Nucl. Instr. Meth. B431 (2018), pp.55-58

Improved atomic displacement cross-sections for proton irradiation of aluminium, iron, copper, and tungsten at energies up to 10 GeV

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Abstract

Displacement cross-sections for an advanced assessment of radiation damage rates were obtained for a number of structural materials irradiated with protons at energies from threshold up to 10 GeV.

The proposed calculation method utilises an athermal recombination-corrected dpa model with corrections obtained from simulations using the binary collision approximation model. Justification of the method was performed using available measured and systematics data.

Keywords: radiation damage, displacement cross-section, protons

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1. Introduction

A reliable estimate of the radiation damage rate of materials irradiated with nucleons is a challenging task relating to accelerator facilities, spallation neutron sources and accelerator driven units [1,2]. Such estimate takes on special significance for the next generation of medium- and high- energy accelerators [3].

The NRT model [4] is traditionally used for the calculation of radiation damage rates in structural materials. Its relative simplicity and implementation in popular codes (NJOY, MCNPX) makes possible to perform the evaluation of the number of defects produced under the irradiation without much hassle. At the same time, available experimental data [5-7] and more rigorous calculations show the difference with NRT estimations. It makes essential the calculation of displacement cross-sections for structural materials using advanced models, which predictions are close to available measurements.

The recently proposed alternative to the NRT model the athermal recombination-corrected dpa (arc-dpa) model [8,9] and the method of derivation of model parameters [10] makes possible the use of results of molecular dynamics simulations (MD) and available measured data for improved calculation of atomic displacement cross-sections and radiation damage rates in materials. Taking into account the potential value and prospects of application of the arc-dpa approach, the calculation of displacement cross sections using the method [8] is of great interest. The relative simplicity of the method and the availability of parameters for different materials [10] distinguish the use of the model [8] from the direct application of the results of MD modeling, as was done in the works [11-13].

The aim of the present work is the calculation of displacement cross-sections for a number of structural materials of special importance [1,2] using the arc-dpa model [8] and the discussion of the possible improvement of the model for a successful evaluation of displacement cross sections in a wide energy range of incident particles.

The method of calculation is briefly discussed in Section 2. Section 3 presents results of calculations.

2. Method of calculation

2.1 Number of stable displacements

According to the arc-dpa concept the number of stable defects produced under irradiation can be parameterized in the following form [8,9]

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

where T_{dam} is the "damage energy" [6], i.e. the energy available to produce atom displacement by elastic collision [4] calculated using the Robinson formula [14], E_d is the displacement energy averaged over all lattice directions [7]. The defect generation efficiency ξ_{arcdpa} in Eq.(1) is approximated as following [8,9]

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

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

The E_d values were taken for Al equal to 27 eV [6], for Fe 40 eV [6], for Cu 33 eV [8], and for W 70 eV [8]. The following b_{arcdpa}, and c_{arcdpa} values were adopted for calculations, correspondingly, for Al: −0.82, 0.443 [10,16], for Fe: −0.568, 0.286 [8], for Cu: −0.68, 0.16 [8], and for W: −0.564, 0.119 [8,15].

Eq.(1) and (2) were applied to correct simulations performed using the binary collision approximation model (BCA) by analogy with combined BCA-MD calculations described in Refs.[11-13]. The idea of such simulation is to "cut off" the BCA modelling at certain energy of the moving ion T_{crit} and calculate the number of defects formed at energies below T_{crit} using the results of MD simulation or arc-dpa model. In the present work the T_{crit} value was assumed equal to the kinetic energy of the ion corresponding to the T_{dam} of 40 keV, as well as in the BCA-MD calculations [11-13].

The BCA calculations were performed using the IOTA code [17], developed in KIT, Karlsruhe, and for comparison using the SRIM code [18]. In both cases the estimation of the number of stable displacements below T_{crit} was performed using Eq.(1) and (2). Calculations using the IOTA code were performed with default input variables using the Lindhard et al approach (LNS) [19] with parameters from Ref.[20]. Details can be found in Refs.[12,21]. The brief explanation of the SRIM simulations using results of MD modelling or arc-dpa calculation is given in Ref.[17].

Figure 1 and 2 show the efficiency of defect generation [6] calculated for Fe+Fe and O+Fe irradiation. The systematics data (Fig.1) and experimental points (Fig.2) were obtained using results of measurements in Ref.[5].

