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Comparative study of survived displacement damage defects in iron irradiated in IFMIF and fusion power reactors

S.P. Simakov *, A.Yu. Konobeyev, U. Fischer, V. Heinzel

Forschungszentrum Karlsruhe, Institute for Reactor Safety, D-76021 Karlsruhe, Germany

ABSTRACT

The assessment of the primary survived defects rates in iron such as vacancies-interstitials pairs and simplest clusters have been performed for the IFMIF, fusion power plant and research reactor. This was achieved by a modified version of the NJOY code, when processing evaluated nuclear cross section file. The modifications accounted for the reduction of the available damage energy predicted by the standard NRT model by the surviving defects fractions. These fractions were picked-up from the molecular dynamics and binary collisions simulation results available in the literature. The number of primary survived and clustered defects in the α-iron irradiated in the high flux test module of IFMIF was estimated as 10 and 6 dpa/fpy or several times less than standard NRT estimates at the level of 30 dpa/fpy. The comparison with damages in iron calculated for irradiation in the first wall of fusion power plant gave however the same reduction factors, that supports the qualification of IFMIF as a fusion material irradiation facility.

1. Introduction

The mission of International Fusion Material Irradiation Facility (IFMIF) [1] is to provide the neutron source to test samples of candidate materials for fusion power reactors (FPR). The most challenge goal is to achieve an annual radiation dose in the High Flux Test Module (HFTM) up to 20 displacements per atom for the low activation steel to predict its radiation behaviour in the first wall (FW) of a Fusion Power Reactors (FPR) [2].

Many efforts have been already applied to evaluate the expected damage rate and show that IFMIF will represent irradiated materials properties for fusion technology [1,3]. All these assessments relied on the model of the Norgett, Robinson and Torrens (NRT) [4], which predicts only the number of initial displaced atoms produced in neutron induced reactions and then in the cascades of atom–atom collisions. Recently new theoretical considerations based on molecular dynamics model (MD) analyses have shown that during the cascade evolution many initial vacancies and interstitials will recombine (see [5,6] and many references in the latest review [7]). The survival ratio (number of survived defects to NRT predictions) is less than one and depends on the energy of primary knock-on atom (PKA). This means that the number of survived displacements averaged over the neutron spectrum will decrease in comparison with standard NRT estimate and may be different for irradiations in IFMIF and FPR, since their neutron spectra are different in shape and extend to the different highest energies 55 MeV and 15 MeV, correspondingly.

In the present work the absolute number of survived radiation defects is evaluated for α-iron irradiated in the HFTM/IFMIF in comparison with FW/FPR as well as research fission reactor. This is achieved by calculating the PKA spectra in the different irradiation environments and applying the defect survival ratios based on MD simulations. This procedure allows the assessment of the radiation induced displacement damage on the basis of the advanced knowledge of the defect formation mechanisms.

2. Neutron and PKA spectra

In the present analyses the irradiation conditions for iron were compared in the following three nuclear facilities:

- High Flux Test Module of IFMIF with two deuteron beams impinging the lithium jet target [1],
- outboard center of the First Wall (FW) of Fusion Power Reactor (FPR) with Helium Cooled Pebble Bed (HCPB) and Lithium Lead (HCLL) blankets at 3.4 GW thermal power [2],
- sample column 5 of the High Flux Reactor (HFR/C5)at Petten [8].

The energy differential neutron fluxes in these facilities were calculated by appropriate computational tools, geometrical models and nuclear data [3,9]. They are shown in upper parts of Figs. 1 and 2 using logarithmic and linear energy scales, whereas the energy integrated neutron fluxes are summarized in Table 1. It is seen that in the energy domain below 1 MeV the IFMIF facility will

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* Corresponding author. Tel.: +49 7247 823761; fax: +49 7247 823718.
E-mail address: simakov@irs.fzk.de (S.P. Simakov).

