Evaluation of Tungsten as Divertor Plasma-Facing Material: Results from Ion-Irradiation Experiments & Computer Simulations

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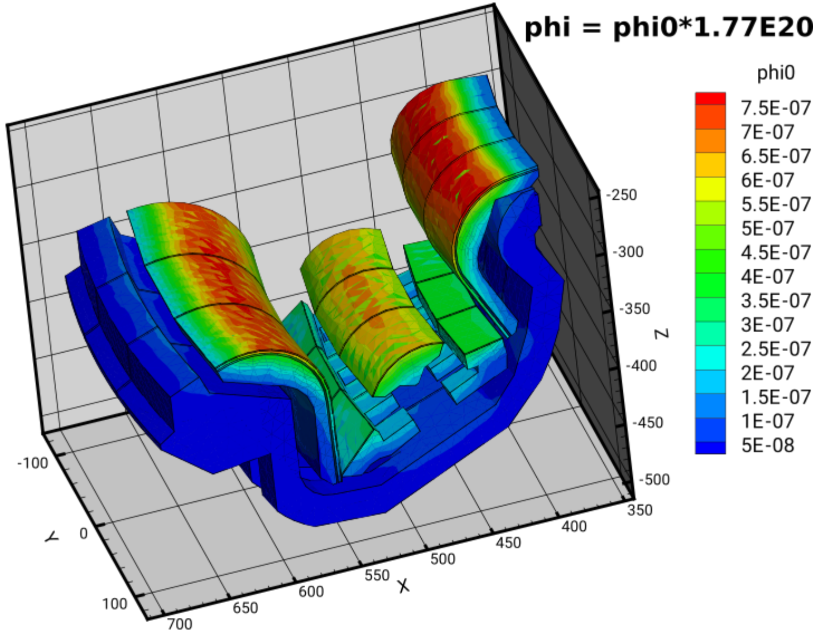
Tungsten as Plasma-Facing Material

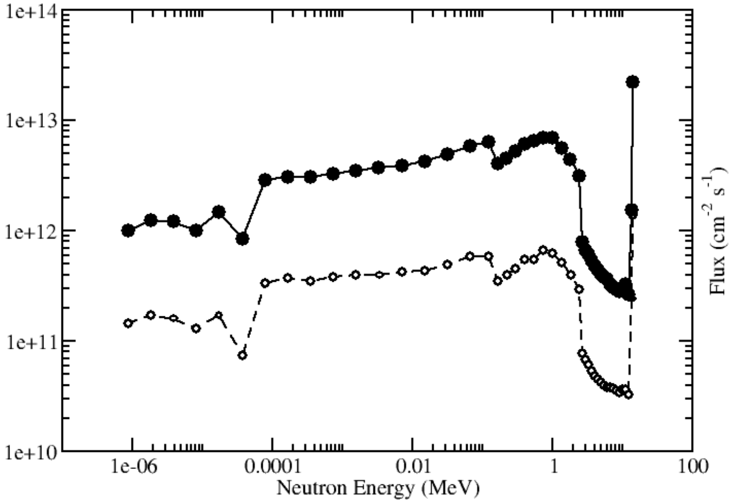
- Low T-retention
- High melting point
- Low erosion
- Low dust formation
- Low Z_{eff}
- High heat flux handling

