Karlsruhe Institute of Technology

EUROfusion

Neutron Displacement Cross-Sections for Materials from Be to U Calculated Using the Arc-dpa Concept

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Objective

- preparation of the data set for improved estimation of the number of defects produced in materials from Be to U
- calculation of atomic displacement cross-sections for neutron incident energies 10^{-11} to 200 MeV using data from actual versions of ENDF/B, JEFF, JENDL, and TENDL

Atomic displacement cross-section

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

$d\sigma/dT$: recoil energy distribution
N_d : number of stable displacements produced by PKA

$$N_d(T) = \frac{0.8}{2E_d}\ \xi(T)\ T_{dam}(T)$$

Robinson formula (NJOY, MCNP, SPECTER)

$$T_{dam}(T) = \frac{T}{1 + k(Z_{PKA}, A_{PKA}, Z_T, A_T) g(Z_{PKA}, A_{PKA}, Z_T, A_T)}$$

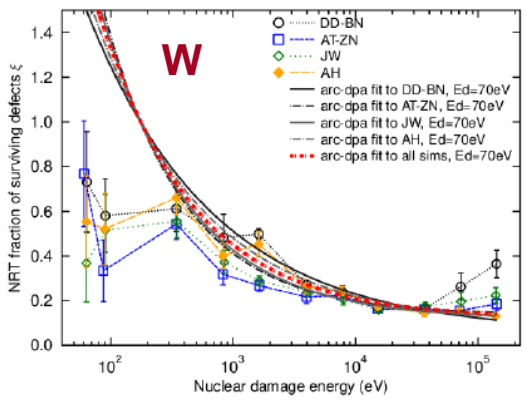
NRT : reference model (poor agreement with experiments and MD)

$$\xi(T_{dam}) = 1$$

Athermal recombination-corrected dpa (arc-dpa) concept*

$$N_d(T_{dam}) = \begin{cases} 0 & \text{when } T_{dam} < E_d \\ 1 & \text{when } E_d < T_{dam} < 2E_d / 0.8 \\ \dfrac{0.8}{2E_d}\xi_{arcdpa}(T_{dam})T_{dam} & \text{when } 2E_d / 0.8 < T_{dam} \end{cases}$$

$$\xi_{arcdpa}(T_{dam}) = \frac{1 - c_{arcdpa}}{(2E_d / 0.8)^{b_{arcdpa}}} T_{dam}^{b_{arcdpa}} + c_{arcdpa}$$



arc-dpa: Fe, Ni, Cu, Pd, Ag, W, Pt, Au

*K.Nordlund et al, NEA/NSC/DOC(2015)9

Estimation of parameters of arc-dpa equations

I. Parameter c_{arcdpa} : asymptotic value of defect generation efficiency

$$c_{arcdpa} = \frac{E_d}{E_{deff}}$$

E_{deff} : the effective threshold displacement energy

$\langle\xi\rangle = 1$ for neutron irradiation in reactors

E_d : the averaged displacement threshold energy

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

E_{dmin} : the minimum displacement threshold energy

The first systematics (1983)

$E_{deff} = C_1 E_{dmin}$ (P.Jung) and $E_d = C_2 T_{melt}$ (Yu.Konobeev,Yu.Korovin)

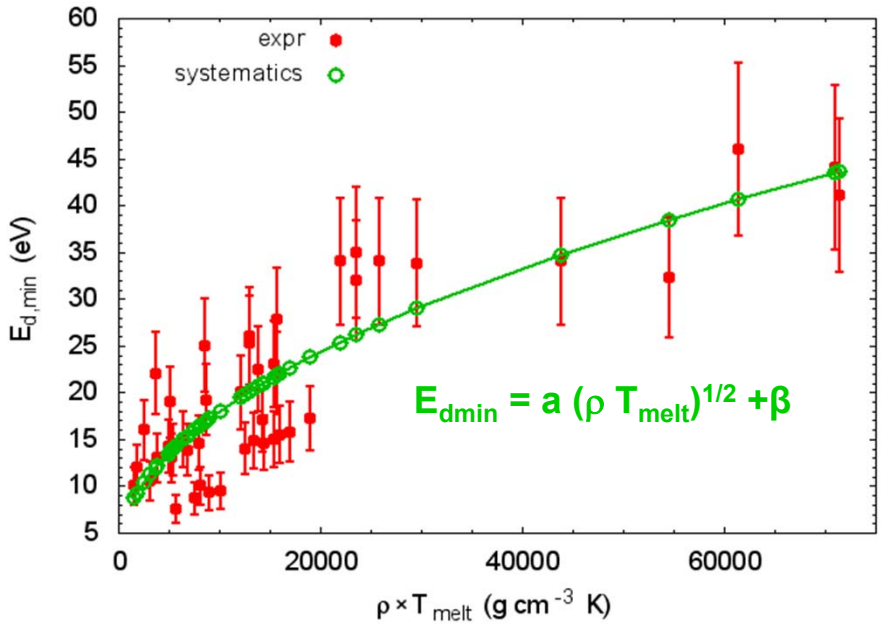
"Blind" search for correlation for E_{dmin}

