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What we can improve in the calculation of displacement cross-sections

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Objectives

- to review problems concerning displacement cross-section calculations in a wide energy range of primary particles
- to discuss possible solutions and improvements

I. NRT model

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

Number of defects

$$N_{NRT}(T) = \frac{0.8}{2E_d} T_{dam}, \qquad T_{dam}(T) = \frac{T}{1 + k(Z_1, A_1) g(Z_1, A_1, Z_2, A_2)}$$

Robinson formula (LSS: Lindhard, Scharff, Schiott, 1963)

$$T_{dam}(T) = \frac{T}{1 + k(Z_1, A_1, Z_2, A_2) g(Z_1, A_1, Z_2, A_2)}$$

Defect production efficiency

$$\xi(T) = N_D / N_{NRT}$$

N_D : MD, BCA, experiment

Wide and rather successful use of NRT

Codes

NJOY code

SPECTER, SPECOMP

LAHET

MCNPX

- simplicity
- in particular cases ξ is "independent" on neutron irradiation conditions in various units

(Stoller et al, Simakov et al, Broeders et al.)

Comparison radiation damage by different radiation sources

“Internal” problems

i. Monatomic materials

compounds: use of NJOY can be incorrect

ii. $Z_1 \approx Z_2$, $A_1 \approx A_2$

iii. $T < 25\, Z_1^{4/3} A_1$, keV; $(dE/dx)_e \propto T^{1/2}$

iv. unified value $\kappa = 0.8$

Influence of limitations on σ_d : JNST, Suppl.2 (2002) p.1236

Example of questionable use: ESS

Measurements vs. NRT

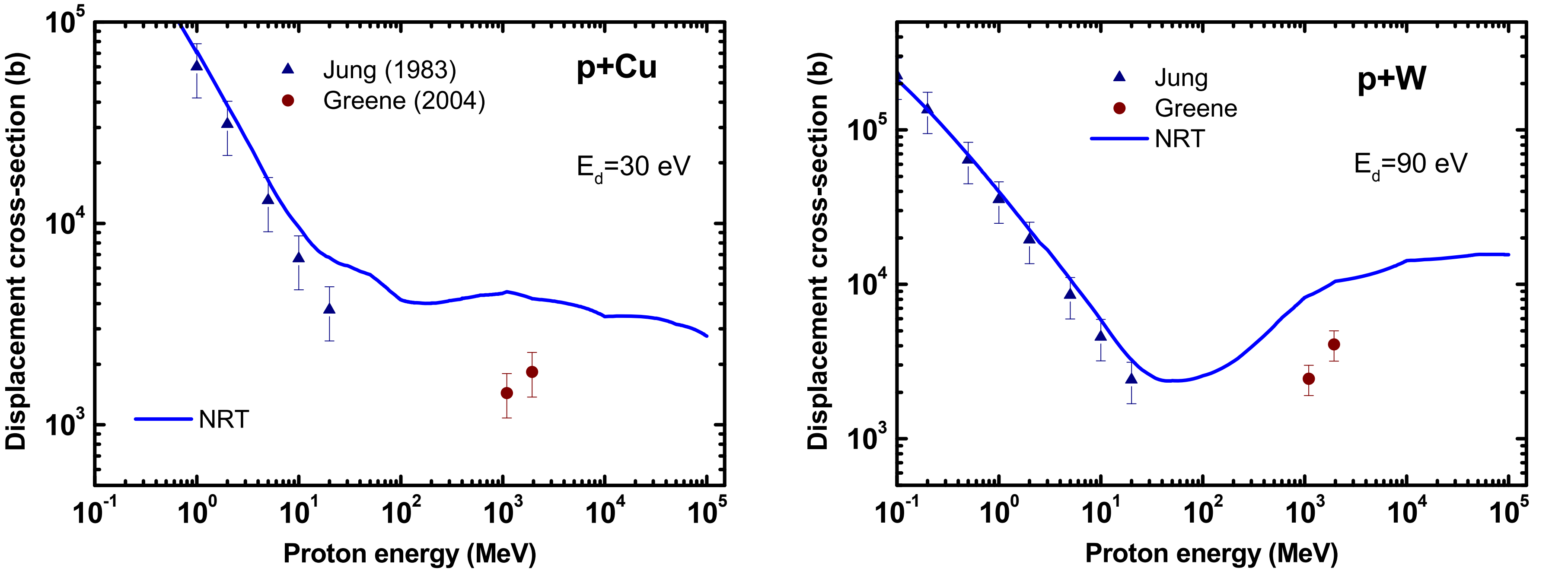
I. Neutron irradiation at relative low energies

P.Jung: redefined E_d values (JNM 117 (1983) p.70)

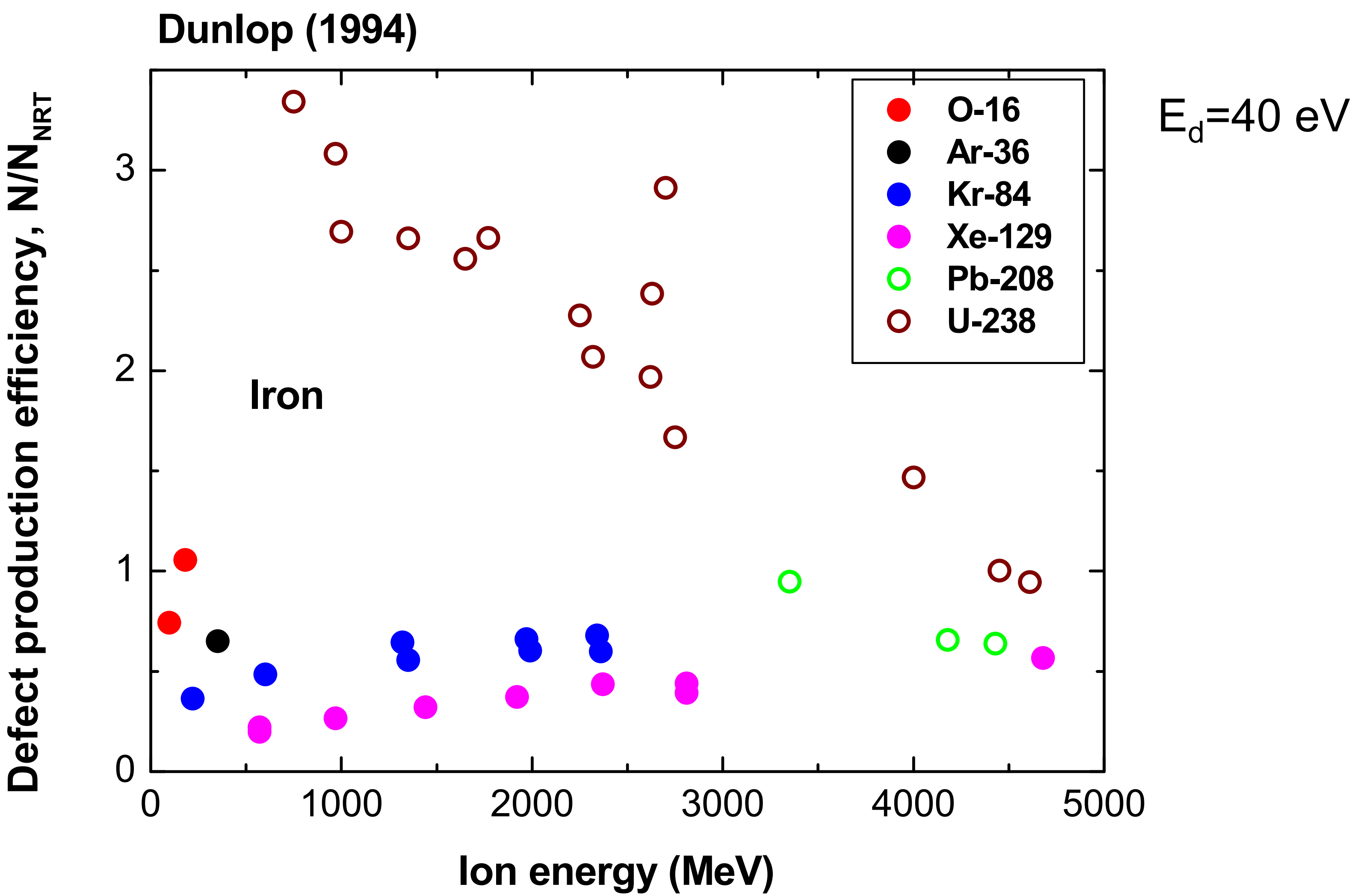
	ρ_F ($\mu\Omega$m)	$T_{d,min}$ (eV)	$T_{d,eff}$ (eV)	$T_{d,eff}/T_{d,min}$
Al	4	16	75	4.7
V	22	25	121	4.8
Fe	30	17	183	10.8
SS	25	18 [a]	120	6.7
Ni	7 [b]	23	142	6.2
Cu	2	19	100	5.3
Nb	16	28	150	5.4
Mo	14	34	159	4.7
Pd	9	34	138	4.1
Ag	2.1	24	113	4.7
Ta	17	32	148	4.6
W	18	40	107	2.7
Pt	10	34	138	4.1
Au	2.5	34	110 [c]	3.2

II. High energy of light projectiles

G.A.Greene et al (AccApp'03): proton energy 1.1 and 1.94 GeV



III. High energy of heavy ions



Success of NRT is not due to the agreement with measurements, probably due the absence of the strong dependence of average defect production for iron on the shape of neutron energy distributions in reactors

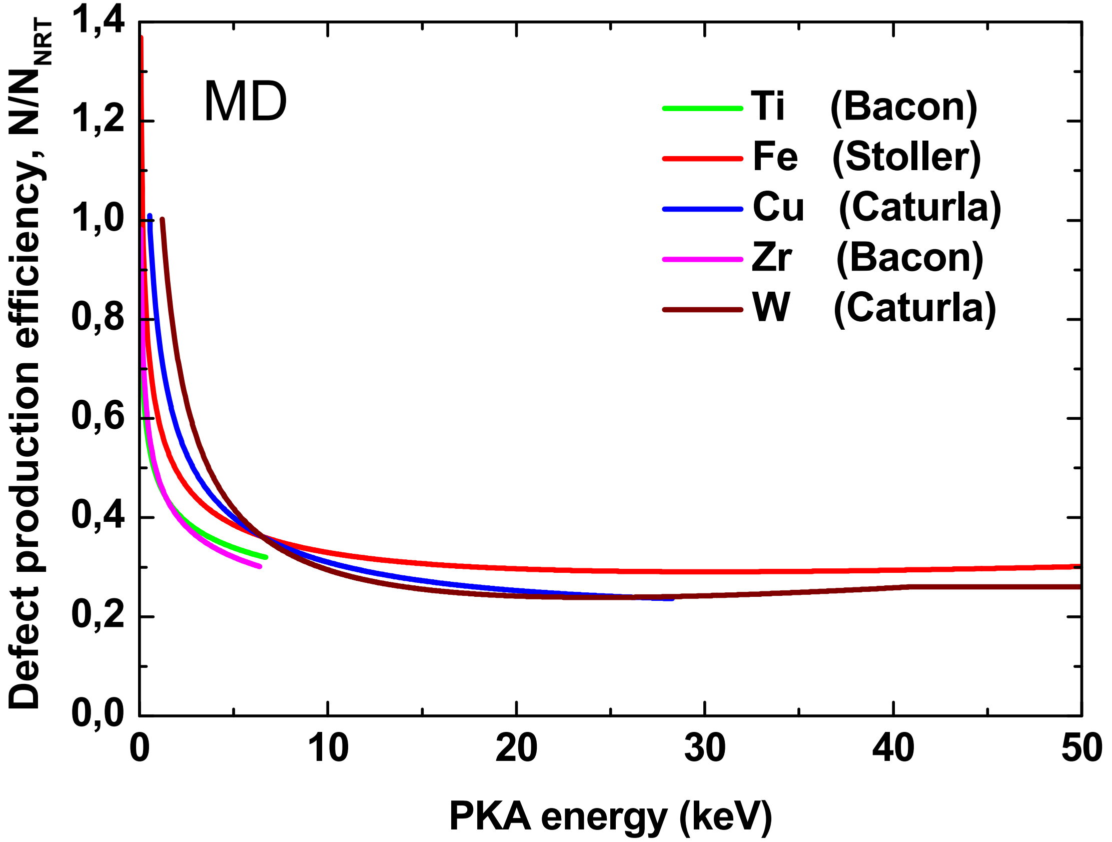
The averaged defect production efficiency ⟨ξ⟩ calculated using various neutron spectra.

