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Evaluation of effective threshold displacement energies and other data required for the calculation of advanced atomic displacement cross-sections

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Abstract

Minimum displacement threshold energy, averaged displacement threshold energy, effective displacement energy, and parameters of arc-dpa equations were estimated for 70 materials from Li to U using available experimental data.

Obtained data can be used for approximate calculation of the radiation damage rate for materials irradiated with neutrons in the different facilities.

Keywords: Radiation damage; Displacement energy; Molecular dynamics.

Introduction

A reliable assessment of radiation induced damage rate of materials assumes the use of atomic displacement cross-sections obtained with well justified nuclear models and advanced methods for calculation of the number of stable defects produced under irradiation. The usage of molecular dynamics simulation method (MD) to calculate the number of defects for a wide number of materials is restricted by the complexity of the method. Currently, such simulation was carried out for a limited number of materials [1].

The goal of this work is the utilisation of available experimental information to get a data set for estimation of the number of stable displacements in materials and calculation of atomic displacement cross-sections.

It is assumed that the number of stable defects is parameterized in the form adopted in the arc-dpa concept [2,3]

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

where $T_{\rm dam}$ is the "damage energy", i.e. the energy available to produce atom displacement by elastic collision [4] calculated using the Robinson formula [5]. The value of E_d is displacement energy averaged over all lattice directions [6], which is often named as "the effective displacement threshold energy" [7]. It is called below "the averaged displacement threshold energy", to distinguish it from the effective threshold energy $E_{\rm deff}$ used in the analyses of irradiation in reactors [8].

The defect generation efficiency is approximated [2,3]

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

where $b_{\rm arcdpa}$ and $c_{\rm arcdpa}$ are parameters.

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In the present work the b_{arcdpa} and c_{arcdpa} values were estimated for most solids from Li to U.

Data obtained can be applied for the correction of NRT [4] prediction for the number of stable defects produced under irradiation and for advanced calculations of the atomic displacement cross-sections and radiation damage rates in the irradiated materials.

The estimation of parameters of Eqs. (1) and (2) is briefly discussed below.

Estimation of parameters of arc-dpa equations

In Eq. (2) parameter c_{arcdpa} represents the asymptotic value of defect generation efficiency and the b_{arcdpa} parameter describes the rate of decrease of $\xi(T_{\mathrm{dam}})$ with the increase of T_{dam}. Although, Eq. (2) may ignore the increase of ξ at relatively high values of T_{dam} [9–11], it does not play an essential role for the use of Eqs. (1) and (2) for nuclear reactor and fusion applications.

Parameter c_{arcdpa}

The analysis shows that the asymptotic value of defect generation efficiency can be calculated for most materials as following

$$c_{\mathrm{arcdpa}} = \frac{E_d}{E_{\mathrm{deff}}} \tag{3}$$

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 (see discussion below and in Ref. [7]), the value E_d is the averaged displacement threshold energy.

The E_{deff} values obtained from the neutron irradiation in reactors are available for a limited number of materials [7]. Approximate evaluation of E_{deff} and E_d for solids can be made using the systematic dependence on values concerning the physical properties of materials. The first systematic for E_{deff} was obtained in Ref. [8,12]: $E_{\mathrm{deff}} = C_1\ E_{\mathrm{dmin}}$ and for the averaged displacement energy in Ref. [13]: $E_d = C_2 T_{\mathrm{melt}}$, where E_{dmin} is the "displacement energy" [6,14] or minimum displacement threshold energy and T_{melt} is the melting temperature, C_i are parameters.

In the present work the systematic dependence of E_d and E_{dmin} was further investigated. The results were used to estimate E_{deff} values for materials from Li to U. Details are discussed below.

As a first step to get the systematics of threshold energies, correlations were studied between investigated values and various physical quantities, which values are known for many materials.

The estimation of minimum displacement energy E_{dmin}

Displacement energy obtained from measured data and compiled in Refs. [6,14] were adopted after the analysis for the further use. Correlation coefficients were calculated for these $E_{\mathrm{dmin}}^{(\mathrm{adopt})}$ values and the atomic number (Z), material density (ρ), melting temperature (T_{melt}), cohesive energy (E_{coh}), and some their combinations. Examples are given in Table 1. The data show, in particular, that the correlation of displacement energy with the atomic number is weak, however the correlation with the cohesive energy and melting temperature is rather strong.

Table 1
Example of correlation coefficients $\mathrm{cov}(x,y)/\sigma_x\sigma_y$ calculated for $E_{\mathrm{dmin}}^{(\mathrm{adopt})}$ from Table 2 and various quantities. See details in the text.