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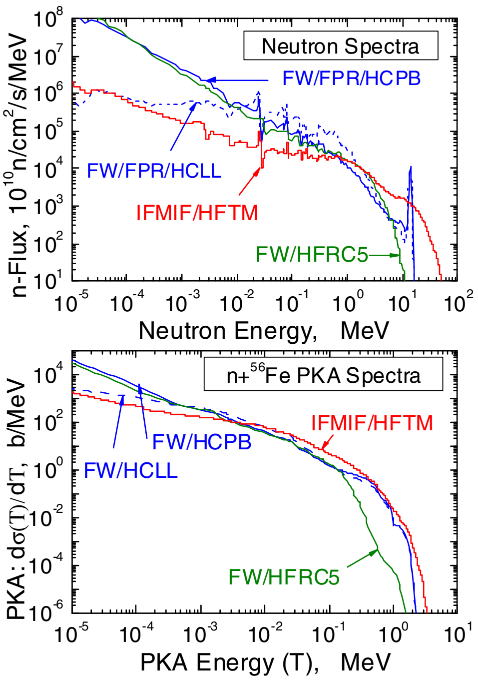

Fig. 1. Neutron energy differential flux (top) for different nuclear systems and spectrum-weighted distribution of PKAs produced by neutrons in iron (bottom).

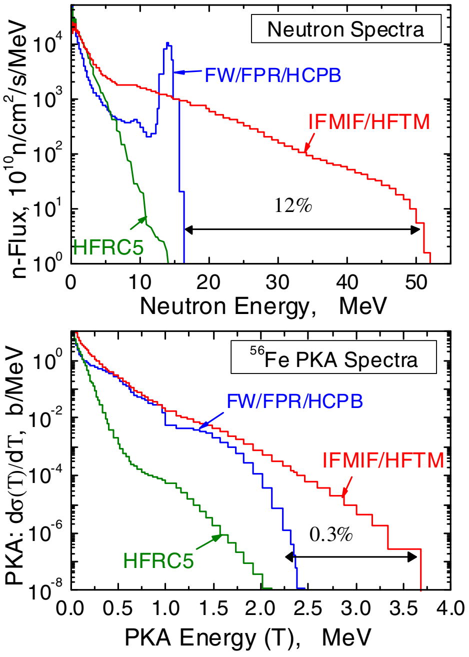

Fig. 2. The same as Fig. 1, but with a linear scale for the energy.

reasonably represent the neutron flux inside the first wall of DEMO reactor with the HCLL blanket but underestimate it in the case of HCPB blanket producing more epithermal neutrons. This difference, however, is not so critical since damage and gas productions are caused mainly by fast neutrons. Most essential differences are observed at high energies, where the neutron spectrum in fusion facilities cuts off at 15 MeV while for IFMIF it extends up to 55 MeV. As Table 1 shows, the fraction of such neutrons will amount to about 12%.

The energy differential cross sections of primary knock-on atoms (PKAs) with atomic mass *A* more than four produced by monoenegetic neutrons incident on iron were calculated by the latest version 99.259 of the NJOY code [10] during the processing of the ENDF/B-VII files. The obtained recoil matrices were weighted by neutron spectra to get an averaged primary PKA energy distribution specific for each energy system under consideration. They are displayed in the bottoms of Figs. 1 and 2 and clearly show that the difference in neutron spectra results to the difference in the PKAs spectra. It is relatively small in the low energy domain ($T < 1$ MeV), but becomes essential above this recoil energy: in the fusion reactor the maximal energy will reach 2.4 MeV, whereas in IFMIF the spectrum extends up to 3.7 MeV. It is worthwhile to notice that the fraction of these IFMIF PKAs is relatively small, i.e. about 0.3%.