Source	Fe	W
TRIGA	0.33	0.34
PWR	0.32	0.35
TLLWR	0.32	0.37
SNR-2	0.34	0.47
TTB, FRM	0.33	0.35
Fission	0.31	0.31
Fusion reactor, first wall	0.32	0.31
14.8 MeV neutrons	0.31	0.27
Be(d,n), 40 MeV deuterons	0.31	0.27

JNM, 328 (2004) p.197

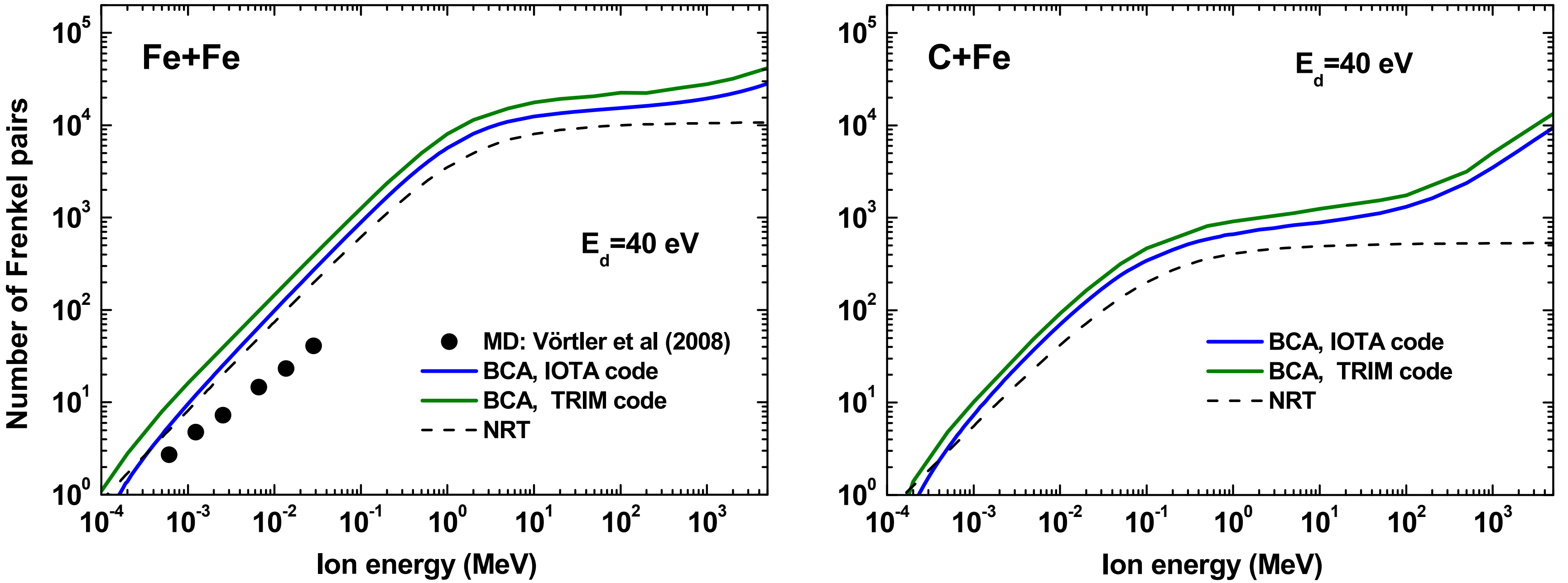
MD vs. NRT

ξ(T) shows strong energy dependence

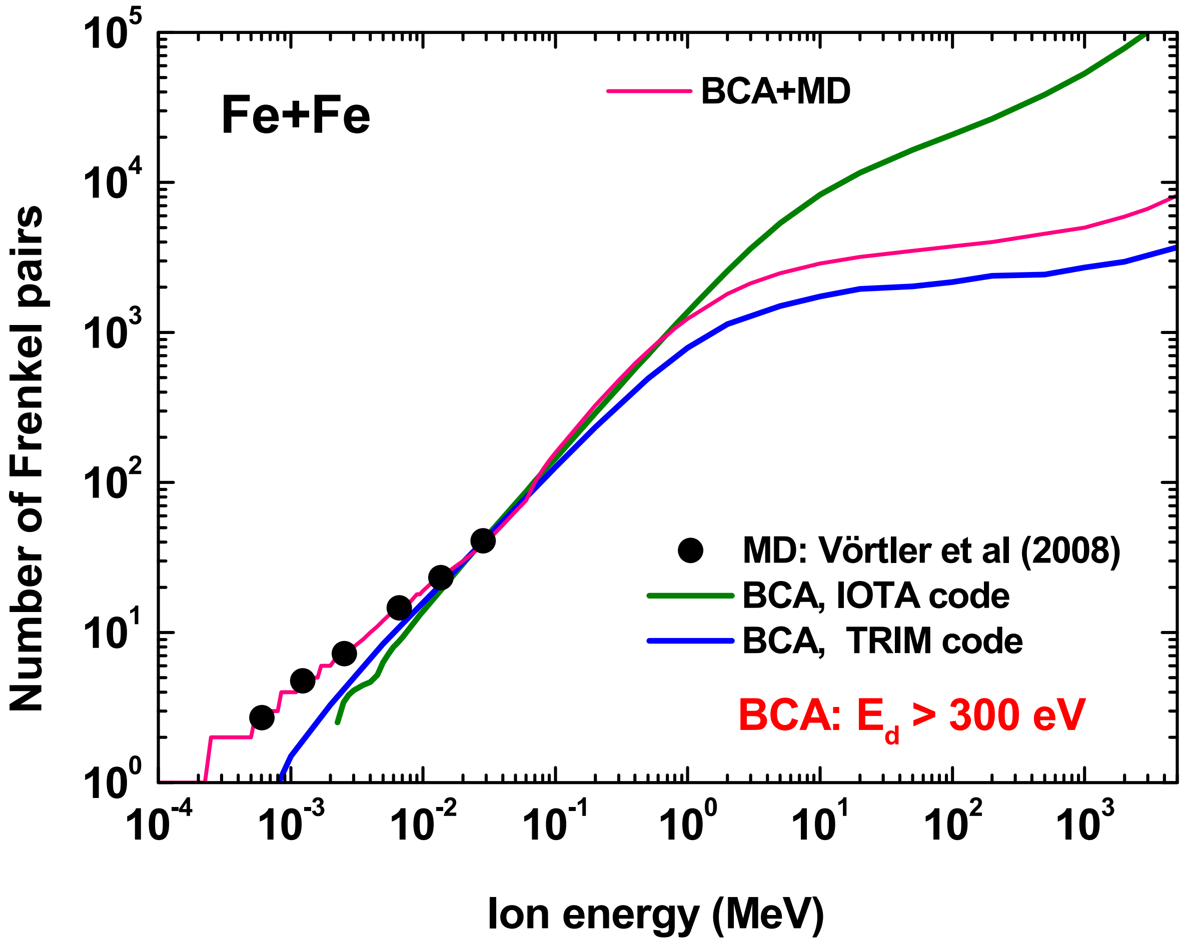


II. BCA simulation

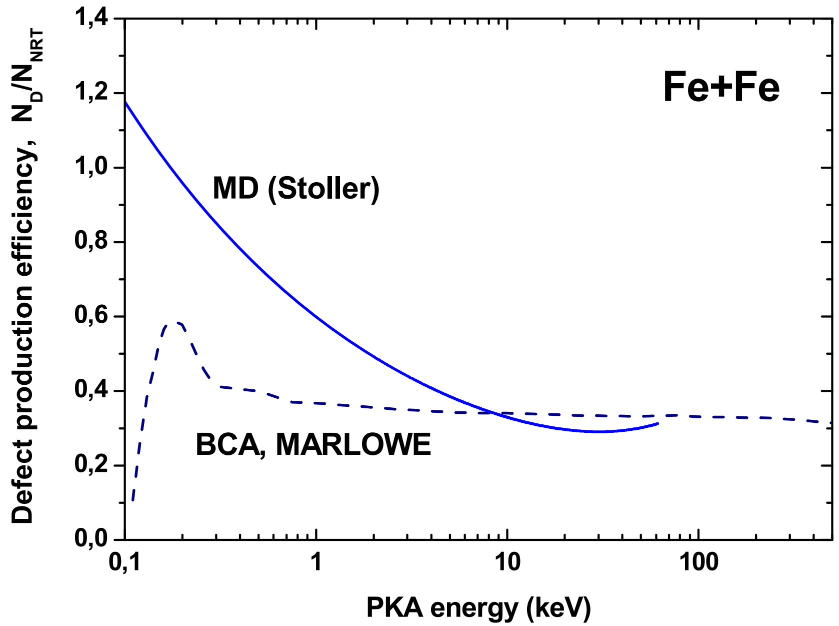
“usually” overestimates NRT results

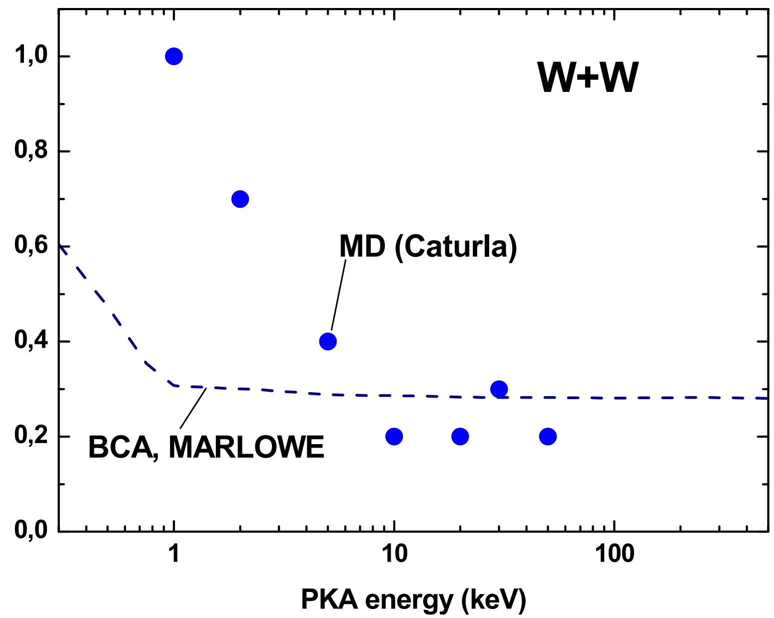


Attempt to use BCA



Attempt to use BCA





"Pure" BCA: high uncertainty of results

III. MD calculations

Comparison with experiments

Experimental damage rates for materials irradiated with neutrons at 4-5 K

Metal	Source	$(d\Delta\rho/d\Phi)\|_{\Delta\rho=0}$ [10-31 Ω·m3]	⟨σTd⟩ [b·keV]	Reference	Efficiency	Ed(η=1) [eV]
V	LTIF,ORNL	7.17	98.05	[43,38,65]	0.449	126.9
V	RTNS,LLL	18.01	257.1	[65]	0.430	132.5
V	LPTR (FNIF-10)	6.56	79.2	[65]	0.509	112.0
V	Be(30 MeV-d,n)	14.03	200.	[65]	0.431	132.3
V	LHTL,JPR-3	8.0	98.5	[63]	0.499	114.3
V	TTB(2),FRM	7.3	90.78	[7,73]	0.494	115.4
Fe	CP-5 (VT53),ANL	3.33	50.7	[47]	0.267	149.8
Fe	LHTL,JPR-3	6.5	84.6	[63]	0.312	128.1
Fe	TTB(1),FRM	6.39	70.9	[7]	0.366	109.2
Nb	CP-5 (VT53),ANL	2.19	55.7	[47]	0.548	142.4
Nb	LTIF,ORNL	3.43	80.25	[43,38,65]	0.595	131.0
Nb	Be(30 MeV-d,n)	7.38	197.	[65]	0.522	149.5
Nb	Be(40 MeV-d,n)	10.1	223.9	[47,65]	0.628	124.1
Nb	LPTR (FNIF-10)	3.47	60.3	[65]	0.802	97.3
Nb	RTNS,LLL	11.44	283.3	[65]	0.562	138.7
Nb	LHTL,JPR-3	6.5	80.2	[63]	1.129	69.1
Nb	TTB(2),FRM	2.7	68.8	[7,73]	0.547	142.7