Quantity	Correlation coefficient
Z	0.22
ρ	0.76
T_{melt}	0.70
$\rho\ T_{\mathrm{melt}}$	0.83
$(\rho\ T_{\mathrm{melt}})^{1/2}$	0.85
E_{coh}	0.78
$E_{\mathrm{coh}}\ /T_{\mathrm{melt}}$	−0.09
$\rho\ E_{\mathrm{coh}}$	0.85

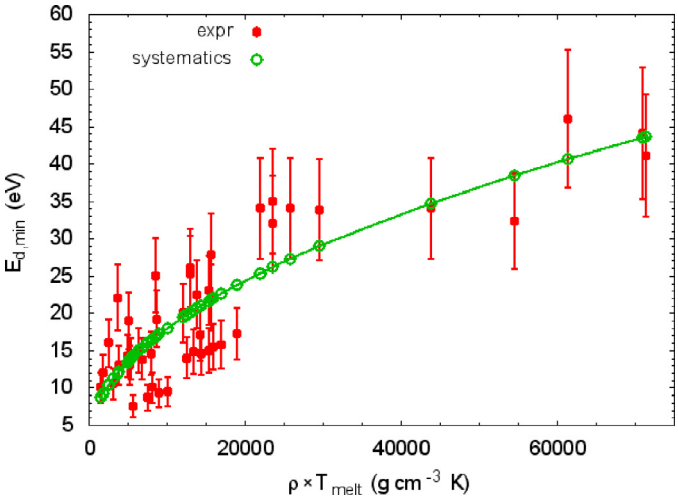

Fig. 1. The systematics $E_{\mathrm{dmin}} = \alpha\ (\rho\ T_{\mathrm{melt}})^{1/2} + \beta$ (green curve). The $E_{\mathrm{dmin}}^{(\mathrm{adopt})}$ values are shown as "expr". See details in the text.

Calculations show that the systematics obtained based on different quantities, such as density, cohesive energy and others, which exhibit the strong correlation with $E_{\mathrm{dmin}}^{(\mathrm{adopt})}$, predict slightly different values of E_{dmin} for materials. The choice of the single "appropriate" systematics for the evaluation of displacement energy is hardly possible, and it is reasonable to use different systematic dependencies with the appropriate weights [15].

In the present work the coefficients of the linear regression and corresponding standard deviations s_i $(i = 1,\ldots,m)$ were calculated for the "m" different cases with strong correlations, which results to "m" different systematics of minimum threshold energy $E_{\mathrm{dmin}}^{(\mathrm{syst})}$. As an example, Fig. 1 shows the systematics obtained using $(\rho T_{\mathrm{melt}})^{1/2}$. Fig. 2 shows the same $E_{\mathrm{dmin}}^{(\mathrm{syst})}$ values for different Z-numbers.

Finally, the E_{dmin} values for materials from Li to U were estimated by averaging the values, obtained using "m" different sets of $E_{\mathrm{dmin}}^{(\mathrm{syst})}$, with s_i^{-2} weights. A special

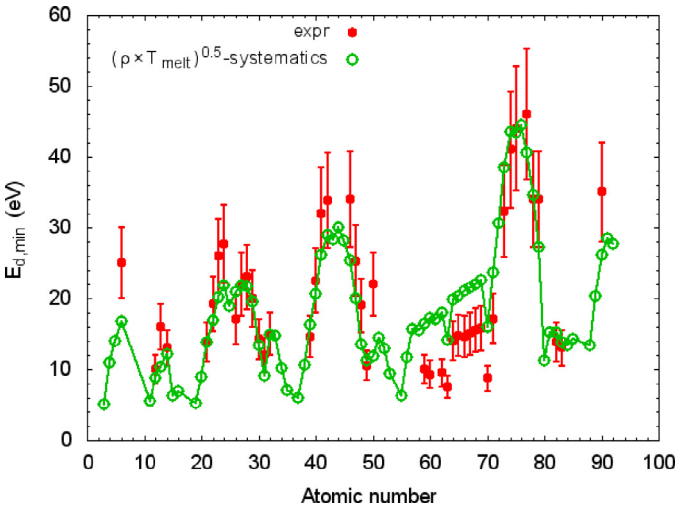

Fig. 2. The same values as in Fig. 1 but as a function of atomic number (Z). Points are connected for better visibility.

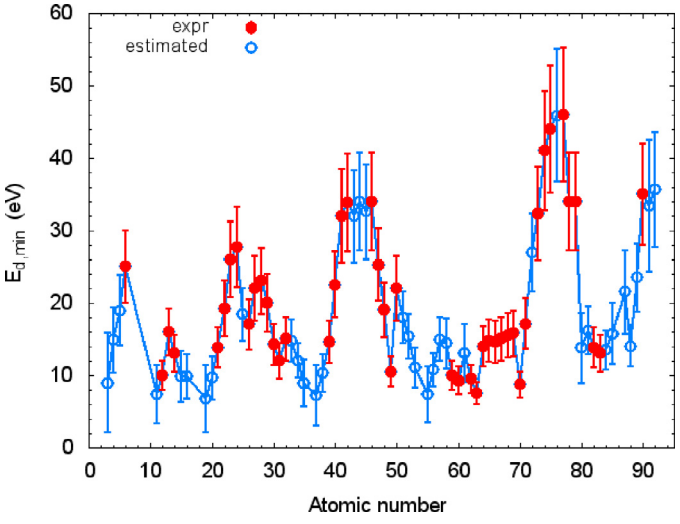

Fig. 3. Estimated values of E_{dmin} (Table 2). The $E_{\mathrm{dmin}}^{(\mathrm{adopt})}$ values are shown as "expr".