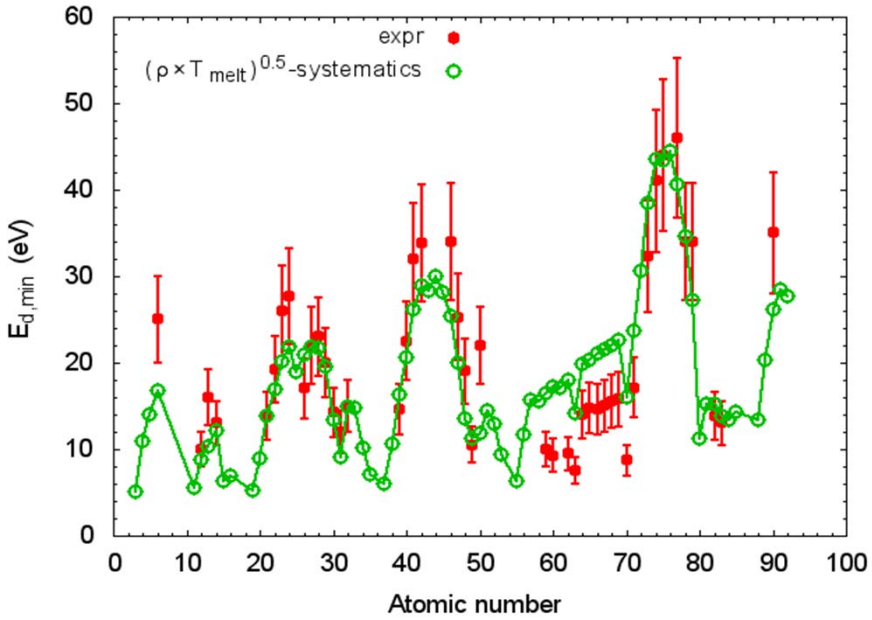
E_{dmin} data: Jung, Eckstein compilations (45 materials)

Quantity	Correlation coefficient
Z	0.22
ρ	0.76
T_{melt}	0.70
$\rho\ T_{melt}$	0.83
$(\rho\ T_{melt})^{1/2}$	0.85
E_{coh}*	0.78
E_{coh}/T_{melt}	-0.09
$\rho\ E_{coh}$	0.85

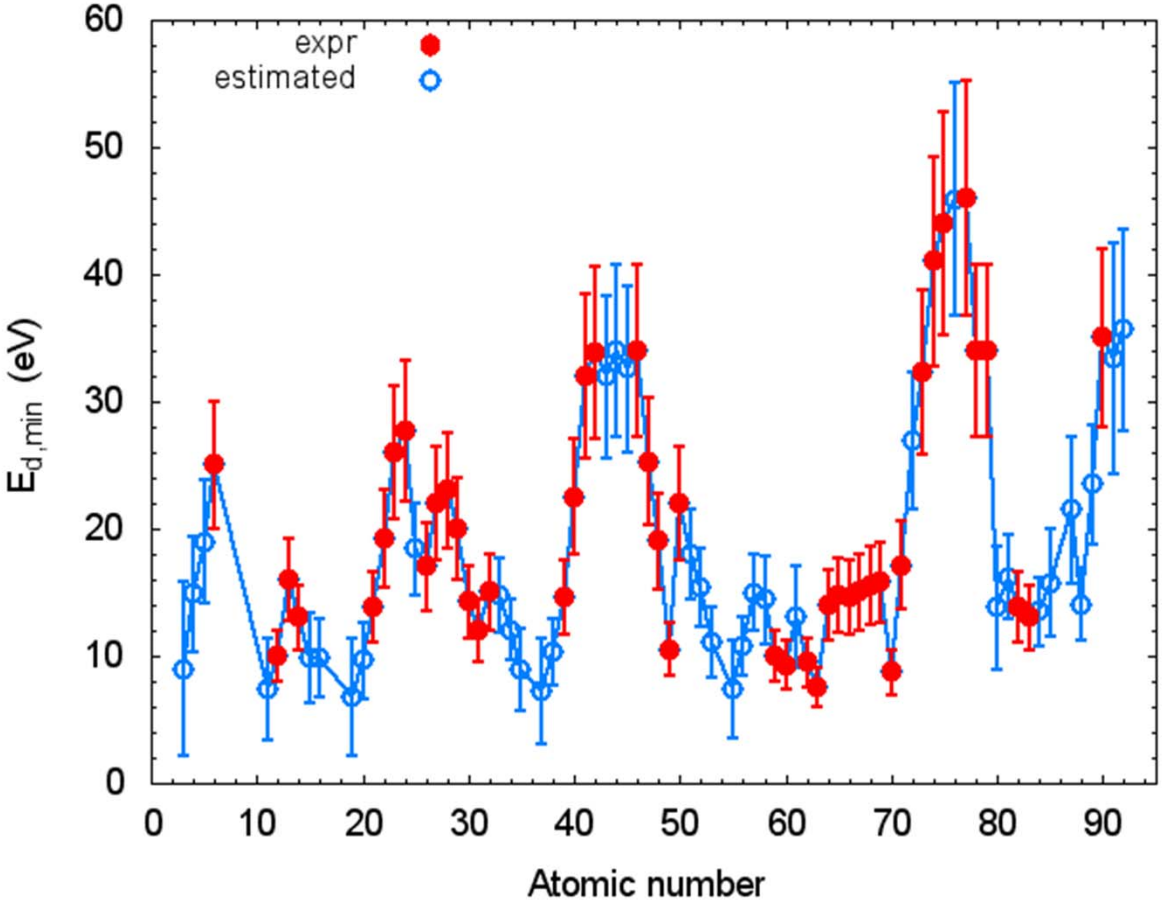
*cohesive energy: difference between the energy of free atoms and the energy of atoms in solid