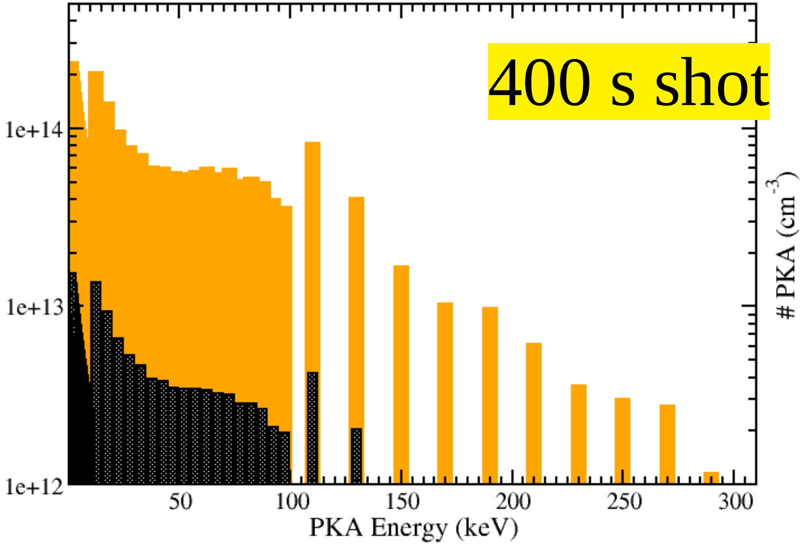
Neutron Irradiation & T-retention

What will be the T-retention in reactor environment?

Neutron flux & PKA spectrum for “ITER-like” reactor







Neutron transport calculations using ATTILA combined with SPECTER

PKA/neutron ~ 0.4

Even if only one D/T-atom was trapped at each defect ...

Machine	Power (MW)	Γ_n (cm^{-2} s^{-1})	FPY§ (lifetime)	Φ_n (cm^{-2})	PKA$ (cm^{-3})	FP$§ ($cm^{-3}$)	T atom - trapped&&
ITER-like**	500	1.7 $x10^{13}$	0.4	2 x 10^{20}	8 x 10^{19}	$8x10^{19}$	$4x10^{25}$ (200 gm)
DEMO*	2000	7 x 10^{13}	14	3 x 10^{22}	1.2 x 10^{22}	1.2 x 10^{22}	**$0.6x10^{28}$ (30 kg!!!)**

* DEMO based on ITER-like
** Surface area ~1000 m^2
§ 1 FPY = 3 x 10^7 s
$ PKA/n = 0.4
$§ FP/PKA = 1
&& 100 m^2 n-wetted area (OVT+dome+IVT)

Assuming 20 years – 1.5kg/year

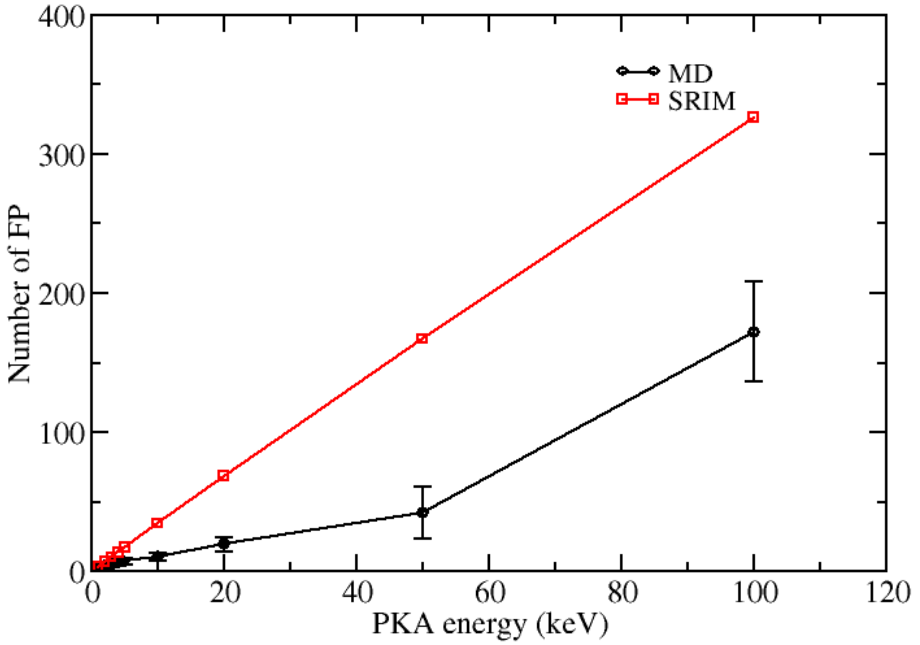
Regulatory limit may force a de-tritiation/change

From the point of view of trapping it is crucial to understand the nature of defect and its relation to PKA

