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Assessment of survived radiation defects by a modified version of NJOY

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Objectives / Introduction

Cascade initiation (≈ 10^{-15} -10^{-13} s) – predicted by the Norgett, Robinson & Torrens (NRT) model:

- incident neutrons produce Primary Knock on Atoms (PKA) in material
- PKAs travel in media and produce a thermal spike by
  - lose energy due to interaction with electrons
  - creation a cascade of PKAs due to ion-ion collisions

Cascade relaxation (till ≈ 10^{-9} s) - simulated by the Molecular Dynamics (MD) model / D.Bacon, R.Stoller and now many others/:

- created initial vacancies and interstitials may recombine or survive (isolated Frenkel pairs or point defects)
- survived interstitials tend to combine in clusters (ICL) having ≥ 2 defects
- cascade tracks cool down till reaching the thermal equilibrium

Important: survived point defects and clusters contribute to radiation induced microstructural evolutions, damage accumulation and eventually make rise to the mechanical property changes

Fusion plant, IFMIF & fission research reactor

	Accelerator source HFTM of IFMIF	Fusion Plant FW of PPCS/HCPB	Fission Reactor HFR/Column 5
Facility power and Neutron flux intensity			
Thermal power	40MeV @ 250mA = 10 MW	3.4 GW	45 MW
n- flux, total	7.3 10^{+14} n/cm^2/s	11 10^{+14} n/cm^2/s	12 10^{+14} n/cm^2/s
n- flux, E >15MeV	12 %	-	-

- Neutron spectra were taken from original studies
- PKA spectra (matrixes) for Fe were calculated by NJOY code (‘groupr’ module) from ENDF/B-VI.8 file in 211 groups structure up 55 MeV
- NJOY output file was processed to get PKA spectra weighted in neutron spectra