Example


expr
systematics
$E_{dmin} = a\,(\rho\, T_{melt})^{1/2} + \beta$
$E_{d,min}$ (eV)
$\rho \times T_{melt}$ (g cm^{-3} K)


expr
$(\rho \times T_{melt})^{0.5}$-systematics
$E_{d,min}$ (eV)
Atomic number

Estimated E_{dmin} values

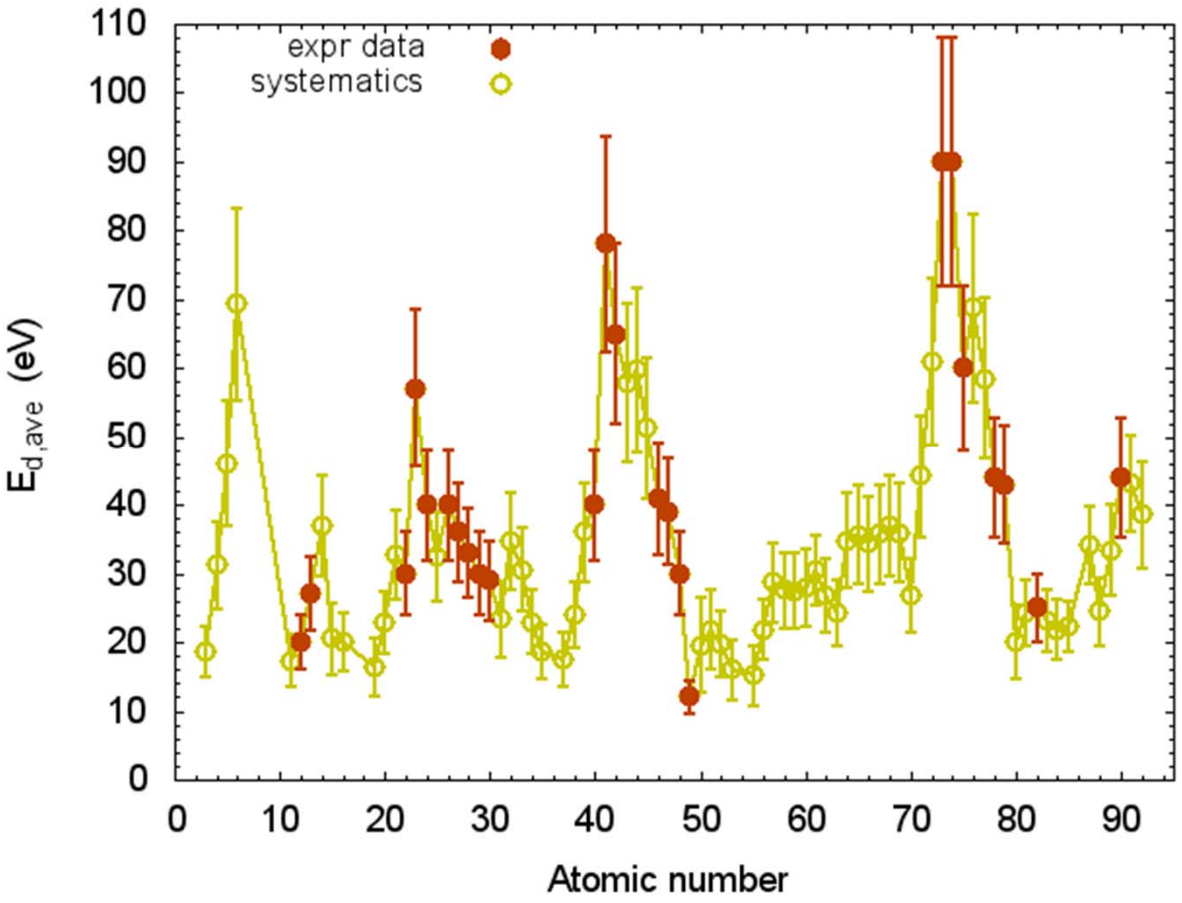


Search for correlation for E_d

E_d: Jung, Broeders compilations (24 materials)

