General displacement function for displacement damage cross-section calculation

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Abstract: The estimation of displacement damage rate requires the prior knowledge of displacement damage cross-section and displacement function is one part in the displacement damage cross-section calculation. The NRT model, which is used to calculate the displacement function for many years, always overestimates the number of displaced atoms in material. Although the arc-dpa model proposed recently can give correct results for the materials irradiated by neutron, there is still no suitable displacement function that can be used to accurately obtain both neutron and charged particles displacement cross-section comparing with experimental data. In the present work, a general displacement function is proposed, which is composed by power function model, arc-dpa model and BCA model. The model parameters are obtained for aluminum, iron, copper and tungsten. The displacement damage cross-sections for the materials irradiated by neutron and charged particles calculated using the general displacement function agree well with available experimental data.

Keyword: displacement function; displacement damage cross-section; neutron irradiation; charged particle irradiation; radiation damage

1. Introduction

A reliable estimation of displacement damage of material is an essential part of the work for the safety of the neutron and charged particle facilities. Displacement damage rate is usually used to estimate the displacement damage. The displacement damage rate can be calculated by folding the product of displacement damage cross-section and flux according to the definition. Therefore, accurate displacement damage cross-section calculation is vital for the reliable displacement

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damage estimation.

Recoil energy spectrum and displacement function are two parts of displacement damage cross-section calculation. Recoil energy spectrum can be obtained from evaluated nuclear data libraries by nuclear data processing codes, such as NJOY [1], NECP-Atlas [2], and also can be calculated by the Monte Carlo codes like MCNP [3], CASCADE [4]. Because the calculation of recoil energy spectrum is reliable to some extent, the main source of the uncertainty of displacement damage cross-section is from the uncertainty of displacement function [5]. NRT model [6], which was developed from Kinchin-Pease model [7], is used to get displacement function since 1970s. Compared with the molecular dynamics (MD) simulations results and experiment data, the displaced atom numbers are always overestimated by the NRT model. A lot of work was done to improve the accuracy of displacement function. Jung et al. [8] derived realistic displacement function for various cubic transition metals from experimental electron, ion and neutron damage rate data. Apart from the directly derivation of the realistic displacement function, another method to improve the accuracy is introducing an efficiency function to correct displacement function obtained by NRT model. Bacon et al. [9] proposed using power function to describe the efficiency function and the model parameters were obtained by fitting based on MD simulations data. Recently, Nordlund et al. [10] proposed arc-dpa model to calculate displacement function and the model parameters were also obtained by fitting based on MD simulations data. Due to the lack of MD simulation data, Konobeyev et al. [11] evaluated the arc-dpa model parameters for 70 materials from Li to U using available experimental data based on systematics. Although these displacement functions or efficiency functions can improve the displacement damage cross-section calculation to some extent, some obvious limitations still exist. For example, arc-dpa model can give good results for neutron or middle energy proton irradiations (from tens of keV to tens of MeV) but not for low energy proton (less than tens of keV) and high energy proton irradiations (lager than tens of MeV) [12]. Other displacement functions and efficiency functions also have similar problems. Thus, it is necessary to develop a general displacement function for displacement cross-section calculation.

In the present work, a general displacement function was proposed to get accurate displacement damage cross-section for materials irradiated by neutron and proton. The general displacement function is composed by a power function model in low damage energies, the arc-dpa model in middle damage energies and the BCA (Binary Collision Approximation) model in high damage

energies. The model parameters were obtained for aluminum, iron, copper and tungsten based on detailed calculations and analysis. Finally, the neutron and proton displacement damage cross-sections were calculated using the general displacement function for these materials. The accuracy of the general displacement function is proved by comparing with the experimental data.

The calculation method of the displacement damage cross-section and the general displacement function are briefly described in Section 2. Section 3 presents the results of calculations and comparisons with the reference data.