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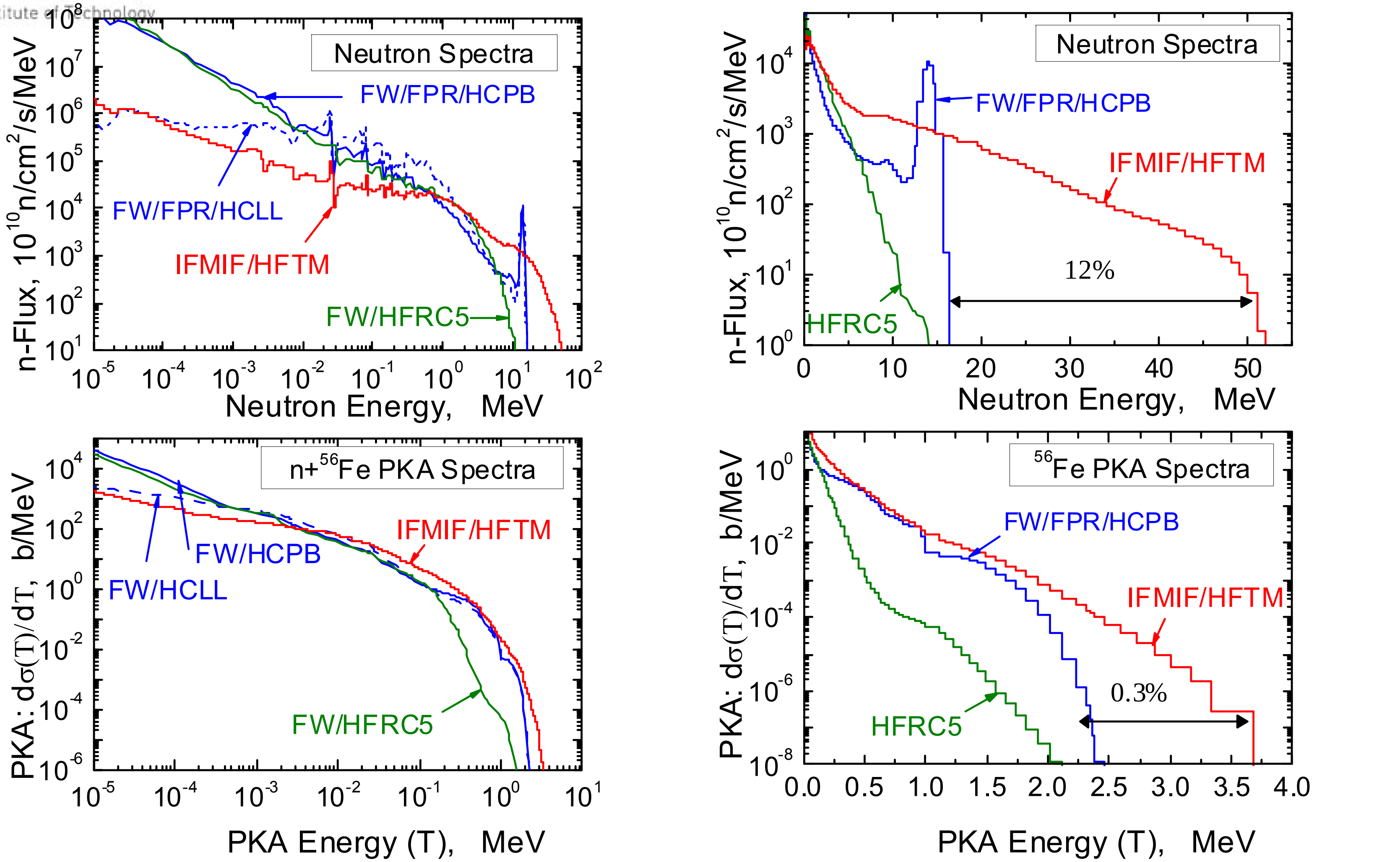
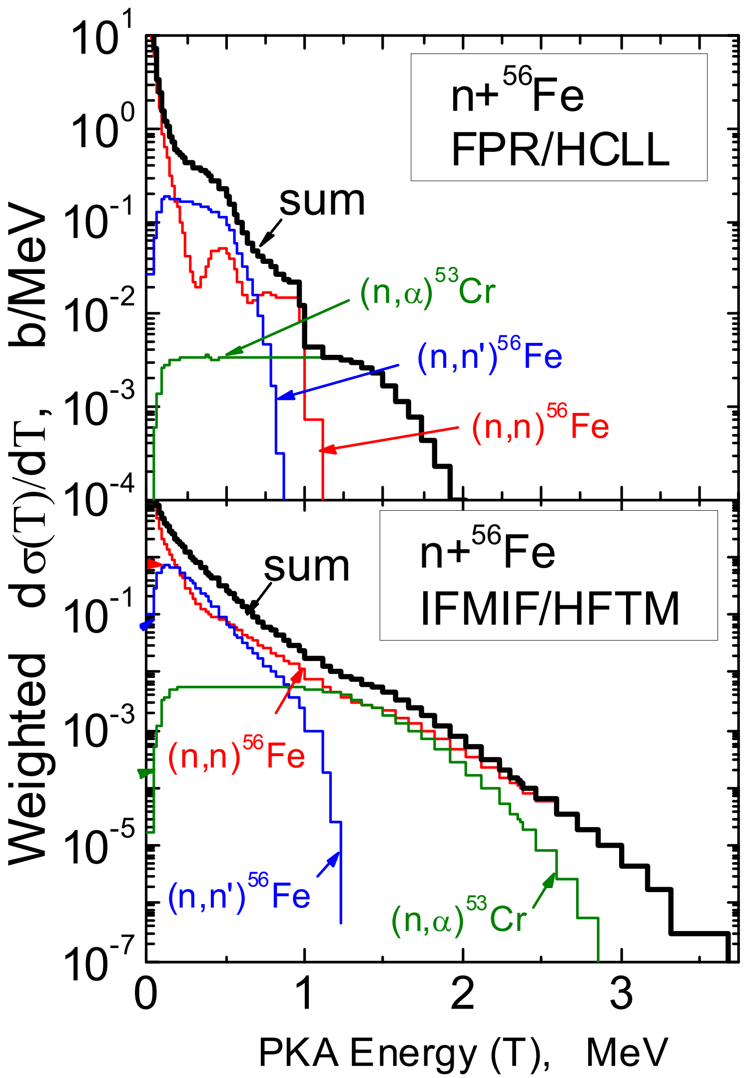
Neutron & PKA spectra in fusion, IFMIF & fission facilities



IFMIF radiation test facility comparison with Fusion Plant:

- ***12% of neutrons have energy above fusion cut-off 15 MeV***
- ***but only 0.3% of knock-on atoms have energy above fusion cut-off 2.2 MeV***

PKA spectra in fusion and IFMIF (reaction contributions)



