DPA AND GAS PRODUCTION IN INTERMEDIATE AND HIGH ENERGY PARTICLE INTERACTIONS WITH ACCELERATOR COMPONENTS

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Abstract

A brief overview of methods for the calculation of the number of stable defects in irradiated materials is presented. Special attention is given to the evaluation of gas production cross-sections performed using nuclear models, experimental data, and systematics. The perspective of the use of evaluated data files for dpa and gas production calculations is discussed.

INTRODUCTION

A calculation of radiation damage and gas production rates in materials is a challenging task combining the modelling of nuclear interactions, the simulation of the material behaviour, and taking into account, as far as possible, experimental data.

The calculation of atomic displacement cross-section consists of two independent parts: the calculation of recoil energy distributions for involved nuclear reactions and the evaluation of the number of stable displacements in materials. The report presents a brief overview of methods of calculation and main important results obtained for the number of defects produced in materials under irradiation. Special attention is given to the evaluation of gas production cross-sections using results of nuclear model calculations, experimental data, and systematics predictions.

DPA PRODUCTION

The dpa production (radiation damage) rate is calculated by summing of integrals of particle- and energy-dependent displacement cross-section σ_d and particle flux over all particle types. The displacement cross-section for incident particle with the kinetic energy E_p is calculated as follows:

$$\sigma_d(E_p)=\sum_i \int_{E_d}^{T_i^{max}} (d\sigma_i(E_p,T_i)/dT_i)\, N_D(T_i)\, dT_i \qquad (1)$$

where $d\sigma_i/dT_i$ is the recoil atom energy distribution for i-th reaction; $N_D(T_i)$ 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 in *i*-th reaction; E_d is the effective threshold displacement energy of material.

Estimating the Number of Stable Defects

The number of stable displacements N_D can be calculated using different approaches with varying degrees of complexity of code implementation and accuracy of predictions.

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The NRT displacement model [1] remains popular in spite of well known shortcomings such as neglecting of an athermal recombination and the use of isotropic displacement energy [2]. The model in more general form [3] is implemented in NJOY [4], LAHET [5], MCNP [6] and other codes, which maintains its popularity for applications. According to the model the number of stable defects produced by the ion with the kinetic energy T_{PKA} is equal to

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

where T_{dam} is the energy transferred to lattice atoms reduced by the losses for electronic stopping of atoms in displacement cascade.

The measure of deviations of the N_D number obtained experimentally or theoretically from one predicted by NRT is quantified as "defect production efficiency"

$$\xi=N_D(T_{PKA})/N_{NRT}(T_{PKA}), \qquad (3)$$

The NRT model has "internal" limitations like for the maximal kinetic energy of PKA [1,7]. Predicted N_{NRT} numbers differs with some exceptions from the measured values for neutron irradiation in reactors [8,9] as for high energy protons [8], and results of molecular dynamics (MD) simulations. For example, the typical ξ value obtained using MD for iron and nickel at T_{dam} below 100 eV exceeds one, and is about 0.3 at 10 -100 keV [2].

The binary collision approximation model (BCA) is a popular method for the simulation of ion interactions with materials, which should be used with care for the estimation of realistic number of stable defects produced under irradiation.

An attempt to reproduce results of MD simulations by a proper choice of BCA parameters leads in many cases to an uncertainty of predictions at ion energies outside MD modelling [8,9]. The recent evaluation of popular BCA code SRIM [10] stated the problem of the calculation of correct number of stable displacements "in any absolute sense" [11].

One of advantages of BCA is the relative simplicity of the direct implementation in codes for the simulation of the particle transport using the Monte Carlo method.

The molecular dynamics simulation is the most adequate method to get realistic number of stable defects produced in irradiated materials.

The electronic losses and interatomic potential are still crucial points concerning the reliability of simulations. At least for iron and copper the total number of stable displacements calculated using MD with modern interatomic potentials are in agreement with experimental

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data [2,8]. However, the fraction of defects in clusters calculated using different potentials varies significantly [2].

