

Investigation of radiation damage rates in a LWR vessel using results of molecular dynamics simulations

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Introduction

The idea is to get displacement cross-sections using

- binary collision approximation model (BCA)
- molecular dynamics simulations (MD).

The displacement cross-section is equal to

$$\sigma_d(E_p) = \sum_i \int_{E_d}^{T_i^{\max}} \frac{d\sigma(E_p, T_i, Z_T, A_T, Z_i, A_i)}{dT_i} v(T_i) dT_i,$$

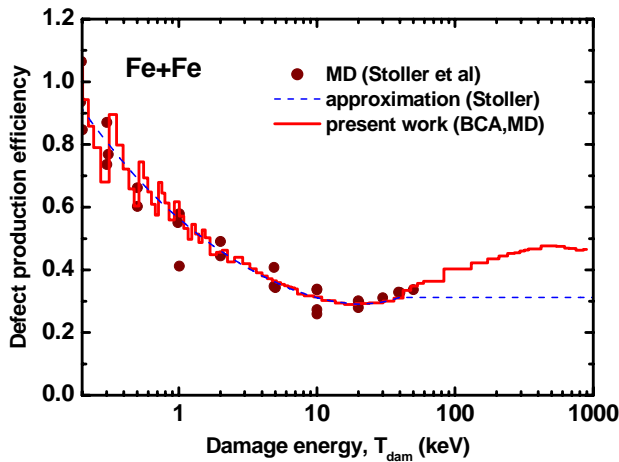
$d\sigma/dT_i$ is the recoil energy distribution,
 $v(T_i)$ is the number of Frenkel pairs produced by PKA,
 $v(T) = \eta(T) \cdot N_{\text{NRT}}(T)$,
 N_{NRT} is the number of defects predicted by NRT,
 $N_{\text{NRT}} = 0.8 \cdot T_{\text{dam}} / (2E_d)$, T_{dam} is the “damage energy”
 $\eta(T)$ is the defect production efficiency.

Calculation of the number of defects produced under irradiation

The BCA calculations are performed up to a certain “critical” energy of the ion, T_{crit} .

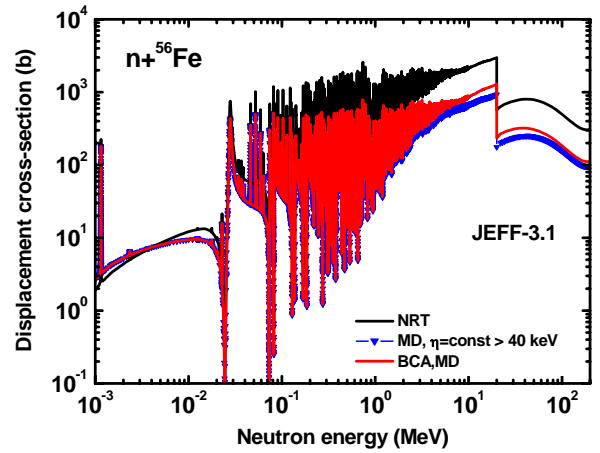
Below T_{crit} the BCA calculation is stopped and the number of defects is evaluated according to results of the MD simulation.

For the self-ion irradiation of iron the T_{crit} was taken equal to 61.2 keV, which corresponds to maximal energy of $E_{\text{MD}} \approx T_{\text{dam}} = 40$ keV.



Defect production efficiency calculated for iron. The maximal T_{dam} (NRT) energy corresponds to the primary energy of Fe-ions equal to 20 MeV.

Displacement cross-sections for neutron irradiation



The elastic displacement cross-section for ^{56}Fe prepared using data from JEFF-3.1

Averaged displacement cross-sections calculated using the NRT model.

Library	$\langle \sigma_d \rangle$ (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

Averaged displacement cross-sections calculated using results of the MD simulations with $\eta = \text{constant}$ above $T_{\text{dam}} = 40$ keV

Library	$\langle \sigma_d \rangle$ (b-keV)	$\langle \sigma_d \rangle / \langle \sigma_d \rangle (\text{NRT})$
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

Averaged displacement cross-sections calculated using BCA, MD

Library	$\langle \sigma_d \rangle$ (b-keV)	$\langle \sigma_d \rangle / \langle \sigma_d \rangle (\text{NRT})$
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