INVESTIGATION OF RADIATION DAMAGE RATES IN A LWR VESSEL USING RESULTS OF MOLECULAR DYNAMICS SIMULATIONS

C.H.M.Broeders, A.Yu.Konobeyev
Institut für Reaktorsicherheit, Forschungszentrum Karlsruhe GmbH, Germany

Abstract

Data for neutron displacement cross-sections were prepared using results of molecular dynamics simulation and results of calculations with the help of the binary collision approximation model. A comparison of various approaches for the determination of number of defects in irradiated materials is discussed.

Introduction

Traditionally, displacement cross-sections using for the calculation of radiation damage rates of materials are obtained using the NRT model [1,2]. The relative simplicity of the model and its implementation in popular codes (NJOY, MCNPX, SPECTER) allows to perform the fast evaluation of displacement cross-sections. At the same time, experimental data [3] and more rigorous calculations of the number of defects produced in materials under the irradiation show the difference with NRT model evaluations. It makes essential the calculation of radiation damage rate for structural materials of nuclear power units using advanced model, which predictions are close to available measured data.

The comprehensive analysis of the radiation damage rate for the LWR vessel using the NRT model and the molecular dynamics (MD) simulation has been performed in Ref.[4]. In addition to results from Ref.[4] the present work deals with the uncertainty of the radiation damage rate calculation using various evaluated nuclear data sets and discusses the use of the method combining the binary approximation model (BCA) and the method of molecular dynamics (MD) for the calculation of the number of defects in irradiated materials.

The calculation of the number of defects at energies exceeding the maximum energy of the MD simulation has been performed using the binary collision approximation model (BCA) [5]. Primary recoil spectra of atoms produced by the neutron irradiation were calculated using data from JENDL-3.3, ENDF/B-VI(8), ENDF/B-VII, JEFF-3.1, and BROND-2.2.

The calculation of the number of defects in irradiated materials using the BCA,MD approach was discussed in details in Refs.[6,7]. Brief description of the method used to obtain the displacement cross-sections is given in the next Section.

Brief description of the method used for the calculation of displacement cross-sections

The displacement cross-section for atoms of irradiated materials is calculated as follows

$$\sigma_d(E_0)=\sum_i \int_{E_d}^{T_i^{max}} \frac{d\sigma(E_0,Z_T,A_T,Z_i,A_i)}{dT_i} \nu(T_i,Z_T,A_T,Z_i,A_i)\,dT_i \quad , \qquad (1)$$

where E_0 is the energy of incidents particles; $d\sigma/dT_i$ is the recoil energy distribution; Z_i and A_i are the atomic number and the mass number of the primary knock-on atom (PKA), correspondingly; Z_T and A_T are the atomic and mass number of the target; $\nu(T_i)$ is the number of Frenkel pairs produced by PKA with the kinetic energy T_i; T_i^{max} is the maximal energy of the recoil spectrum; E_d is effective threshold displacement energy; the summing is for all type of recoil atoms formed in the irradiation.

The number of defects produced by the PKA in material $\nu(T)$ can be written as follows

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

where $\eta(T)$ is the defect production efficiency [3], N_{NRT} is the number of defects predicted by the NRT model [1,2]

$$N_{NRT} = \frac{0.8}{2E_d} T_{dam}(T), \quad (3)$$

$$T_{dam}(T) = \frac{T}{1 + k\left(3.4008\,\varepsilon^{1/6} + 0.40244\,\varepsilon^{3/4} + \varepsilon\right)}, \quad (4)$$

$$k = \frac{32}{3\pi}\left(\frac{m_e}{M_T}\right)^{1/2} \frac{(A_i + A_T)^{3/2} Z_i^{2/3} Z_T^{1/2}}{A_i^{3/2}(Z_i^{2/3} + Z_T^{2/3})^{3/4}}, \quad (5)$$

$$\varepsilon = \left[A_T T/(A_i + A_T)\right]\left[a/(Z_i Z_T e^2)\right], \quad (6)$$

$$a = a_0 (9\pi^2/128)^{1/3}\left(Z_i^{2/3} + Z_T^{2/3}\right)^{-1/2}, \quad (7)$$

here m_e is the mass of an electron; M_T is the mass of the target atom; a_0 is the Bohr radius; “e” is the electron charge; the kinetic energy T is taken in keV.

