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Effect of activation cross section uncertainties in the assessment of primary damage for MFE/IFE low-activation steels irradiated in IFMIF

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ABSTRACT

The present study is mainly aimed to provide the primary damage (displacements per atom, generation of solid transmutants and gas production rates) of structural materials irradiated in the high and medium flux test modules of the International Fusion Materials Irradiation Facility (IFMIF). We have investigated if the change of the composition during the irradiation time has effect on the prediction of the atomic displacements. The effect of the activation cross section uncertainties in the assessment of both solid transmutants and hydrogen and helium production is also analyzed. The results are provided element-by-element, so that the primary damage of any material irradiated in such neutron environments can be easily assessed; in this paper, we have predicted the primary damage of the low activation steel Eurofer.

1. Introduction and problem description

The subject of damage/transmutation calculations in IFMIF facility has been covered extensively. In the primary damage assessment of irradiated materials, the displacements per atom (dpa) and gas production rates during the irradiation time have to be predicted. These quantities are needed for qualifying the material behaviour of some candidate structural materials for Magnetic and Inertial Fusion Energy (MFE/IFE) [1].

In this respect, the IFMIF community has made efforts to validate inventory codes. Our ACAB [2] code has demonstrated a quantitative agreement with such codes. However, very few works have addressed uncertainty analysis to draw conclusions on the reliability of those acceptable results under the potential impact of activation cross section uncertainties. Here, we address this problem in a comprehensive way using a Monte Carlo method implemented in ACAB code.

In this paper, the transmutation/damage behaviour is investigated under different neutron flux spectra corresponding to both the IFMIF high flux test module (HFTM) (7.3×10^{14} n/cm^{2}s, $\langle E \rangle \sim 5.6$ MeV and 97.7% of neutrons having energies above 0.1 MeV) and the medium flux test module (MFTM) (1.2×10^{14} n/cm^{2}s, $\langle E \rangle \sim 2.4$ MeV) [3]. In Section 2, the related methodology involved in ACAB code is presented. In Section 3, we have performed an element-by-element analysis and it has been demonstrated as a helpful tool to easily analyse the damage/transmutation performance of irradiated materials. The contribution of each source-element to the generation of any transmutant product and dpa is obtained in a straightforward way. The primary damage assessment for the low activation steel Eurofer [3] is presented in Section 4.

2. Methodology

The computational system ACAB is able to compute the inventory evolution as well as a number of related inventory response functions useful for safety and waste management assessments. ACAB predicts the H- and He-production by nuclear reactions (n,xH) or (n,xHe) on all nuclei. In addition, ACAB provides the generation/depletion of transmutants and the number of dpas. The prediction of atomic displacements is written as

$$\frac{dpa}{s} = \sum_i \rho^i \cdot \phi \cdot \frac{\sigma_D^i}{2E_d^i}, \tag{1}$$

where ρ^i is the number density of nuclide i, ϕ is the total neutron flux, σ_D^i (eV – b) is the one-group damage energy production cross section of nuclide i and E_d^i is the energy required to displace the atom i from its lattice, being the sum extended over all isotopes. Therefore, ACAB can predict the evolution of the dpa magnitude during the irradiation time using Eq. (1). In order to predict the number of dpas, a multigroup damage library is required to be collapsed with the neutron flux spectra. So, a multigroup damage

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library based on ENDF/B-VII.0 has been processed with NJOY99.220. This library can be requested from the NEA Data Bank.

We have calculated the effect of activation cross section uncertainties in the assessment of H- and He-production and generation/depletion of transmutants using the Monte Carlo method implemented in ACAB. This procedure is based on simultaneous random sampling of all the cross sections involved in the problem. We will make use of the recent EAF2005/UN [4] uncertainty library to perform this job [5].

3. Element-by-element transmutation

An extensive evaluation has been performed to assess the importance of the element-by-element transmutation in both the HFTM [6] and MFTM neutron environments. Firstly, the dpa, H- and He-gas production are analyzed. In Table 1, dpa values for typical intended and impurities steel elements are illustrated after one year of irradiation time. For Fe, we have obtained 38 dpa in HFTM and 3 dpa in MFTM. Moreover, we have seen that the prediction of dpa/s in Fe does not change significantly during the irradiation time. For HFTM, at the initial time composition, we obtain 1.19E−06 dpa/s, and after one year of irradiation time, this value only decreases in 0.4%. The contributions to the generation of H and He are obtained in a straightforward way, and the relative errors are shown in Table 1. For Fe, the H- and He-production relative errors are less than 7%, and similar uncertainty values appear in HFTM and MFTM. It can be seen that the largest uncertainty values (~40%) are obtained for C in the prediction of He. In this case, ~66% of the total He production is due to the reaction $^{12}C(n,n2\alpha)\alpha$, with a relative error in the cross section of ~48%. The data shown in Table 1 for Fe can be used for a preliminary assessment of steels. For instance, in the case of Eurofer, the contribution of Fe after one year of irradiation in HFTM and MFTM is ~89% in dpas, ~91% in the generation of H and ~85% for He.

