Ratio of survived primary defects to NRT (Efficiency Function): Overview of available MD results, fits ….

I. Basic Equations (see, e.g. *K. Nordlund et al [1,2]):*

The number of athermal recombination-corrected (arc) defects or replacements-per-atom" (rpa):

$$N_d(E) = \begin{bmatrix} 0 & \text{when} & E < E_d \\ 1 & \text{when} & E_d < E < 2E_d/0.8 \\ \dfrac{0.8E}{2E_d}\xi(E) & \text{when} & 2E_d/0.8 < E < \infty \end{bmatrix}$$

where the efficiency function $\xi(E)$ is for:

the arc-dpa:
$$\xi_{arcdpa}(E) = \frac{1-c_{arcdpa}}{(2E_d/0.8)^{b_{arcdpa}}} E^{b_{arcdpa}} + c_{arcdpa}$$

the rpa:
$$\xi_{\text{rpa}}(E) = \left(\frac{b_{rpa}{}^{c_{rpa}}}{(2E_d/0.8)^{c_{rpa}}} + 1 \right) \frac{E^{c_{rpa}}}{b_{rpa}{}^{c_{rpa}} + E^{c_{rpa}}}$$

II. Fitting to the MD simulations

Table 1. Reliable fitting parameters with uncertainties for the *arc*-dpa and *rpa* equations *ξ(E)* for metals given in Table (other materials - private communication with K. Nordlund):

Material	Crystal Structure	E_d (eV)	*arc*		*rpa*		Fit Range (keV)	Reference
			b_{arcdpa}	c_{arcdpa}	b_{rpa}	c_{rpa}		
Fe	bcc	40	-0.568 ± 0.020	0.286 ± 0.005	1020 ± 140	0.950 ± 0.039	< 200	[2]
Ni	fcc	39	3107	0.930				[1]
Pd	fcc	41	2877	0.980			< 200	[1]
W	bcc	70	-0.564 ± 0.018	0.119 ± 0.005	12300 ± 1300	0.730 ± 0.010		[2]
Pt	fcc	44	5500	0.881			< 200	[1]
Au	fcc	?	?	?				[2]
Zr	hcp	40	$\xi(E_{PKA}) = 5\ E_{PKA}^{0.75}/(0.8\ E_{PKA})/2E_d)$				< 50	[3]
Fe	fcc	40	$\xi(E_{PKA}) = A\ E_{MD}^{B}/(0.8\ E_{PKA})/2E_d)$: A=4.05, B=0.86				< 100	[4]

Comments: E_d values which are used by authors in their fits (the differences cp. ASTM recommendation are noted).

Reference

1. K. Nordlund, A.E. Sand, F. Granberg et al., Primary Radiation Damage in Materials, OECD/NEA Report *NEA/SC/DOC(2015)9*
2. K. Nordlund, IAEA CRP RCM-2 Summary Report *INDC(NDS)-0691, p. 19*; IAEA, Dec 2015
3. N. Lazarev, IAEA CRP RCM-2 Summary Report *INDC(NDS)-0691, p. 83*; IAEA, Dec 2015
4. D. Terentyev, IAEA CRP RCM-2 Summary Report *INDC(NDS)-0691, p. 87*; IAEA, Dec 2015

III. Extending of the Efficiency function to the higher reaction Recoils energies.

To cover existing and designed materials testing facilities we need efficiency functions for the PKA energy up to, e.g. in the case of Fe:

- 0.7 MeV for Fission, where maximum Neutron Energy 10 MeV,
- 1.0 MeV for Fusion, where maximum Neutron Energy 15 MeV,
- 3.8 MeV for IFMIF, where maximum Neutron Energy 55 MeV,
- 140 MeV for Spallation, if maximum Neutron Energy 2000 MeV.

Contributions:

- A. Konobeev: https://www-nds.iaea.org/CRPdpa/SRIM_MD.pdf
- other contributions ???

IV.1. Published Information for Mono-elemental materials

1. Iron

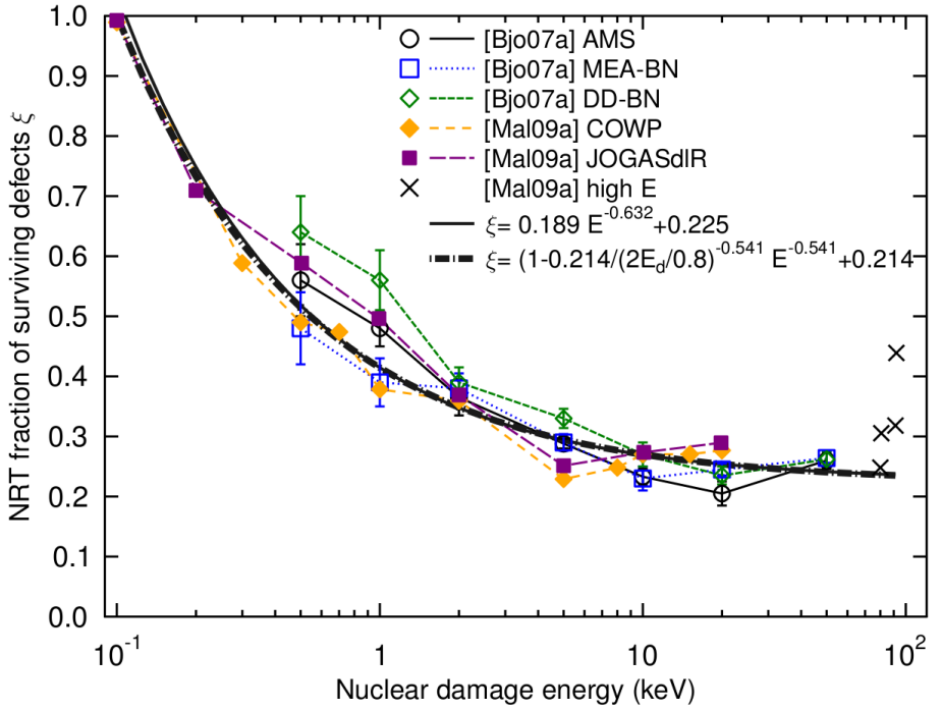


Fig. 1.1. Fraction of surviving defects (Frenkel Pair) vs. **MD energy**.
Fig. from K. Nordlund, INDC(NDS)-0624, p. 17.