procedure from the BEKED code [16] has been used in each case to eliminate possible systematic deviation of $E_{\mathrm{dmin}}^{(\mathrm{syst})}$ values from $E_{\mathrm{dmin}}^{(\mathrm{adopt})}$. The estimated E_{dmin} and $E_{\mathrm{dmin}}^{(\mathrm{adopt})}$ values are shown in Fig. 3 and Table 2.

The estimation of averaged displacement threshold energy E_d

The method used for the estimation of E_d is similar to the one described above. The E_d values derived from measured data and compiled in Refs. [6,7] were adopted as input data to obtain systematics. The search for correlations was carried out for the adopted $E_d^{(\mathrm{adopt})}$ values and number of quantities discussed above. The final E_d values were calculated by a weighted summation of predictions of various systematics obtained.

Table 3 shows examples of correlation coefficients calculated for $E_d^{(\mathrm{adopt})}$ and different quantities. The correlation with the atomic number is the weakest and with E_{dmin}, T_{melt}, and others is rather strong.

Table 2
Estimated and adopted ("A") E_{dmin} values in eV.

3 Li	9 ± 7	39 Y	15 ± 3 A	69 Tm	16 ± 3 A
4 Be	15 ± 5	40 Zr	22 ± 5 A	70 Yb	9 ± 2 A
5 B	19 ± 5	41 Nb	32 ± 6 A	71 Lu	17 ± 3 A
6 C	25 ± 5 A	42 Mo	34 ± 7 A	72 Hf	27 ± 5
11 Na	7 ± 4	43 Tc	32 ± 6	73 Ta	32 ± 6 A
12 Mg	10 ± 2 A	44 Ru	34 ± 7	74 W	41 ± 8 A
13 Al	16 ± 3 A	45 Rh	33 ± 7	75 Re	44 ± 9 A
14 Si	13 ± 3 A	46 Pd	34 ± 7 A	76 Os	46 ± 9
15 P	10 ± 4	47 Ag	25 ± 5 A	77 Ir	46 ± 9 A
16 S	10 ± 3	48 Cd	19 ± 4 A	78 Pt	34 ± 7 A
19 K	7 ± 5	49 In	10 ± 2 A	79 Au	34 ± 7 A
20 Ca	10 ± 3	50 Sn	22 ± 4 A	80 Hg	14 ± 5
21 Sc	14 ± 3 A	51 Sb	18 ± 4	81 Tl	16 ± 3
22 Ti	19 ± 4 A	52 Te	15 ± 3	82 Pb	14 ± 3 A
23 V	26 ± 5 A	53 I	11 ± 3	83 Bi	13 ± 3 A
24 Cr	28 ± 6 A	55 Cs	7 ± 4	84 Po	13 ± 3
25 Mn	18 ± 4	56 Ba	11 ± 2	85 At	16 ± 4
26 Fe	17 ± 3 A	57 La	15 ± 3	87 Fr	21 ± 6
27 Co	22 ± 4 A	58 Ce	14 ± 3	88 Ra	14 ± 3
28 Ni	23 ± 5 A	59 Pr	10 ± 2 A	89 Ac	24 ± 5
29 Cu	20 ± 4 A	60 Nd	9 ± 2 A	90 Th	35 ± 7 A
30 Zn	14 ± 3 A	61 Pm	13 ± 4	91 Pa	33 ± 9
31 Ga	12 ± 2 A	62 Sm	10 ± 2 A	92 U	36 ± 8
32 Ge	15 ± 3 A	63 Eu	8 ± 2 A		
33 As	15 ± 3	64 Gd	14 ± 3 A		
34 Se	12 ± 2	65 Tb	15 ± 3 A		
35 Br	9 ± 3	66 Dy	15 ± 3 A		
37 Rb	7 ± 4	67 Ho	15 ± 3 A		
38 Sr	10 ± 3	68 Er	16 ± 3 A		

Table 3
Example of correlation coefficients calculated for $E_{\mathrm{d}}^{(\mathrm{adopt})}$ from Table 4 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
$T_{\mathrm{melt}}^{3/2}$	0.90
E_{coh}	0.86
E_{coh}^{2}	0.90
E_{coh} T_{melt}	0.91

Fig. 3 shows estimated Ed values for materials from Li to U. The numerical data are given in Table 4.