Secondly, the evolution of solid transmutants is investigated. In Table 2 we have predicted the element-by-element transmutation processes and the relative error in HFTM after one year of irradiation time: the depletion of the initial *Z* element and the generation of new elements are given. The Cr will be transmuted mainly into V with a relative error of 3% and the Mn into Cr with an error of 9%. The W will increase the level of Ta and Re, with a relative error of 11% and 4%, respectively. We have found that the induced uncertainty in the activation performance of most of the generated or depleted intended elements is around 10%. C and Ti have the maximum uncertainties with 25% and 19%, respectively.

4. Comparative study of Eurofer steel transmutation

The element-by-element transmutation results presented in Section 3 can be used to predict the transmutation/damage performance of any material irradiated in these neutron environments. Here, the primary damage is calculated for the low activation steel Eurofer [3]. In Table 3, the dpa values are shown after one year of irradiation time: 38 dpa in HFTM and 3 dpa in MFTM. The main contributions to these values, both in HFTM and MFTM, are Fe (~89%) and Cr (~10%).

Additionally, changes of the Eurofer initial elements are shown in Table 3. The transmutation of the main constituents of Eurofer, Fe, C and Cr, are not significant. For HFTM, the prediction of minor constituents of Eurofer increases in all cases, +7% for B, +25% for Ti, +9% for V, +23% for Mn and +2% for Ta. The maximum relative errors are for Ti and Ta, 11.8% and 17.4%, respectively. In general, new elements are generated during the irradiation time in the vicinity of the initial elements (5 appm for Re). For MFTM, the maximum transmutation (+2%) appears for Ti and Mn.

The total H- and He-production are comparable to some initial constituents. In the case of HFTM we predict 1346 appm and 292 appm, for H and He, respectively. This production is due to (n,xH) and (n,xHe) reactions in Fe. In the case of HFTM, the isotope ^{56}Fe produces ~70% of the total amount of H via (n,p) and (n,np) reactions, and ~73% of He via (n,He) and (n,nHe) reactions.

The relative error in the prediction of H is 6.5% in HFTM and 5.3% in MFTM. In the case of He, similar errors are observed. These small relative errors are a consequence of the low uncertainty of the (n,xH) and (n,xHe) cross sections for ^{56}Fe. The relative errors for the (n,nHe) and (n,nH) cross sections are 8.3%. Lower uncertainties remain for (n,He) and (n,H) reactions, 1.6% and 1%, respectively.

Table 1
Damage (in dpas), gas production rates for hydrogen and helium (appm) and relative error (ε, in %) of typical intended and impurities elements in reduced activation steels after 1 year of irradiation time in the HFTM and MFTM/IFMIF.

Z	Element	HFTM/IFMIF					MFTM/IFMIF				
		dpa	H	ε (%)	He	ε (%)	dpa	H	ε (%)	He	ε (%)
5	B	18	806	7	3474	7	3	58	9	1273	7
6	C	18	423	16	3431	39	3	34	17	278	41
7	N	25	2683	12	2468	12	3	215	12	145	19
8	O	35	359	10	1397	8	4	28	9	93	10
13	Al	47	1084	9	703	10	5	78	9	53	9
14	Si	55	2309	4	1202	4	5	171	4	87	5
15	P	54	3936	17	880	14	4	288	18	62	19
16	S	50	4281	8	2662	13	4	283	10	150	15
22	Ti	44	986	8	415	32	4	76	8	35	33
23	V	24	659	10	81	7	2	49	8	6	4
24	Cr	40	1143	6	300	12	3	86	5	24	9
25	Mn	33	844	17	197	31	3	66	17	16	33
26	Fe	38	1445	7	293	5	3	107	6	23	5
27	Co	37	1249	17	259	27	3	98	17	21	30
28	Ni	50	5787	6	1808	29	4	433	6	170	20
29	Cu	51	2030	17	317	5	4	142	18	25	4
39	Y	51	789	16	52	8	4	60	16	4	5
41	Nb	19	738	15	120	17	2	57	14	9	13
42	Mo	19	1120	12	104	9	2	89	13	8	9
73	Ta	10	193	24	19	26	1	14	24	1	22
74	W	12	224	10	26	12	1	16	10	2	10

Table 2
Transmutants (appm) and relative error (ε, in %) of typical intended and impurities elements in reduced activation steels after 1 year of irradiation in the HFTM/IFMIF.