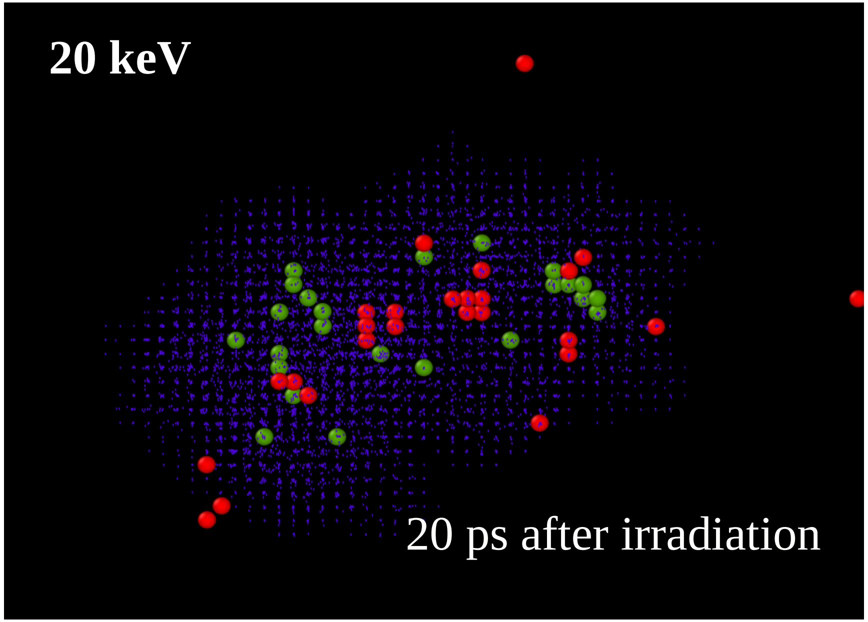
Number of defects & defect cluster size increases with PKA energy

Comparison with SRIM E_d = 90 eV.

Recombination is significant

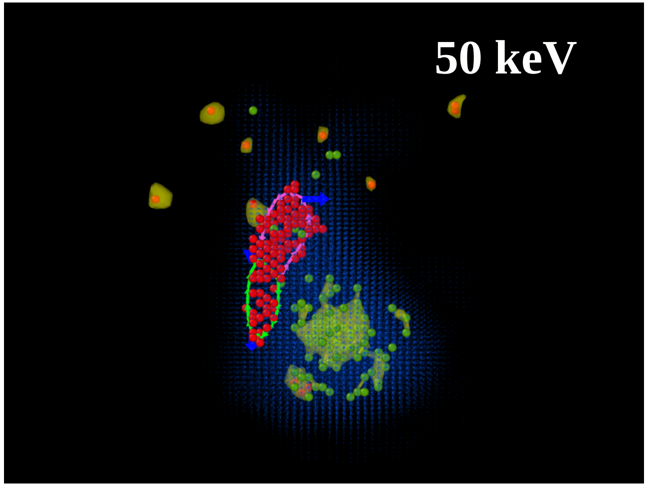


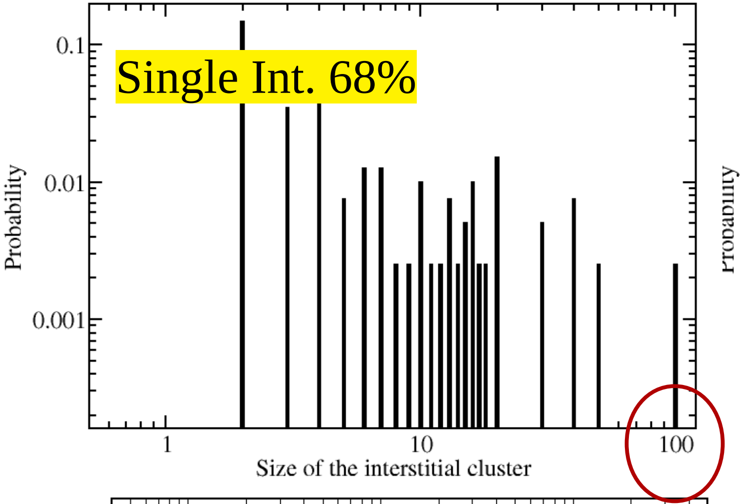
At lower PKA energies, (E_{PKA} < 30 keV) smaller defect clusters are formed