2. Methodology

2.1 Displacement damage cross-section calculation

The formula used to calculate displacement damage cross-section is written as follows:

$$\sigma_d(E)=\sum_i \int_{E_d}^{T_i^{\max}} \nu(T_i)\frac{\mathrm{d}\sigma(E,T_i)}{\mathrm{d}T_i}\mathrm{d}T_i \tag{1}$$

where E is the incident particle energy; $\mathrm{d}\sigma(E,T_i)/\mathrm{d}T_i$ is the recoil energy distribution of *i*-th nuclear interaction. $T_i^{\max}$ is the maximum energy of recoil atom produced in the *i*-th nuclear interaction; E_d is the threshold displacement energy of target material; $\nu(T_i)$ is the displacement function, which stands for the number of displaced atoms at damage energy T_i.

In order to obtain displacement cross-section by Eq. (1), the recoil energy distribution $\mathrm{d}\sigma(E,T_i)/\mathrm{d}T_i$ and displacement function $\nu(T_i)$ should be calculated firstly. The nuclear data processing code, such as NJOY or NECP-Atlas, can be used to calculate the recoil energy distribution for incident neutron from evaluated nuclear data libraries. The calculation method of the recoil energy spectrum for incident proton was described by Konobeyev et al. [12]. They will not be repeated here again. Although a lot of models, such as arc-dpa model, can be used for displacement function calculation, they cannot provide enough precision for neutron and proton irradiation at the same time as mentioned in the beginning. Thus, the general displacement function was proposed and described in the following part.

2.2 General displacement function

A new general displacement function was proposed in this paper. It is made up of three different

models in different damage energy ranges, except that the number of displaced atoms is zero when the damage energy is less than the minimum threshold damage energy. These models include a power function model, the arc-dpa model and BCA model. The proposed general displacement function can be written as:

$$\nu(E_a)=\begin{cases} 0, & E_a < E_{d,\min} \\ AE_a^n, & E_{d,\min} < E_a < E_{crit1} \\ \xi(E_a)\nu_{NRT}(E_a), & E_{crit1} < E_a < E_{crit2} \\ BCA \text{ simulation}, & E_{crit2} < E_a \end{cases} \tag{2}$$

where $\nu(E_a)$ is the number of displaced atoms. E_a is the Lindhard's damage energy [13]. $E_{d,\min}$ is the minimum threshold damage energy. When damage energy is less than minimum damage energy, the number of displaced atoms is zero. E_{crit1} and E_{crit2} are critical damage energy to divide damage energy into three parts. When the damage energy less than E_{crit1} and lager than $E_{d,\min}$, power function is used to describe the displacement function. A and n are model parameters in the power function. The power function instead of one displaced atom produced in the low energy can improve the precision of displacement cross section because it is close to the reality more. When the damage energy less than E_{crit2} and lager than E_{crit1}, arc-dpa model is adopted. $\xi(E_a)$ is the efficiency function of arc-dpa model, which can be described as:

$$\xi(E_a)=(1-c_{arc})\left(\frac{0.8E_a}{2E_d}\right)^{b_{arc}}+c_{arc} \tag{3}$$

where E_d is the threshold displacement energy of target material, b_{arc} and c_{arc} are arc-dpa model parameters.

Analytical formulas are always used in damage energies lower than E_{crit2}. However, when the damage energy is larger than E_{crit2}, the displacement function is obtained from BCA simulations. It should be noticed that the BCA simulation here is not pure BCA simulation as usual but BCA simulation coupling with analytical displacement function in energies lower than E_{crit2} as Eq (2). It means that in the simulation process of the BCA code, the number of displacement atoms is directly calculated using Eq. (2) when the damage energy of the recoil atom is less than E_{crit2}.

Because the energy loss for high energy recoil atom is mainly due to ionization effect, it is reasonable to use BCA method to simulate the cascade process for high energy recoil. The method coupling BCA method with analytical displacement function has been realized in the IOTA code [14].

