DISPLACEMENT CROSS-SECTIONS

Obtained E_d, b_{arcdpa}, and c_{arcdpa} values and data from Table II were used for the calculation of atomic displacement cross-sections for solids from beryllium to uranium. The NJOY code [14] with implemented Eq.(1),(2) was applied for calculations.

Displacement cross-sections were obtained using the data from JEFF-3.3T3 [10], ENDF/B-VIII.beta4 [11], JENDL-4.0 [12], and TENDL-2015 [13].

Fig.5 and Fig.6 show typical examples of displacement cross-sections calculated using Eq.(1),(2) and the NRT model. Data plotted were obtained by averaging over a number of neutron energy groups.

The data obtained on the basis of JEFF-3.3T3, ENDF/B-VIII.beta4, and JENDL-4.0 were extended up to the incident neutron energy 200 MeV using the data prepared with TENDL-2015. Fig.7 shows typical examples. It is important to note that the data for the energy above 100 MeV were not yet verified using the high energy INC models, which are implemented, for example, in the MCNP code [19].

The displacement cross sections in ENDF-6 format were processed using the NJOY code and recorded in the ACE format. The data in both formats, obtained using ENDF/B-VIII.beta4, JENDL-4.0, and TENDL-2015 data are ready for download [20-22].

Special efforts were made to estimate an uncertainty of obtained cross-sections. Calculations of covariance matrices were performed using the Monte Carlo method described in Ref.[23]. It was assumed that the main source of uncertainty of displacement cross-section is the spread of the total reaction cross section and parameters of arc-dpa model.

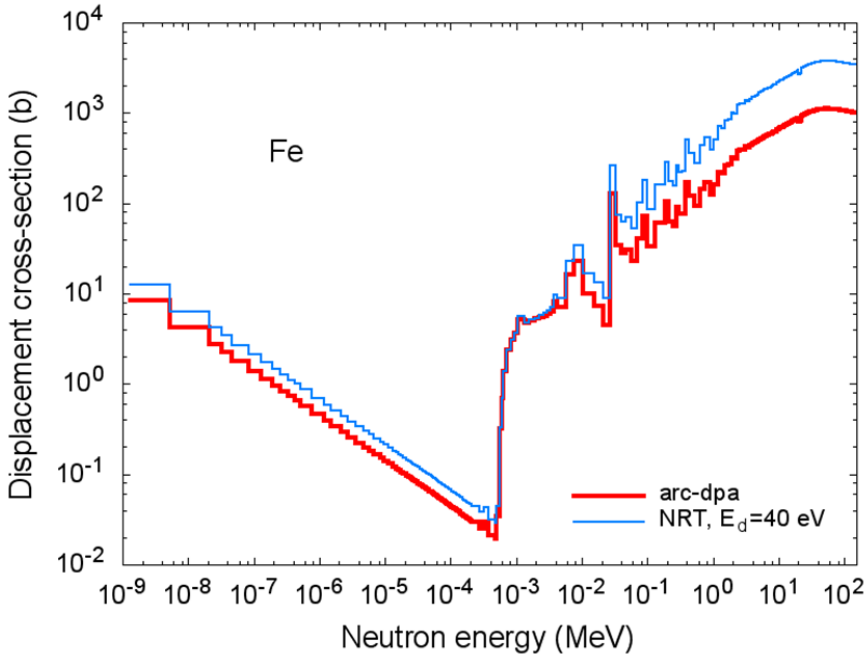

Figure 5. Displacement cross-section for iron calculated using data from ENDF/B-VIII.beta4 and using the arc-dpa model with parameters from Table II, and the NRT model.

