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TRANS_MU computer code for computation of transmutant formation kinetics in advanced structural materials for fusion reactors

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Abstract

A method of controlling a systematic error in transmutation computations is described for a class of problems, in which strictly a one-parental and one-residual nucleus are considered in each nuclear transformation channel. A discrete-logical algorithm is stated for the differential equations system matrix to reduce it to a block-triangular type. A computing procedure is developed determining a strict estimation of a computing error for each value of the computation results for the above named class of transmutation computation problems with some additional restrictions on the complexity of the nuclei transformations scheme. The computer code for this computing procedure – TRANS_MU – compared with an analogue approach has a number of advantages. Besides the mentioned quantitative control of a systematic and computing errors as an important feature of the code TRANS_MU, it is necessary to indicate the calculation of the contribution of each considered reaction to the transmutant accumulation and gas production. The application of the TRANS_MU computer code is shown using copper alloys as an example when the planning of irradiation experiments with fusion reactor material specimens in fission reactors, and processing the experimental results.

1. Introduction

In studies of alloy property changes due to radiation and on determinate of their fitness for fusion reactors, an reliable calculation of radiation effects is of great importance.

The main part of the investigations of reactor material properties is carried out in research reactors with plenty of special irradiation channels and methodical provisions for conducting irradiation experiments.

When planning and performing irradiation of fusion reactor materials, a comparative analysis of irradiation conditions in a fission reactor and those in a fusion reactor is required for the correspondence of their basic radiation parameters: damage rates, hydrogen and helium isotope accumulation rates and chemical composition change due to transmutation.

The TRANS_MU computer code (developed in SSC RF RIAR) is presented here in order to estimate isotope composition changes in alloys under irradiation with the control mathematical and computing errors. The basic mathematical model of the computer code is described and examples given of its application to estimate radiation effects in advanced fusion reactor materials.

2. Statement of the task

In the given work the transmutation computation tasks are considered at constant neutron-physical parameters. These tasks are reduced to solving the Cauchy problem for a linear ordinary differential system (ODS) with constant coefficients. The nuclear transformation scheme of such computations is an oriented graph with loaded edges. The nodes correspond to variables in ODS, and the edges to the nuclear transformations.

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Each edge is characterised by the rate value (nondiagonal element of the ODS matrix) in the corresponding transformation channel under irradiation conditions under computation.

The range of the rate values for different transformation reactions is very wide. The greatest values exceed 10^{15} s^{-1} (short-lived isotopes decay), the smallest ones are in the range 10^{-20}–10^{-25} s^{-1}. Though, in theory one isotope could produce all others existing in nature (>2200), very few isotopes (usually no more than 5) are accumulated in significant quantities. Therefore the nuclear transformation scheme of a certain material includes a limited number of isotopes and channels. The limitation of the scheme causes a systematic error in the transmutation computation.

The proposed mathematical model of isonucleus transmutation [1] with definitions stated in the paper [2], and the theorem of an enclosed task on isonucleus transmutation computation make it possible to find a two-way estimation of the solution of the isonucleus transmutation methodical standard through the solution of a particular computation in a specified subclass of tasks.

The computation procedure is developed for a certain subclass of tasks for isonucleus transmutation computation. The implementation of calculations in terms of interval arithmetic for the described procedure gives guaranteed estimations of computation error for each value of the computation results.

3. Control of the methodical error in a class of tasks for isonucleus transmutation computation

For the control of a systematic error in the computations of structural material transmutations a mathematical model of isonucleus transmutation [1] is proposed, where, according to the definition, in each channel of nuclear transformations there is exactly one target isotope and one residual isotope.

Definition 1. A task of isonucleus transmutation computation (TITC) is the Cauchy task of dimension n

$$\frac{dA(t)}{dt} = RA(t), \quad A(0) = A_0 \geqslant 0. \tag{1}$$

The elements of a matrix R are constant and satisfy the following equations:

$$\begin{aligned} &r_{ii} \leqslant 0, && 1 \leqslant i \leqslant n, \\ &r_{ij} \geqslant 0, && 1 \leqslant i \neq j \leqslant n, \\ &\sum_i r_{ij} = 0, && 1 \leqslant j \leqslant n. \end{aligned} \tag{2}$$