The estimation of effective displacement energy E_{deff}

The E_{deff} values obtained from reactor measurements at low temperatures were taken from the compilation Ref. [7]. Observed correlations between these $E_{\mathrm{deff}}^{(\mathrm{adopt})}$ values and different variables are weaker than in the case of E_{dmin} and E_d discussed above.

The E_{deff} values were estimated using systematics obtained with E_{dmin}, E_d, and T_{melt} (see Table 5.) The final values are shown in Fig. 5 and Table 6.

Estimated values of c_{arcdpa}

The c_{arcdpa} values were calculated according Eq. (3) and using data from Tables 4 and 6. Obtained values are shown in Fig. 6 and Table 7.

Table 4
Estimated and adopted ("A") averaged displacement threshold energy E_d values in eV.

3 Li	19 ± 4	37 Rb	17 ± 4	65 Tb	36 ± 7
4 Be	31 ± 6	38 Sr	24 ± 5	66 Dy	34 ± 7
5 B	46 ± 9	39 Y	36 ± 7	67 Ho	36 ± 7
6 C	69 ± 14	40 Zr	40 ± 8 A	68 Er	37 ± 7
11 Na	17 ± 4	41 Nb	78 ± 16 A	69 Tm	36 ± 7
12 Mg	20 ± 4 A	42 Mo	65 ± 13 A	70 Yb	27 ± 5
13 Al	27 ± 5 A	43 Tc	58 ± 12	71 Lu	44 ± 9
14 Si	37 ± 7	44 Ru	60 ± 12	72 Hf	61 ± 12
15 P	20 ± 5	45 Rh	51 ± 10	73 Ta	90 ± 18 A
16 S	20 ± 4	46 Pd	41 ± 8 A	74 W	90 ± 18 A
19 K	16 ± 4	47 Ag	39 ± 8 A	75 Re	60 ± 12 A
20 Ca	23 ± 5	48 Cd	30 ± 6 A	76 Os	69 ± 14
21 Sc	33 ± 7	49 In	12 ± 2 A	77 Ir	58 ± 12
22 Ti	30 ± 6 A	50 Sn	20 ± 10	78 Pt	44 ± 9 A
23 V	57 ± 11 A	51 Sb	22 ± 6	79 Au	43 ± 9 A
24 Cr	40 ± 8 A	52 Te	20 ± 5	80 Hg	20 ± 5
25 Mn	33 ± 7	53 I	16 ± 4	81 Tl	24 ± 5
26 Fe	40 ± 8 A	55 Cs	15 ± 4	82 Pb	25 ± 5 A
27 Co	36 ± 7 A	56 Ba	22 ± 4	83 Bi	23 ± 5
28 Ni	33 ± 7 A	57 La	29 ± 6	84 Po	22 ± 4
29 Cu	30 ± 6 A	58 Ce	28 ± 6	85 At	22 ± 4
30 Zn	29 ± 6 A	59 Pr	27 ± 5	87 Fr	34 ± 6
31 Ga	23 ± 5	60 Nd	28 ± 6	88 Ra	24 ± 5
32 Ge	35 ± 7	61 Pm	30 ± 5	89 Ac	33 ± 7
33 As	31 ± 6	62 Sm	27 ± 5	90 Th	44 ± 9 A
34 Se	23 ± 5	63 Eu	24 ± 5	91 Pa	43 ± 7
35 Br	19 ± 4	64 Gd	35 ± 7	92 U	39 ± 8

Table 5
Example of correlation coefficients calculated for $E_{deff}^{(adopt)}$ from Table 6 and various quantities. See details in the text.

Quantity	Correlation coefficient
E_{dmin}	0.47
E_d	0.58
Z	0.25
ρ	0.44
T_{melt}	0.50
E_{coh}	0.42

Alternative c_{arcdpa} values obtained using the method of molecular dynamics for Fe and W [2,3] and for Ni, Cu, Pd, Ag, Pt, and Au in Ref. [17] are listed in Table 8 together with b_{arcdpa} and E_d values used in the analysis [2,3,17].

A direct comparison of the data from Tables 7 and 8 is possible after taking into account the difference in values of E_d from Tables 4 and 8. Although the results from Table 7 are based on experimental data, this does not guarantee their accuracy, see, for example, the brief discussion in Ref. [7].

Parameter b_{arcdpa}

The first calculations of the damage rate in reactors using the results of MD simulation for Fe [18,7,19], Ti, Cu, Zr, and W [7] showed a relatively weak sensitivity of the values obtained to the shape of the neutron spectrum and hence to the $\xi(T_{dam})$ values at relatively low T_{dam} energies for all materials except tungsten.

Table 6
Estimated and adopted ("A") effective displacement energy E_{deff} values in eV.