The number of works relating to MD simulations is definitely large and only a limited part concerns the information on stable displacements in materials relevant to the present report. The following works presenting calculated N_D values for different materials are to be mentioned, for metals: Al [12-14], Ti [13], V [15-17], Fe [18-24], Ni [13,14,25-27], Cu [13,14,28-33], Zr [13,30,34,35], Mo [36], W [15,28,37,38], Pt [14], Au [14], alloys: Fe-Cr [22,39,40], Fe-Cr-C [41], Ni_3Al [13], Ni-Fe [25], Cu-Au [42], U-Mo [43], semiconductors: Si [14,44], Ge [14], GaN [45], carbides: SiC [46,47], Fe_3C [48], WC [49], oxides: MgO [50], UO_2 [51], spinels: $MgAl_2O_4$ [52], $MgGa_2O_4$ [52], $MgIn_2O_4$ [52], and zirconolite, $CaZrTi_2O_7$ [53]. Other important papers concerning materials discussed can be found in reference sections of corresponding publications.

Apparently, the range of MD application is limited by ion energies, where energetic losses are properly treated. Ref.[54] presents a brief discussion. With an exception of Ref.[19] where the maximal energy of simulation for iron, E_{MD} is equal to 200 keV and the corresponding PKA energy about 425.5 keV, other works have focused on simulations with E_{MD} energies up to several tens of keV.

The N_D values obtained in MD simulations demonstrate rather weak temperature dependence [11]. In general, N_D decreases with the increase of temperature [18,29]; whereas the comparison some results, for example, for copper in Ref.[28] at 10K Ref. and Ref.[29] at 300 K does not show any significant difference.

The modelling using MD is complicate enough and restricted by the ion-energies to be directly implemented in high energy particle codes.

The N_D values obtained in Refs.[12-53] and experimental data [8,55-58] can be applied for evaluation of the radiation damage in materials after an extrapolation of MD results to the range of higher energies of PKA.

Extrapolation of MD results to higher energies outside the range of simulations is necessary to estimate radiation damage rate of materials irradiated with intermediate and high energy particles in different units.

The simple solution is to use a "constant efficiency" approximation, where the ξ value at the maximal energy of MD simulation $E_{MD}^{(max)}$ is used for all energies above $E_{MD}^{(max)}$.The approximation was applied in Ref.[28] for the analysis of the damage production in Cu and W irradiated with 1.1 and 1.94 GeV protons [57].

Recently proposed alternative to the NRT formula [2,59] also assumes the constant efficiency at high PKA energies. An athermal recombination corrected displacement damage (arc-dpa) [2,59] is calculated with the following efficiency value

$$\xi(E) = (1\text{-}c)\,(2E_d/0.8)^{-b}\,E^b + c, \qquad (3)$$

where "b" and "c" are parameters, "c" corresponds to the saturation at high energies [2], and it supposed that $b < 0$.

The approximation seems reasonable up to rather high energies of PKA, where deviations from measured data [58] are established [9].

The other way to get the number of stable defects at high PKA energies is the modelling using combined BCA-MD method [60,61].

The BCA-MD simul ation seems to be an effective approach for the evaluation of the number of defects produced in materials under the irradiation with intermediate and high energy particles.

The idea is to perform BCA simulations for atomic collisions caused by all PKAs produced in the nuclear reaction up to a certain "critical" energy of ions. Below this energy, which is usually taken equal to 30-60 keV [9], the BCA modelling is stopped and the number of defects is estimated according to results of MD simulations.

Figure 1 shows the example of combined BCA-MD modelling. Other examples and details can be found in Refs.[9,60-64].

As well as the "pure" BCA" model, the combined BCA-MD method is rather easily implemented in Monte Carlo particle transport codes.