Fig. 1 shows the efficiency function for copper, which is the ratio of the displaced atoms calculated from the general displacement function to that obtained by the NRT model. Compared with the arc-dpa model, the new efficiency function shows the incremental pattern in low and high energy range.

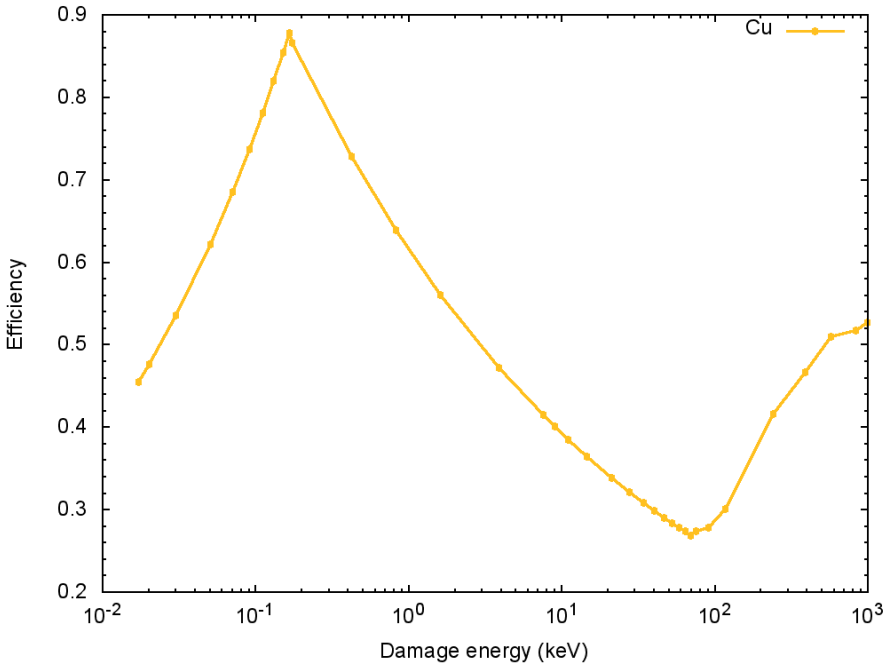

Fig. 1 Efficiency function for copper.

2.2.1. Obtaining of model parameters in the general displacement function

As shown in Eq (2) and (3), there are eight model parameters in the general displacement function. They include $E_{d,\min}$, E_d, E_{crit1}, E_{crit2}, A, n, b_{arc} and c_{arc}. In this section, the obtaining of these model parameters for aluminum, iron, copper and tungsten are described.

Firstly, $E_{d,\min}$ and E_d are common displacement damage parameters. $E_{d,\min}$ for aluminum, iron, copper and tungsten are 16 eV, 17 eV, 19 eV and 40 eV [15], respectively. E_d for aluminum, iron, copper and tungsten are 27 eV [15], 40 eV [15], 33 eV [10], 70 eV [10], respectively.

b_{arc} and c_{arc} are arc-dpa model parameters, which can be got from Ref. [10] or [11]. b_{arc} and c_{arc} for Fe are -0.568 and 0.286 [10], and for Al are -0.820 and 0.443 [11]. Because some calculations [12] show that the arc-dpa model with b_{arc} and c_{arc} from Refs. [10] and [11] cannot give well agreement with the experimental data, new b_{arc} and c_{arc} are fitted for Cu and W based on experimental data in this work. For Cu, b_{arc} and c_{arc} are -0.195 and 0.000. And for Al, they are -0.60 and 0.280.