3 Li	56 ± 13	37 Rb	56 ± 11	65 Tb	73 ± 15
4 Be	68 ± 17	38 Sr	63 ± 14	66 Dy	74 ± 15
5 B	79 ± 20	39 Y	71 ± 18	67 Ho	77 ± 15
6 C	97 ± 27	40 Zr	57 ± 11 A	68 Er	79 ± 16
11 Na	54 ± 13	41 Nb	124 ± 28 A	69 Tm	81 ± 16
12 Mg	45 ± 9 A	42 Mo	141 ± 28 A	70 Yb	70 ± 14
13 Al	61 ± 12 A	43 Tc	123 ± 25	71 Lu	88 ± 18
14 Si	74 ± 15	44 Ru	128 ± 26	72 Hf	106 ± 21
15 P	58 ± 12	45 Rh	121 ± 24	73 Ta	125 ± 25 A
16 S	56 ± 13	46 Pd	129 ± 26 A	74 W	150 ± 30 A
19 K	49 ± 17	47 Ag	124 ± 61 A	75 Re	69 ± 14 A
20 Ca	55 ± 21	48 Cd	67 ± 13 A	76 Os	111 ± 22
21 Sc	62 ± 25	49 In	52 ± 15	77 Ir	117 ± 23
22 Ti	36 ± 8 A	50 Sn	28 ± 6 A	78 Pt	123 ± 25 A
23 V	111 ± 22 A	51 Sb	54 ± 25	79 Au	100 ± 20 A
24 Cr	109 ± 22	52 Te	52 ± 23	80 Hg	71 ± 14
25 Mn	100 ± 20	53 I	49 ± 20	81 Tl	77 ± 15
26 Fe	129 ± 26 A	55 Cs	48 ± 18	82 Pb	76 ± 15
27 Co	138 ± 29 A	56 Ba	55 ± 20	83 Bi	74 ± 15
28 Ni	142 ± 38 A	57 La	61 ± 21	84 Po	74 ± 15
29 Cu	99 ± 20 A	58 Ce	60 ± 20	85 At	76 ± 15
30 Zn	79 ± 16 A	59 Pr	60 ± 19	87 Fr	87 ± 17
31 Ga	70 ± 14	60 Nd	61 ± 19	88 Ra	78 ± 16
32 Ge	80 ± 16	61 Pm	65 ± 18	89 Ac	90 ± 18
33 As	76 ± 15	62 Sm	63 ± 17	90 Th	106 ± 21
34 Se	66 ± 13	63 Eu	61 ± 16	91 Pa	103 ± 21
35 Br	60 ± 12	64 Gd	71 ± 16	92 U	100 ± 20

Table 7
The c_{arcdpa} values calculated using the data from Tables 4 and 6.

3 Li	0.34 ± 0.10	37 Rb	0.31 ± 0.09	65 Tb	0.49 ± 0.14
4 Be	0.46 ± 0.14	38 Sr	0.38 ± 0.11	66 Dy	0.46 ± 0.13
5 B	0.58 ± 0.19	39 Y	0.50 ± 0.16	67 Ho	0.46 ± 0.13
6 C	0.71 ± 0.24	40 Zr	0.70 ± 0.20	68 Er	0.47 ± 0.13
11 Na	0.32 ± 0.10	41 Nb	0.63 ± 0.19	69 Tm	0.44 ± 0.13
12 Mg	0.44 ± 0.13	42 Mo	0.46 ± 0.13	70 Yb	0.38 ± 0.11
13 Al	0.44 ± 0.13	43 Tc	0.47 ± 0.13	71 Lu	0.50 ± 0.14
14 Si	0.50 ± 0.14	44 Ru	0.47 ± 0.13	72 Hf	0.57 ± 0.16
15 P	0.36 ± 0.12	45 Rh	0.42 ± 0.12	73 Ta	0.72 ± 0.20
16 S	0.36 ± 0.11	46 Pd	0.32 ± 0.09	74 W	0.60 ± 0.17
19 K	0.33 ± 0.14	47 Ag	0.31 ± 0.17	75 Re	0.87 ± 0.25
20 Ca	0.41 ± 0.18	48 Cd	0.45 ± 0.13	76 Os	0.62 ± 0.17
21 Sc	0.53 ± 0.24	49 In	0.23 ± 0.08	77 Ir	0.50 ± 0.14
22 Ti	0.83 ± 0.25	50 Sn	0.70 ± 0.29	78 Pt	0.36 ± 0.10
23 V	0.51 ± 0.15	51 Sb	0.40 ± 0.21	79 Au	0.43 ± 0.12
24 Cr	0.37 ± 0.10	52 Te	0.38 ± 0.19	80 Hg	0.28 ± 0.09
25 Mn	0.33 ± 0.09	53 I	0.33 ± 0.16	81 Tl	0.32 ± 0.09
26 Fe	0.31 ± 0.09	55 Cs	0.32 ± 0.15	82 Pb	0.33 ± 0.09
27 Co	0.26 ± 0.08	56 Ba	0.40 ± 0.17	83 Bi	0.31 ± 0.09
28 Ni	0.23 ± 0.08	57 La	0.47 ± 0.19	84 Po	0.29 ± 0.08
29 Cu	0.30 ± 0.09	58 Ce	0.46 ± 0.17	85 At	0.30 ± 0.08
30 Zn	0.37 ± 0.10	59 Pr	0.46 ± 0.17	87 Fr	0.39 ± 0.10
31 Ga	0.33 ± 0.10	60 Nd	0.46 ± 0.17	88 Ra	0.31 ± 0.09
32 Ge	0.43 ± 0.12	61 Pm	0.47 ± 0.15	89 Ac	0.37 ± 0.11
33 As	0.40 ± 0.11	62 Sm	0.42 ± 0.14	90 Th	0.42 ± 0.12
34 Se	0.35 ± 0.10	63 Eu	0.40 ± 0.13	91 Pa	0.42 ± 0.11
35 Br	0.31 ± 0.09	64 Gd	0.49 ± 0.15	92 U	0.39 ± 0.11