The data in Fig.1 and 2 shows the agreement between arc-dpa-BCA calculations performed using IOTA and SRIM, measured data and systematics. An essential difference from pure arc-dpa predictions is observed at ion energies above 200-400 keV. The influence of these energies on calculated displacement cross-sections is discussed in Section 3. In order to simplify the use of the obtained results (Fig.1), the efficiency calculated using the arc-dpa-BCA method for Fe-Fe irradiation can be approximated as following:

$$\xi_{arcdpa}(T_{dam}) = \begin{bmatrix} \dfrac{1-c_{arcdpa}}{(2E_d/0.8)^{b_{arcdpa}}} T_{dam}^{b_{arcdpa}} + c_{arcdpa} & \text{when } T < T_{crit} \\ \alpha_1 T^{1/4} + \alpha_2 T^{-1/4} + \alpha_3 & \text{when } T \geq T_{crit} \end{bmatrix}, \qquad (3)$$

where T is the kinetic energy of Fe-ion in MeV, E_d= 40 eV, b_{arcdpa}= -0.568, c_{arcdpa}= 0.286 [8], T_{crit} = 0.075 MeV, and the fitting parameters α_i are as follows: $\alpha_1=7.04\times10^{-4}$, α_2 = -0.0195, α_3 =0.442

The expression Eq.(3) repeats Eq.(2) below the critical kinetical energy of ion T_{crit} and at higher energies approximates the increasing value of ξ_{arcdpa} (Fig.1) predicted by the IOTA calculations.

2.2 Displacement cross-section

The displacement cross-section is calculated using the following expression [22]

$$\sigma_d(E_p) = \sum_i \int_{E_d}^{T_i^{max}} \frac{d\sigma(E_p, Z_T, A_T, Z_i, A_i, T_i)}{dT_i} N_d(Z_T, A_T, Z_i, A_i, T_i) dT_i \qquad (4)$$

where E_p is the incident particle energy; $d\sigma/dT_i$ is the kinetic energy distribution of *i*-th primary knock-on atom (PKA), where *i* refers to elastic scattering or nuclear reaction ; Z and A are the atomic and the mass numbers, “T” and “*i*” relates to the target and the recoil atom, correspondingly, for the elastic scattering $Z_i = Z_T$, $A_i = A_T$; N_d is the number of stable displacements; T_i^{max} is the maximal kinetic energy of the PKA produced in *i*-th reaction; the summation is over all recoil atoms produced by the irradiation.

The calculation of elastic component of σ_d is discussed in Refs.[11-13]. The energy distribution of recoils produced in proton elastic scattering contains contributions of screened Coulomb scattering, the nuclear scattering and their interference. The LNS formula [19,21] with parameters obtained by Winterbon et al Ref.[20] was applied for dσ/dT calculation at proton incident energies below several MeV. At higher energies, calculations were performed using the optical model with parameters of Koning and Delaroche [23] and Madland [24]. Above 500 MeV dσ/dT was calculated using the relativistic formula [25,26]. Fig.3 shows a typical example of the elastic component of σ_d calculated using different approaches. Various calculations "pass one into another", just in the area of their joint applicability [11], which simplifies the evaluation of the elastic part of the displacement cross-section.

The contribution of nonelastic nuclear processes to σ_d was calculated using the CEM03 code [27]. Due to a special combination of models implemented in the code, CEM03 can be used to simulate nuclear processes in the energy range from several MeV to several GeV.

Fig.4 shows a typical contribution of elastic and nonelastic processes to the displacement cross-section. The contribution of elastic scattering dominates at relatively low proton energies below 20 MeV, with increasing energy it is inferior to nonelastic processes, which become dominant at energies above 100 MeV.

3. Results and discussion

Displacement cross-sections were calculated using different approaches for the evaluation of the number of stable displacements N_d: i) Eqs.(1),(2) were applied for all energies of recoil atoms produced under irradiation, ii) the combined arc-dpa-BCA simulation applying the IOTA code was used to get N_d values, as discussed in Section 2.1, iii) N_d was calculated using the standard NRT model with the threshold energies E_d described above.