E_{crit1}, A and n are obtained at this same time. A and n are fitted based on the electron displacement damage cross-sections which are got from Jung's paper [8]. E_{crit1} is the energy corresponding to the intersection of the power function and the efficiency function of arc-dpa model. The calculation method of electron displacement damage cross-section was described in Oen's paper [16]. In order to realize the fitting, new code is developed based on the theory of electron displacement damage cross-section calculation to implement the analytical displacement function including the power function model and arc-dpa model. The following E_{crit1}, A and n were fitted in this work, correspondingly, for Al: 92.2eV, 0.07, 0.52, for Fe: 105.7eV, 0.02, 0.83, for Cu: 126.2eV, 0.20, 0.29, and for W: 237.4eV, 0.01, 0.82.

E_{crit2} is an empirical model parameter. Konobeyev et al. [12] took 40 keV as the critical energy for all materials and it showed good accuracy for high energy proton displacement damage cross-section. But the results for neutron irradiation are not always good enough. To balance the accuracy between neutron and high energy proton irradiation, E_{crit2} are redetermined and they are 40 keV, 40 keV, 70 keV, 40 keV for Al, Fe, Cu and W.

All model parameters used in the general displacement function for Al, Fe, Cu and W are concluded in Table 1.

Table 1 Model parameters in general displacement function

Model parameters	Al	Fe	Cu	W
$E_{d,\min}$ (eV)	16	17	19	40

E_d (eV)	27	40	33	70
E_{crit1} (eV)	92.2	105.7	126.2	237.4
E_{crit2} (keV)	40	40	70	40
A	0.07	0.02	0.20	0.01
n	0.52	0.83	0.29	0.82
b_{arc}	-0.82	-0.568	-0.195	-0.60
c_{arc}	0.443	0.286	0.000	0.28

3. Results and discussion

3.1. Averaged neutron displacement damage cross-section

The low temperature damage-resistivity rates for Al, Fe, Cu and W irradiated by several different neutron spectra were measured in a number of past experimental studies. These neutron spectra are concluded in Table 2. The experimental displacement damage cross-sections can be obtained by:

$$\sigma_d^e = \frac{1}{\rho_F}\frac{\Delta\rho}{\Delta\phi} \tag{4}$$

where $\Delta\rho/\Delta\phi$ the damage rate which is measured in experiments; ρ_F is the Frenkel pair resistivity taken equal to 3.7, 24.6, 2.2 and 27 $\mu\Omega\cdot m$ for Al, Fe, Cu and W, respectively [15].

Table 2 Summary of the spectrum of neutron irradiation sources

Spectrum name	Explanation
CP-5(VT53), ANL	VT53 fast neutron cryogenic facility of the Argonne CP-5 reactor
Be(40MeV-d,n)	Neutrons produced by the (40 MeV-d,n) reaction of Be
LTIF, ORNL	Low-temperature irradiation facility at Oak Ridge National Laboratory
RTNS, LLL	Rotating target neutron source facility at Lawrence Livermore National Laboratory
LHTL, JRR-3	Liquid helium temperature loop in the Japan Research Reactor-3
TTB, FRM	Low-temperature irradiation facility at the Research Reactor Munich

Averaged neutron displacement damage cross-sections for Al, Fe, Cu and W irradiated by the neutron spectra summarized in Table 2 were calculated using the general displacement function and arc-dpa model. The evaluated nuclear data library is JEFF 3.3 [17]. Table 3 shows the calculated results. For Al, Fe and Cu, the ratios of calculations to experimental data (C/E ratio) are larger than

0.8 and less than 1.2 as using general displacement function. When the arc-dpa model is used, the vast majority of C/E ratios are between 0.8 and 1.2, but some C/E ratio are larger than 1.2 or less than 0.8. For W, all of the C/E ratios are less than 0.9 and even some of them are less than 0.7. The similar conclusion was also pointed out in Ref. [15]. Broeders et al. [15] described that the observed discrepancy between the theoretical calculated and experimental displacement cross-sections for tungsten should be related to the problems of the measurement of the initial damage rate in Refs. [18-21] or to the MD calculations and further studies are needed to understand the observed difference. In this research, the problems of the measurement of the initial damage rate are regarded as the reason and the detailed explanations will be described in relation to the results of the proton displacement damage cross-section in the next chapter.