Table 8
Data obtained using the method of molecular dynamics in Refs. [2,3,17].

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

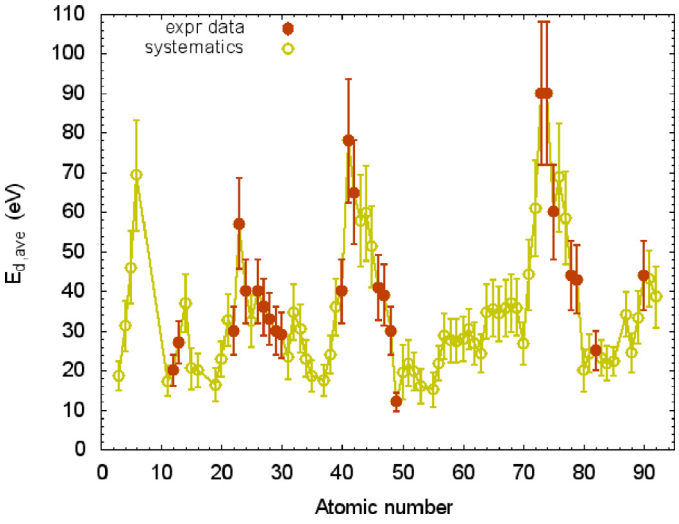

Fig. 4. Estimated values of averaged displacement threshold energy E_d. The $E_d^{(adopt)}$ values are shown as "expr".

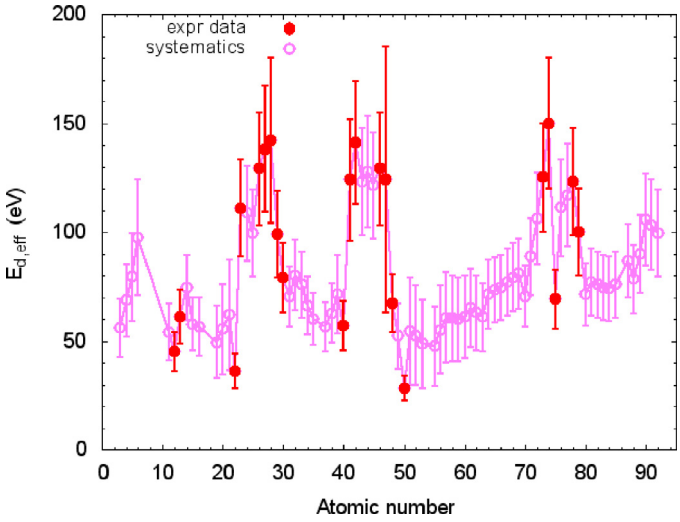

Fig. 5. Estimated values of effective displacement energy E_{deff}. The $E_{deff}^{(adopt)}$ values are shown as "expr".

In the present work, the influence of b_{arcdpa} parameter, concerning the rate of decrease of ξ, on the value of radiation damage rate was studied for 70 materials from Li to U.

The averaged value of defect generation efficiency was calculated as follows

$$\langle \xi \rangle = \int \sigma_{d,arcdpa}(E)\varphi(E)dE / \int \sigma_{d,NRT}(E)\varphi(E)dE, \quad (4)$$

where $\sigma_{d,arcdpa}$ is displacement cross-section calculated according Eqs. (1),(2), $\sigma_{d,NRT}$ is calculated using the NRT model, $\varphi(E)$ is a neutron spectrum.

The $\sigma_{d,arcdpa}$ values were calculated for different materials using Eqs. (1),(2) and c_{arcdpa} were taken from Tables 7 and 8.

Table 9
The $\langle \xi \rangle$ values for tungsten calculated with b_{arcdpa} and c_{arcdpa} from Table 8 for different irradiation conditions [7,20] using various nuclear data libraries. See details in the text.