Compilation of measurements
JNM, 328 (2004) p.197

Iron

Experiment	MD (Stoller)
T=4-5 K	T=100-900 K
$\langle\xi\rangle = 0.32 \pm 0.05$	$\langle\xi\rangle = 0.32 \pm 0.1$

Copper

Experiment	MD (Caturla)
T=4-5 K	T=10 K
$\langle\xi\rangle = 0.32 \pm 0.03$	$\langle\xi\rangle = 0.27 \pm 0.03$

Tungsten

Experiment	MD (Caturla)
T=4-5 K	T=10 K
$\langle\xi\rangle = 0.61 \pm 0.08$	$\langle\xi\rangle = 0.34 \pm 0.06$

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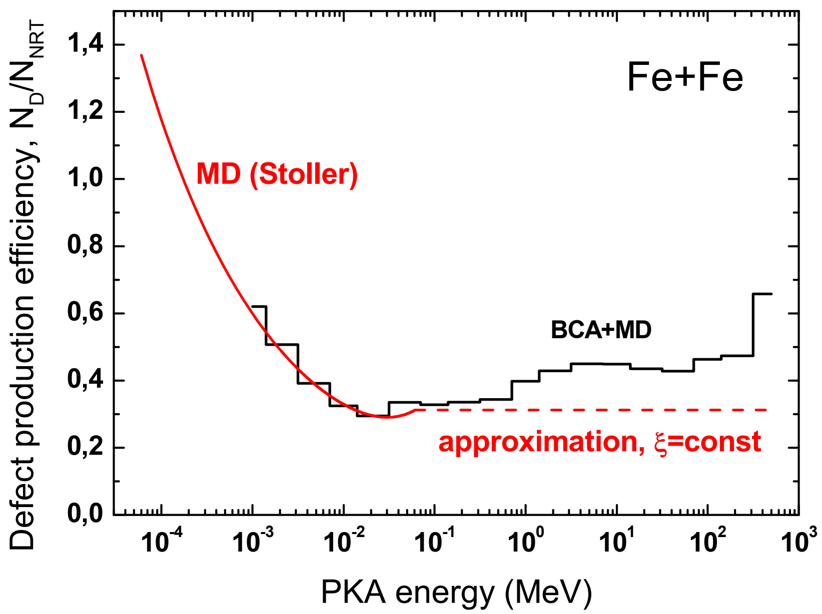
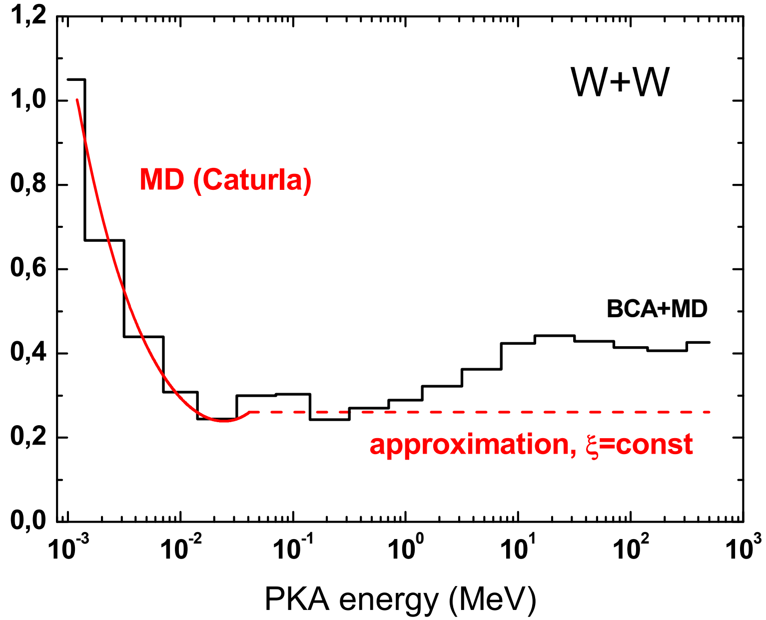
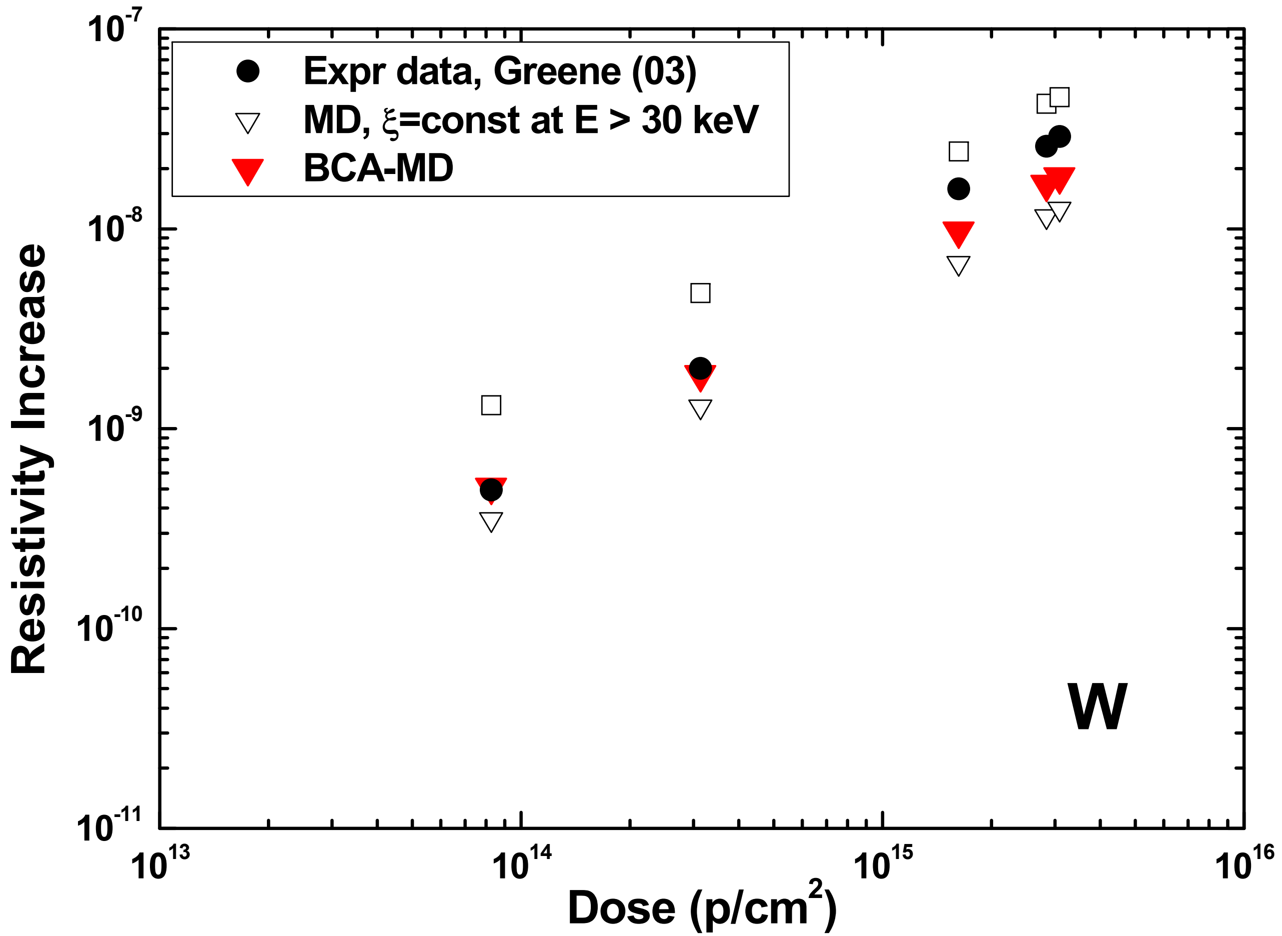
Irradiation with intermediate and high energy protons

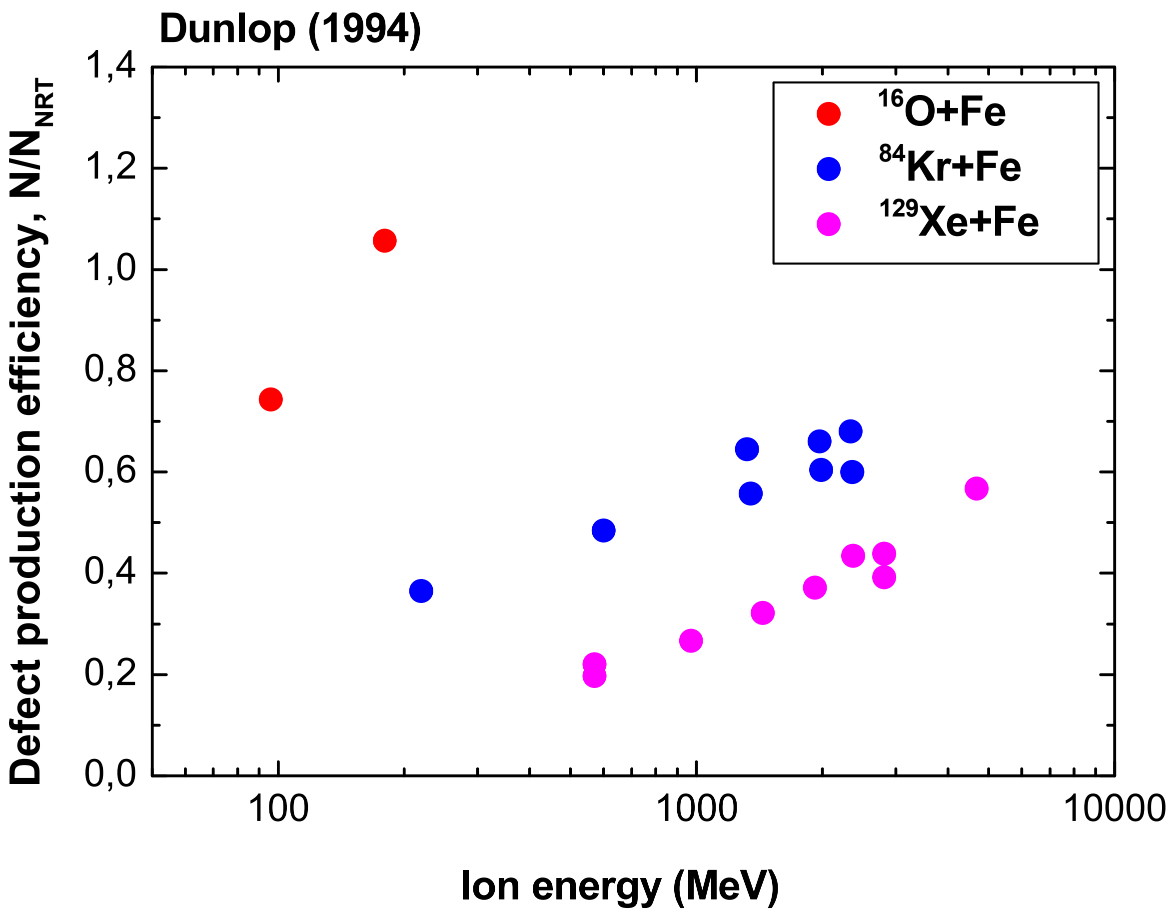
MD: is the information enough? ξ = const at T> 30-50 keV (?)