Table 3 Experimental proton displacement damage cross-section

Material	Source	Damage rate (10^{-31} Ω m^3/proton) [15]	Experimental displacement cross section (b)	Calculated Displacement damage cross-section(b)		C/E value	
				General displacement function	arc-dpa model	General displacement function	arc-dpa model
Al	CP-5(VT53), ANL	1.49	402.7	342.6	379.3	0.851	0.942
	LTIF, ORNL	2.19	591.9	663.2	754.8	1.120	1.275
	RTNS, LLL	4.18	1129.7	1054.9	1010.6	0.934	0.895
	LHTL, JRR-3	2.20	594.6	663.2	754.8	1.115	1.269
	TTB, FRM	2.57	694.6	608.9	684.0	0.877	0.985
Fe	CP-5(VT53), ANL	3.33	135.4	123.7	117.3	0.914	0.866
	LHTL, JRR-3	6.5	264.2	289.5	265.7	1.096	1.006
	TTB, FRM	6.39	259.8	242.0	226.7	0.931	0.873
Cu	CP-5(VT53), ANL	0.424	192.7	161.2	158.5	0.837	0.823
	Be(40MeV-d,n)	2.11	959.1	1136.0	701.9	1.184	0.732
	LTIF, ORNL	0.723	328.6	310.0	299.0	0.943	0.910
	RTNS, LLL	2.48	1127.2	1109.0	701.1	0.984	0.622
	LHTL, JRR-3	0.70	318.2	310.0	299.0	0.974	0.940
	TTB, FRM	0.71	322.7	285.4	279.1	0.884	0.865
W	LTIF, ORNL	4.2	155.6	97.3	96.6	0.625	0.621
	RTNS, LLL	11.55	427.8	382.9	341.8	0.895	0.799
	LHTL, JRR-3	3.9	144.4	97.3	96.6	0.674	0.669
	TTB, FRM	3.3	122.2	86.8	86.5	0.710	0.708

3.2. Proton displacement damage cross-section

Proton displacement damage cross-sections were calculated using the method proposed in Ref [12] based on general displacement function. The results from NRT model, arc-dpa model and previous evaluation by Konobeyev et al. are also included for comparison. Some experimental proton displacement cross-section summarized in Ref [22] and from Jung [8] are used as reference.

Figs. 2 – 5 show the proton displacement damage cross-sections for Al, Fe, Cu and W up to 10 GeV. From the comparison with Jung's experimental reference data, it is found that the proton displacement cross-sections at low energies are improved a lot, because the power function model used in the low PKA (Primary Knock-on Atom) energies gives more physically realistic description than one defect generation in this energy range. In Konobeyev's previous evaluation, original arc-dpa model parameters from Nordlund et al. [10] give good agreement with Jung's data for Al, Fe and W, but the proton displacement damage cross-sections of copper were underestimate as using original arc-dpa model parameters. New arc-dpa model parameters for copper are fitted based on experimental data [23] here to reduce this deviation. As shown in Fig. 3, new evaluation for copper is better than previous evaluation. At high energies, the arc-dpa model always underestimate the displacement damage cross-sections. Konobeyev et al. [12] proposed to combine BCA model with arc-dpa model to improve the calculation. The same combination is also used in the general displacement function which is used in the following proton displacement damage cross-section calculation. The difference is that a flexible critical damage energy, which is the symbol E_{crit2} in the general displacement function, is used. Konobeyev et al. used 40 keV as the critical damage energy between arc-dpa model and BCA calculation. The BCA calculation is used to get displacement function for the following two reasons. Firstly, the energy loss of high energy protons is mainly due to the ionization and so it contributes little to the displacement. Secondly, some MD simulations also show that the efficiency function has a tendency of growth when it reaches a certain energy [24].