Figs.5-8 show calculated displacement cross-sections and data from Refs.[28-30]. Results of measurements for tungsten [29] were renormalized using the Frenkel pair resistivity (ρ_{FP}) equal to 27 $\mu\Omega$ m [6,12]. Data shown in figures as "Jung (83)" were obtained from the analysis of integral experiments in Ref.[28] and normalized using the following ρ_{FP} values: Al: 3.7 [6], Fe: 24.6 [6], Cu: 2.0 [29,30], and W: 27 $\mu\Omega$ m [6].

Figures show the good agreement between the arc-dpa Eq.(1),(2) and arc-dpa-BCA calculations for Al at all proton incident energies, and for Fe, Cu, and W at proton energies below 20-50 MeV. At higher energies, the results of arc-dpa-BCA calculations are in better agreement with experimental data for Cu and W (Fig.7,8). The cross sections calculated using the NRT model exceed the results of both calculations at almost all proton energies.

At energies below 20 MeV, the σ_d values calculated using the arc-dpa model are in good agreement with the data [28] for all materials except copper (Fig. 7). One possible explanation is the likely inconsistency of data [28] for copper, since the NRT calculations are close to the data [28] (Fig.7), and on the other hand, the work [28] applies the value of effective threshold energy for copper equal to 100 eV [28], which should result to about three times smaller displacement cross-sections comparing with NRT-calculations. See details in Ref.[6].

At relatively low proton energies, below 20 MeV, and for Al for all energies, the use of Eq.(1),(2) without BCA correction is quite reasonable.

The agreement of the arc-dpa-BCA calculations with the experimental data for copper and tungsten [29,30] are arguments in favour of using this calculation method to obtain the number of stable defects. Such agreement with measurements at proton energies above 100 MeV is observed apparently only for calculations with taking into account the increase of defect generation efficiency in consistence with systematics and measured data [5] (Fig.1,2).

Displacement cross sections obtained using arc-dpa model combined with BCA calculations as described in Section 2.1 were recorded in ENDF-6 format and processed using the NJOY code [31]. The data can be downloaded on Ref.[32].

4. Conclusion

Displacement cross-sections were calculated for proton irradiation of aluminium, iron, copper, and tungsten at proton incident energies from threshold up to 10 GeV. The number of stable defects was estimated using the arc-dpa model with corrections obtained using BCA calculations.

Data obtained [32] can be used for an advanced evaluation of radiation damage rates for examined materials.

The proposed calculation method can be used to obtain displacement cross sections for other materials from beryllium to uranium, for which model parameters are available [10].

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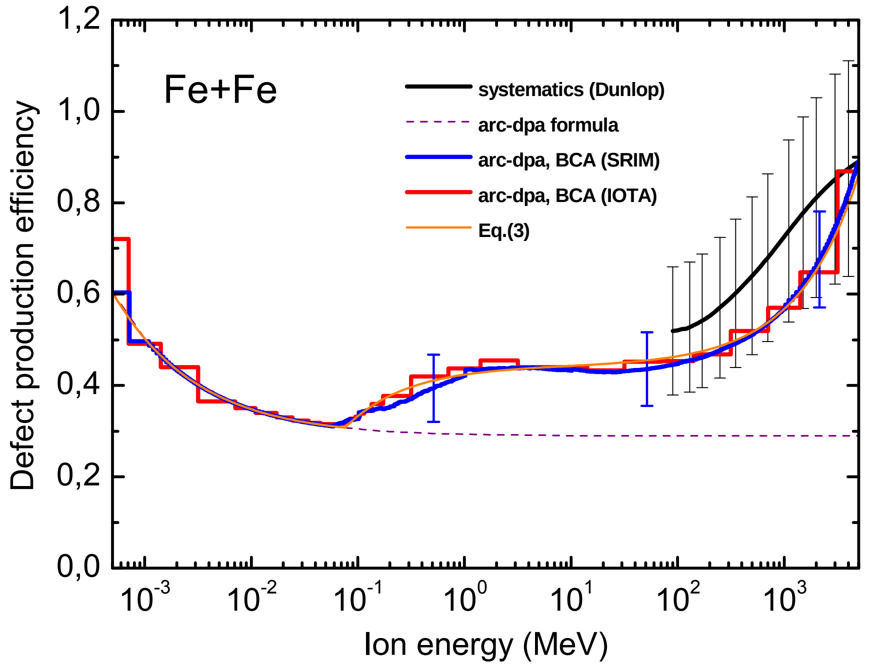

Fig.1 The ratio of the number of stable defects calculated with the IOTA code and the SRIM code using arc-dpa formulas Eq.(1),(2), and estimated using the systematics [5] to the number of defects predicted by the NRT model for Fe+Fe irradiation, and approximate curve Eq(3). See explanations in the text.