Definition 2. Enclosed in TITC of dimension n Eq. (1) by the first m variables is the TITC of dimension $m + 1$

$$\frac{dB(t)}{dt} = SB(t), \quad B(0) = B_0, \tag{3}$$

where the matrix S is determined by the first m columns of the matrix R:

$$\begin{aligned} &S_{ij} = r_{ij}, && 1 \leqslant i,\ j \leqslant m, \\ &S_{im+1} = 0, && 1 \leqslant i \leqslant m = 1, \\ &S_{m+1,j} = \sum_{i=m+1}^{n} r_{ij}, && 1 \leqslant j \leqslant m. \end{aligned}$$

Vector B_0 is determined by the vector A_0:

$$b_{0,j} = a_{0,j}, \quad 1 \leqslant j \leqslant m,$$

$$b_{0,m+1} = \sum_{j=m+1}^{n} a_{0,j}.$$

Only the first m of variables from n in the initial TITC is considered in the enclosed TITC. The last variable in the enclosed TITC has the meaning of a collector for all transformation in the initial TITC, where a target isotope variable has number $\leqslant m$, and a residual one $>m$.

In the TITC class, an adequate description of nuclear fission and reactions of nuclear synthesis is impossible. For the lightest nuclei, the choice of a residual isotope from the decay or reaction products is ambiguous. However, for the nuclei with the atomic charge from 10 up to 80, a hypothetical TITC (STITC) can be accepted as the systematic standard of isonucleus transmutation computations. STITC includes all natural isotopes and reactions of nuclear transformations.

To consider a particular transmutation computation as TITC enclosed in STITC, it is necessary:

- to consider strictly one target and one residual isotope in each transformation channel;
- to determine full elimination rate for all isotopes included in the scheme;
- to add a collector variable to the isotope variables under consideration and a difference between the full elimination rate of a given isotope and the sum of rates of transformations for all the reaction included in the scheme and to take it as a transformation rate of a given isotope into the collector.

The way of controlling a systematic error proceeds from the following theorem.

The enclosed TITC theorem. If $A(t)$ is the solution of a TITC (1), and $B(t)$ the solution of enclosed TITC Eq. (3), at $t \geqslant 0$ the following inequalities hold true:

$$b_j(t) \leqslant a_j(t) \leqslant b_j(t) + b_{m+1}(t) \quad \text{at } 1 \leqslant j \leqslant m, \tag{4}$$

$$0 \leqslant a_j(t) \leqslant b_{m+1}(t) \quad \text{at } m+1 \leqslant j \leqslant n. \tag{5}$$

Thus, the current value of the enclosed TITC collector variable is equal to the width of an interval of the double-sided estimations (4) and (5) of the STITC solution.

4. Computing procedure for computation tasks of isonucleus transmutation

The TITC matrix is brought to a block-triangular form by means of the discrete-logic analysis of the nuclear transformations scheme [2]. By simplification of the scheme (excluding the accumulation in the low-rate reactions from consideration), it is possible to ensure the fulfilment of the condition: the dimension of diagonal blocks does not exceed the given maximum value. For TITC enclosed in STITC, the systematic error caused by simplification of the scheme will be computed in the two-way estimations (4) and (5).

The problem of eigenvalues of matrix R is factorized with diagonal blocks. The important additional information on the spectrum and eigenbasis of TITC matrixes, determined by equalities (2), can be obtained from the simple relation with stochastic matrixes:

$$\frac{1}{k}R^{\mathrm{T}} + E = S, \tag{6}$$

where R^{T} is the transposed TITC matrix, E the matrix 1 of dimension n, S the stochastic matrix of dimension n, and k the constant, satisfying an inequality $k \geqslant \max|r_{ii}|$.

All known spectral properties of stochastic matrixes are easily transferred to the TITC matrixes taking account of equality (6).

Based on the complete solution of the eigenvalue problem of matrices, the computer implementation of the proposed procedure of the numerical TITC solution [2] is applicable to the TITC subclass, where matrices satisfy the conditions:

- dimension of each diagonal block presented as a block-triangular matrix does not exceed 10;
- all eigenvalues of matrix R are real;
- matrix R eigenvectors number is equal matrix R dimension.

The eigenvalues are found from the characteristic equation. All calculations are implemented in terms of interval arithmetic. In test variants the relative interval width of the calculated nonzero eigenvalues in the test computations did not exceed 10^{-10}, while the stiffness coefficient reached 10^{30}. As the TITC solution is defined as a linear combination of exponents, the computing expenses do not depend on the value of the time coordinate which determines the solution. The computation time of the test variants did not exceed several tens of seconds using a high-performance PC-computer.