For an ion moving in the material the simulation of atomic collisions was performed by BCA up to a certain minimal “critical” energy (T_{crit}) of the ion. Below this energy the BCA calculation was interrupted and the number of defects was estimated using results of MD simulations. The procedure was performed for all PKAs formed in atomic collision cascades.

For iron the number of Frenkel pairs created by ions with the energy below T_{crit} has been estimated according to the empirical equation obtained in Refs.[8,9], which approximates results of the MD simulation

$$\eta = 0.5608 E_{MD}^{-0.3029} + 3.227\times10^{-3} E_{MD}, \quad (8)$$

where E_{MD} is the initial energy in the MD simulation taken in keV. It is supposed that the effective threshold energy for iron is equal to 40 eV.

Eq.(8) has been used up to the maximal energy of $E_{MD} \approx T_{dam} = 40$ keV, which corresponds to the critical energy T_{crit} equal to 61.2 keV for the self-ion irradiation of iron.

Fig.1 shows the efficiency of the defect generation η for the Fe-Fe irradiation. The η value is expressed as a function of the damage energy T_{dam} in the energy range which corresponds to the primary kinetic energy of Fe-ions up to 20 MeV. Calculations were performed using the IOTA code [5]. Also Fig.1 shows the defect production efficiency calculated in Refs.[8-10] by MD.

Recoil spectra $d\sigma/dT$, Eq.(1) were obtained using angular and energy distributions of particles produced in neutron irradiation of natural iron taken from various data libraries. Spectra were recovered using the NJOY code.

Results and discussion

Displacement cross-sections averaged using typical LWR neutron spectrum and calculated using the NRT model and nuclear data from JENDL-3.3, ENDF/B-VI(8), ENDF/B-VII, JEFF-3.1, and BROND-2.2 are shown in Table 1. There is a good agreement between cross-sections obtained using data from various nuclear data sets. The maximal difference in $\langle\sigma_d\rangle$ values does not exceed 4.2 %.

Table 2 shows the averaged displacement cross-sections calculated using the results of MD simulations [8,9] and the approximation of the efficiency of the defect generation above T_{dam} = 40 keV by the constant. At present this approximation is widely used [3,4,8,9] for the evaluation of the number of defects at energies exceeding the maximal energy of MD simulations.

Table 3 shows the displacement cross-section calculated using $\eta(T)$ values obtained from combined BCA,MD simulations (Fig1.) The comparison of the data from Table 2 and Table 3 shows that the use of BCA,MD instead of the constant approximation of $\eta(T)$ results in the increase of $<\sigma_d>$ values up to 10-11 %. The difference between displacement cross-sections evaluated using NRT and MD simulations is substantial (Table 2,3)

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 [8-10] (dots).

