New Data Files for the Calculation of Neutron and Proton Induced Radiation Damage Rates in Structural Materials of High Energy Systems

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Abstract

Displacement cross-sections were obtained for chromium, iron, and nickel using results of the molecular dynamics simulations and calculations using the binary collision approximation model at incident neutron and proton energies from 10^{-5} eV up to 1 GeV. The IOTA code was applied to obtain the number of defects in irradiated materials. At low energies of incident particles nuclear recoil spectra were calculated using ENDF/B-VII data and the NJOY code. Displacement cross-sections are stored using the ENDF-6 format. The first intended application of obtained cross-sections is the calculation of radiation damage dose for materials irradiated in MEGAPIE.

1. Introduction

The calculation of the radiation damage rate in structural materials using results of molecular dynamics simulations (MD) is one of the actual tasks of evaluating of the primary damage of structral materials irradiated in reactors and advanced nuclear energy systems. The first attempts to get displacement cross-sections usable for such calculations have been made for tantalum, tungsten, and iron in Refs.[1,2].

In the present work displacement cross-sections were obtained for chromium, iron, and nickel at the incident nucleon energies from 10^{-5} eV up to 1 GeV using the results of MD simulations and calculations using the the binary collision approximation model (BCA). Data for proton irradation of iron [2] were revised and improved.

The displacement cross-section is calculated as follows

$$\sigma_d(E_p) = \sum_i \int_{E_d}^{T_i^{max}} d\sigma(E_p, Z_T, A_T, Z_i, A_i, T_i)/dT_i \times \nu(T_i, Z_T, A_T, Z_i, A_i)\, dT_i \qquad (1)$$

where E_p is the energy of the incident particle; $d\sigma/dT_i$ is the recoil atom energy distribution depending on Z_T, A_T, Z_i, and A_i which are atomic and mass numbers of the target and the recoil atom produced in the ***i***-th reaction channel, correspondingly, for the elastic scattering $Z_i = Z_T$, $A_i = A_T$; $\nu(T_i)$ is the number of Frenkel pairs produced by the primary knock-on atom (PKA) with the kinetic energy T_i; T_i^{max} is the maximal kinetic energy of the PKA produced in ***i***-th reactions.

The number of defects produced in irradiated material is equal to

$$\nu(T_i) = \eta(T_i)\, N_{NRT}(T_i), \qquad (2)$$

where η is the defect production "efficiency" [1,2] and N_{NRT} is the number of defects calculated accroding to the NRT model

$$N_{NRT} = 0.8 \cdot T_{dam}/(2E_d), \qquad (3)$$

where T_{dam} is the energy transferred to lattice atoms in collision cascades reduced by the losses for electronic stopping of moving atoms; E_d is the effective threshold displacement energy.

2. Simulation of the defect production in irradiated materials

The idea of the simulation is to combine BCA calculations with the results of the MD modelling.

For an ion produced in the nuclear reaction and moving in the material the simulation of atomic collisions is performed by BCA down to a certain minimal kinetic energy (T_{crit}) of the ion. Below this energy the BCA simulation is stopped and the number of defects is estimated using results of the MD modelling.

The energy T_{crit} is about 30-60 keV depending from the target and the highest energy in the MD simulations [1,2].

In the present work the number of defects produced by ions with the kinetic energy below T_{crit} was estimated for chromium and iron according to MD simulations of Vörtler et al. [3], and for nickel according to Bacon et al. [4]. The BCA calculations were performed using the IOTA code [5].

The efficiency of the defect generation $\eta(T)$ is shown in Fig.1 for the self-ion irradiation of iron.

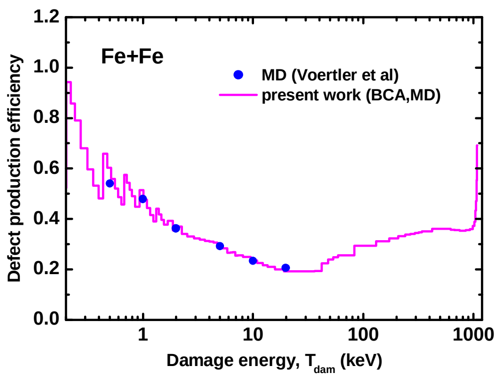

Fig. 1: The efficiency of the defect production for the Fe-Fe irradiation obtained using the combined BCA,MD method (histogram) and results of the MD simulation [3] (dots).

The η value is shown in Fig.1 as a function of the damage energy T_{dam} in the energy range of the primary kinetic energy of Fe ions up to 5 GeV.

The possible explanation of the energy dependence of $\eta(T)$ is presented in Refs.[1,2].

3. Calculation of displacement cross-sections

The total value of the displacement cross-section was calculated as the sum of the displacement cross-section corresponding to the proton or neutron elastic scattering σ_{del} and the displacement cross-section for nucleon nonelastic interactions with target nuclei σ_{dnon}.

The effective threshold displacement energy E_d, Eqs.(1),(3) for chromium, iron, and nickel was taken equal to 40 eV.

3.1 Elastic scattering of nucleons

The σ_{del} values for primary neutrons were calculated using the Koning, Delaroche, and the Madland optical potentials. The example of calculated displacement cross-sections is shown in Fig.2 for natural iron.

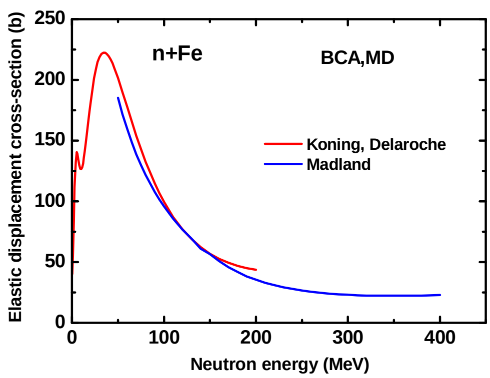

Fig. 2: The displacement cross-section for the elastic neutron scattering on iron calculated using various optical potentials. The number of Frenkel pairs was calculated using BCA,MD approach.