	Accelerator source HFTM/IFMIF	Fusion Plant FW of PPCS/HCPB	Fission Reactor HFR/Column 5
Primary Knock-on Atoms			
Maximal PKA energy	3.9 MeV	2.7 MeV	1.2 MeV
PKAs fraction T > 2.3 MeV	0.3 %	-	-
Sigma ^{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 %

Dominant reaction channel contributors:
elastic and inelastic produce 98-99% of PKAs

NRT and MD models formalism

Norgett, Robinson & Torrens (NRT) model assesses initial no. of knock-on atoms:

Available Energy for lattice damage : $$E_a(E) = \sum_i \int_{E_d}^{T} \frac{d\sigma(E,T_i)}{dT_i} P(T_i)\ dT_i$$

where $P(T_i)$ - the portion of initial recoil energy T_i transferred to lattice atom

Displacement XS: $$\sigma = \frac{0.8}{2E_d} E_a$$

where E_d – energy needed to eject atom from lattice (= 40 eV for Fe)

Molecular Dynamics (MD) assesses survived defects after cascade cooling:

Point defects (Frenkel pairs), N_{FP}: $$\eta_{FP}(T) = \frac{N_{FP}}{N_{NRT}}$$

Interstitial Clusters, N_{IC}: $$\eta_{IC}(T) = \frac{N_{IC}}{N_{NRT}}$$

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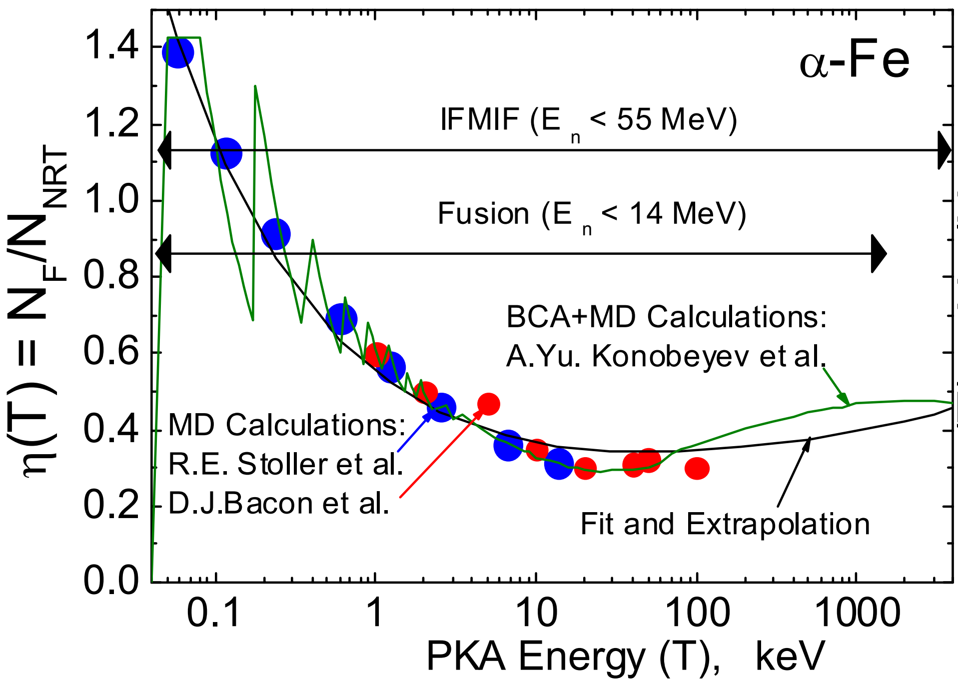
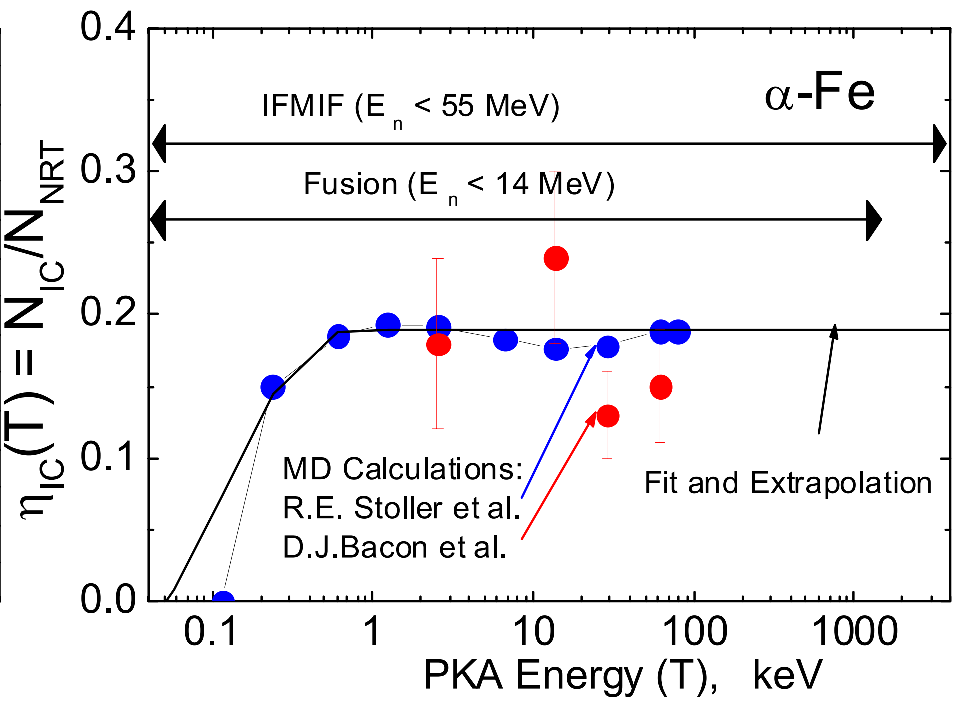
MD results for survived defects fractions in α-Fe