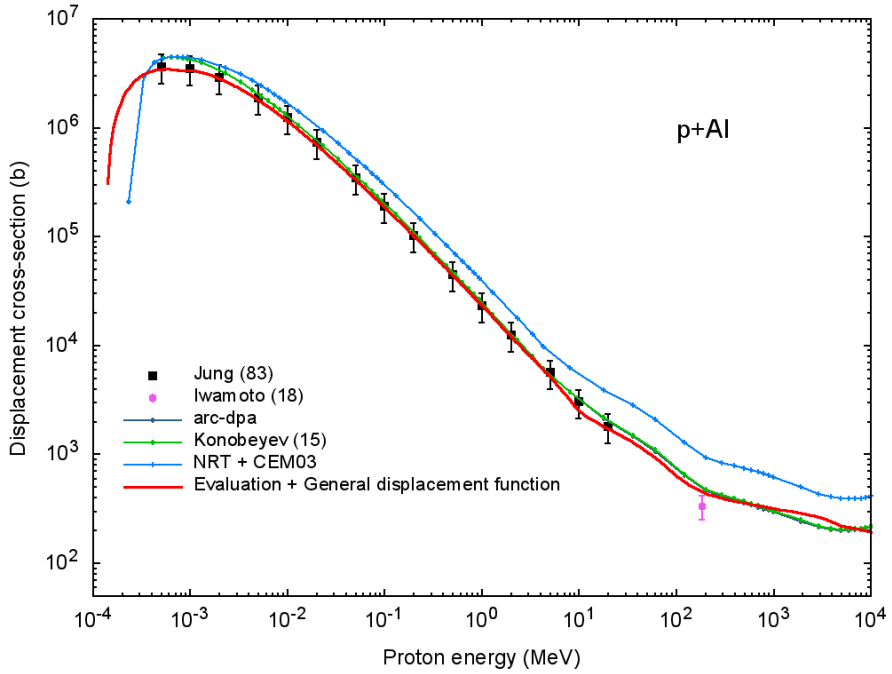

Fig. 2 Displacement damage cross-section for p+Al irradiation. All points are experimental data, which can be found in our paper [22] and Jung's paper [8]; all lines are the calculated values. Arc-dpa, Konobeyev (15) and NRT + CEM03 are the proton displacement damage cross-sections calculated using arc-dpa model, arc-dpa coupling BCA model and NRT model, respectively, from Ref. [21]. "Evaluation + General displacement function" is the evaluated proton displacement damage cross-sections calculated using general displacement function.