		Transmutants (appm) and relative error (in %)									
		$Z-2$		$Z-1$		Z		$Z+1$		$Z+2$	
Z	Initial element	ε (%)	appm	ε (%)	appm	ε (%)	appm	ε (%)	appm	ε (%)	ε (%)
5	B	2466	9	351	7	−3362	7	0	16	0	22
6	C	475	6	357	19	−1845	25	0	30	0	68
7	N	1823	5	2671	12	−4817	8	0	60	0	22
8	O	1364	8	216	14	−1610	7	0	48	0	51
13	Al	231	5	1124	10	−1382	8	13	12	0	15
14	Si	1255	5	926	4	−2202	4	1	15	0	33
15	P	254	49	3610	18	−3907	17	23	29	0	68
16	S	2838	13	1502	18	−4371	10	1	12	0	22
22	Ti	390	34	317	9	−709	19	1	14	0	17
23	V	5	36	666	12	−726	11	54	11	0	22
24	Cr	350	10	1930	3	−2282	3	0	19	0	21
25	Mn	121	50	1562	9	−1773	9	86	10	0	68
26	Fe	395	8	1081	7	−1511	7	0	13	0	21
27	Co	149	47	2961	8	−3132	8	14	15	0	15
28	Ni	4099	5	2360	3	−6941	5	1	10	0	12
29	Cu	258	4	4165	8	−4925	7	482	3	0	51
39	Y	8	11	3105	5	−3232	5	111	15	0	21
41	Nb	60	14	2267	5	−2348	5	2	15	0	15
42	Mo	230	14	1038	12	−1935	7	604	7	30	15
73	Ta	9	44	4695	10	−7036	8	2332	10	0	11
74	W	102	26	1692	11	−3461	6	1663	4	4	11

Table 3
Elemental composition (appm) of Eurofer steel and transmutation (appm) and relative error (ε, in %) after 1 year of irradiation time in the HFTM and MFTM/IFMIF.

Element (dpa)	Initial appm	HFTM/IFMIF 38		MFTM/IFMIF 3	
		appm	ε (%)	appm	ε (%)
H	0	1346	6.5	101	5.3
He	0	292	5.2	23	4.6
B	51	4	9.6	0	17.3
C	4860	−4	52.6	0	59.6
N	1191	−5	7.8	0	9.3
O	348	−1	7.3	0	8.5
Al	206	1	7.3	0	7.3
Si	990	−2	6.3	0	5.9
P	90	−0.2	31.8	−0.02	34.7
S	87	−0.3	11.0	−0.02	12.4
Ti	116	29	11.8	2	8.0
V	2183	207	3.1	17	2.2
Cr	96 233	128	22.3	7	28.0
Mn	4048	918	7.0	76	5.9
Fe	885 883	−1282	6.8	−102	5.2
Co	47	0.1	12.0	0.1	1.6
Ni	47	−0.1	17.5	−0.01	21.5
Cu	44	−0.2	7.2	−0.03	6.1
Nb	6	0.02	25.3	0.01	23.3
Mo	29	−0.1	7.6	−0.01	9.1
Ta	215	4	17.4	0	44.9
W	3327	−10	6.8	−1	7.6
Re	0	5	4.2	1	6.8
Os	0	0.01	0.00	0	0.0

5. Conclusions

In order to assess the primary damage behaviour of low activation steels irradiated in IFMIF, the ACAB code has been used. It provides the generation/depletion of solid and gaseous transmutants coupled with the number of dpas. We have concluded that the dpa rate is nearly constant in one year of irradiation time.

In addition, the impact of potential activation cross section uncertainties on the transmutation calculations has been analyzed. We have calculated the effect of the cross section uncertainties in all steel elements under different neutron IFMIF environments, and we can conclude that the errors in transmutants depend on neutron flux and spectrum. For HFTM we have found significant uncertainties in the transmutation responses for C, P, Cr, Ni, Nb and Ta. In the case of H- and He-gas production the maximum uncertainty is below 7%, both in HFTM and MFTM.

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