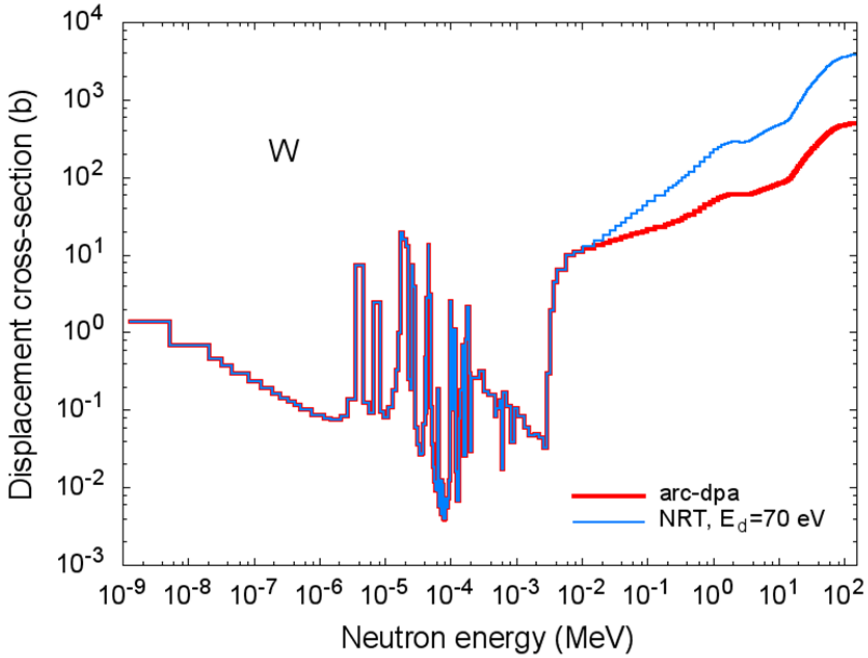

Figure 6. Displacement cross-section for tungsten calculated using data from ENDF/B-VIII.beta4 and using the arc-dpa model with parameters from Table II, and the NRT model.