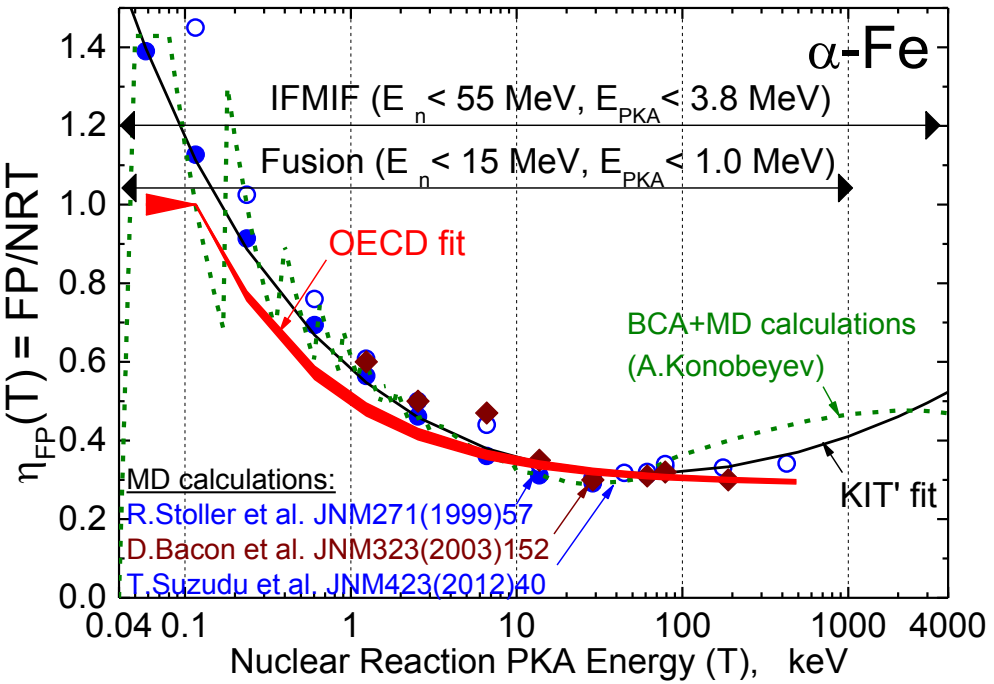


Fig. 1.2. Fraction of surviving defects (Frenkel Pair) vs. **PKA initial energy**.
Symbols: MD data: from Ref. shown in Fig.
Curves: BCA+MD by A. Konobeyev, Acc. App. 2011 (- - -)
K. Nordlund' fit to available MD results by formula
$\varepsilon_{FP}(T(E_{MD})) = \frac{1-c}{(2E_d/0.8)^b} E_{MD}^b + c$ incl. uncertainties (—)

1. Iron (cont.)

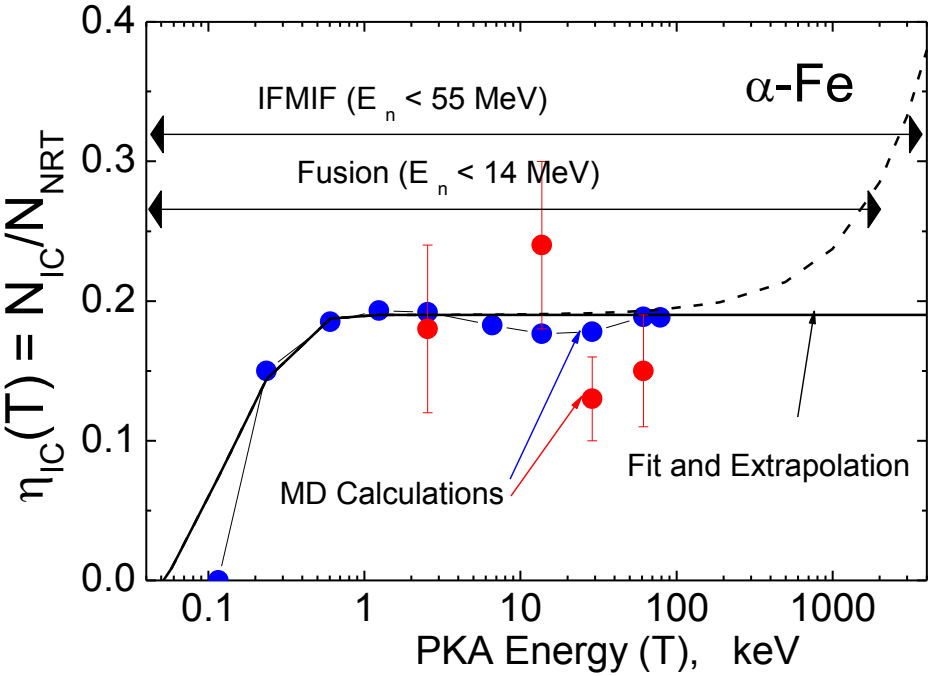


Fig. 1.3. Efficiency function for Interstitial Clusters:
MD results from R.E. Stoller, L.R. Greenwood, JNM 271(1999)57;
and D.J. Bacon, Yu.N. Osetsky et al., JNM 323(2003)152