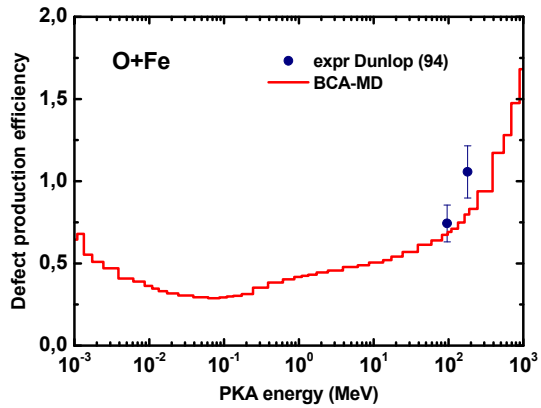

Figure 1: The ξ values the O+Fe irradiation.

Kinetic Monte Carlo (KMC) [65] is the method for the simulation of the long-term defect evolution. While the MD technique provides the information about atomistic processes up to nanoseconds, the KMC method is able to track the cascade damage up to seconds [28,66] and hours [67]. In the KMC method the primary defects such as individual point defects, clusters, and impurities are considered as "objects", which evolution is tracked over time [65]. Various approaches in KMC modelling like object KMC, event KMC, and atomic KMC differ in the details of simulation, description of object interaction and treatment of time scales [65,66].

It may seem reasonable to apply for the evaluation of radiation damage the N_D values predicted by KMC, as it is done, for example, for iron in Ref.[67], and not ones estimated with MD or BCA-MD simulations. At the same time, the uncertainties concerning KMC simulations make the direct use of KMC results rather premature [68].

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Calculation of Recoil Energy Distributions

The calculation of recoil energy distributions in nuclear reactions is another integral part of displacement cross-section computations.

The dσ/dT values can be obtained using an information from evaluated data files such as ENDF/B or calculated using theoretical models suitable for the description of elastic and non-elastic interaction of primary particles with material.

Figure 2 shows an example of dσ/dT values calculated using various nuclear models [6,69] for non-elastic interactions of 1 GeV protons with ^{56}Fe. The difference in corresponding σ_d values calculated using the NRT model is illustrated in Fig. 3. Other examples of energy recoil distributions calculated using evaluated data libraries and nuclear model codes can be found in Ref.[70].

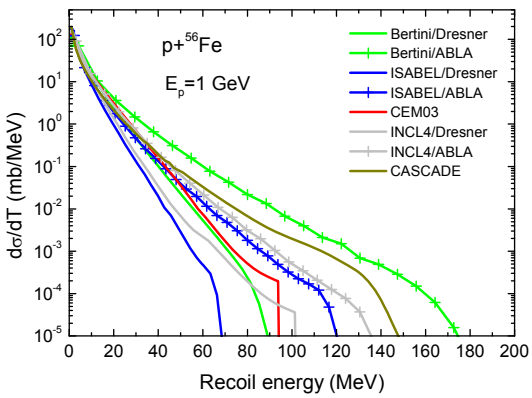

Figure 2: Example of calculated dσ/dT values.

The difference in calculated recoil energy distributions using various models leads to statistically different results of σ_d cross-section. In this case the evaluated value of displacement cross-section is calculated as a weighted sum of results obtained using different models [60,61]. Weights reflect the "quality" of corresponding nuclear models in describing experimental data relevant to the task and can be calculated as inverse values of deviation factors, discussed e.g. in Ref.[71].

Modelling Using High Energy Particle Transport Codes

Three general approaches can be used for improved calculations of radiation damage rate using particle transport codes. In the first approach the simulation of nuclear and atomic interactions with primary particles are supplemented by direct BCA or BCA-MD modelling. An advantage of the method is complete sequential simulation of damage production during the irradiation. Problems concern the possible use of experimental information for defect production and the computational time. In most cases, the approach has no advantage over less time-consuming methods discussed below.