The interval implementation of the eigenbasis computation and decomposition of the vector of initial values on it, will allow one to obtain a guaranteed estimation of a computation error of the TITC solution calculated this way.

5. Computation results of transmutation in copper alloys using TRANS_MU computer code

5.1. Input data and methods of computations

The computations were carried out for natural copper with 100 appm ^{10}B impurity for six variants of neutron spectra (values of thermal, fast and integral neutron flux are shown in Table 1). The neutron spectra (given in the 100-group energy scale) are shown in Fig. 1.

A mathematical model of isonucleus transmutation and the TRANS_MU computer code were used for computations. In the nuclear transformations scheme for copper alloys, 16 isotopes and 220 transformation channels were included (using the decay data from the file ENDF-B/V and cross sections from the library ADL-3 [3]). The accumulation of residual nuclei from transformations was refined for 68 channels. The systematic error for this scheme is 1 appm for all neutron spectra variants and irradiation up to a damage dose of 5 dpa.

The SPECTERD computer code [4] was used for damage computation.

Table 1
Basic parameters for neutron spectra, 10^{14} cm^{-2} s^{-1}

Variant	$F_{E\,<\,0.55\ \mathrm{eV}}$	$F_{E\,>\,0.1\ \mathrm{MeV}}$	$F_{E\,>\,0}$
1	2.662	2.427	8.772
2	2.989	3.928	12.35
3	2.11	15.78	31.36
4	1.72	12.92	25.66
5	0.514	3.951	9.94
6	0.459	2.527	6.89

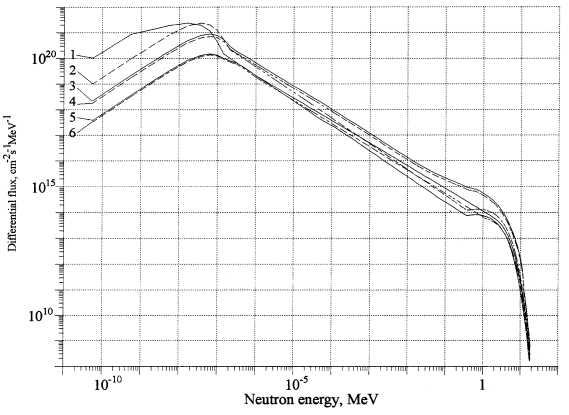

Fig. 1. Neutron spectra variations (solid line – odd number variants, dashed line – even number variants).

5.2. Nickel and zinc accumulation rates

The computation results showed that for irradiation doses to 5 dpa the nonlinearity of nickel and zinc accumulation dynamics did not exceed 1%. In this case, the accumulation of a chemical element for each neutron spectrum variant can be characterised by one parameter – accumulation rate in appm/dpa units. The results are given in Table 2. Special computations proved that transmutation rates of copper alloys presented in appm/dpa give 1–3% accuracy.

5.3. Gas production rates

The nonlinearity of hydrogen accumulation does not exceed 1% at an irradiation doses to 5 dpa. The calculated hydrogen accumulation rates are shown in Table 2.

Helium production in the irradiated samples is provided mainly by the reaction ^{10}B (n,α), contribution of all other reactions with α-particle emission being extremely small. ^{10}B burn out (especially for spectra 1 and 2) achieves large values at an irradiation doses of 1 dpa. For this reason, the helium production rate is not constant during irradiation. Fig. 2 shows the dynamics of helium production in copper samples with 100 appm ^{10}B impurity on irradiation to a dose of 5 dpa.

5.4. Rates of transmutants accumulation caused by each of four spectrum energy groups

As the transmutation process in copper with 100 appm ^{10}B impurity is not linear in neutron spectrum (transmutation in a summarised spectrum is not equal to the sum of transmutations in the addends of the spectrum), the definition of the accumulation rate contribution of each of four energy groups of the spectrum is rather approximate. The nuclear reaction rates (as well as the displacement rate of atoms in the radiation damage model used) are linear in neutron spectrum. This fact makes a basis for a contribution estimation of each neutron spectrum group.