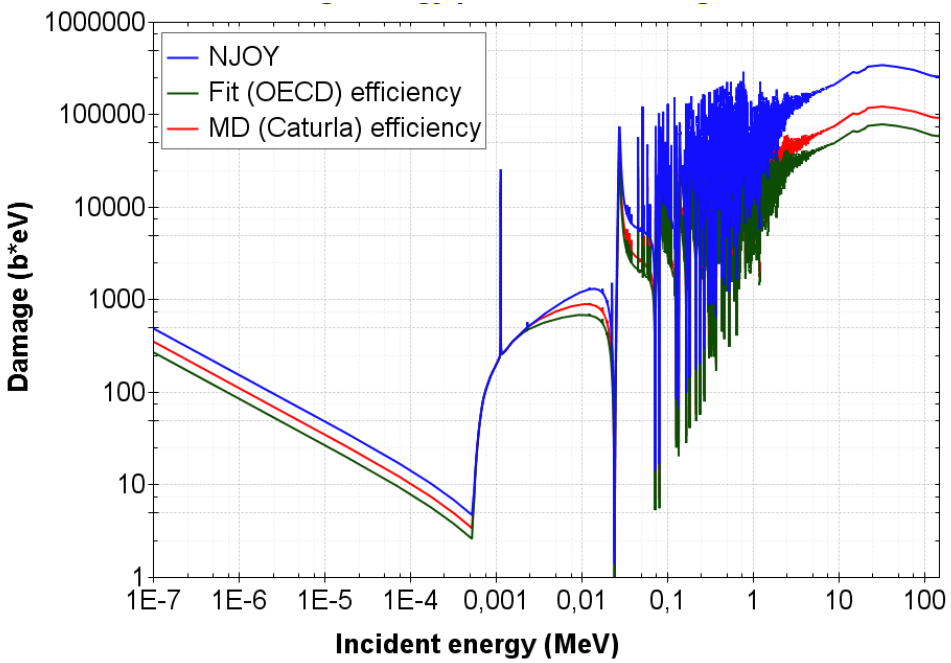


Fig. 1.4. Impact of FP Efficiency on the arc-dpa.
Fig. from O. Cabellos' presentation at RCM-1
(see https://www-nds.iaea.org/CRPdpa/RCM1_Presentations.htm)

2. Copper

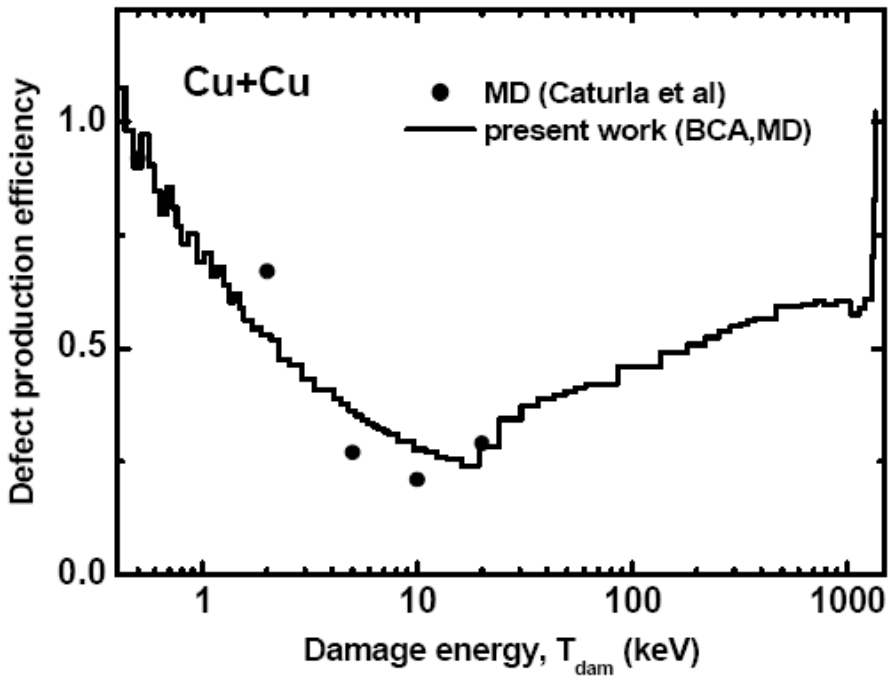


Fig. 2.1. FP vs. PKA Energy.
Fig. from A. Konobeev et al., AccApp-2007, p. 241
MD results - M.J. Caturla et al., J. Nucl. Mat. 296(2001)90