The next approach uses N_D values calculated using BCA-MD(+KMC) and corrected applying available experimental data. The ξ(E) obtained in a parameterized form or pointwise is used for all PKAs generated after elastic and non-elastic interactions of particles with atoms. The approach is implemented in MARS15 [72], FLUKA [73], and PHITS [74] codes. For light targets, it seems reasonable to use individual ξ(E) values for PKAs with different Z and A produced in nuclear reactions.

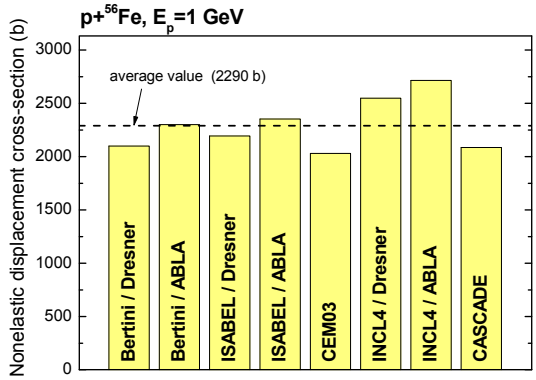

Figure 3: Example of calculated σ_d values.

The third approach applies evaluated atomic displacement cross-sections. It is the most flexible way to use available experimental data for defect production and to apply advanced nuclear models for calculation of recoil energy distributions and systematics data.

Recently displacement cross-sections were evaluated for neutron and proton interactions with Al, Ti, V, Cr, Fe, Ni, Cu, Zr, and W at incident energies from 10^{-5} eV to 3 GeV [75]. The evaluated data can be supplemented by estimated covariance matrices relating to uncertainties of applied model parameters [76].

GAS PRODUCTION

A reliable estimation of gas production rate in nuclear reactions is performed either by using well tested nuclear models describing the emission of light fragments in nuclear reactions, or by using evaluated data properly combining available measured and systematics data with results of model calculations with optimized parameters.

The progress in the accuracy of gas production cross-sections calculations at intermediate and high energies of primary particles is primarily associated with the constant development and improvement of computational methods implemented in MARS15 [72], CEM03 [77], Geant4 [78], FLUKA [73] , INCL4 [79], and CASCADE [69,80] codes. At incident nucleon energies below 100-200 MeV an important role plays the development of models implemented in TALYS [81,82] and EMPIRE [83] codes. Illustrations of the difference in gas production cross sections calculated using different models can be found in Ref.[70].

The use of evaluated H- and He-isotopes production cross-sections is the most flexible and reliable way to get gas production rates under irradiation. As a rule, the cross-section evaluation procedure comprises an analysis

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of measurements, calculations using nuclear models relevant for specific energy ranges, and the proper statistical combination of theoretical and experimental data, taking into account calculated and experimental uncertainties.

Recently, proton-, deuteron-, triton-, ^{3}He-, and ^{4}He-production cross-sections for neutron and proton induced reactions were evaluated for Al, Cr, Fe, Ni, W [75], and Ti [84] at incident energies from 10^{-5} eV to 3 GeV.

Even if no experimental data are available for the investigated target, the calculated H and He-isotope production cross sections can be corrected using "reference data for gas production cross-sections" obtained in Ref.[85]. The data [85] concern information on proton, deuteron, triton, ^{3}He, and ^{4}He production cross-sections for 278 stable target nuclei from Li to B at fixed incident proton energies 62, 90, 150, 600, 800, and 1200 MeV. To obtain such data [85], the atomic mass dependence of corresponding cross sections was evaluated using available experimental data and results of calculations using different nuclear models, in contrast to the usual evaluation of the energy dependence of cross sections for investigated reactions.

CONCLUSION

The methods for the calculation of the number of stable defects, N_D in irradiated materials, the NRT model, the BCA model, the simulations using MD, and KMC are briefly discussed. In most cases, the calculation of radiation damage rate in materials requires the information on N_D values at the energies outside MD simulations. The use of combined BCA-MD method for the estimation of N_D at such energies is promising.

Various approaches including the use of evaluated data files for reliable assessment of radiation damage and gas production rates are discussed.

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