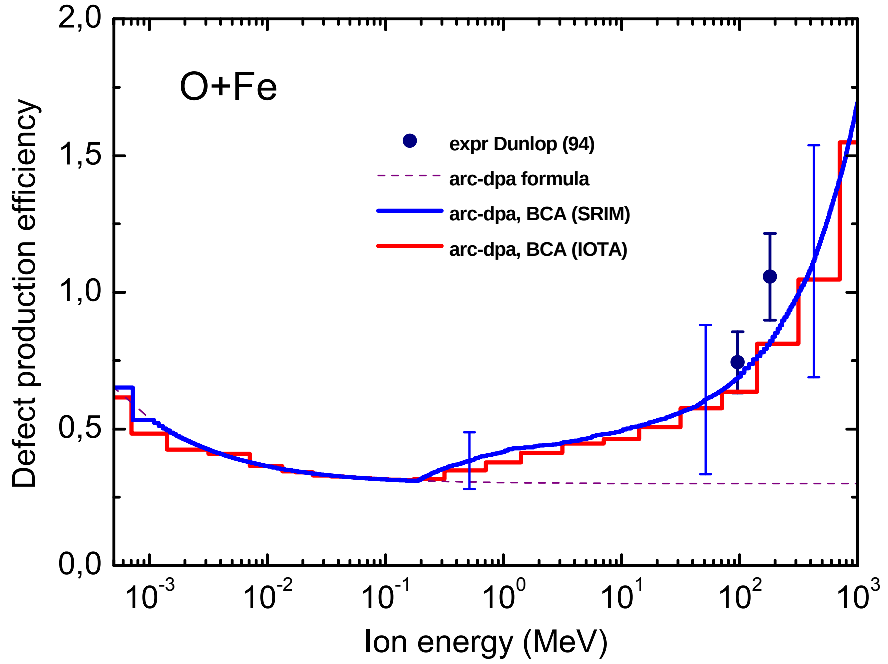

Fig.2 The same as in Fig.1 for O+Fe irradiation. Experimental values are derived from Ref.[5] with E_d values equal to 40 eV.