(bcc lattice form exists up to 910°C in pure ferrite or mild steels)

Primary Frenkel pairs



Primary Interstitial Clusters



Status of MD results:

- ***Frenkel pairs: decreasing function then levelling off; Clusters - threshold function***
- ***lack of MD results above 100 keV and for other recoils except Fe ions in Fe lattice***
- ***extrapolation up to 3 MeV supposing each cascade breaks out in subcascades with low surviving fraction (proved by BCA simulations for Frenkel pairs)***

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NJOY modification

Module HEATR calculates:

$$(MT = 444) = E_a(E) = \sum_i \int_{E_d}^{T} \frac{d\sigma(E,T_i)}{dT_i} P(T_i)\ dT_i \qquad \sigma = \frac{0.8}{2E_d} E_a$$

where $P(T_i)$ – partition function = the portion of recoil energy T_i transferred to lattice atom

function df(e,zr,ar,zl,al):

```
c    *******************************************************************   heatr.1707
c    damage function using the lindhard partition of                      heatr.1708
c    energy between atomic and electronic motion                          heatr.1709
c    call with e=0 for each reaction to precompute the constants          heatr.1710
c    *******************************************************************   heatr.1711
```

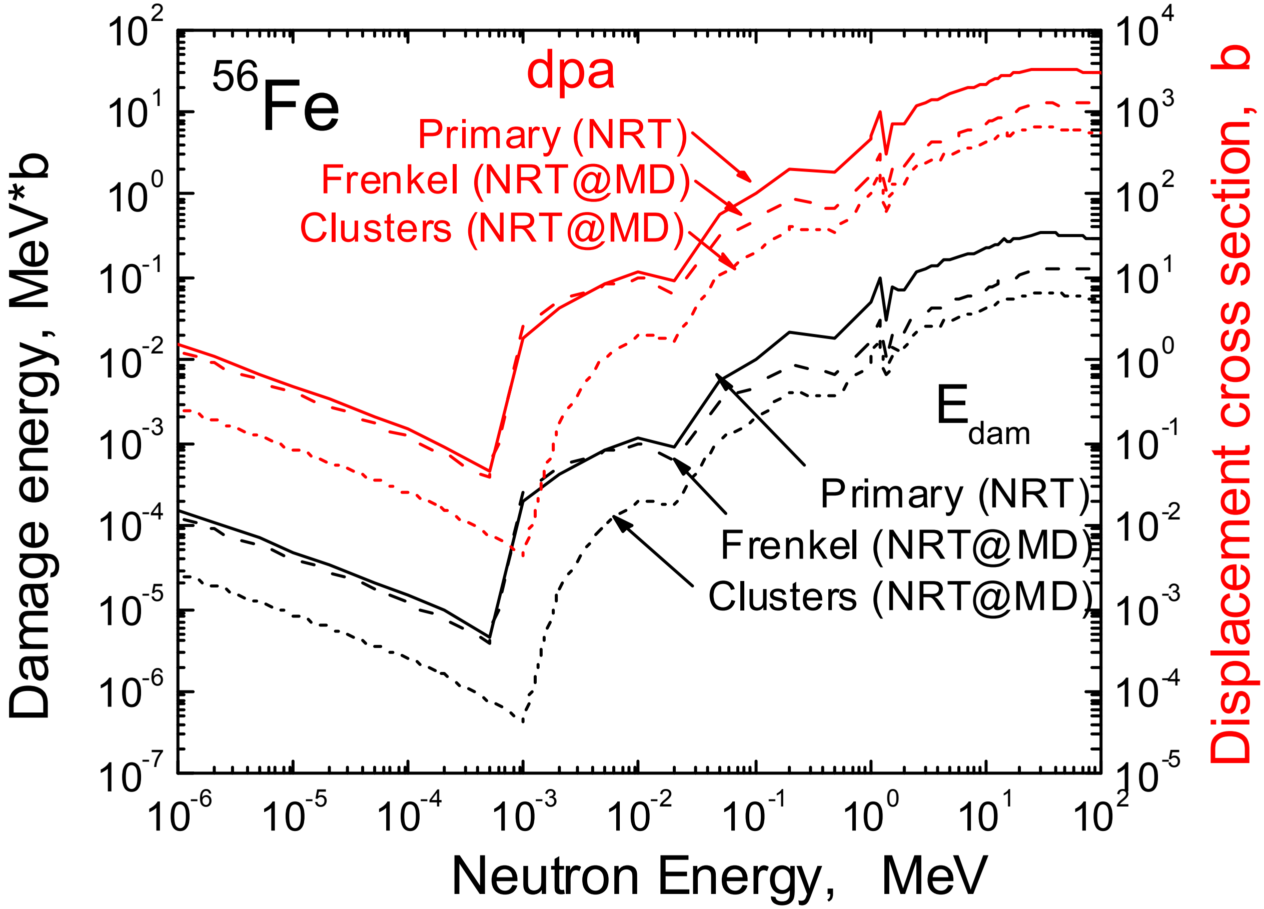
This function returns damage energy for every recoils having energy *e = T*

To account for MD results the df-function could be multiplied by surviving fraction η as:

either *a function of e = T:* $df = df * \eta(T)$

or a function of $df = E_{md}$: $df = df * \eta(df)$

Results: NRT and MD Damage energy and Displacement XS



NRT damage energy and displacement cross sections turn to be reduced:
- by factor of 3 above 100 keV neutron energy for Frenkel pairs
- by factor of 3 in the whole neutron energy range for interstitial Clusters

Results: damage rate in IFMIF and Fusion Plant

	Accelerator source HFTM of IFMIF	Fusion Plant FW of PPCS/HCPB	Fission Reactor HFR/Column 5
Facility power and Neutron flux intensity			
Thermal power	40MeV @ 250mA	3.4 GW	45 MW
n- flux, total n- flux fraction with E > 15MeV	7.3 10^{+14} n/cm^2/s 12 %	11 10^{+14} n/cm^2/s -	12 10^{+14} n/cm^2/s -
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) *ratio survived to initial*	9.7 dpa/fpy *0.33*	6.7 dpa/fpy *0.33*	3.3 dpa/fpy *0.33*
Interstitials clusters defects (NRT+MD) *ratio survived to initial*	5.6 dpa/fpy *0.19*	3.8 dpa/fpy *0.19*	1.9 dpa/fpy *0.19*

Conclusions

- the NJOY's code module has been modified to account for survived defects during processing of the evaluated data
- a lack of the MD calculation results for the PKAs energies above 100 keV necessitates the extrapolation for surviving fractions up to 2-3 MeV relying on BCA/MD approach and general considerations
- the damage rates caused in the α-iron inside the HFTM of IFMIF are found to be 10 dpa/fpy (Frenkel pairs) and 5.6 dpa/fpy (interstitial clusters) instead of 30 dpa/fpy (initial NRT knock-on atoms)
- however, the ratios of survived damages to the initial NRT pairs turn out to be the same for all three considered systems
- this means that the IFMIF, from the view of survived defects in Fe, remains to be an appropriate neutron source for simulation of material radiation damage effects expected in fusion power reactors

The results will be presented as a contributed paper (# 23) at ICFRM-13, Nice, 10-14 December 2007