Fig. 3 shows the contributions of different reactions to the PKA spectra. In all facilities elastic scattering Fe(n,n) dominates (78–97%), than followed by inelastic scattering ^{56}Fe(n,n')^{56}Fe (correspondingly 20–3%), ^{56}Fe(n,2n)^{55}Fe reaction (1.5–1.0%) and helium production ^{56}Fe(n,α)^{53}Cr (<0.2%). The later is exothermic one with $Q = 0.326$ MeV, that explains the excess of the ^{53}Cr recoil energy above the ^{56}Fe one.

3. Assessment of the defects production rate

The created reaction residuals will slow down in iron lattice and kick off the atoms producing in such a way a cascade of initial displaced atoms and vacancies. These displacements are accounted for by the Norgett, Robinson and Torrens model (NRT), which is a standard option of NJOY code. It calculates an available damage energy production cross section E_a (further will be called as 'damage energy') produced by all *i* recoils with energy T_i:

$$E_a(E) = \sum_i \int_{E_d}^{T} \frac{d\sigma(E,T_i)}{dT_i} P(T_i)\, dT_i \tag{1}$$

The formula takes into account that only the portion $P(T_i)$ of recoil energy can be transferred to lattice atoms (damage efficiency), while the other part will be dissipated among electrons. The partition function *P* was obtained by Torrens basing on the electronic screening theory of Linhard [11]. The damage energy (1) is used then for estimation of displacement cross sections:

$$\sigma = \frac{0.8}{2E_d} E_a \tag{2}$$

where E_d is an energy needed to eject an atom from its lattice position. The damage energy and displacement cross section for ^{56}Fe calculated by NJOY from ENDF/B-VII file using NRT model and $E_d = 40$ eV are shown in Fig. 4.

Extensive molecular dynamics (MD) calculations [5–7] deliver the information on (i) survived point defects, i.e. vacancies and self-interstitial atoms (Frankel pairs), N_{FP}, and (ii) interstitial clusters, N_{IC}, accumulated in the host lattice at the end of the cooling phase of the thermal spike in the cascade zone. The corresponding ratios to the NRT number of primary PKAs, N_{NRT}, are the functions of recoil energy *T*: (but are practically independent on the crystal structure and ambient temperature):

$$\eta_{FP}(T) = \frac{N_{FP}}{N_{NRT}} \quad \text{or} \quad \eta_{IC}(T) = \frac{N_{IC}}{N_{NRT}} \tag{3}$$

The summary of MD results for α-iron lattice are depicted in Figs. 5 and 6, demonstrating that the fraction of survived point defects decreases as PKAs energy increases and reaches its minimum 0.3 at 100 keV, whereas the probability to form the clusters opens above 0.1 keV and saturates above 1 keV. Above 100 keV the MD simulations are still not available, whereas PKAs energies extend up to 2400 keV in the FPR and 3700 keV in IFMIF (Figs. 1 and 2). To get $\eta_{FP}(T)$ and $n_{IC}(T)$ in this energy domain we extrapolated

Table 1
Irradiation conditions and correlations of dpa rates produced in iron irradiated in IFMIF, Fusion power plant and fission reactor.

Parameter	Facility and irradiation spot		
	Accelerator source HFTM of IFMIF	Fusion plant FW of PPCS/HCPB	Fission reactor HFR/Column 5
Facility power and neutron flux intensity			
Thermal power	10 MW	3.4 GW	45 MW
n-flux, total	$7.3 \times 10^{+14}$ n/cm^2/s	$11 \times 10^{+14}$ n/cm^2/s	$12 \times 10^{+14}$ n/cm^2/s
n-flux fraction with $E > 15$ MeV	12%	–	–
Primary Knock-on Atoms (PKA)			
Maximal PKA energy	3.7 MeV	2.7 MeV	1.2 MeV
PKAs fraction with $T > 2.3$ MeV	0.3%	–	–
Cross section ^{56}Fe(n,x)PKA	3.1 b	5.2 b	7.2 b
Contribution of (n,n)^{56}Fe	77.5%	93.8%	97.3%
contribution of (n,n′)^{56}Fe	19.8%	4.6%	2.6%
Contribution of (n,2n)^{55}Fe	1.5%	1.1%	–
Contribution of (n,α)^{53}Cr	0.2%	0.1%	0.1%
Displacement damage to iron lattice			
Initial vacancies-interstitials (NRT)	29.4 dpa/fpy	19.9 dpa/fpy	10.0 dpa/fpy
Frankel pairs defects (NRT + MD)	9.7 dpa/fpy	6.7 dpa/fpy	3.3 dpa/fpy
Ratio survived to initial	0.33	0.33	0.33
Interstitials clusters defects (NRT + MD)	5.6 dpa/fpy	3.8 dpa/fpy	1.9 dpa/fpy
Ratio survived to initial	0.19	0.19	0.19