More than 99% of helium production is provided by the ^{10}B (n,α) reaction. More than 95% of nickel accumulation is provided by the following chain of transformations

$$^{63}\mathrm{Cu} \rightarrow (\mathrm{n},\gamma) \rightarrow {}^{64}\mathrm{Cu} \rightarrow \beta^{+} \text{ decay} \rightarrow {}^{64}\mathrm{Ni}.$$

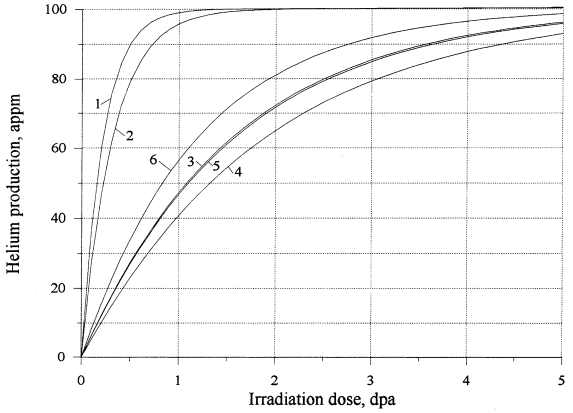

Fig. 2. Helium production dynamics.

All zinc is accumulated by two transformation chains:

$$^{63}\mathrm{Cu} \rightarrow (\mathrm{n},\gamma) \rightarrow {}^{64}\mathrm{Cu} \rightarrow \beta^{-} \text{ decay} \rightarrow {}^{64}\mathrm{Zn},$$

$$^{65}\mathrm{Cu} \rightarrow (\mathrm{n},\gamma) \rightarrow {}^{66}\mathrm{Cu} \rightarrow \beta^{-} \text{ decay} \rightarrow {}^{66}\mathrm{Zn}.$$

For the variants of neutron spectra considered, the zinc accumulation by these two chains occurs at a ratio from 1:2.26 to 1:2.81 (the second chain gives from 69% to 74% of the accumulated zinc). Table 3 gives the percentage contribution of each of four energy groups for 3 neutron spectra variants corresponding to the rates of three nuclear reactions mentioned above.

6. Conclusions

The TRANS_MU computer code provides a guaranteed systematic error estimation for each value of the transmutation computation results in an increasing reliability and validity of the computations.

The investigations carried out (using the TRANS_-MU computer code) have confirmed the possibility of a correct calculation of transmutation processes in copper

Table 2
Transmutation rates

Spectrum variant	H production rate (appm/dpa)	Ni accumulation rate (appm/dpa)	Zn accumulation rate (appm/dpa)	Ni/Zn rate ratio
1	7.8	862	2146	0.40
2	7.9	616	1488	0.41
3	6.7	175	377	0.46
4	5.5	143	309	0.46
5	6.5	215	449	0.48
6	6.8	253	540	0.47

Table 3
The contributions (%) of 4 energy groups to the nuclear reaction rates

Variant	Reaction	Group $0 < E < 0.255$ eV	Group $0.255 < E < 0.84$ eV	Group 0.84 eV $< E < 0.11$ MeV	Group 0.11 MeV $< E$
2	^{10}B (n,α)	82.00	8.47	9.51	0.02
	^{63}Cu (n,γ)	74.29	5.26	20.08	0.37
	^{65}Cu (n,γ)	76.86	5.45	17.11	0.58
3	^{10}B (n,α)	58.95	16.93	23.98	0.14
	^{63}Cu (n,γ)	37.67	8.00	52.39	1.95
	^{65}Cu (n,γ)	41.94	8.91	45.98	3.17
5	^{10}B (n,α)	43.96	23.20	32.67	0.16
	^{63}Cu (n,γ)	22.24	8.74	67.36	1.66
	^{65}Cu (n,γ)	26.17	10.29	60.67	2.87

alloys applying the developed methods of mathematical simulation.

It is useful to state the following firm results of the computations carried out.

1. The influence of the reactor schedule on transmutation rates is insignificant, therefore presentation of the results in appm/dpa is valid.
2. The maximum Ni and Zn accumulation rate are observed in spectrum 1 and reaches 862 and 2146 appm/dpa, respectively, primarily caused by the lowest thermal flux in neutron spectrum.
3. The minimum Ni and Zn accumulation rate are observed in spectrum 4 and reaches 143 and 309 appm/dpa, respectively, primarily caused by the lowest thermal flux in neutron spectrum.
4. The ratio of Ni and Zn accumulation rates varies insignificantly (0.4–0.48) for all neutron spectra variations considered.
5. The total accumulation rate of all other chemical elements (except Ni and Zn) does not exceed 0.1 appm/dpa.
6. The hydrogen accumulation rate does not exceed 8 appm/dpa for the neutron spectra considered.

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