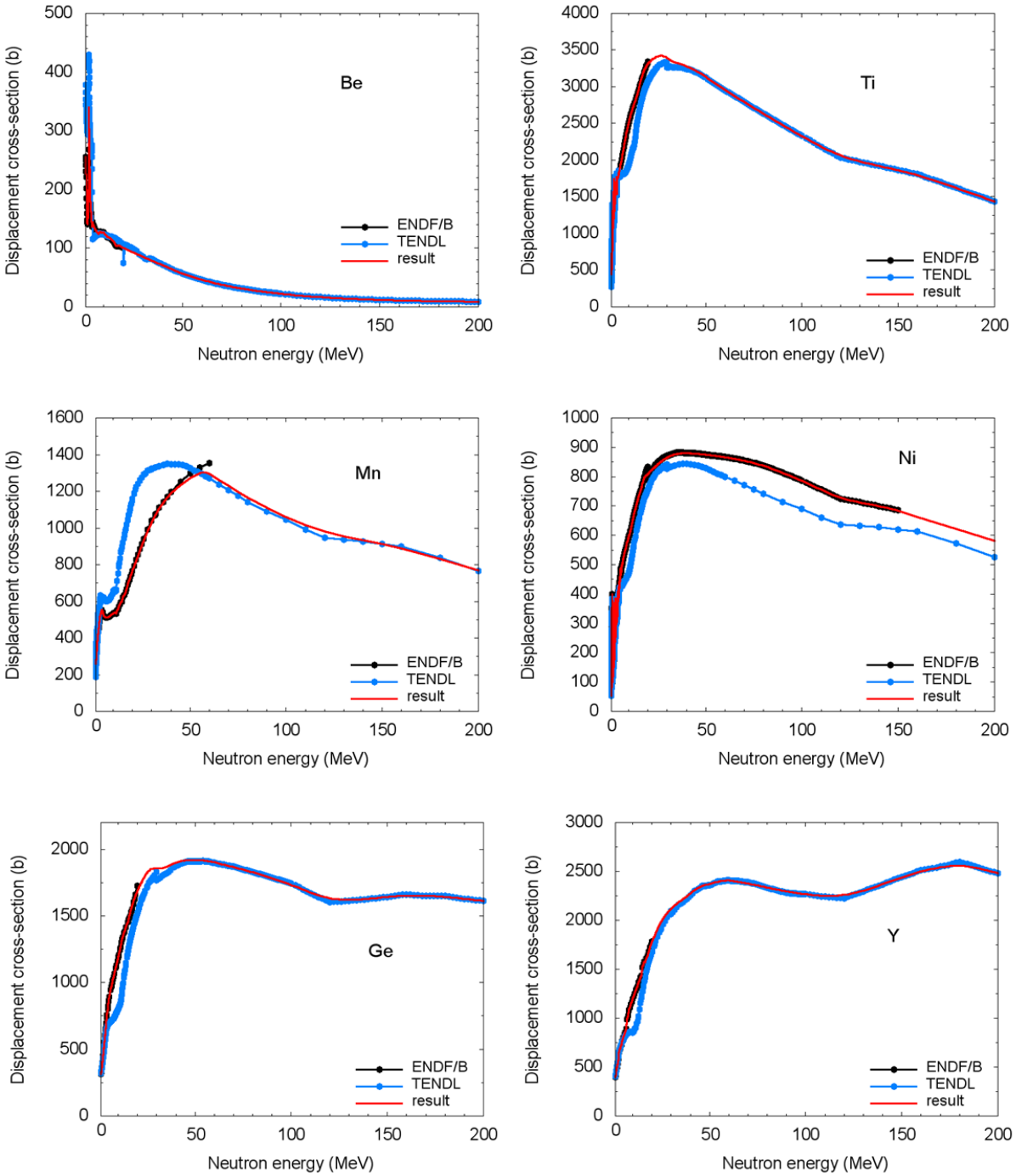

Figure 7. Examples of the use of data prepared with TENDL-2015 for the extension of displacement cross-sections obtained using data from ENDF/B-VIII.beta4 up to 200 MeV. The number of produced defects was calculated using Eq.(1),(2).

The total cross section was sampled using available covariance information [10-13]. The sampling of b_{arcdpa} and c_{arcdpa} parameters is discussed in Ref.[24]. As an illustration, Fig.8 shows relative standard deviation (RSD) for displacement cross-sections obtained for neutron irradiation of iron. The b_{arcdpa} and c_{arcdpa} parameters were varied with the RSD value equal to 20%. The total cross sections, recoil energy distributions, and covariance matrix were taken from TENDL-2015 after the NJOY processing. For comparison, Fig.8 shows the result of the estimation [24], which additionally takes into account the uncertainty of recoil energy distributions. Obtained covariance matrices can be used for improved estimation of errors in calculating the radiation damage rate.

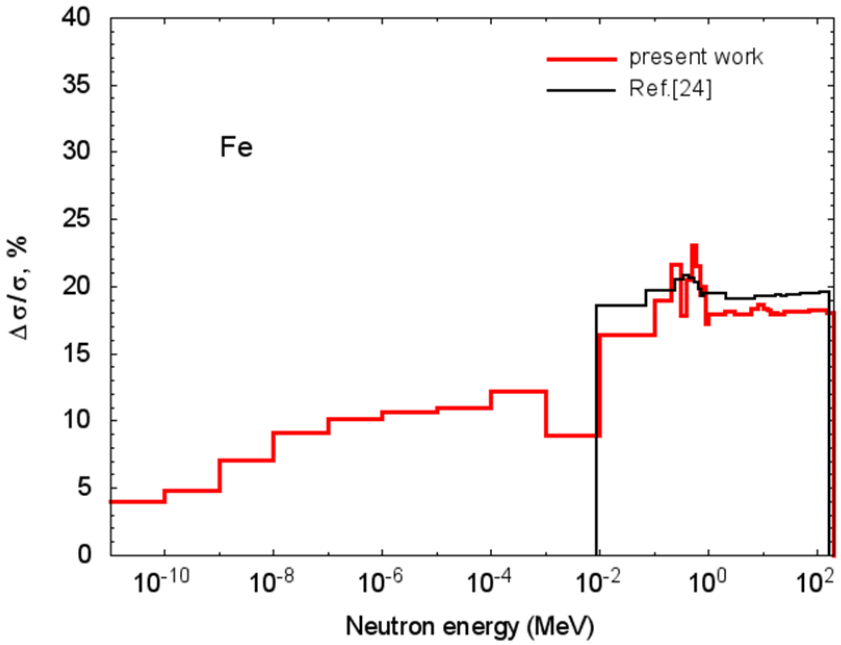

Figure 8. Estimated RSD values for displacement cross-sections for iron and results obtained in Ref.[24] at neutron energies above 0.1 MeV. See explanations in the text.

4. CONCLUSIONS

Atomic displacement cross-sections were calculated using the arc-dpa model [2,3] for a number of materials ranging from Be to U. For Fe, Ni, Cu, Pd, Ag, W, Pt, and Au the parameters included in the arc-dpa formalism were taken from Refs.[2,3,8] (Table II) and for other materials were estimated using a semi-empirical systematic approach. The approach utilizes the correlations between minimum, averaged, and effective threshold displacement energy and a number of quantities such as melting temperature, material density, cohesive energy, and others.

The NJOY code was applied to generate improved displacement cross-sections using data of JEFF-3.3T3, ENDF/B-VIII.beta4, JENDL-4.0, and TENDL-2015. Displacement cross-sections, based on the first three above mentioned libraries, were extended up to incident neutron energy 200 MeV using the TENDL data. The produced data files [20-22] are available in the ENDF-6 and ACE format. Files contain also the displacement cross-sections calculated using the NRT model.

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