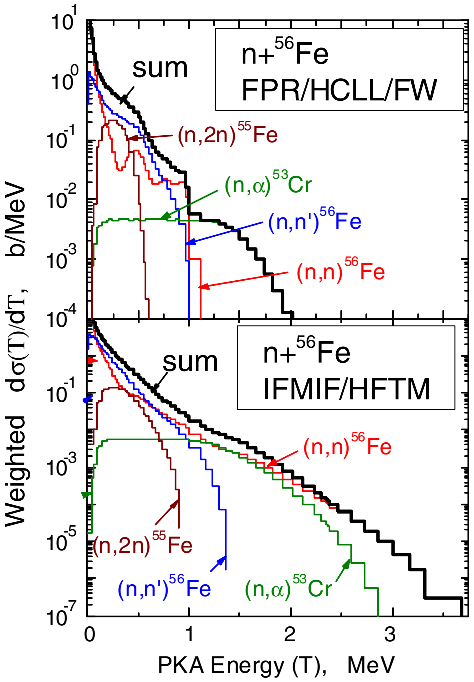

Fig. 3. Neutron spectrum-weighted PKA's differential cross sections for n + ^{56}Fe for specific reaction channels and their sum.

the fit curves obtained to the MD results below 100 keV, supposing the moderate increasing for the Frenkel pairs (this reflects the tendency for cascade to break up into sub-cascades as it was observed in MD simulations) and saturation for clustering surviving functions. This is supported as well by binary collision approximation (BCA) calculations [12], where the MD surviving fraction for Frenkel pairs was applied for cascade species when its energies drop below 100 keV.

To calculate the number of survived defects the HEATR module of the NJOY code was modified in such a way that it reduces the specific contribution to the total damage energy (1) from every recoil by multiplying the available damage energy $P(T_i)$ by the relevant surviving function (3) for every species and energy T_i. These functions for all residual nuclei were assumed to be the same as for Fe atoms, because MD results are not available for other recoils. This suggestion seems will not affect the final results, since the contribution of other recoils besides Fe is less than 2% (Table 1).

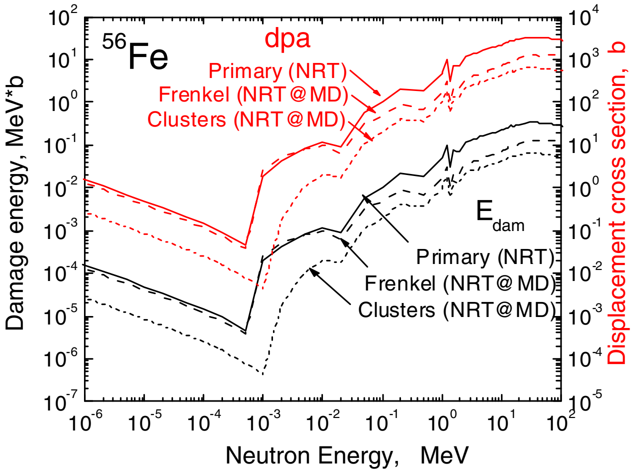

Fig. 4. Damage energy and displacement cross sections for the neutron induced reaction on iron.