Quantity	Correlation coefficient
E_{dmin}	0.77
Z	0.38
ρ	0.54
T_{melt}	0.89
$T_{melt}^{3/2}$	0.90
E_{coh}	0.86
E_{coh}^2	0.90
$E_{coh}\ T_{melt}$	0.91

Estimated E_d values



^{9}Be: systematics: 31 ± 6 eV MD DFT*: 30 - 35 eV (unknown before analysis)

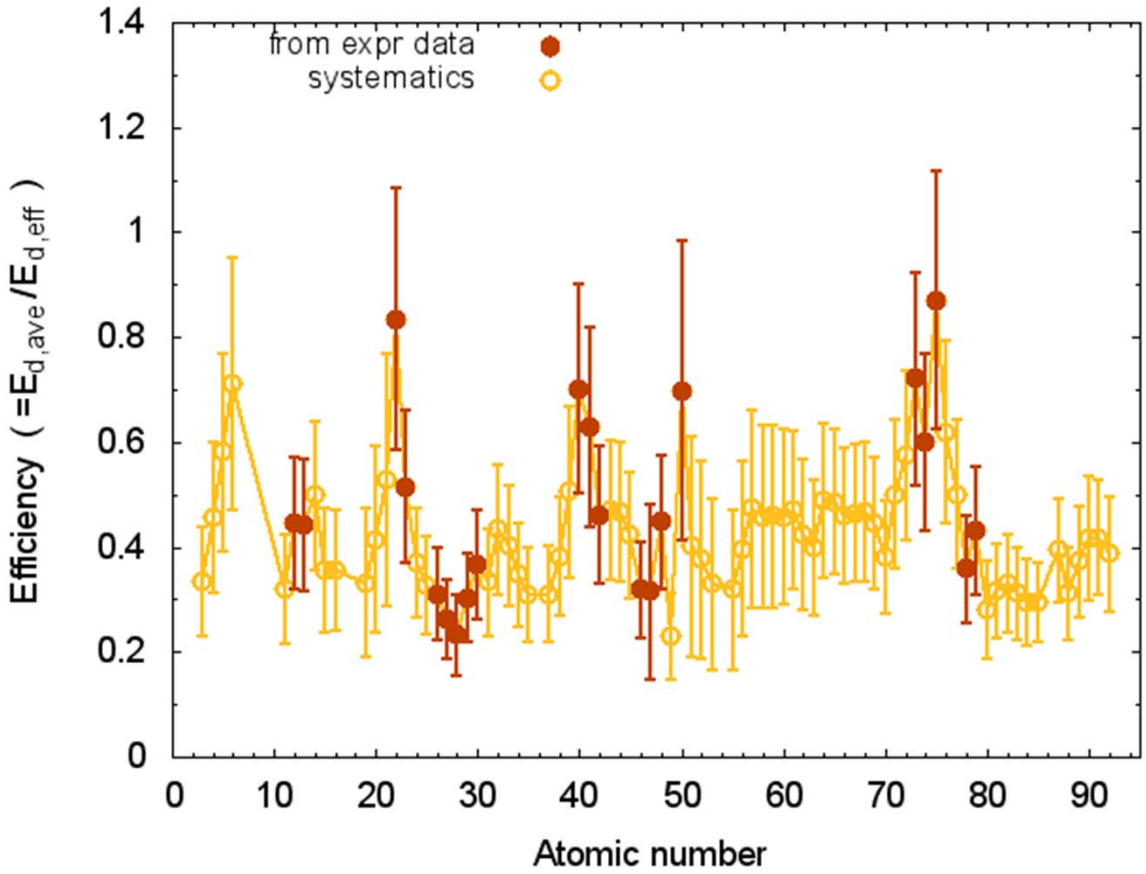
* Vladimirov, Borodin (KIT), NIMB (2017)

Search for correlation for E_{deff}

E_{deff}: Broeders compilations (21 materials)

Quantity	Correlation coefficient
E_{dmin}	0.47
E_d	0.58
Z	0.25
ρ	0.44
T_{melt}	0.50
E_{coh}	0.42