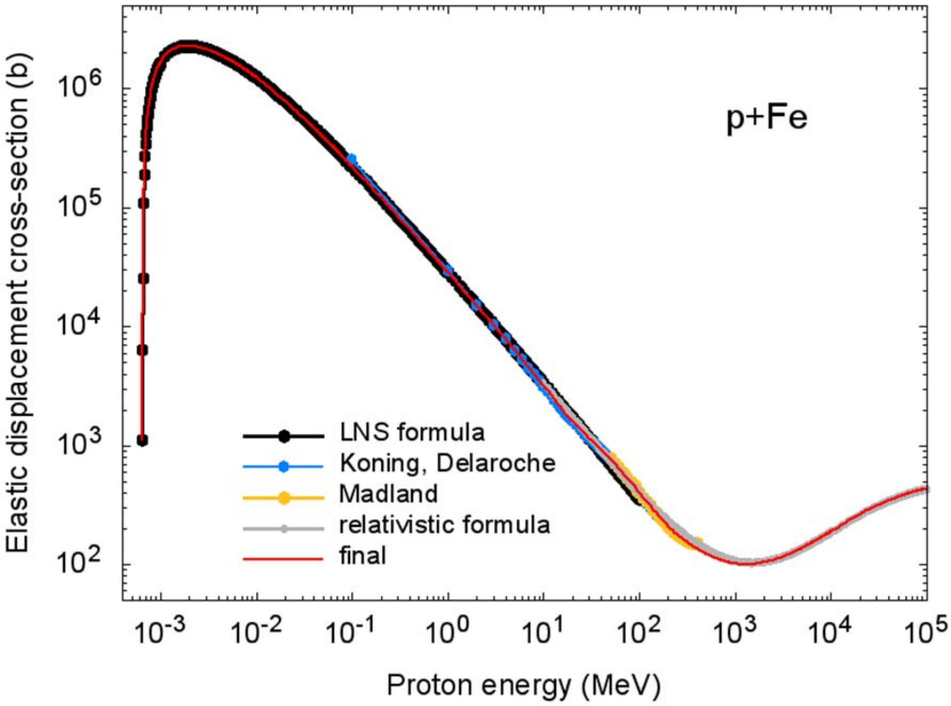

Fig.3 Displacement cross-section for elastic proton scattering on Fe calculated using the LNS formula with parameters from Ref.[19], the optical model with parameters from Ref.[23] ("Koning") and Ref.[24] ("Madland"), and relativistic formula [25,26] and the final estimated data. See explanations in the text.

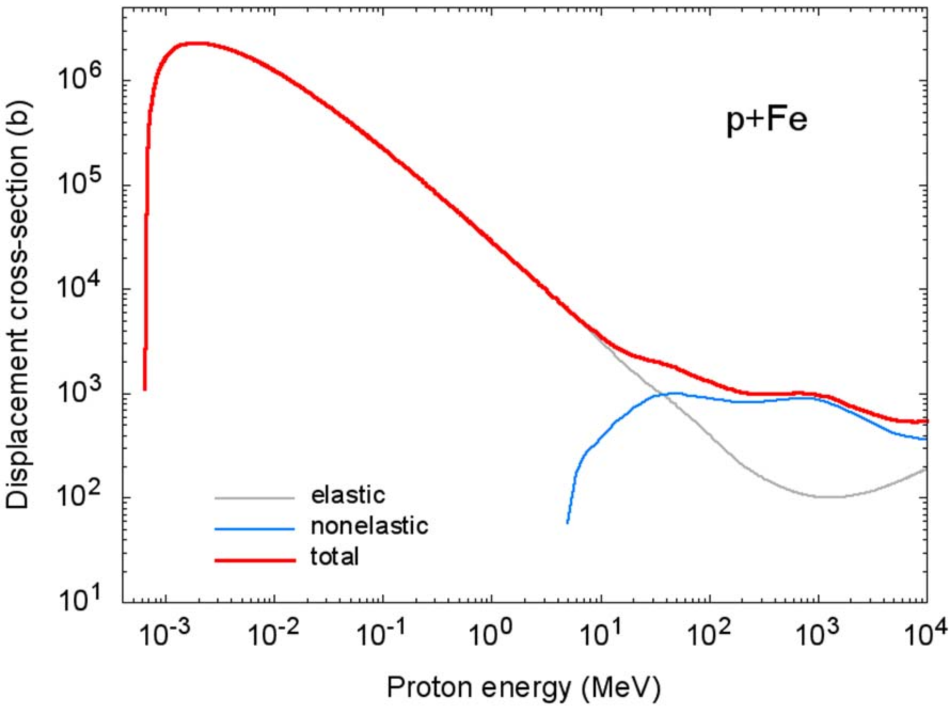

Fig.4 The contribution of elastic scattering and nonelastic nuclear processes to the total displacement cross-section for p+Fe irradiation.