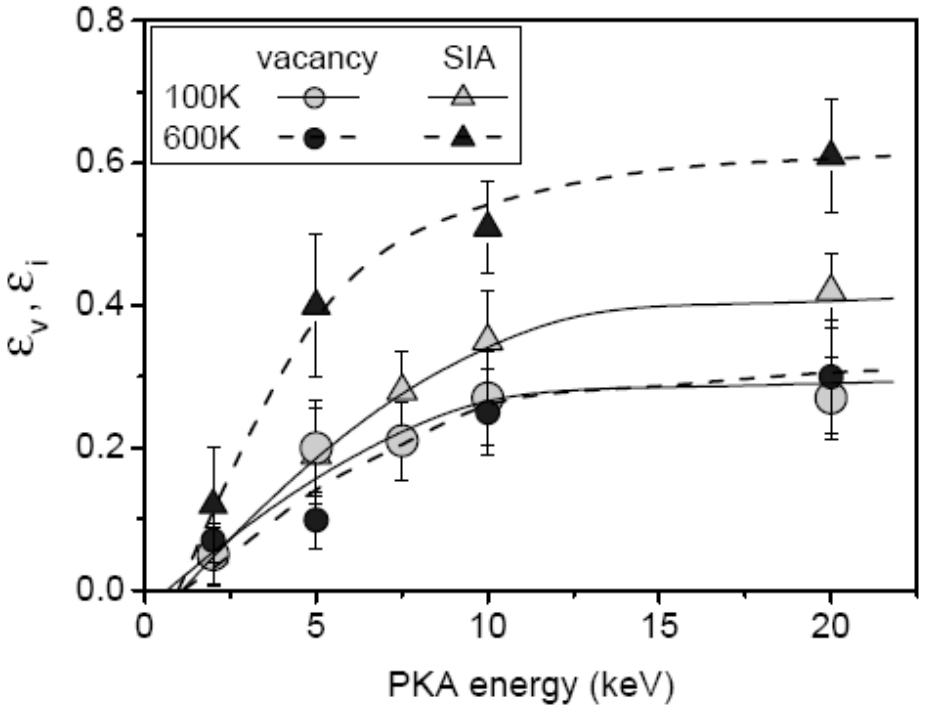


Fig. 2.2. Fraction of Vacancies and Interstitials Clusters vs. PKA energy and impact of Temperature.
Fig. from D.J. Bacon et al., JNM 365(2004)46

2. Copper (cont.)

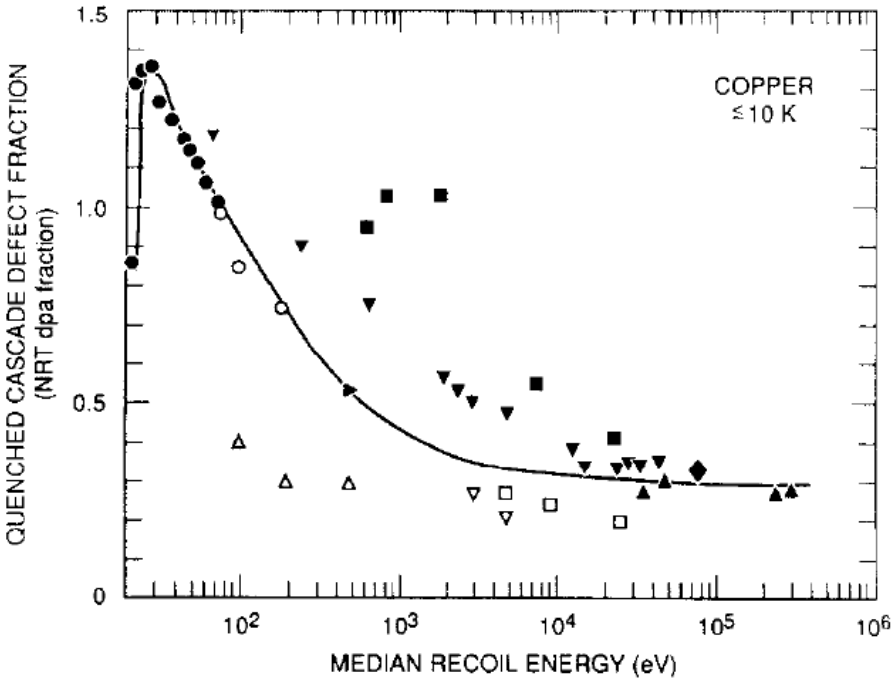


Fig. 2. Dependence of the quenched cascade defect fraction (QDF) on median PKA energy in copper. The open symbols [6,20,54,55] refer to MD calculations whereas the filled symbols refer to experimental measurements as the result of electron (●) [48], ion (▼ ■) [9,47], fission fragment (◆) [53] and neutron (▶ ▲) [11,49–52] irradiation at low temperatures.