The calculation of σ_{del} for protons with energies up to several MeV has been carried out using the formula for the recoil energy distribution taking into account screening effects in the ion scattering in materials (see details in Ref.[2])

$$d\sigma(E_p,T)=\pi a^2 f(t^{1/2})\frac{dt}{2t^{3/2}}, \qquad (4)$$

where the "a", $f(t^{1/2})$, and "t" are the screening lenght, the screening function, and the reduced energy, correspondingly.

At incident proton energies above 3-4 MeV the displacement cross-section σ_{del} has been calculated using the optical model with Koning, Delaroche, and Madland potentials. Above 0.4 GeV the calculation of σ_{del} has been performed with the help of the relativistic approach (details in Ref.[2]). Fig.3 shows the displacement cross-section for iron irradiated by protons and calculated using various models and approaches.

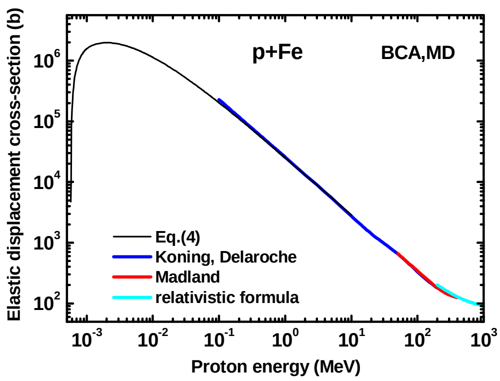

Fig. 3: The displacement cross-section for the elastic proton scattering on iron calculated using Eq.(4), optical model with Koning, Delaroche and Madland potentials, and using the relativistic formula for the recoil energy distribution (see details in Ref.[2]).

The good agreement is observed between various approaches (Figs.2,3) in ranges of their combined applicability.

3.2 Nonelastic interactions of nucleons with nuclei

To estimate the value of displacement cross-sections for nonelastic nucleon interactions σ_{dnon}, the atomic collision cascades in materials were simulated for all residual atoms produced in nuclear reactions induced by primary nucleons using the method described in Section 2.

Calculations of the recoil energy distributions were performed using nuclear models implemented in MCNPX [6], CASCADE [7], and DISCA-C [8] codes. The simulation of atomic collision was performed using the combined BCA,MD approach with the help of the IOTA code [5].

The example of the displacement cross-section calculated for nucleon nonelastic interactions with ^{56}Fe at the primary energy 600 MeV is shown in Table 1.

The scatter of σ_{dnon} values calculated using various nuclear models is observed at any incident particle energy. An appropriate way of evalaution of σ_{dnon} is the averaging of cross-sections obtained by different models with the weights proportional to their predictive abilities [2]. Because the question about the predictive power of various models is still open especially for recoil spectra calculations, in the present work the evaluation of σ_{dnon} was performed using equal weights for all nuclear models. One should note that the list of models used at various incident energies of primary particles is different depending on the applicability of the models.

Table 1: Displacement cross-sections (b) for nonelastic interactions of 0.6 GeV neutrons and protons with ^{56}Fe.

Nuclear model	Neutrons	Protons
Bertini/Dresner	807	727
Bertini/ABLA	864	775
ISABEL/Dresner	815	732
ISABEL/ABLA	857	776
CEM03	781	712
INCL4/Dresner	956	849
INCL4/ABLA	1002	894
CASCADE	796	717
DISCA-C	870	786
Average value	861 ± 75	774 ± 62

4. Evaluated displacement cross-sections

Evaluated values of displacement cross-sections were obtained for natural mixtures of isotopes for chromium, iron, and nickel at the incident energy from 10^{-5} eV to 1 GeV. At energies below 20 MeV nuclear data used for the calculation of the recoil spectra were taken from ENDF/B-VII. Data were processed using the NJOY code with the new subroutine containing tabulated ν(T) data, Eq.(2).

Inconsistencies in nonelastic cross-sections observed in MCNPX calculations at 0.4 GeV were eliminated in the σ_{dnon} evaluation.

Two data sets of displacement cross-sections were prepared for each target basing on BCA, MD and the the NRT model.

Data are stored in the ENDF-6 format. The MF file number 3 and MT section numbers 900 and 901 were used to record displacement cross-sections obtained using the BCA,MD approach and NRT, correspondingly.

Fig. 4 shows the example of evaluated data for iron at intermediate energies.

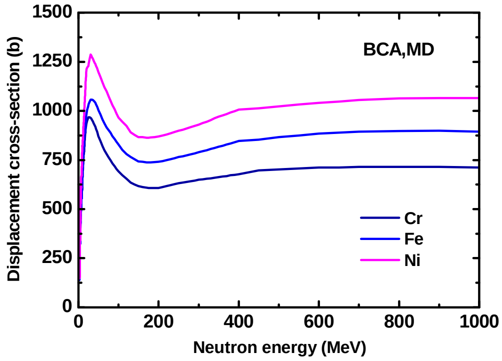

Fig. 4: The evaluated displacement cross-sections for iron irradiated by neutrons at intermediate energies. The number of defects was calculated using the BCA,MD approach.

5. Conclusion

Displacement cross-sections were obtained for chromium, iron, and nickel irradiated with neutrons and protons at energies from 10^{-5} eV up to 1 GeV using the binary collision approximation model and results of molecular dynamics simulations.

The first intended application of the data obtained is the calculation of radiation damage dose for stainless steel irradiated in MEGAPIE.

References

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