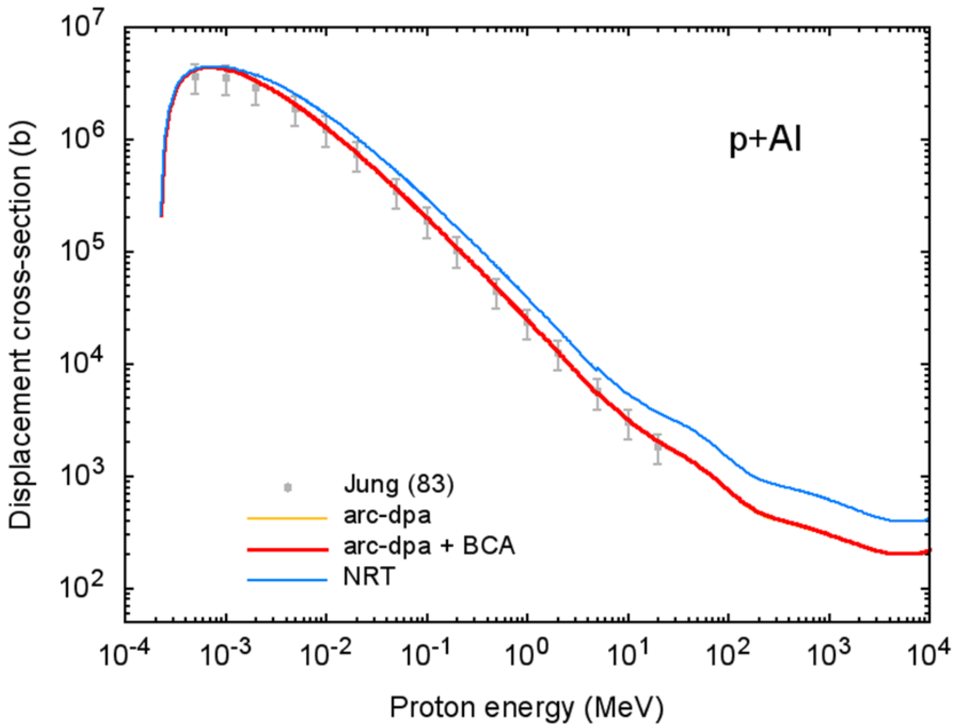

Fig.5 Displacement cross-section for Al irradiated with protons calculated using the arc-dpa model, Eq(1),(2), combined arc-dpa – BCA approach, and the NRT model. Points are obtained from analysis of integral experiments in Ref.[28]. See details in the text.

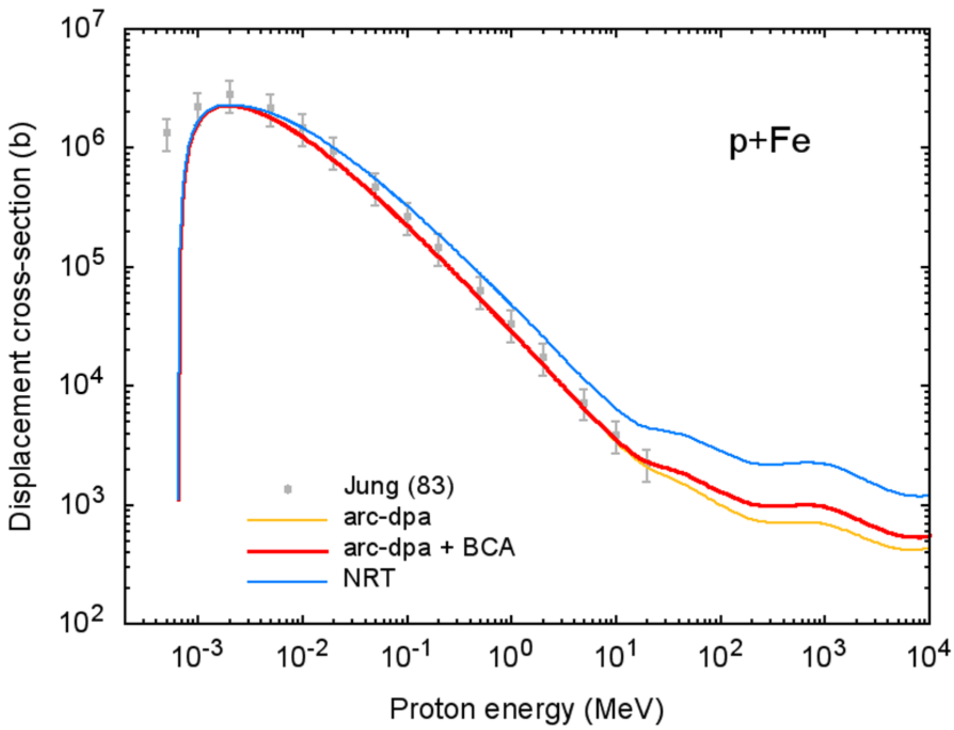

Fig.6 The same as in Fig.5 for p+Fe irradiation.