Fig. 2.3. Taken from S.J. Zinkle and B.N. Singh,. JNM 199(1993)173

3. Tungsten

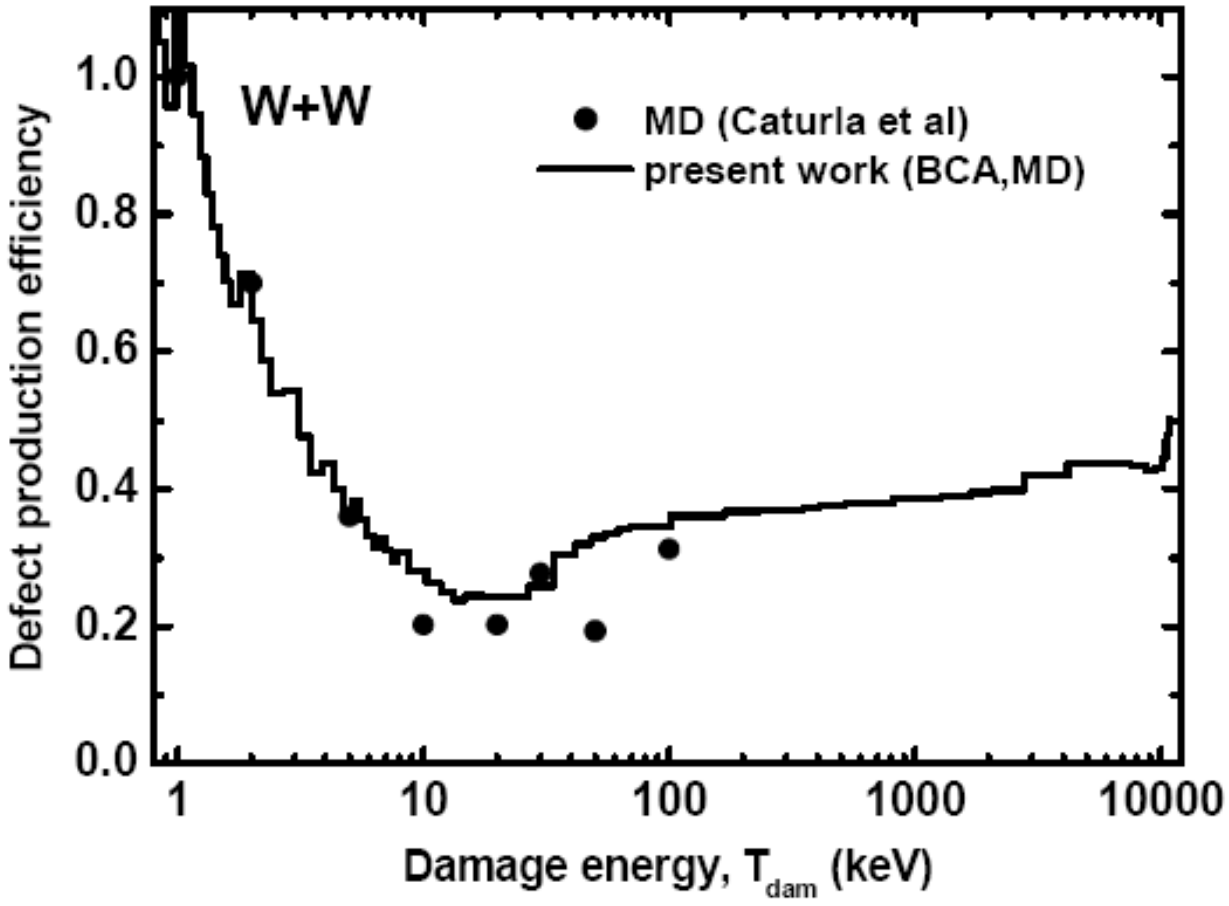


Fig. 3.1. from A. Konobeyev, C.H.M Broeders, U. Fisher, Proc. of AccApp-2007, p. 241.
MD results from M.J. Caturla et al., J. Nucl. Mater. 296(2001)90

4. Aluminium, Titanium, Nickel, Zirconium and alloy Ni_3Al

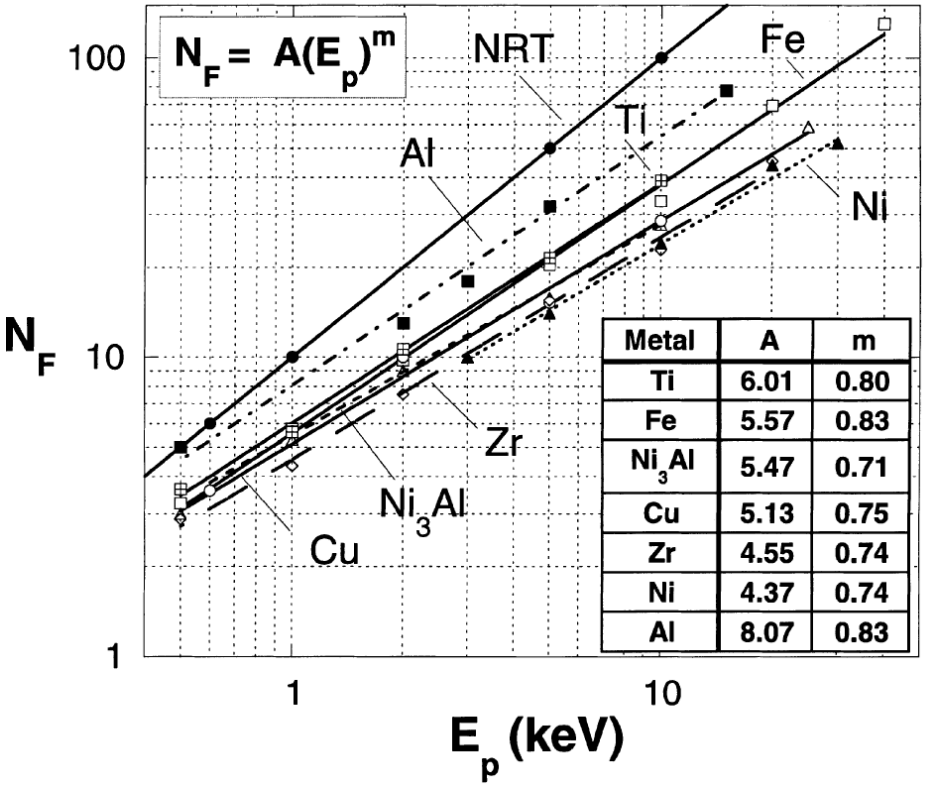


Fig. 4.1. Survived number of Frankel Pairs vs. PKA energy.
Fig. from D.J. Bacon et al., JNM 276(2000)1