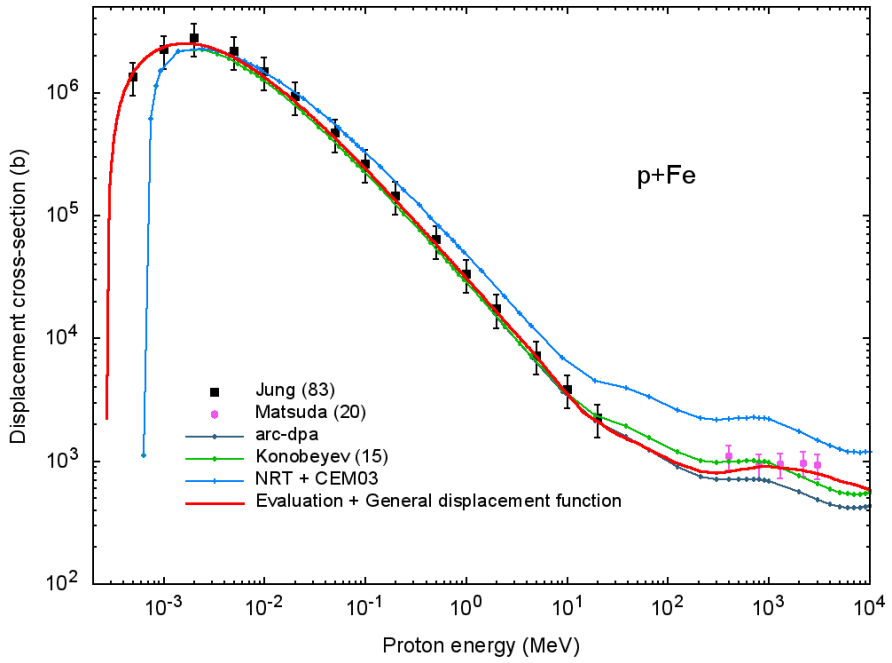

Fig. 3 The same as in Fig.1 for p+Fe irradiation

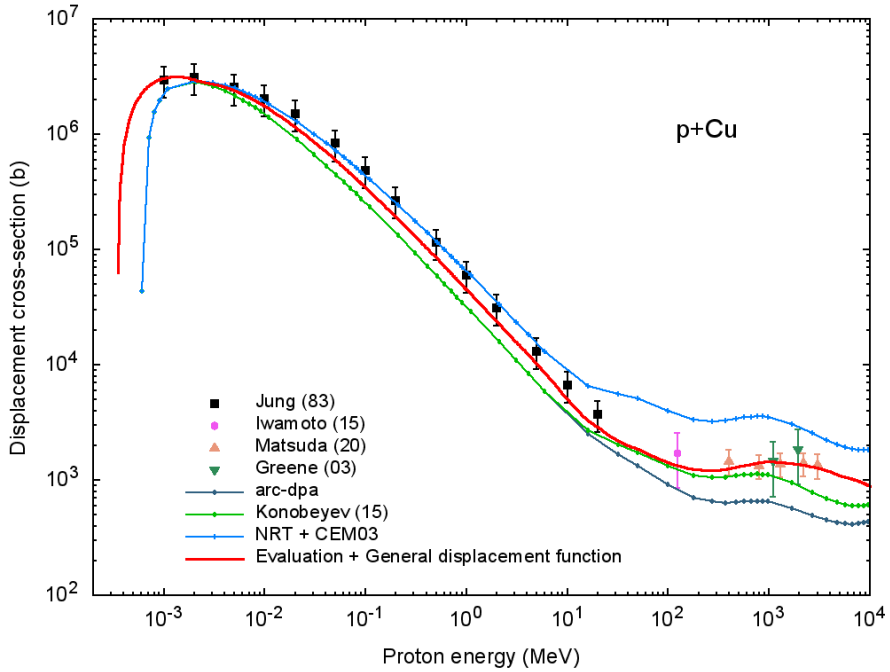

Fig. 4 The same as in Fig.1 for p+Cu irradiation

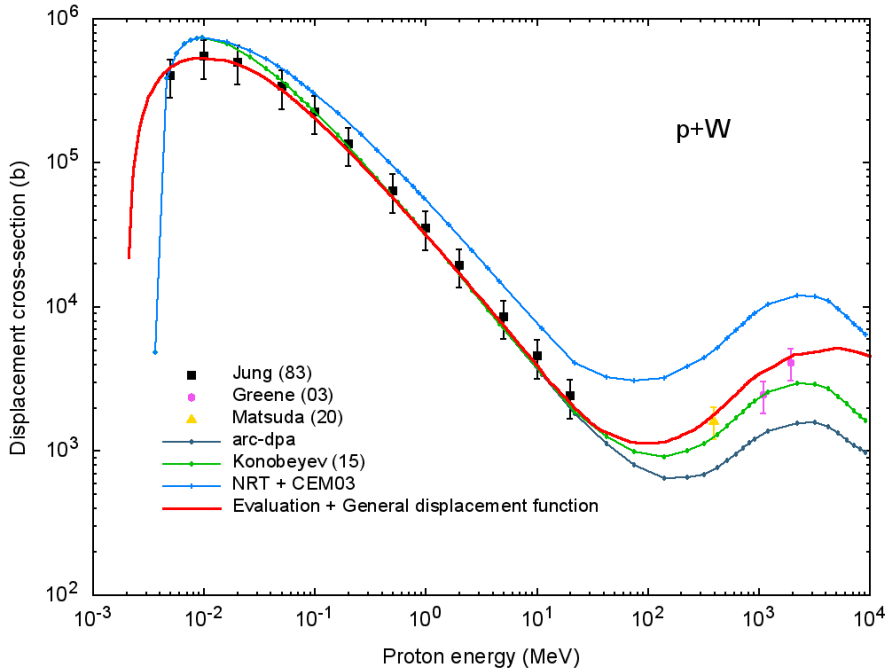

Fig. 5 The same as in Fig.1 for p+W irradiation

It is emphasized that the proton displacement damage cross-section for W agree well with the experimental data as considering the efficiency function increase by combining the BCA calculation. However, as mentioned in Sec. 3.1, the averaged neutron displacement cross-sections for tungsten have obvious difference compared with the experimental data and the reasons for this difference are regarded as the problems of the measurement of the initial damage rate. In order to explain the reasons, the real displacement efficiencies for tungsten in different irradiation conditions are summarized in Table 4. The real displacement efficiency is the ratio of experimental displacement damage cross-section to that calculated using NRT model. For high energy proton irradiation, the efficiencies are between 0.24-0.35. In the high energy proton irradiation, the recoil energies are almost larger than 10 keV and MD simulations shows the efficiencies in this recoil energy range are between 0.2 – 0.4 [24]. It proves that the MD simulation results can be used to fit the arc-dpa model parameters for tungsten and achieve good agreement with proton experimental data. However, for the neutron irradiation, the average defect production efficiencies are larger than 0.5 and they are far away from the MD simulations and proton irradiation experimental data. Therefore, it is deduced that the measurements of the initial damage rate have some problems.

Table 4 Real displacement production efficiency for W

Irradiation sources	Efficiency
LTIF, ORNL	0.555
RTNS, LLL	0.380
LHTL, JRR-3	0.515
TTB, FRM	0.500
389 MeV proton	0.324
1.1 GeV proton	0.246
1.94 GeV proton	0.347

3.3. Discussions about displacement functions

Because the recoil energy spectrum has high level of accuracy, the displacement function calculation becomes very important. To some extent, the displacement function determines the accuracy of displacement damage cross-section calculation. Arc-dpa model is regarded as the physically realistic damage model and also can get better results compared with the NRT model.