p+W, proton energy 1.1, 1.94 GeV





The approximation N_D/N_{NRT}= const at T > T(max MD) is questionable

IV. Combined BCA – MD simulations

Combined approach for the calculation of the number of stable displacements

Moving ion: transition from BCA to MD at the certain "critical" kinetic energy (T_{crit})

$T < T_{crit}$: MD

$T > T_{crit}$: BCA

Critical energy (T_{crit}): 30 – 60 keV

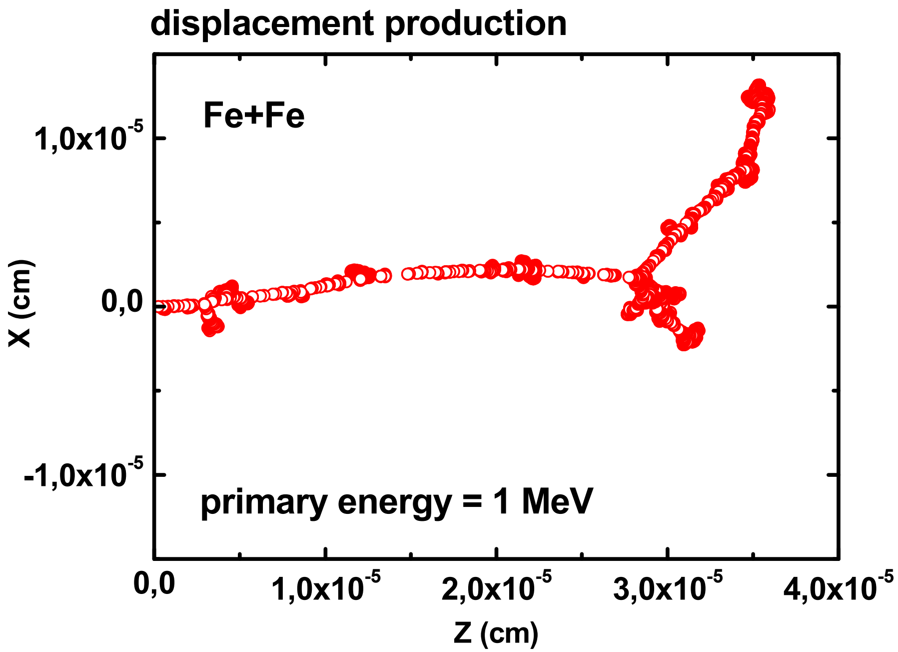
BCA calculations

IOTA code

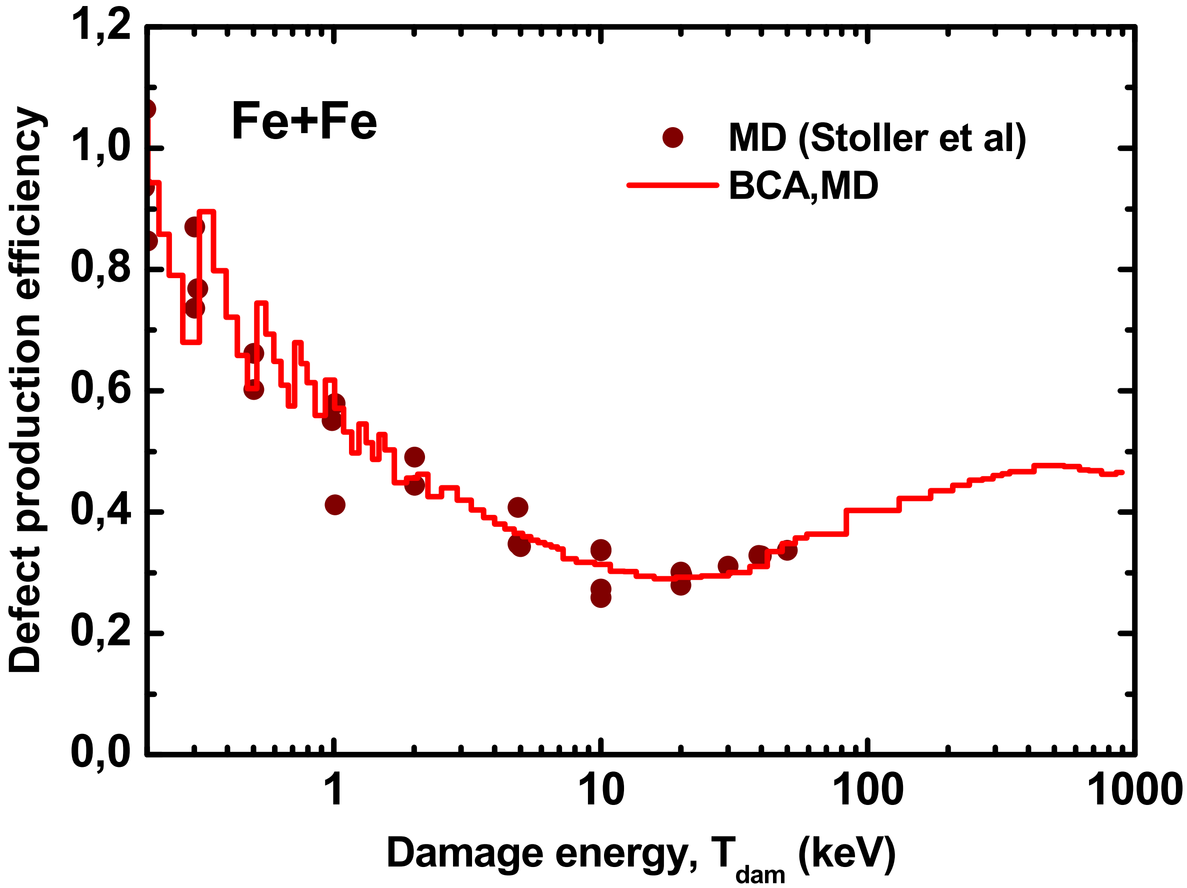
ENEA: 2003

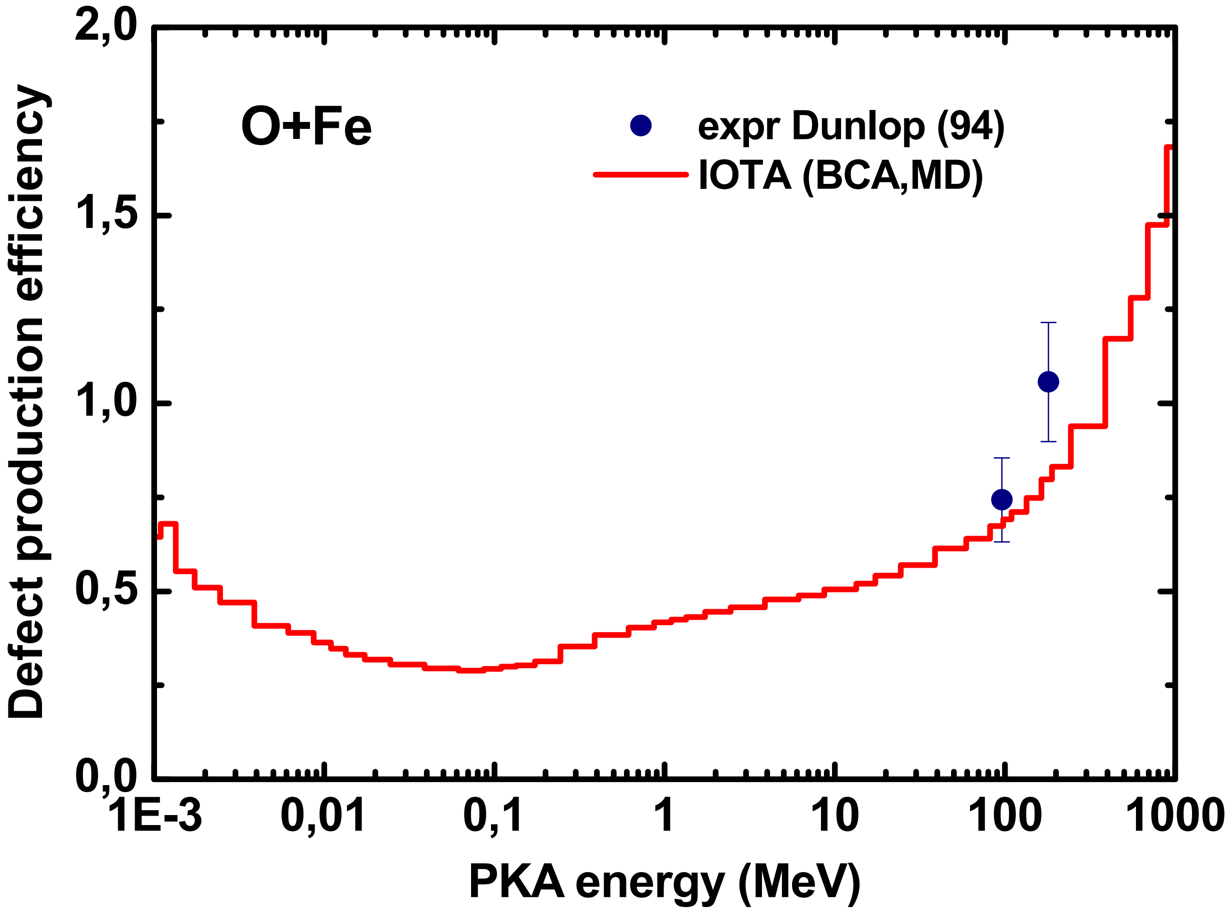
FZK, INR: 2004, (Report FZK6984)