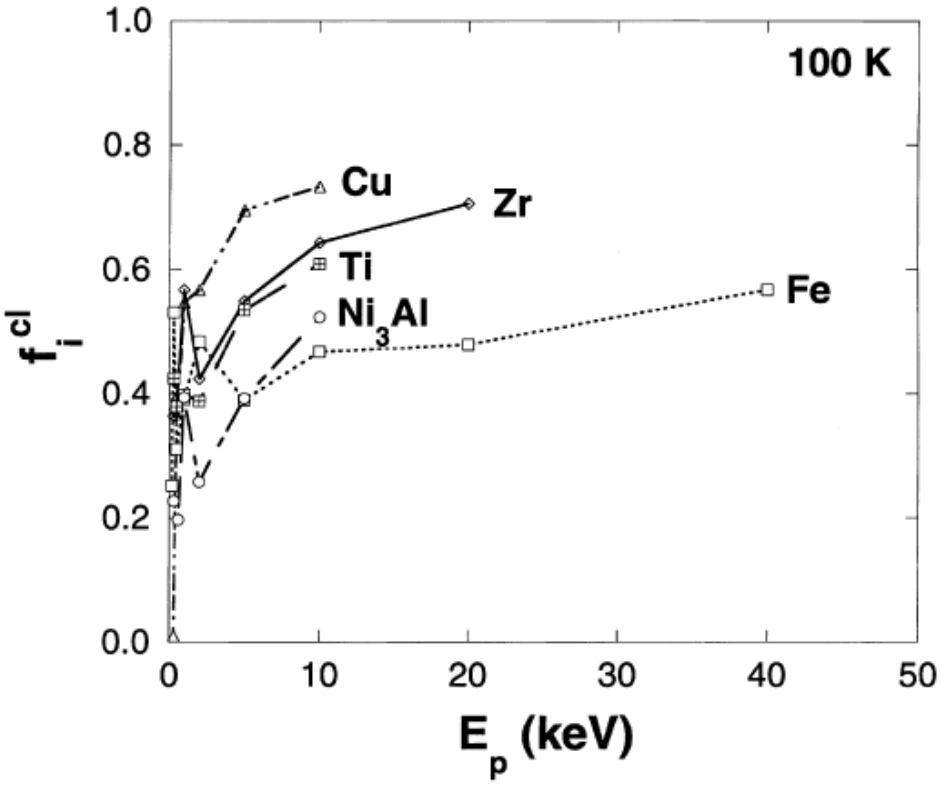
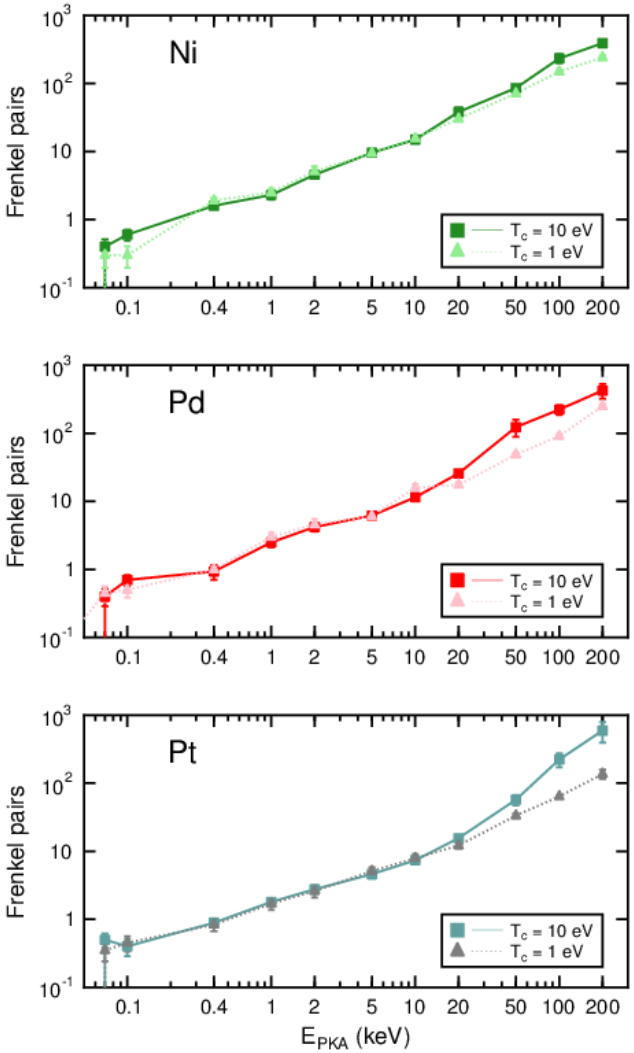


Fig. 4.2. Survived number of Clusters of Interstitials vs. PKA energy.
Fig. from D.J. Bacon et al., JNM 276(2000)1

5. Nickel, Palladium and Platinum



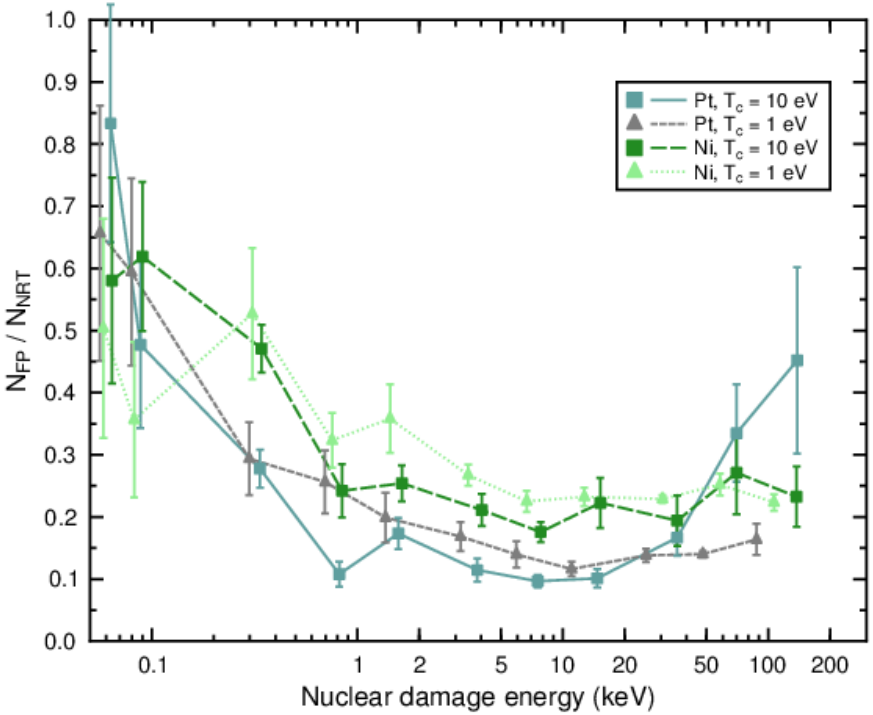


Fig. 5.1. Numbers of surviving defects (FP) from simulations with different T_c and efficiencies functions FP/NRT.