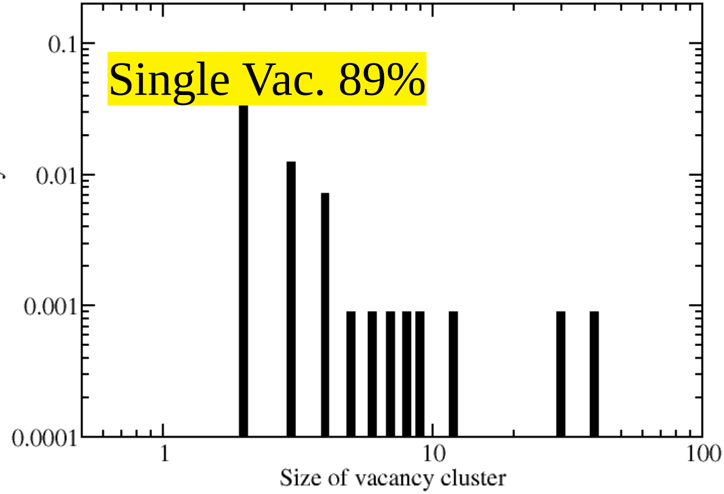


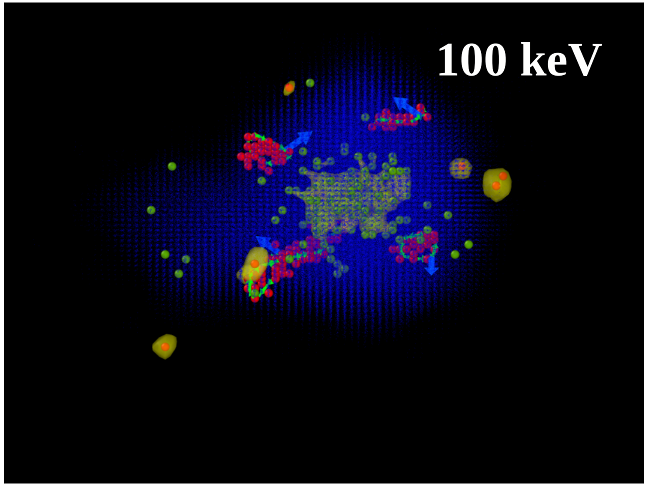
Interstitials in red, Vacancies in green
Atoms participating in the cascade ~1/2 ps have been superposed

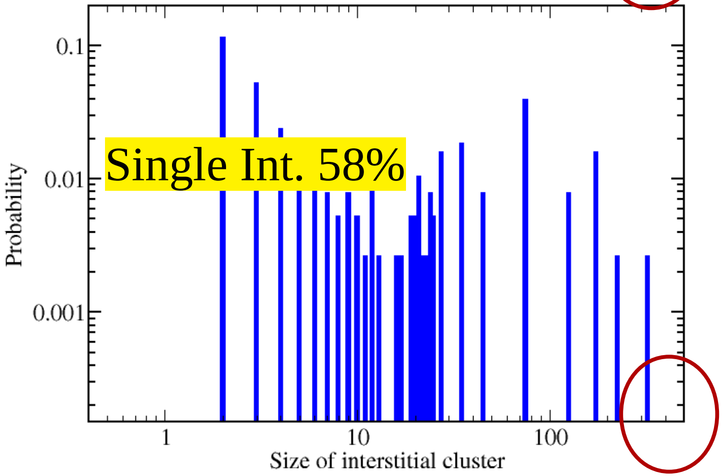
As PKA energy increases larger interstitial & vacancy clusters are formed