last modification: 2011

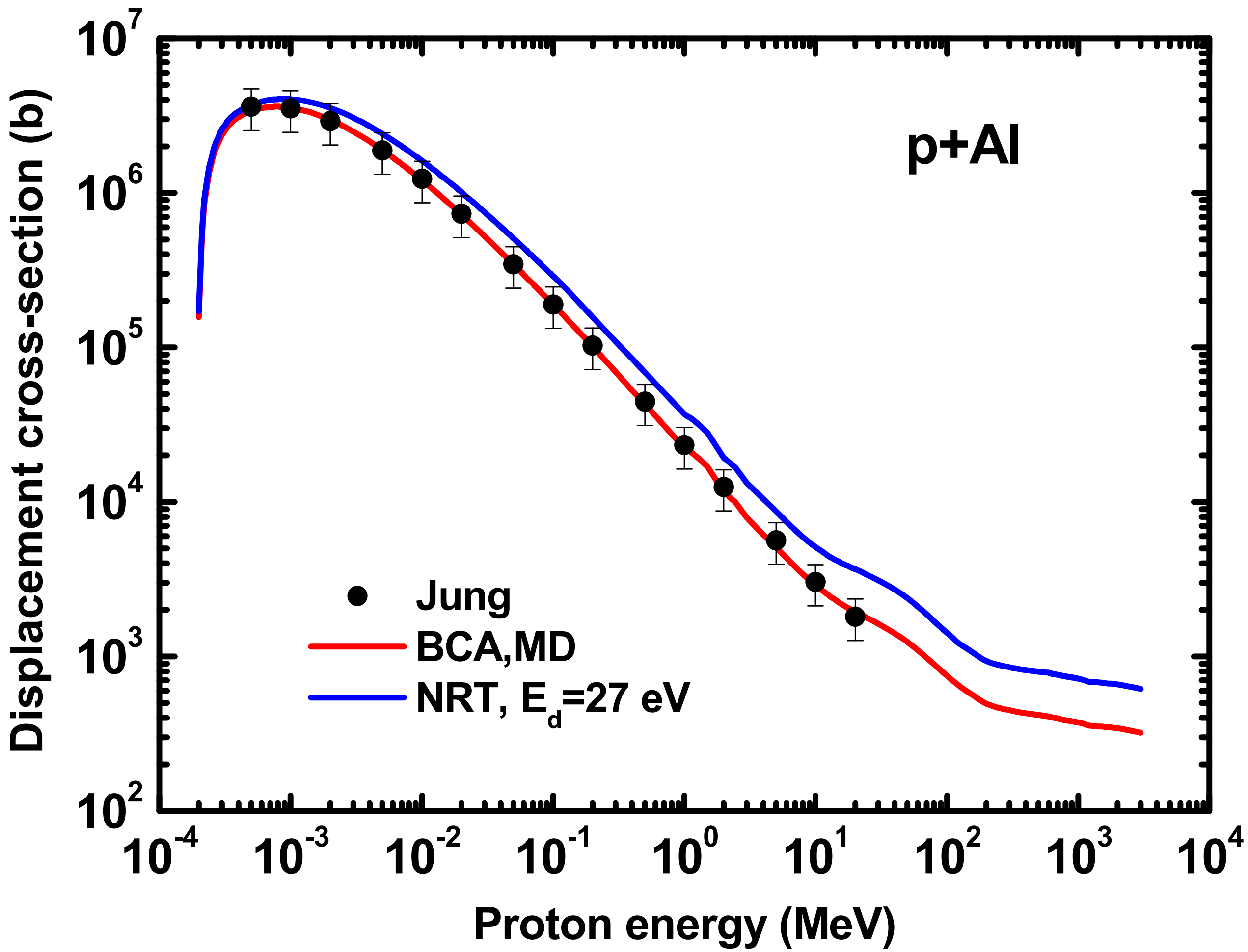


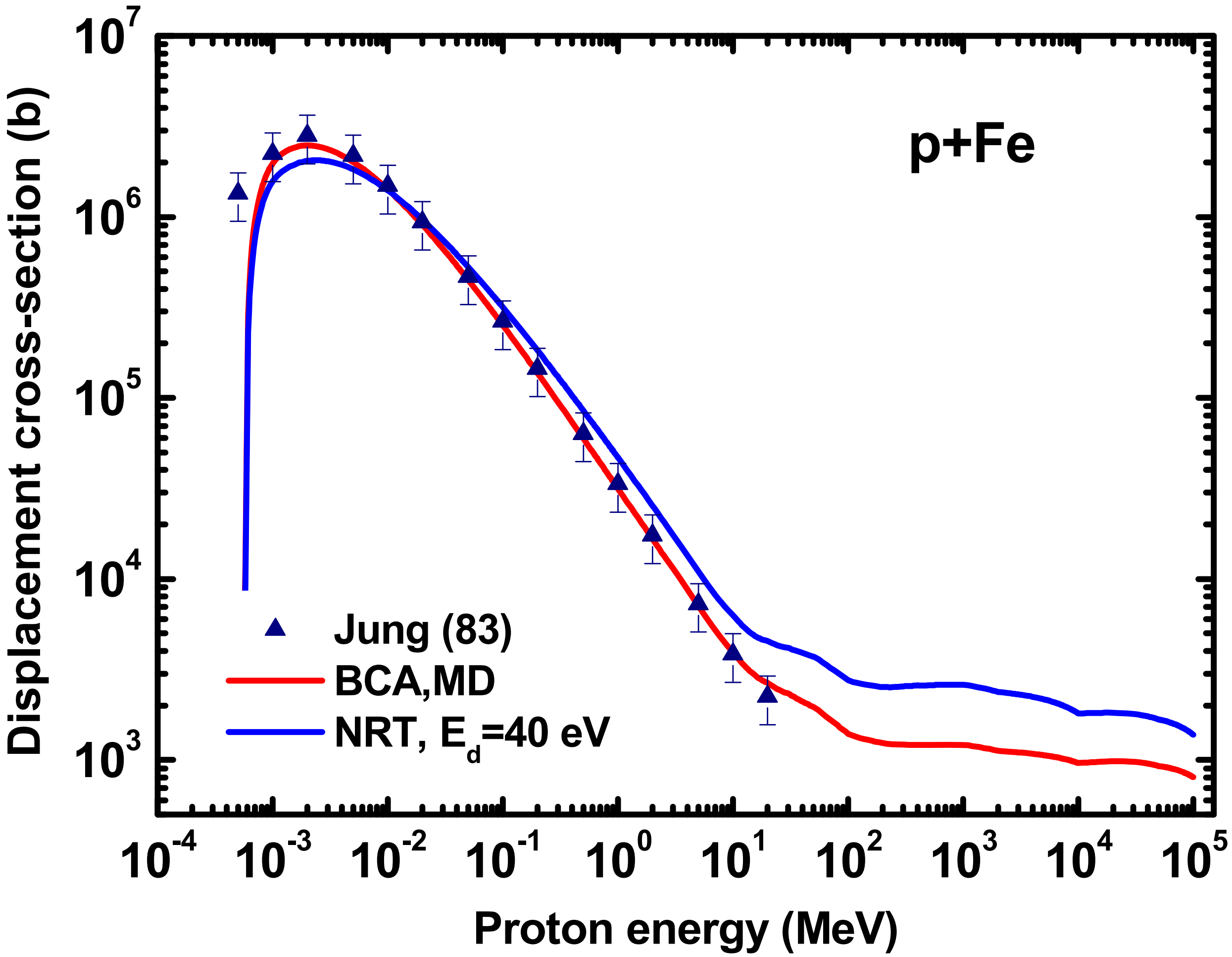
Example of calculated defect generation efficiency N_D/N_{NRT}

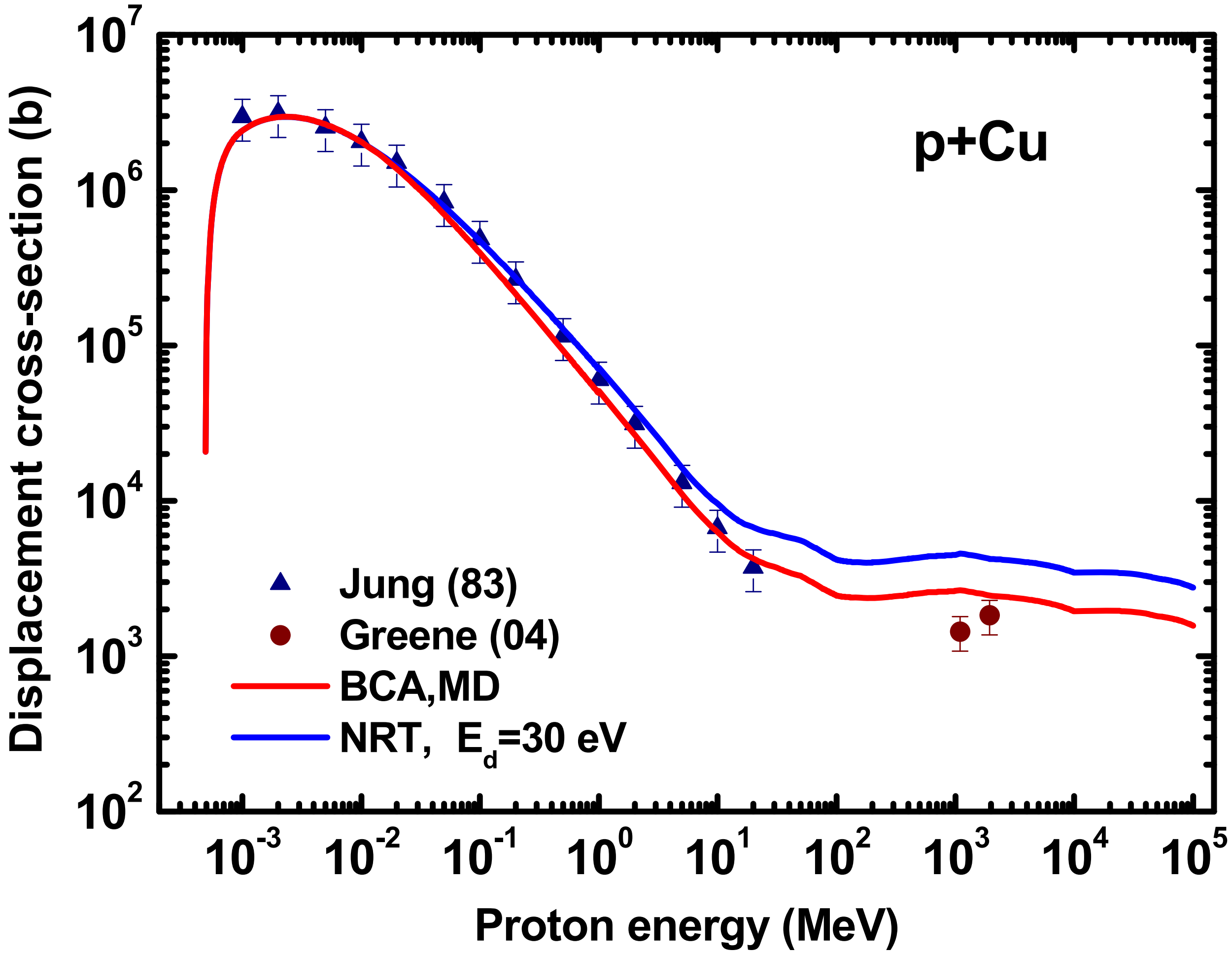


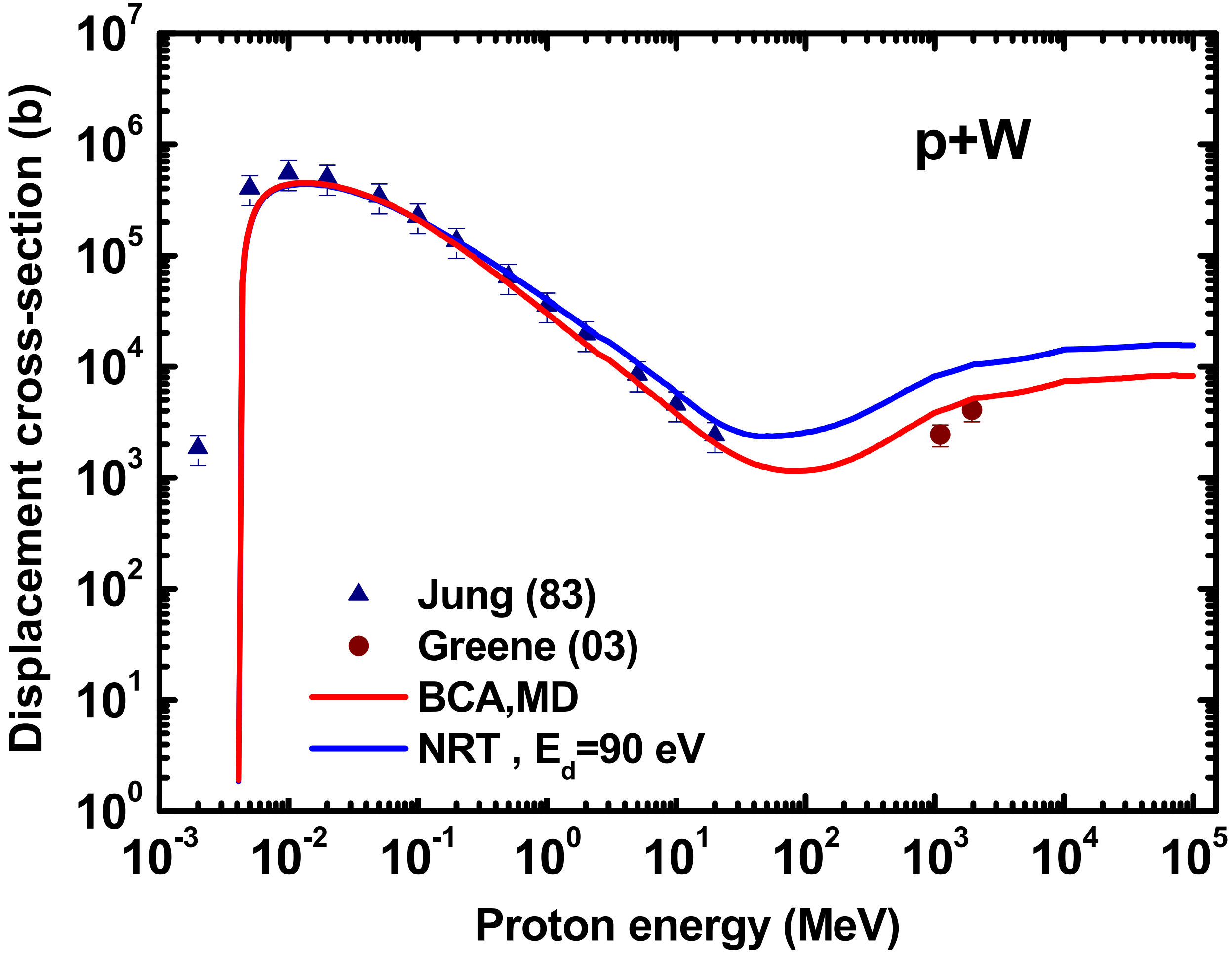

O+Fe
expr Dunlop (94)
IOTA (BCA,MD)
Defect production efficiency
2,0
1,5
1,0
0,5
0,0
1E-3
0,01
0,1
1
10
100
1000
PKA energy (MeV)