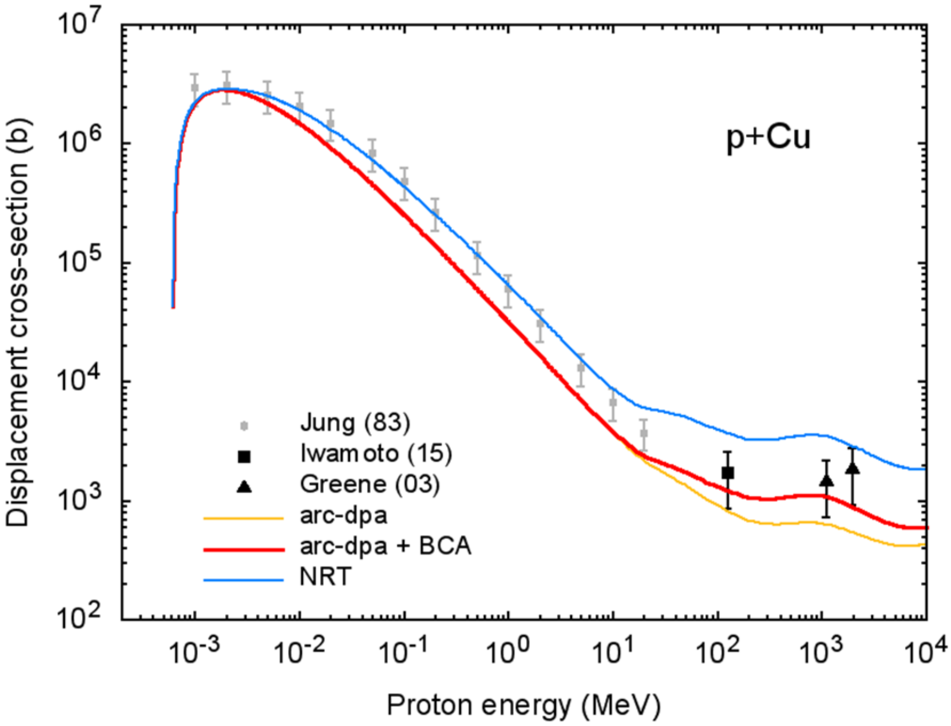

Fig.7 The same as in Fig.5 for p+Cu irradiation. Measured data are from Refs.[29,30].

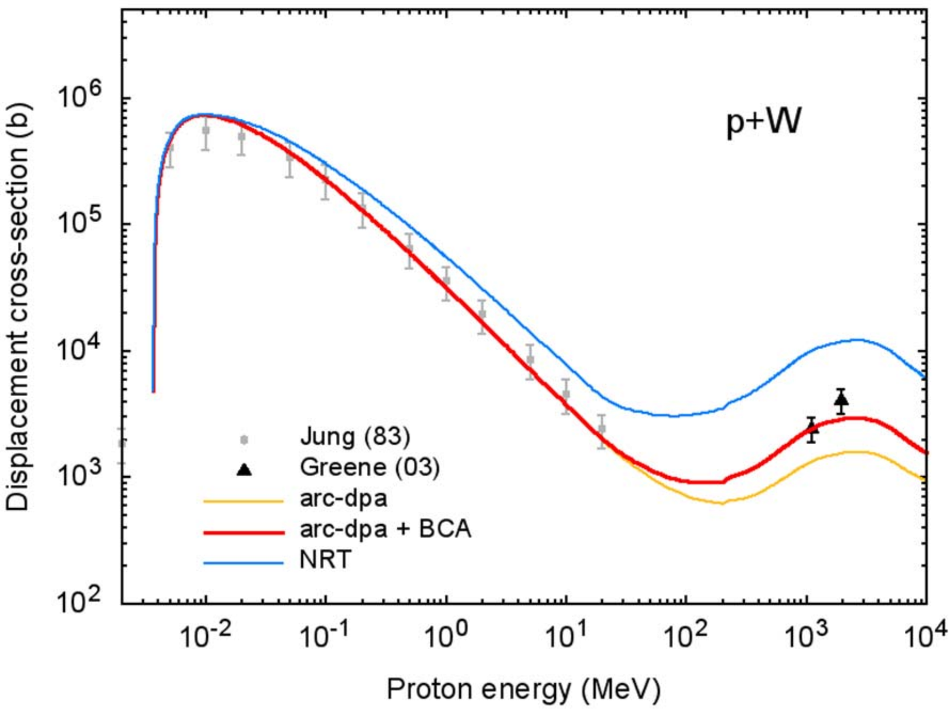

Fig.8 The same as in Fig.5 for p+W irradiation. Measured data are from Ref.[29].