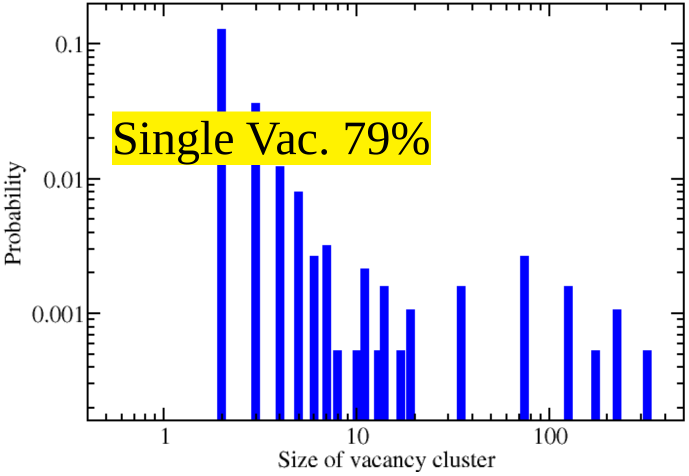




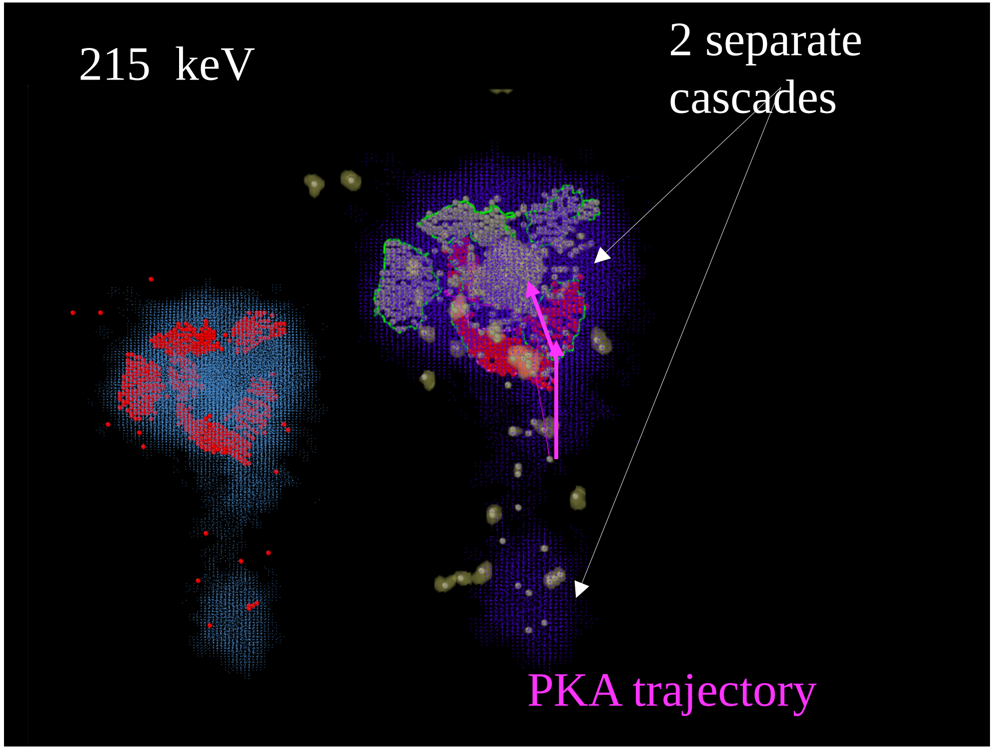




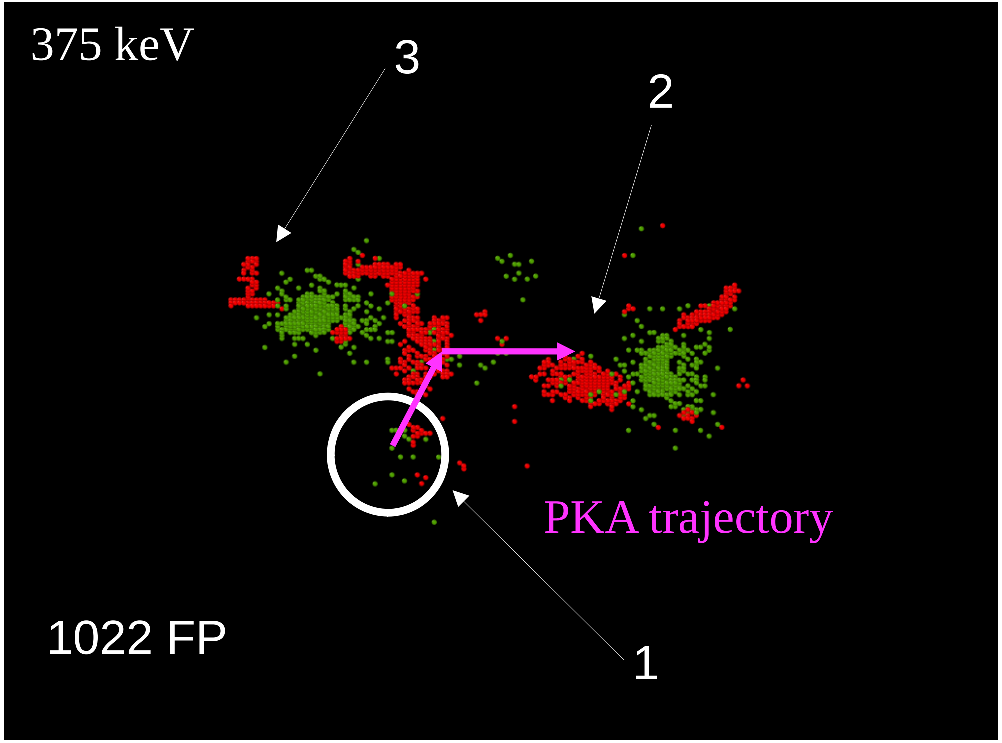




At even higher energies (E_{PKA}>150 keV) splitting of cascades limit the cluster size



Spatially & temporally interacting cascades



100 ps after bombardment

Vacancies leave the imprint of the cascade at room temperature

So far:

Correlation between PKA and defect needs to be studied for estimating T-trapping

Simulations show interstitials are mobile and show clustering at the end of the cascade

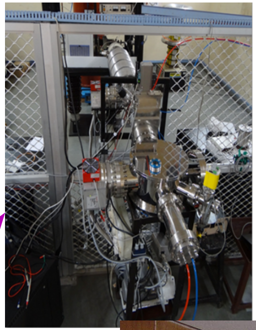