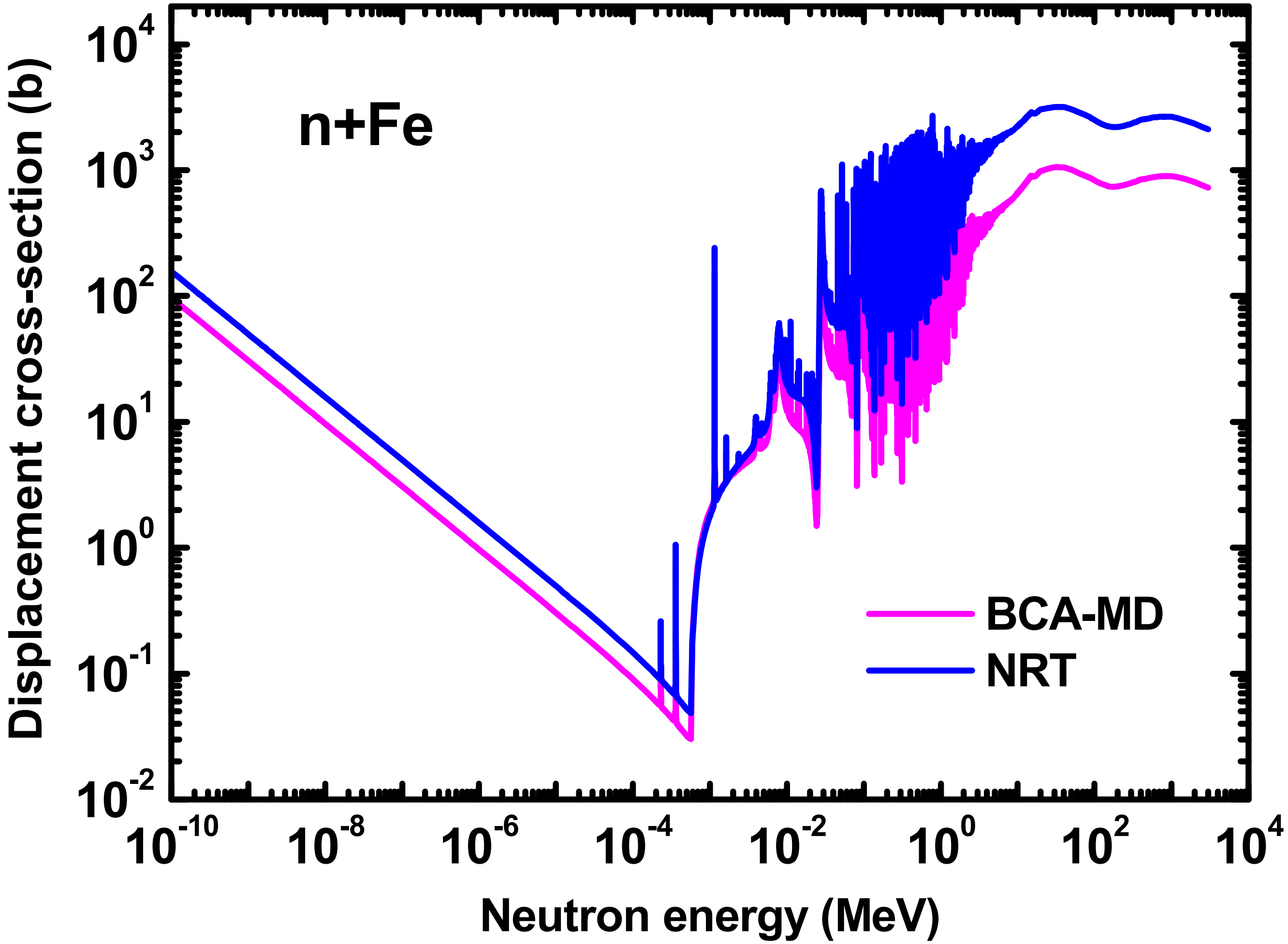
Example of calculated displacement cross-sections



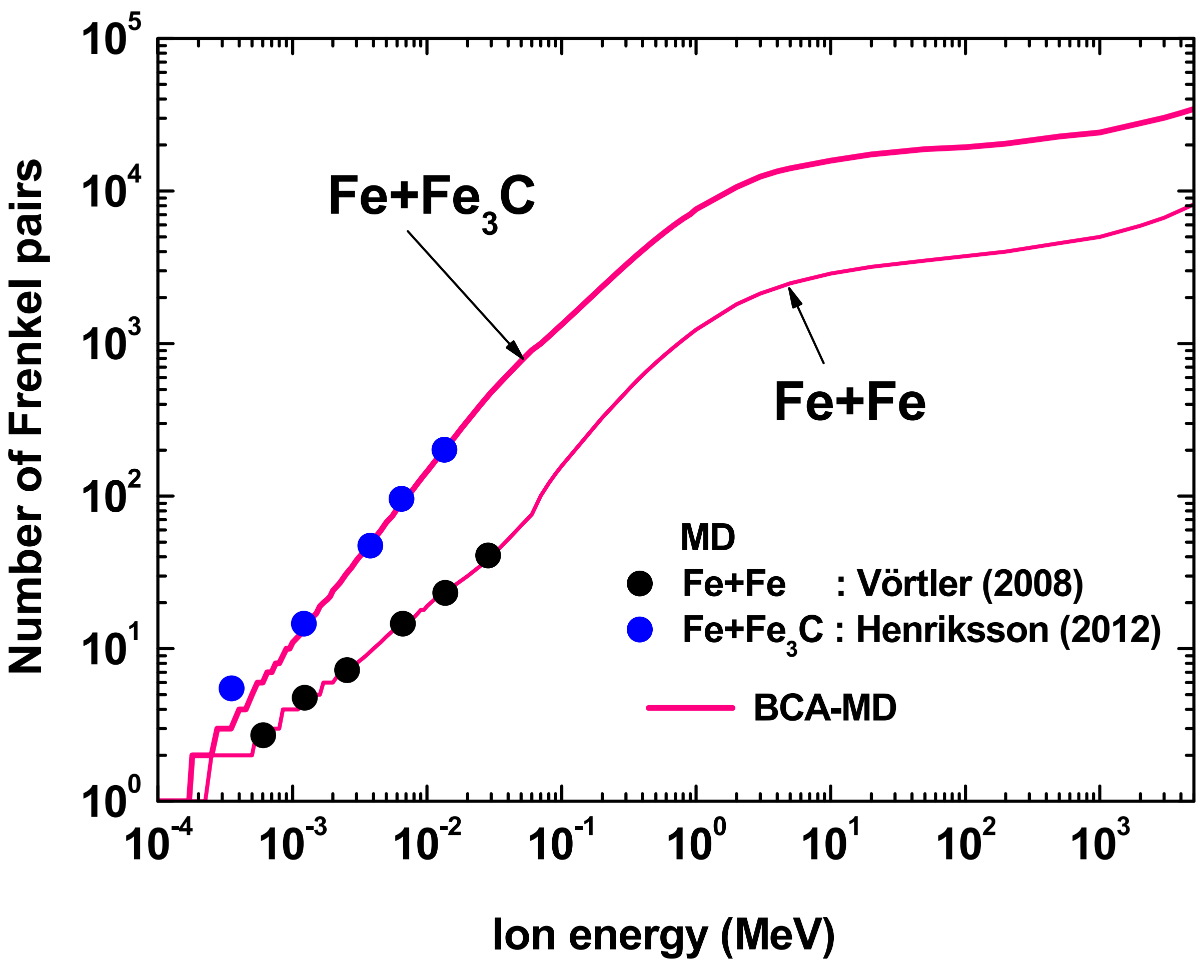

p+Fe
Displacement cross-section (b)
Proton energy (MeV)
Jung (83)
BCA,MD
NRT, E_d=40 eV
10^7
10^6
10^5
10^4
10^3
10^-4 10^-3 10^-2 10^-1 10^0 10^1 10^2 10^3 10^4 10^5


p+Cu
Displacement cross-section (b)
Proton energy (MeV)
Jung (83)
Greene (04)
BCA,MD
NRT, E$_d$=30 eV
10^7
10^6
10^5
10^4
10^3
10^2
10^-3
10^-2
10^-1
10^0
10^1
10^2
10^3
10^4
10^5


p+W
Jung (83)
Greene (03)
BCA,MD
NRT , E$_d$=90 eV
Displacement cross-section (b)
Proton energy (MeV)
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}



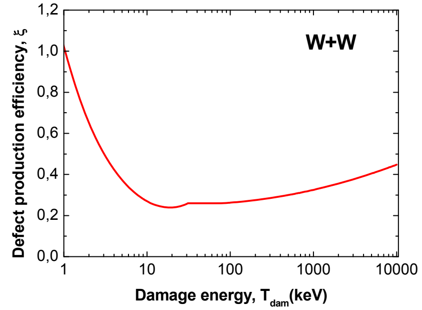
n+Fe
BCA-MD
NRT
Displacement cross-section (b)
Neutron energy (MeV)



Number of Frenkel pairs
Ion energy (MeV)
Fe+Fe$_3$C
Fe+Fe
MD
Fe+Fe : Vörtler (2008)
Fe+Fe$_3$C : Henriksson (2012)
BCA-MD

BCA – MD: improvement of displacement cross-section calculations

Defect production efficiency ξ(T): simple parameterization



Corrections: using <ξ(T)> from experimental damage rates for neutron irradiations at T=4-5 K

NJOY: easy implementation, function DF( )