Estimated values of c_{arcdpa}



II. Parameter b_{arcdpa} : the rate of $\xi(T_{dam})$ decrease

$$<\xi> = \frac{\int \sigma_{d,arcdpa}(E)\varphi(E)dE}{\int \sigma_{d,NRT}(E)\varphi(E)dE}$$

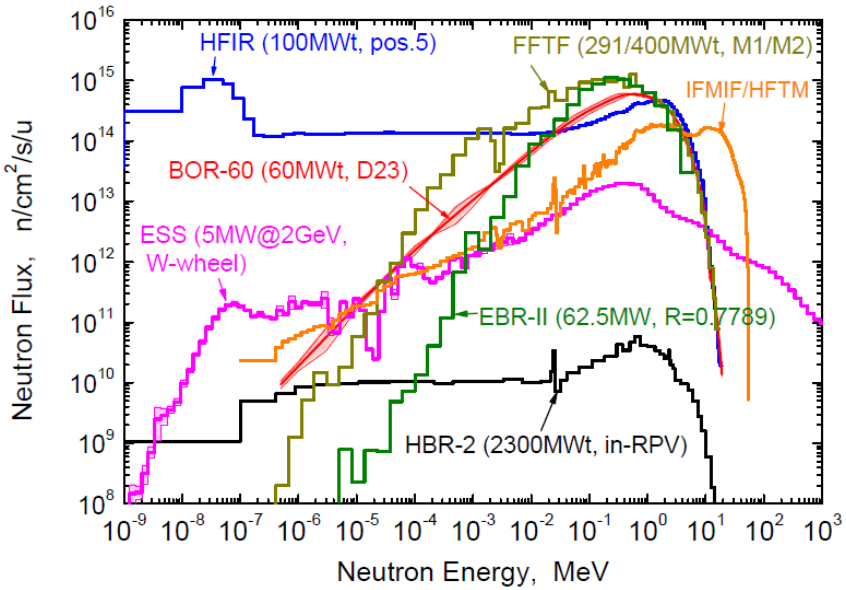
22 neutron irradiation spectra

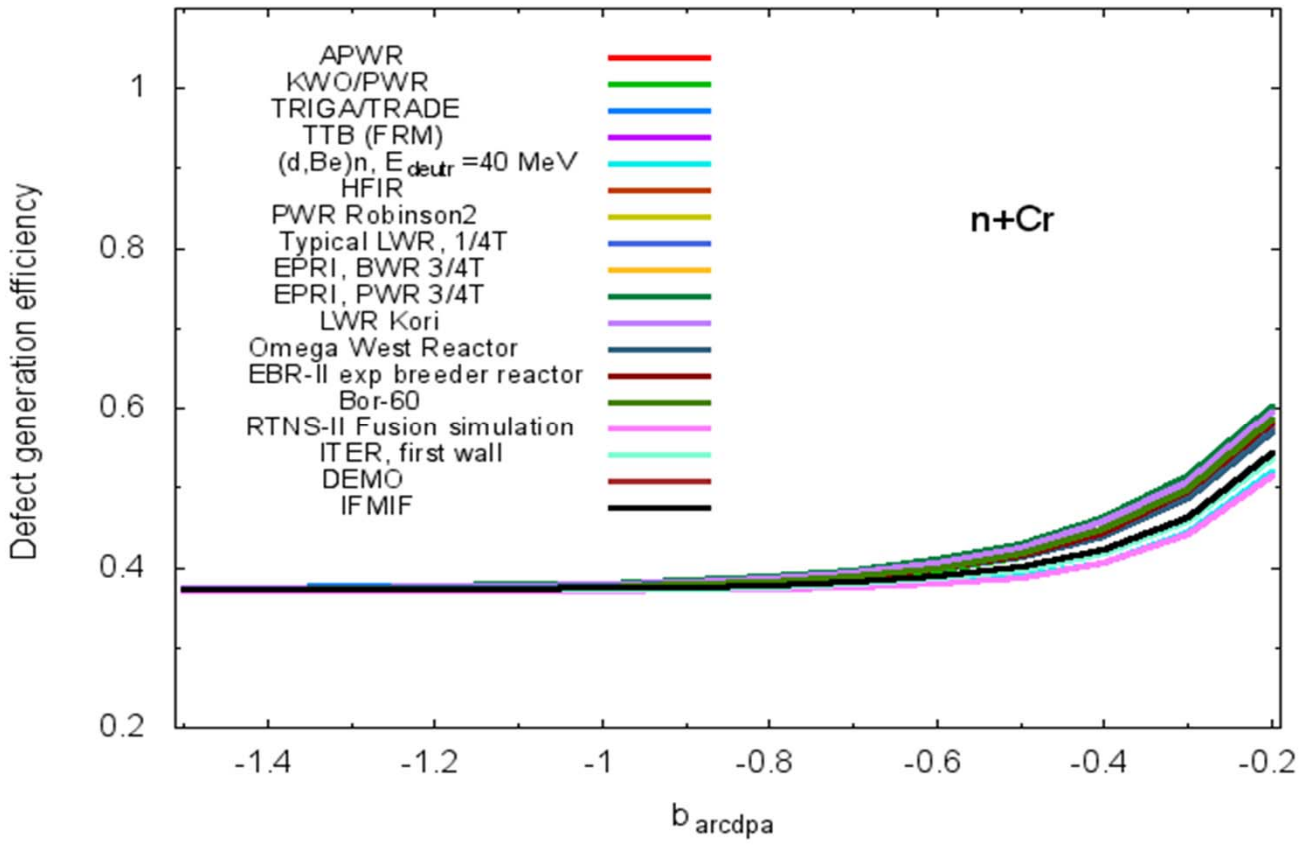
b_{arcdpa} value: from -1.5 to -0.2

Nordlund b_{arcdpa} data

Fe, Ni, Cu, Pd, Ag, W, Pt, Au

S.P.Simakov https://www-nds.iaea.org/CRPdpa




APWR
KWO/PWR
TRIGA/TRADE
TTB (FRM)
(d,Be)n, E deutr =40 MeV
HFIR
PWR Robinson2
Typical LWR, 1/4T
EPRI, BWR 3/4T
EPRI, PWR 3/4T
LWR Kori
Omega West Reactor
EBR-II exp breeder reactor
Bor-60
RTNS-II Fusion simulation
ITER, first wall
DEMO
IFMIF
n+Cr
Defect generation efficiency
1
0.8
0.6
0.4
0.2
-1.4
-1.2
-1
-0.8
-0.6
-0.4
-0.2
b arcdpa

Averaged efficiency values <ξ> for tungsten (b_{arcdpa}, c_{arcdpa}: Nordlund)

Irradiation	ENDF/B-VIII.b4	JEFF-3.3T3	JENDL-4.0	TENDL-2015
APWR	0.26	0.24	0.24	0.25
KWO PWR	0.25	0.23	0.23	0.24
TRIGA/TRADE	0.24	0.22	0.23	0.23
TTB, FRM	0.25	0.23	0.24	0.24