Figs. from A.E. Sand, K. Nordlund, "On the lower energy limit of electronic stopping in simulated collision cascades in Ni, Pd and Pt", JNM 456(2015)99

6. Silver

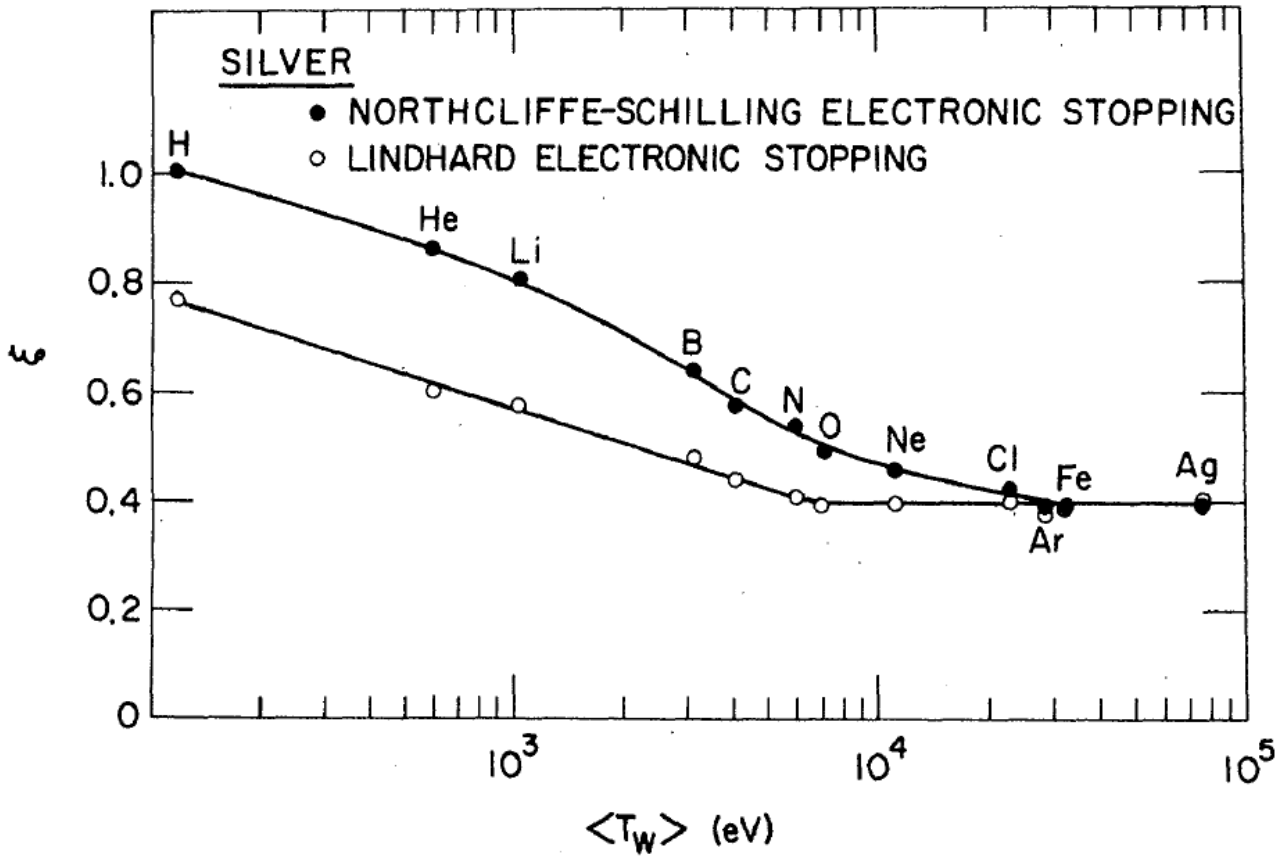


Fig. 6.1. Efficiency for ion irradiation of Silver (*is it an impact of electronic stopping power ?*).
Fig. from R.S. Averbach et al., Phys. Rev. B18 (1978) 4156