Some questions are to be clarified

1. Temperature dependence of N_D

Iron

MD (Stoller): $\langle\xi\rangle = 0.32 \pm 0.1$ T=100-900 K

Neutron experiments: $\langle\xi\rangle = 0.32 \pm 0.05$ T=4-5 K

Copper

MD (Caturla): $\langle\xi\rangle = 0.27 \pm 0.03$ T=10 K

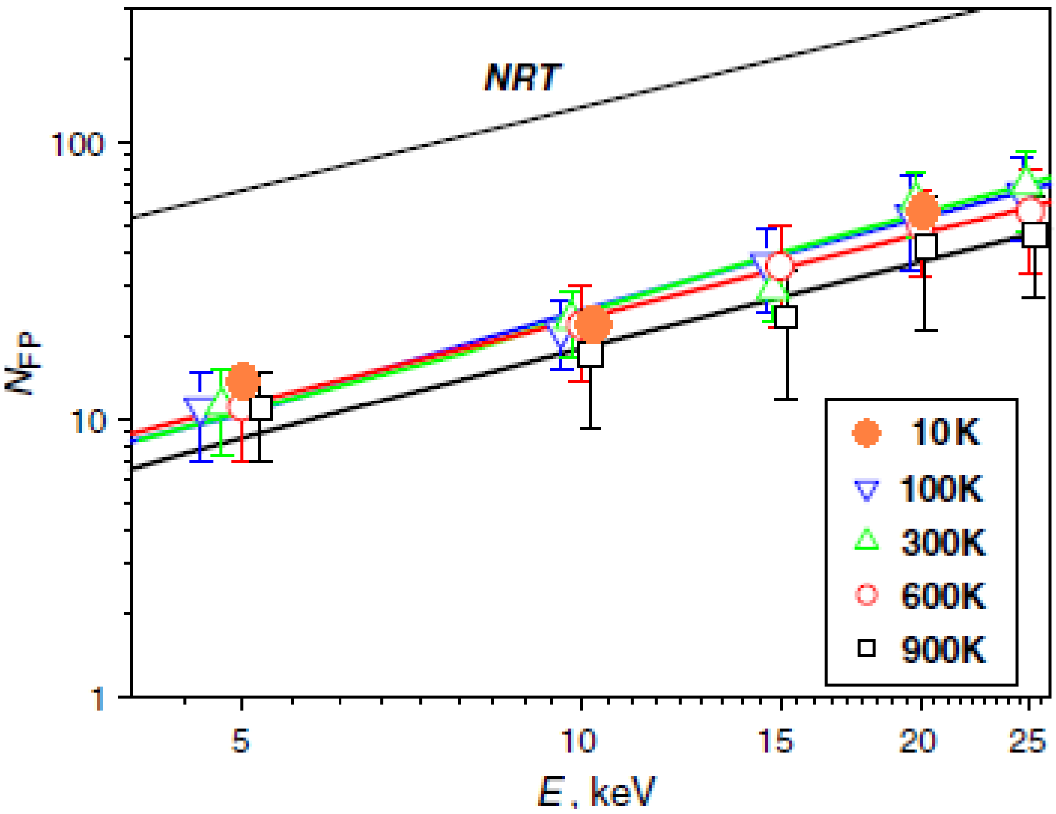
Neutron experiments: $\langle\xi\rangle = 0.32 \pm 0.03$ T=4-5 K

Is there agreement or disagreement ?

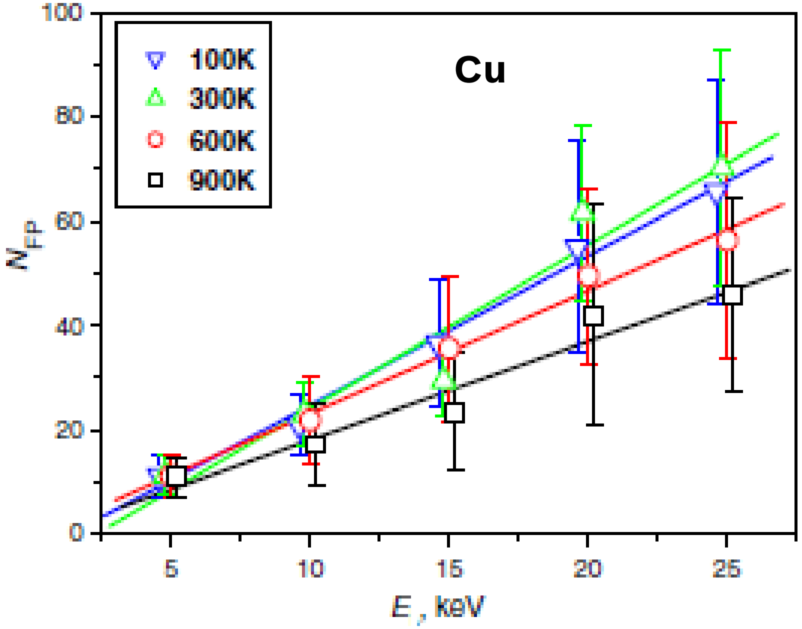
Copper

Caturla el al (2001): 10 K

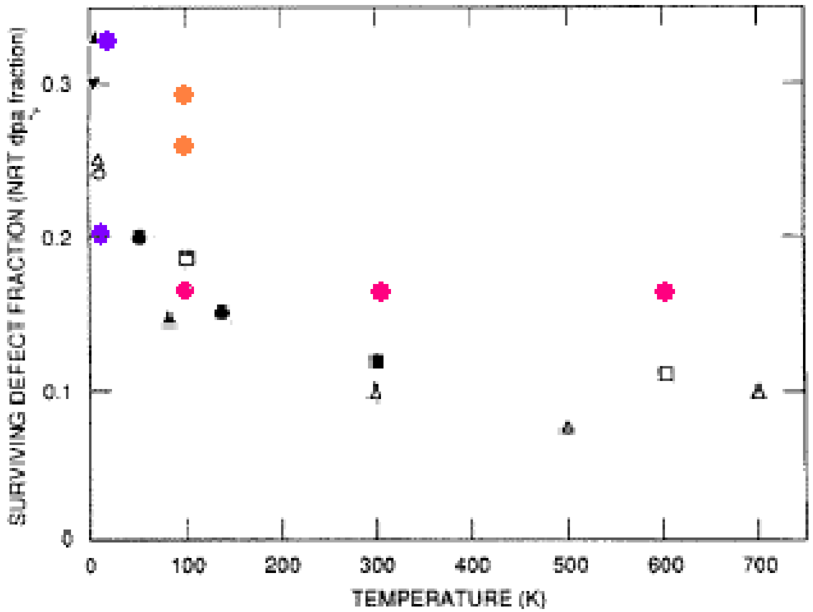
Voskoboinikov et al (2008): 100-900 K



Voskoboinikov et al (JNM 377 (2008) 385)

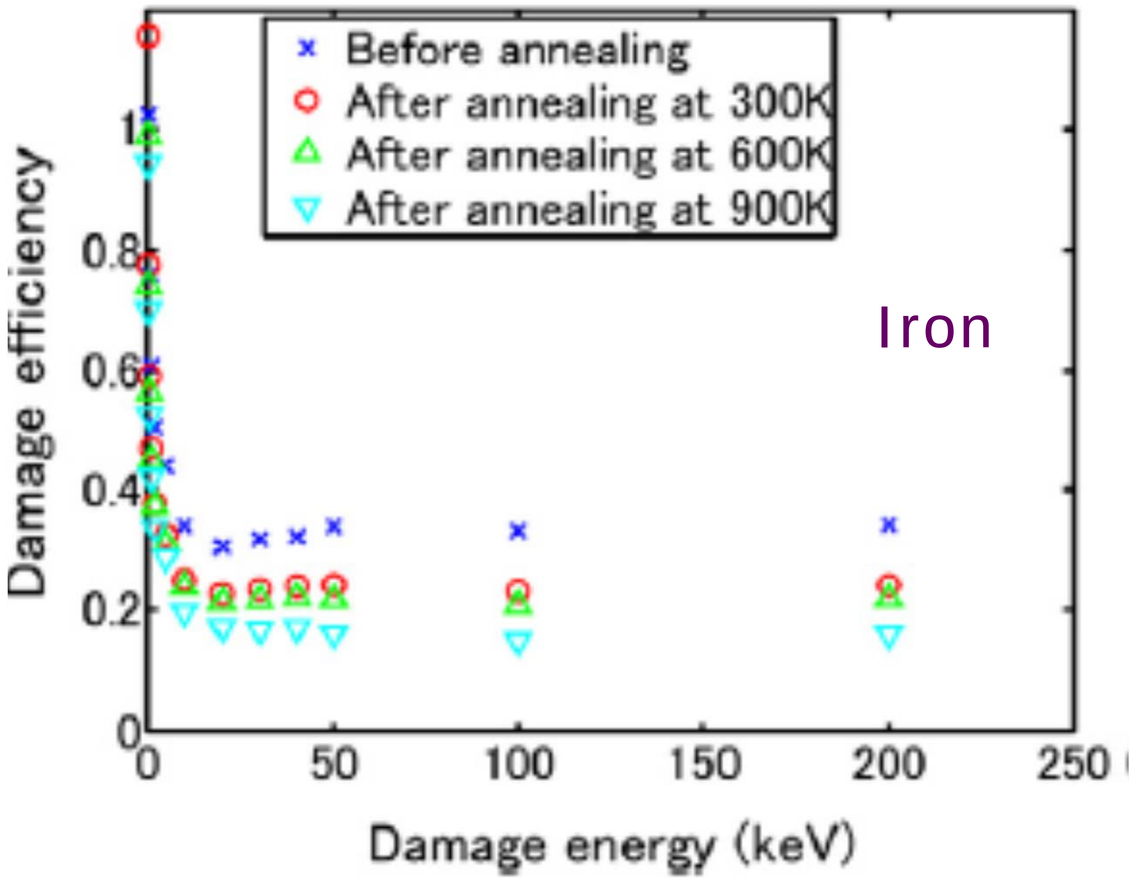


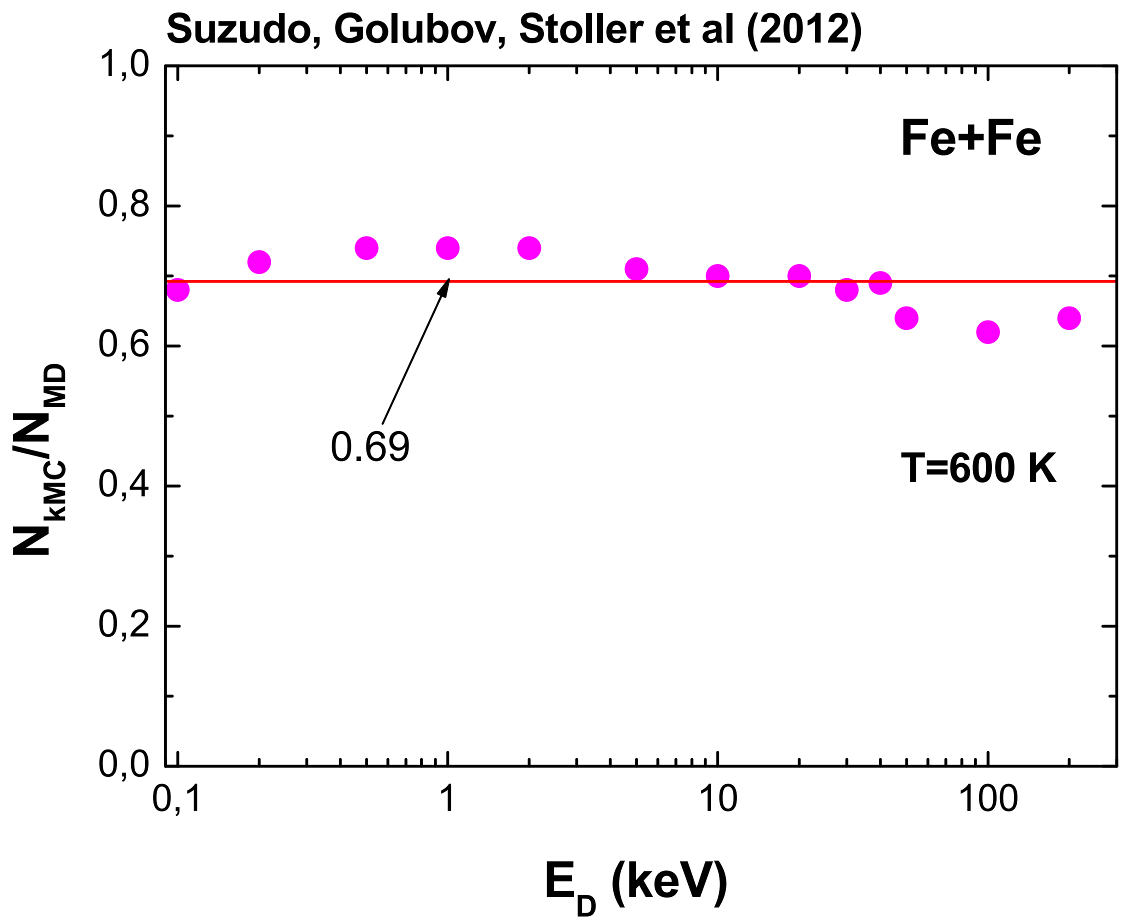
Zinkle, Singh (JNM 199 (1993) 173) (black symbols)
new data: Caturla (2003), Voskoboinikov (2008), Bacon (2000)



2. MD and kMC

T.Suzudo, S.I.Golubov, R.E.Stoller et al: JNM 423 (2012) p.40.