Fission	0.22	0.21	0.20	0.21
14.8 MeV neutrons	0.17	0.15	0.15	0.16
(d,Be) 40 MeV deuterons	0.16	0.14	-	0.16
HFIR	0.25	0.23	0.24	0.24
PWR Robinson2	0.26	0.25	0.26	0.26
Typical LWR	0.26	0.25	0.25	0.26
EPRI, BWR 1/4T	0.24	0.24	0.23	0.24
EPRI, BWR 3/4T	0.27	0.25	0.26	0.26
EPRI, PWR 1/4T	0.26	0.25	0.24	0.25
EPRI, PWR 3/4T	0.30	0.28	0.29	0.29
LWR Kori	0.28	0.27	0.28	0.28
Omega West Reactor	0.24	0.22	0.23	0.23
EBR-II expr breeder reactor	0.26	0.25	0.25	0.25
Bor-60	0.27	0.26	0.25	0.26
RTNS-II Fusion simulation	0.17	0.15	0.15	0.16
ITER, first wall	0.21	0.18	0.18	0.18
DEMO	0.22	0.19	0.19	0.19
IFMIF	0.19	0.14	-	0.18

Material	$D = \frac{<\xi>_{max} - <\xi>_{min}}{<\xi>_{ave}} 100\ \%$			
	ENDF/B-VIII.b4	JEFF-3.3T3	JENDL-4	TENDL-2015
Co	< 20	31	31	<20
Cu*	33	32	32	33
Rh	<20	<20	43	<20
Pd*	20	<20	<20	<20
Ag*	30	<20	<20	<20
Cd	31	70	31	72
In	38	31	38	33
Sm	64	65	64	65
Eu	51	73	59	60
Gd	59	61	60	62
Dy	26	21	28	23
Er	29	<20	29	<20
Lu	32	<20	–	<20
Hf	<20	<20	32	<20
W*	56	68	59	61
Pt*	–	28	–	28
Au*	112	112	62	40
Hg	86	45	83	44