However, it has to be mentioned that arc-dpa model does not perform satisfactorily in calculating the displacement damage cross-section of materials irradiated by low and high energy protons and individual neutron energy spectra. The reasons for the limitation of arc-dpa model are regarded as the following two aspects. Firstly, the maximum energy for MD simulations is limited to a few hundred keV due to the limitation of computational resources. Secondly, the variation of the efficiency function is rather complex and simple power efficiency function in arc-dpa model is difficult to describe the real displacement function. Jung proposed to use electron, ion and neutron experimental displacement damage cross-section to derive the displacement function. Usually, the displacement damage cross-sections of materials irradiated by different types of irradiation sources are contributed from the PKA in different energy range. Therefore, theoretically, the method deriving displacement function from Jung should achieve more physically realistic results than others because the displacement function is got in different energy range separately using corresponding irradiation sources in Jung's method. The general displacement function is also divided into three parts to improve the accuracy. Apart from the consideration in Jung's paper, high energy proton irradiation data is also concluded here. The accuracy of displacement function was further improved.

4. Conclusions

General displacement function was proposed for the calculation of displacement damage cross-section. The model parameters in the general displacement function for aluminum, iron, copper and tungsten were obtained and summarized in Table 1. Neutron and proton displacement damage cross-sections were calculated for aluminum, iron, copper and tungsten. Numerical results show that these displacement damage cross-sections agree well with the experimental data. Data obtained [25] can be used for an advanced evaluation of radiation damage rates for examined materials.

Acknowledgements

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