Irradiation	ENDF/B-VII.1	JEFF-3.3T2	JENDL-4.0	TENDL-2015
APWR	0.26	0.25	0.24	0.25
KWO PWR	0.25	0.24	0.23	0.24
TRIGA/TRADE	0.24	0.24	0.23	0.23
TTB, FRM	0.24	0.25	0.24	0.24
Fission	0.22	0.21	0.20	0.21
14.8 MeV neutrons	0.17	0.15	0.15	0.16
(d,Be) 40 MeV deuterons	0.16	0.14	–	0.16
HFIR	0.25	0.26	0.24	0.24
PWR Robinson2	0.26	0.27	0.26	0.26
Typical LWR	0.26	0.25	0.25	0.26
EPRI, BWR 1/4T	0.24	0.24	0.23	0.24
EPRI, BWR 3/4T	0.27	0.26	0.26	0.26
EPRI, PWR 1/4T	0.26	0.25	0.24	0.25
EPRI, PWR 3/4T	0.30	0.29	0.29	0.29
LWR Kori	0.28	0.29	0.28	0.28
Omega west reactor	0.24	0.25	0.23	0.23
EBR-II expr breeder reactor	0.26	0.25	0.25	0.25
Bor-60	0.27	0.26	0.25	0.26
RTNS-II Fusion simulation	0.19	0.15	0.15	0.16
ITER, first wall	0.21	0.18	0.19	0.18
DEMO	0.22	0.19	0.19	0.19
IFMIF	0.19	0.14	–	0.18

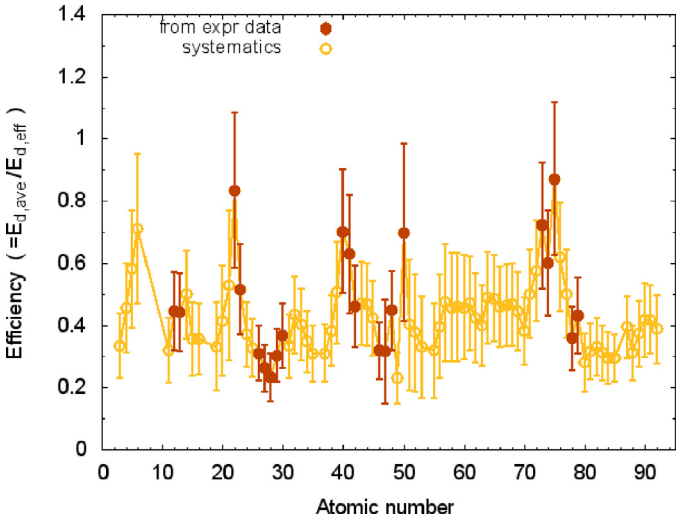

Fig. 6. The c_{arcdpa} values calculated using the data from Tables 4 and 6. Data for elements, for which $E_{\mathrm{deff}}^{(\mathrm{adopt})}$ values are available (see Table 6), are shown as "expr".

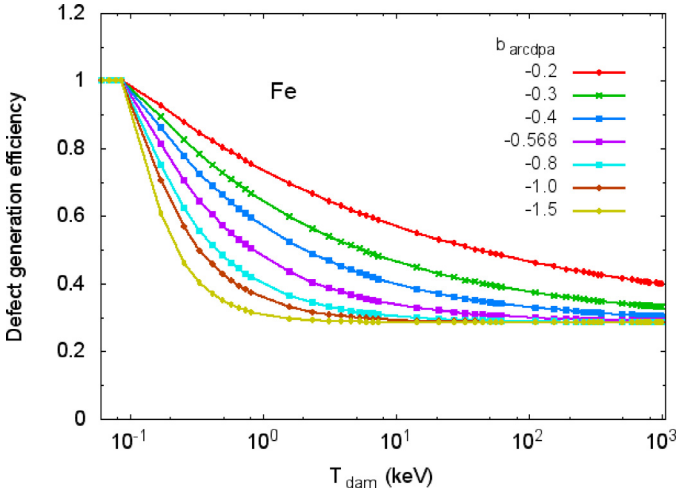

Fig. 7. Defect generation efficiency $\xi(T_{\mathrm{dam}})$ calculated with different b_{arcdpa} for iron. The value −0.568 corresponds to the data from Table 8.

The data from Table 7 were applied in cases, where results of MD simulation (Table 8) are not available. The b_{arcdpa} value varied from −1.5 to −0.2. Typical values $\xi(T_{\mathrm{dam}})$ calculated with different b_{arcdpa} values are shown in Fig. 7 for iron.

Calculations of $\langle\xi\rangle$ were performed for 22 various neutron spectra [7,20] corresponding to the irradiation of materials in nuclear and fusion reactors, and other facilities. Nuclear data for calculation of recoil energy distributions were taken from ENDF/B-VII.1 [21], JEFF-3.3T2 [22], JENDL-4 [23], and TENDL-2015 [24]. Numerical calculations were performed using the NJOY-2012 code [25] after the implementation of Eqs. (1),(2).