IV.2. Published Information for Multi-elemental (crystalline) materials

1. Fe-xCr systems

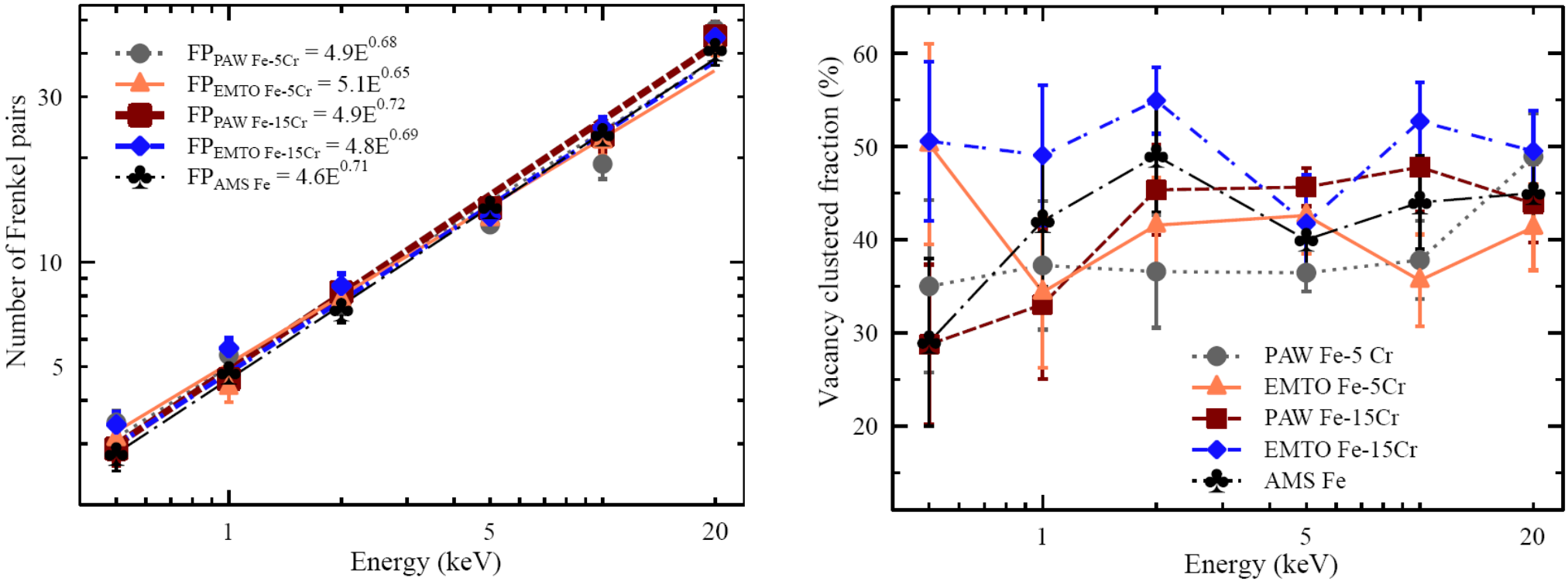


Fig. 1.1. The averaged number of surviving Frankel Pairs (left) and fraction of Vacancies in Clusters vs PKA energy in Fe-xCr and pure Fe vs. PKA energy. Figs. from K. Vörtler, C. Björkas, D. Terentyev, L. Malerba, K. Nordlund., JNM 382(2008)24 (see there more details and results).

2. Fe-xCu systems

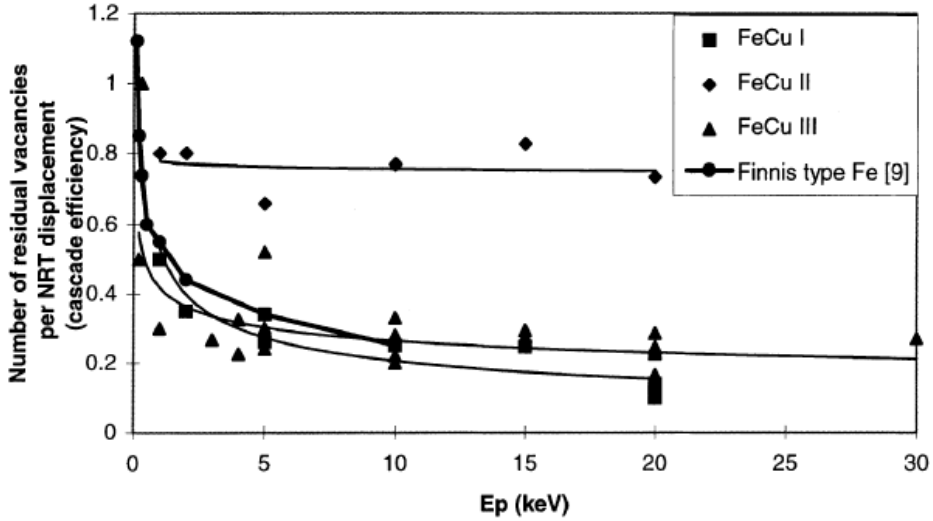


Fig. 4. Number of residual vacancies per NRT displacement (cascade efficiency) versus PKA energy at 600 K. The result of each cascade is represented instead of simulation averages. The drawn lines are only guidelines to show the trends.

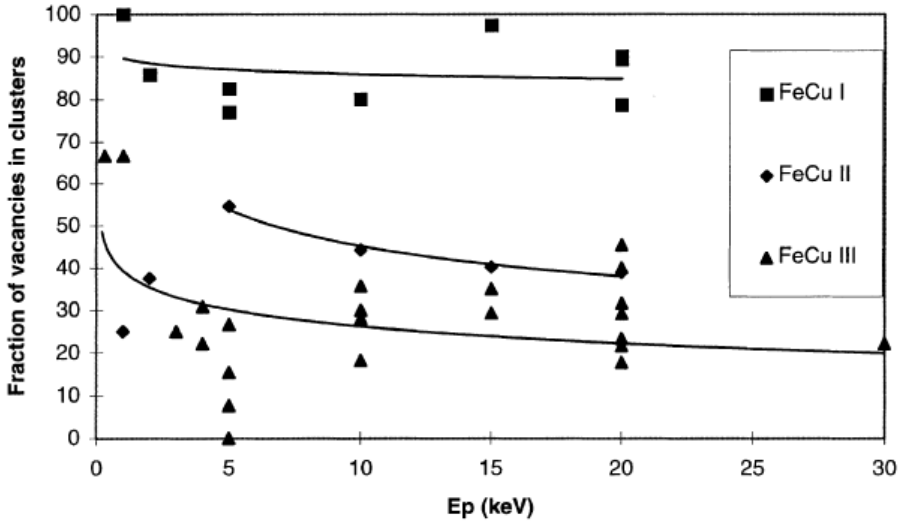


Fig. 7. Amount of vacancies in clusters versus PKA energy at 600 K for FeCu I, FeCu II and FeCu III. The result of each cascade is represented instead of simulation averages. The drawn lines are only guidelines to show the trends.

Fig. 1.2. The example figures for FeCu from C.S. Becquart C. Domain, A. Legris, J.C. Van Duysen, JNM 280(2000)73.

3. Fe-xMn-yNi-zCr systems

Table 3.1. Reliable fitting parameters for the *arc*-dpa *ξ(E)* for alloys:

Material	Crystal Structure	E_d (eV)	*arc*		*rpa*		Fit Range (keV)	Reference
			b_{arcdpa}	c_{arcdpa}	b_{rpa}	c_{rpa}		
alloys Fe-xMn-yNi-zCu	fcc	40	$\xi(E_{PKA}) = A\ E_{MD}^{B}/(0.8\ E_{PKA})/2E_d$): see parameters in [4]				< 100	[4]

Reference

4. D. Terentyev, IAEA CRP RCM-2 Summary Report *INDC(NDS)-0691, p. 97, Annex 1*, IAEA, Dec 2015