* b_{arcdpa} : Nordlund, b_{arcdpa} = –0.8 in other cases

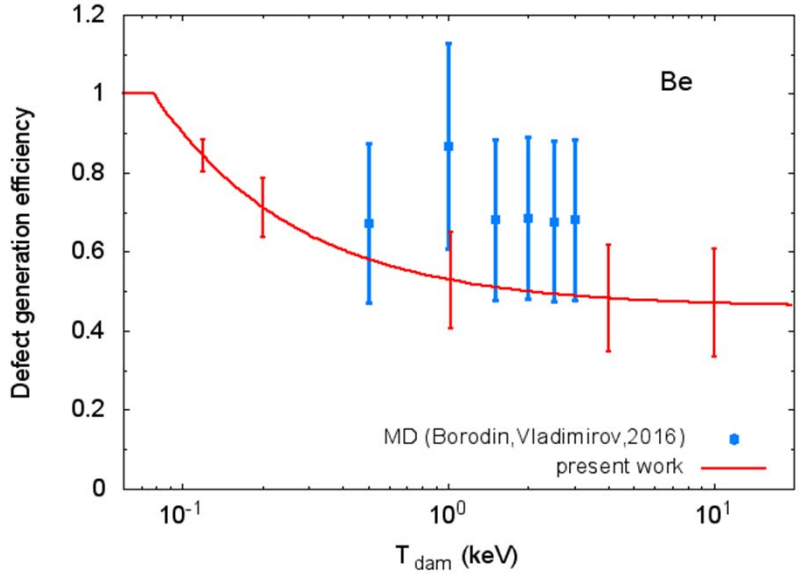
Li to U : 70 materials

Fe, Ni, Cu, Pd, Ag, W, Pt, Au: Nordlund data or c_{arcdpa}, b_{arcdpa} obtained

Co, Cd, In, Sm, Eu, Gd, Dy, Hg: c_{arcdpa} obtained, b_{arcdpa} is very approximate

other materials: c_{arcdpa}, b_{arcdpa} obtained

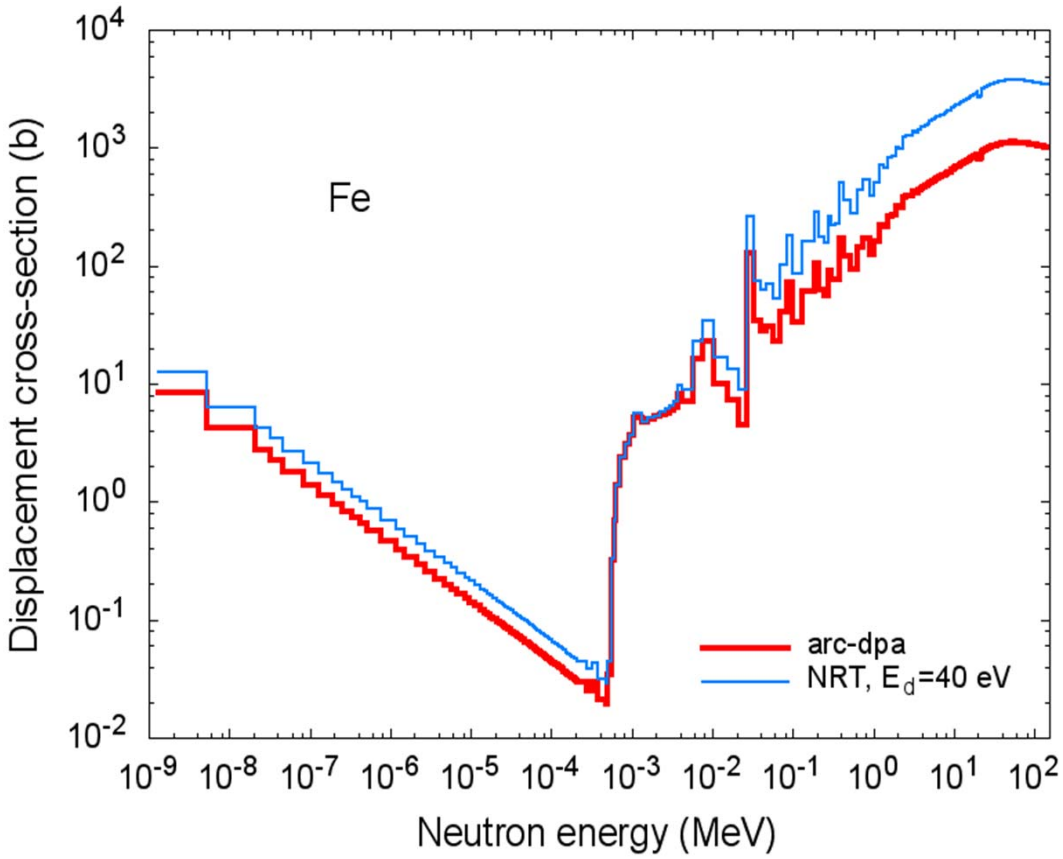
Example



MD: Borodin, Vladimirov (KIT), Nucl. Mat. Energy (2016)