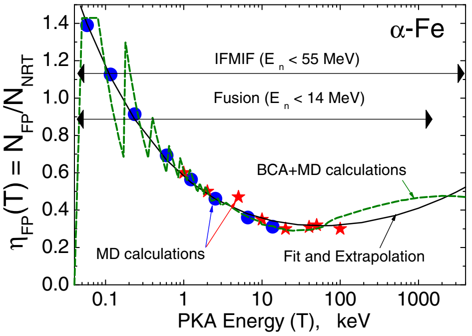

Fig. 5. Fraction of survived Frenkel pairs to the NRT initial PKAs versus the recoil kinematic energy: blue points and red stars – MD simulations [5] and [6], green dashed curve – BCA/MD simulations [11], black solid curve – fit used in present calculations. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

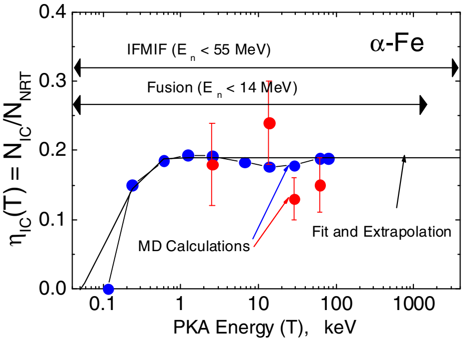

Fig. 6. Thee same as Fig. 5, but for fraction of survived clusters to the NRT initial PKAs.

Table 1 lists the displacement rate in iron matrix caused by irradiation in the different nuclear facilities operating at scheduled power. The rates of the initial generated displacements as calculated by NRT model amounts to 30, 20 and 10 dpa per full power year (fpy) in HFTM of IFMIF, first wall of FR with HCPB blanket and in the sample column #5 of HFR, respectively. The production rate of survived primary point and clustered defects after recombination phase of initial ones will be 3 and 5 times less for all facilities under consideration. Such insensitivity to the neutron spectra could be explained by the dominant contribution of the neutrons with energies above 0.1 MeV to the total displacement damage. As Fig. 4 shows in this energy domain the displacement cross sections for the survived defects are proportional to NRT one. The present results are in agreement with those for Frenkel pairs obtained in the similar analysis for fusion and fission reactors [5,12].

The results of calculations depend on extrapolation of surviving ratios which presently can be predicted by the MD simulations only up to PKA energies 100 keV. In the case of Frankel pairs the extending of ratios up to 4000 keV is guided by the BCA calculations, whereas for the interstitial clusters remains to be a guess. To assess the sensitivity of results to the possible variation of surviving ratio, the $n_{IC}(T)$ was linearly increased from 0.19 to 0.38 in the energy range from 100 keV to 4000 keV. This results to the increasing of the number of survived interstitial clusters by factor 1.8, which turns out to be practically the same for all neutron spectra used.

4. Conclusions

In the present work the attempt was made to estimate the number of survived Frenkel pair defects and interstitial clusters produced in the iron under irradiation in the accelerator driven facility (IFMIF) in comparison with fusion power plants as well as a fission research reactor. This was done in a similar way which usually used to estimate the initial number of interstitial-vacancy pairs (NRT model): folding of the corresponding neutron differential flux with a damage energy obtained during processing of the evaluated data by the NJOY code. The main problem on this way was found to be a lack of the MD calculation results for the PKAs energies above 100 keV, that necessitates the extrapolation and guessing for surviving fractions up to 4 MeV relying on BCA calculations and general considerations.

Applying this approach, it was found that the mean damage rates caused in the mild iron steels during irradiation inside the HFTM of IFMIF will be 10 dpa/fpy and 5.6 dpa/fpy for the survived interstitial-vacancies pairs and those collapsed in the clusters in the cascade zone after its cooling, correspondingly. The important finding is that the ratios of survived damages to the initial NRT pairs turn out to be the same for all three considered systems. This means that from this view of survived defects IFMIF remains to be an appropriate neutron source to simulate material radiation damage effects expected in fusion power reactors.

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