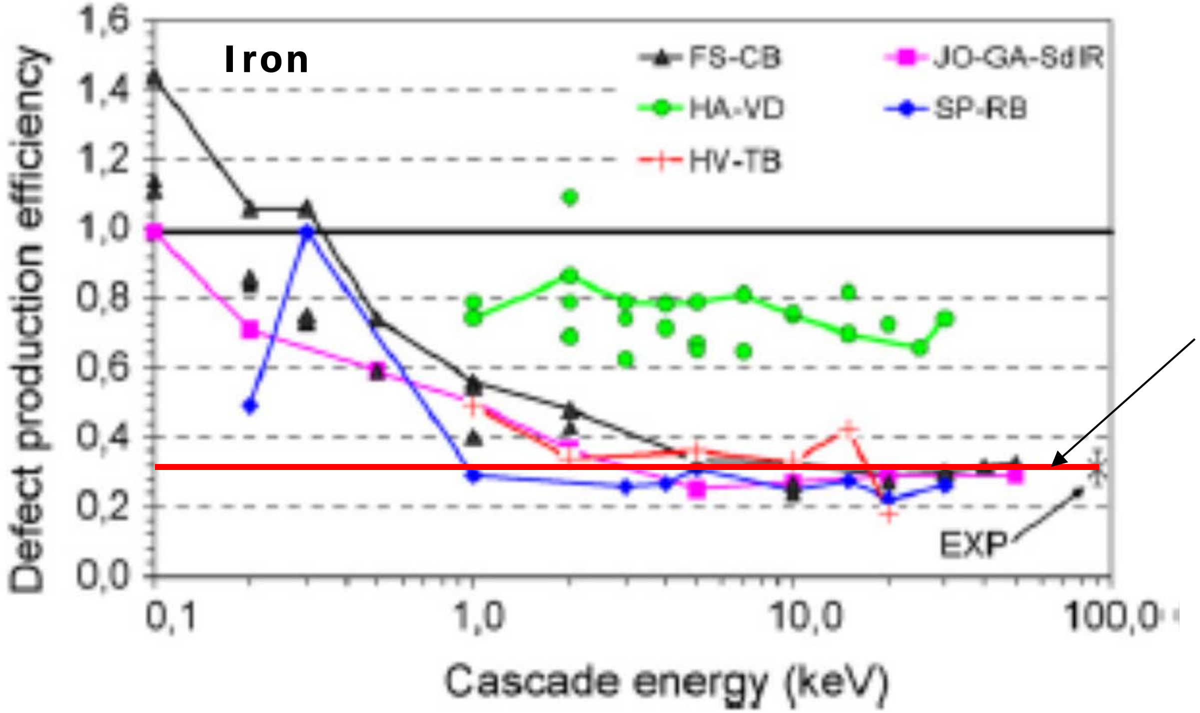




What corrections should be applied for other materials ?

3. Uncertainty of N_D calculations

L.Malerba, JNM 351 (2006) 28; M.Victoria et al, FED 82 (2007)2413



<ξ>$_{exp}$ from neutron irradiation

The uncertainty can be reduced using experimental damage rates for materials irradiated with neutrons at T=4-5 K

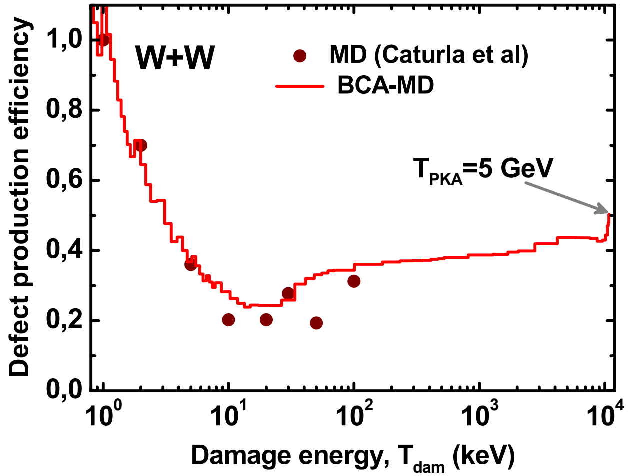
V. Proposed improvements

1. Materials: **Fe, Al, Ti, V, Ni, Cu, Zr, W**

MD results are available

Experimental damage rates are available, T=4-5 K

Modeling: BCA+MD up to hundreds MeV of T_{PKA}



Corrections: kMC

Improvement: use of $<N_D/N_{NRT}>$ values extracted from experimental damage rates for neutron irradiation in reactors

Compilation: JNM 328 (2004) p.197

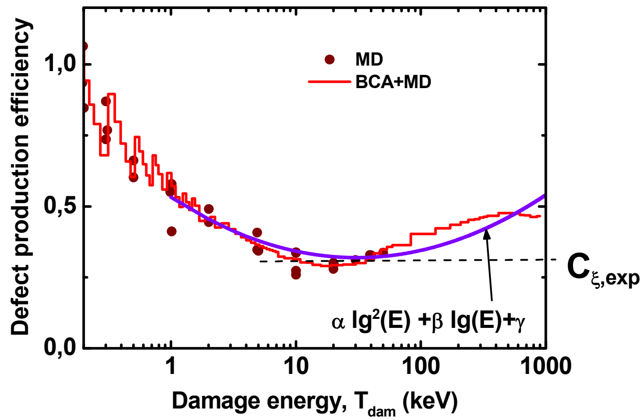
Metal	<ξ>
Al	0.45 ± 0.07
Ti	0.87 ±0.22
V	0.52 ±0.04
Fe	0.32 ±0.05
Ni	0.25 ±0.06
Cu	0.31 ±0.03
Zr	0.72 ±0.13
W	0.61 ±0.08

Compounds: **Fe_3C , Fe_xCr_y, Ni_3Al, WC**

2. Other materials: **Mg, Mo, Ta, …**

MD results are not available

$N_D/N_{NRT}(T)$: parameterization



$C_{\xi,exp}$: $<N_D/N_{NRT}>$ experimental damage rates

Metal	$<\xi>$
Nb	0.67 ±0.21
Mo	0.47 ±0.07
Ta	0.73 ±0.09
Mg	0.45 ±0.04
Ti	0.87 ±0.22
Co	0.27 ±0.06

VI. Processing of nuclear data, NJOY

Total displacement cross-section

a. Explicit form

Realistic displacement cross-sections obtained using MD, BCA-MD :

barns

MF=3, unassigned MT (e.g.=901)

Uncertainties:

MF=33, MT=901

b. Calculations using NJOY

Function DF (NRT)+ calculation of efficiency of defect generation $\xi(T)$

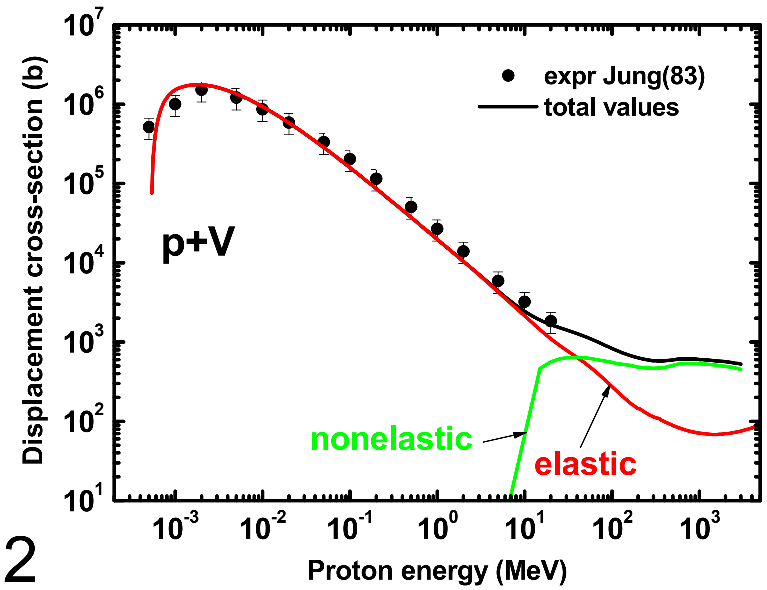
$\xi(T)$: parameterized form

Built-in information: parameters, $C_{\xi,exp}$

Input data: user defined parameters for $\xi(T)$

Elastic displacement cross-sections for incident charged particles

Today omitted in evaluated data files



Variant 1 (+)

Special section: MF=3, MT=902

Variant 2 (-)

Built-in calculations (NJOY): *approximate* calculations

Built-in calculations

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$$\sigma_{d,el}(E_p)=\int_{E_d}^{T_{max}}\frac{d\sigma(E_p,Z_T,A_T,T)}{dT}N_D(T,Z_T,A_T)dT$$

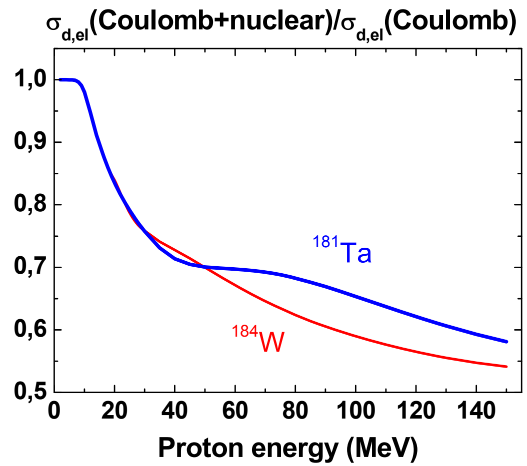
Winterbon, Sigmund, Sanders

$$d\sigma_i(E,Z_T,A_T,T)=\pi a^2 f(t^{1/2})\frac{dt}{2t^{3/2}},$$

$f(t^{1/2})$: the screening function
“a”: the screening length
“t” : the reduced energy

Contirbutions to $\sigma_{d,el}$

- screened Coulomb scattering (+)
- nuclear scattering (-)
- interference (-)



Displacement cross-sections for compounds

Reasonable improvements

Current calculations for Fe_3C: 3 (Fe+Fe) + (C+C)

Special ENDF/B sections (MT) for components

Fe in Fe : MF=3 MT=X_1, e.g. 901

Fe in Fe_3C : MF=3, MT=X_2

Fe in SS_1 : MF=3, MT=X_3

Fe in SS_2 : MF=3, MT=X_4

<…>

Special ENDF/B file (MF) for components (more flexible)

Example: MF=16

The structure close to MF=10

Single MT number, IZAP defines the material

Fe in Fe : MF=16, MT=901, $IZAP_1$

Fe in Fe_3C : MF=16, MT=901, $IZAP_2$

Fe in SS_1 : MF=16, MT=901, $IZAP_3$

Fe in SS_2 : MF=16, MT=901, $IZAP_4$

<…>

Conclusion

Possible improvements of displacement cross-section calculations were discussed

- advanced model calculations of the number of stable defects produced under irradiation
- corrections using experimental data
- parameterization of defect production efficiency
- implementation in NJOY