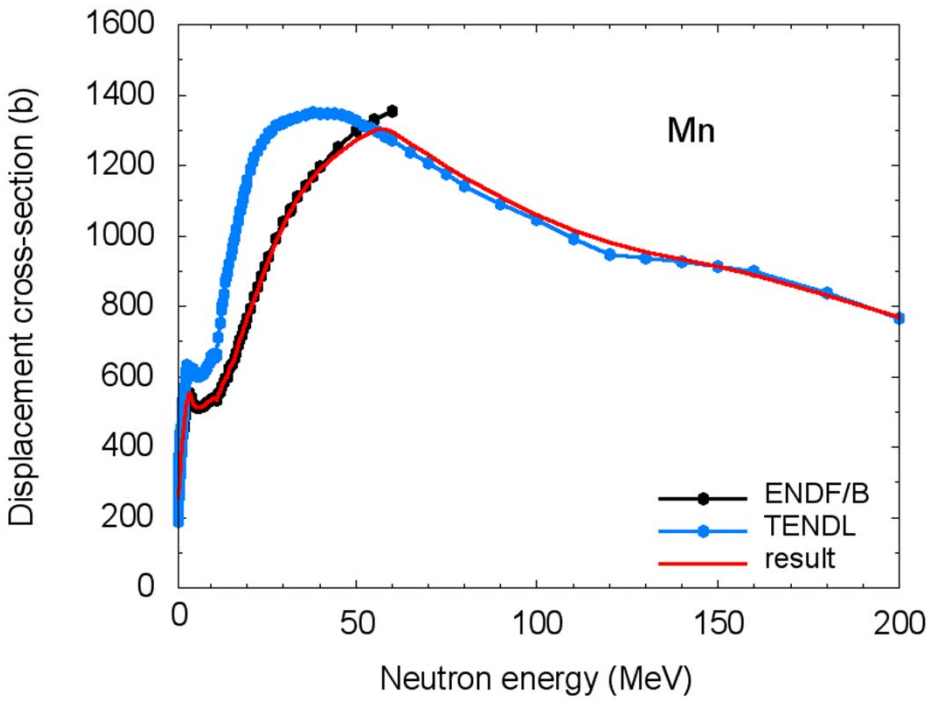
Calculation of displacement cross-sections

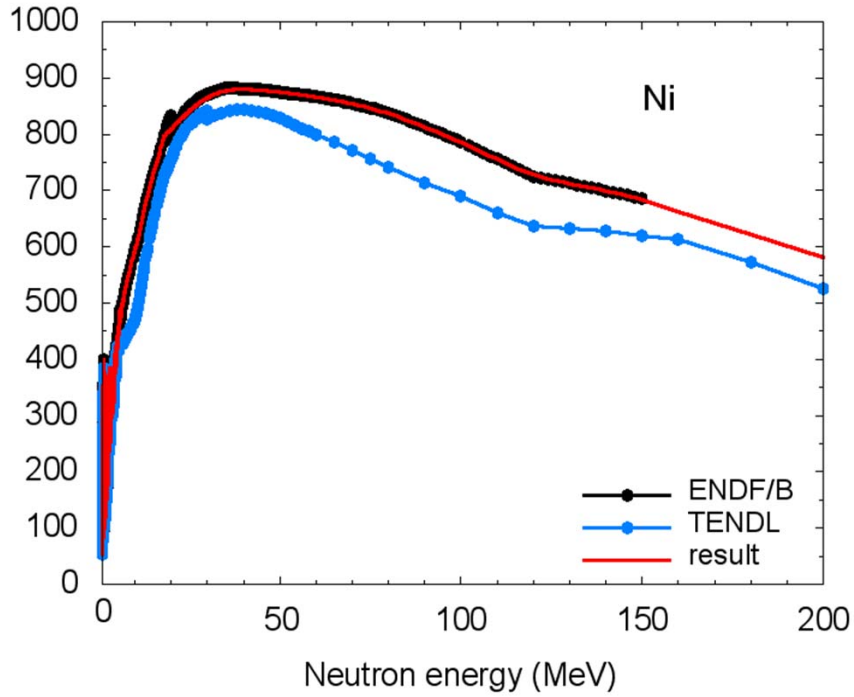
ENDF/B-VIII.beta4, JEFF-3.3T3, JENDL-4.0, TENDL-2015



Extension of the data up to 200 MeV

Examples





Atomic displacement cross-sections for materials from Be to U

Neutron incident energy: from 10^{-11} to 200 MeV

Format: ENDF-6 and ACE

arc-dpa (MT=900) and NRT model (MT=901)

ENDF/B-VIII.beta4: https://goo.gl/RkAbvk

JENDL-4.0: https://goo.gl/FwLqPi

TENDL-2015: https://goo.gl/9YgwCQ

Conclusion

Atomic displacement cross-sections were calculated for materials from Be to U at neutron energies up to 200 MeV using arc-dpa model

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