Examples of calculated $\langle\xi\rangle$ values are shown for tungsten in Table 9.

Quantification of the difference in $\langle\xi\rangle$ obtained for various spectra and selected material and the library is performed

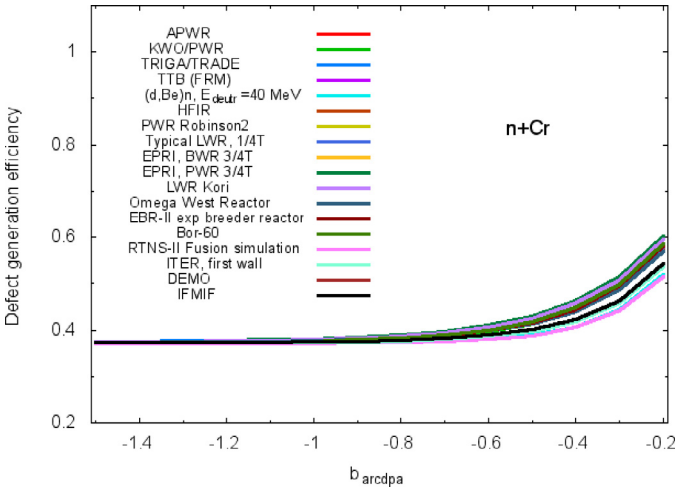

Fig. 8. The $\langle\xi\rangle$ values calculated for chromium with different b_{arcdpa} values and for different irradiation conditions. Nuclear data are taken from ENDF/B-VII.1.

Table 10
The list of materials with D values exceeding 20% obtained using data from different libraries. The D values were calculated with b_{arcdpa} from Table 8 for materials marked with an asterisk and with $b_{\mathrm{arcdpa}} = -1.0$ for other materials.

Material	D-value (%)			
	ENDF/B-VII.1	JEFF-3.3T2	JENDL-4	TENDL-2015
Co	26	26	27	<20
Cu*	33	33	32	33
Rh	<20	<20	39	<20
Pd*	20	<20	<20	<20
Ag*	30	<20	<20	<20
Cd	24	69	24	71
In	28	28	28	32
Sm	64	65	65	66
Eu	46	74	60	60
Gd	59	61	60	63
Dy	26	25	28	22
Er	29	<20	29	<20
Lu	31	<20	–	<20
Hf	<20	<20	32	<20
W*	56	70	59	61
Pt*	–	28	–	28
Au*	112	112	62	40
Hg	84	44	80	43

using the following formula

$$D = \frac{\langle\xi\rangle_{\max} - \langle\xi\rangle_{\min}}{\langle\xi\rangle_{\mathrm{ave}}} 100\ \% \qquad (5)$$

where $\langle\xi\rangle_{\max}$ and $\langle\xi\rangle_{\min}$ the maximal and minimal value of $\langle\xi\rangle$ calculated using one of the neutron spectra, correspondingly. $\langle\xi\rangle_{\mathrm{ave}}$ is the arithmetic mean of results obtained using all 22 neutron spectra.

Calculations show that the shape of the neutron spectrum and, accordingly, the value of b_{arcdpa} has a significant impact on $\langle\xi\rangle$ for a range of materials. List of materials for which the D value exceeds 20%t, are given in Table 10. Approximate estimation of parameter of b_{arcdpa} in these cases is rather difficult.

For most materials the influence of the b_{arcdpa} parameter value on the calculated $\langle\xi\rangle$ value is relatively small. In these cases the $\langle\xi\rangle$ value for different type of irradiation can be estimated with b_{arcdpa} parameter equal to -1. Fig. 8 shows a typical dependence of $\langle\xi\rangle$ on the b_{arcdpa} parameter.

Conclusion

Minimum displacement threshold energy E_{dmin}, averaged displacement threshold energy E_d, and effective displacement energy E_{deff}, corresponding to neutron irradiation in different facilities, were estimated for 70 materials from Li to U using available experimental data. Results are given in Tables 2,4,6 and shown in Figs. 3–5.

The values of b_{arcdpa} and c_{arcdpa} parameters, Eqs. (1) and (2), used for calculation of the number of stable displacements, were estimated for different materials.

Obtained data and data from Refs. [2,3,17] can be used for approximate calculation of radiation damage rate using Eqs. (1) and (2) for materials irradiated with neutrons in different facilities. The b_{arcdpa} and c_{arcdpa} are taken as following

- for Fe, Ni, Cu, Pd, Ag, W, Pt, and Au data from Table 8 are applied
- for other materials except Co, Cd, In, Sm, Eu, Gd, Dy, and Hg the value of c_{arcdpa} parameter is taken from Table 7, the parameter b_{arcdpa} is equal to -1
- for Co, Cd, In, Sm, Eu, Gd, Dy, and Hg c_{arcdpa} can be taken from Table 7, the b_{arcdpa} value is not well defined at present.

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