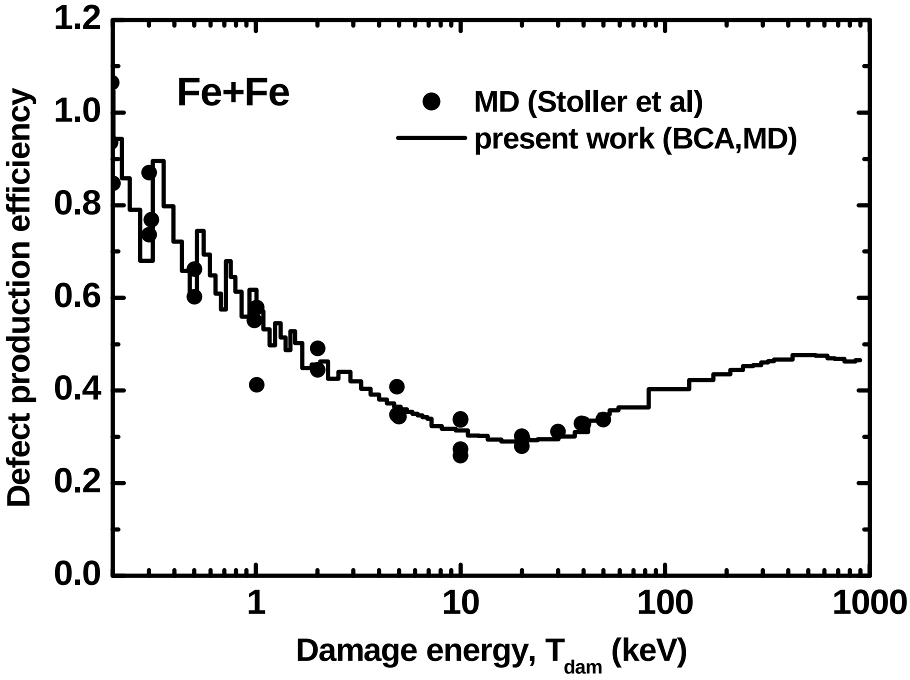

Table 1

Averaged displacement cross-sections calculated using the NRT model.

Library	$<\sigma_d>$ (b·keV)
ENDF/B-VII	18.31
ENDF/B-VI(8)	18.31
JEFF-3.1	17.98
JENDL-3.3	18.73
BROND-2.2	18.46

Table 2
Averaged displacement cross-sections calculated using results of the MD simulations with η=constant above T_{dam} = 40 keV

Library	$<\sigma_d>$ (b·keV)	$<\sigma_d>/<\sigma_d>$(NRT)
ENDF/B-VII	6.02	0.329
ENDF/B-VI(8)	6.02	0.329
JEFF-3.1	5.89	0.328
JENDL-3.3	6.15	0.328
BROND-2.2	6.15	0.333

Table 3
Averaged displacement cross-sections calculated using BCA,MD

Library	$<\sigma_d>$ (b·keV)	$<\sigma_d>/<\sigma_d>$(NRT)
ENDF/B-VII	6.68	0.365
ENDF/B-VI(8)	6.68	0.365
JEFF-3.1	6.53	0.363
JENDL-3.3	6.83	0.365
BROND-2.2	6.80	0.369

References

[1] M.J.Norgett, M.T.Robinson, I.M.Torrens, Nucl. Eng. Des. **33** (1975) 50.

[2] M.T.Robinson, J. Nucl. Mater. **216** (1994) 1.

[3] C.H.M. Broeders, A.Yu. Konobeyev, J. Nucl. Mater. **328** (2004) 197.

[4] V.A.Pechenkin, Yu.V.Konobeev, I..V.Pyshin, E.E.Petrov, V.A.Khoromskii, V.P.Kryuchkov, A.M.Voloshchenko, V.I.Tsofin, K.G.Rozanov, Atomic Energy **100** (2006) 332.

[5] C.H.M. Broeders, A.Yu. Konobeyev, K. Voukelatou, FZKA 6984, 2004; http://bibliothek.fzk.de/zb/berichte/FZKA6984.pdf

[6] C.H.M. Broeders, A.Yu.Konobeyev, J. Nucl. Mater. **336** (2005) 201.

[7] C.H.M. Broeders, A.Yu. Konobeyev, C. Villagrasa, J. Nucl. Mater. **342** (2005) 68

[8] R.E.Stoller, L.R.Greenwood, J. Nucl. Mater. **271&272** (1999) 57.

[9] R.E. Stoller, Nucl. Eng. Des. **195** (2000) 129.

[10] R.E. Stoller, J. Nucl. Mater. **276** (2000) 22.