Vacancies are immobile at room temperature – leave the imprint of cascade

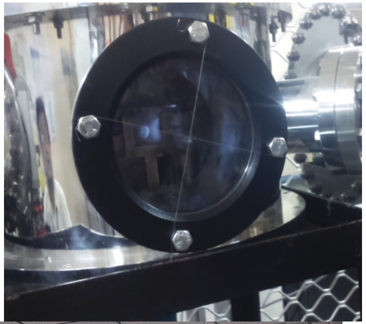
Ion-Irradiation Experiments

Effect of PKA spectrum

Parameters of irradiation experiments

Ions (m) Energy	Mean Range (µm)	Fluence (cm^2)	dpa E_d=90eV	Facility
D^+ (2) 100 keV	0.6	5 x 10^{17}	0.85	14 MeV n- generator, IPR
He^+ (4) 250 keV	0.6	5 x 10^{15}	0.02	LEIBF, IUAC, Delhi
B^{3+} (11) 10 MeV	4.5	1.3 x 10^{14} 1.0 x 10^{15}	0.001, 0.01	3 MeV Tandem accelerator, Bilaspur
Au^{7+}(197) 80 MeV	4.5	1.3 x 10^{14}	0.22	15 MeV pelletron, IUAC, Delhi



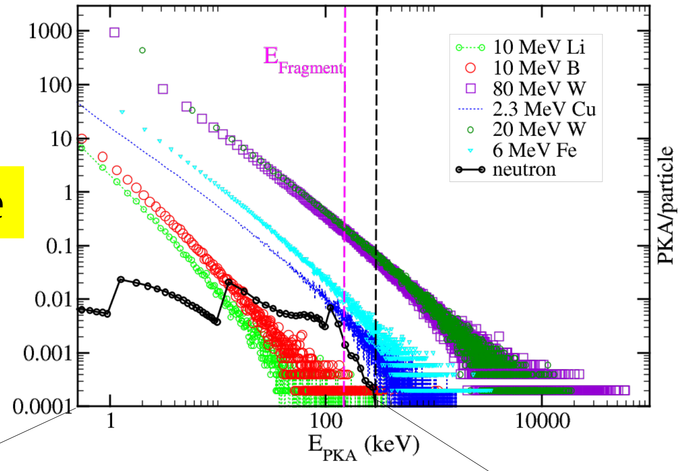


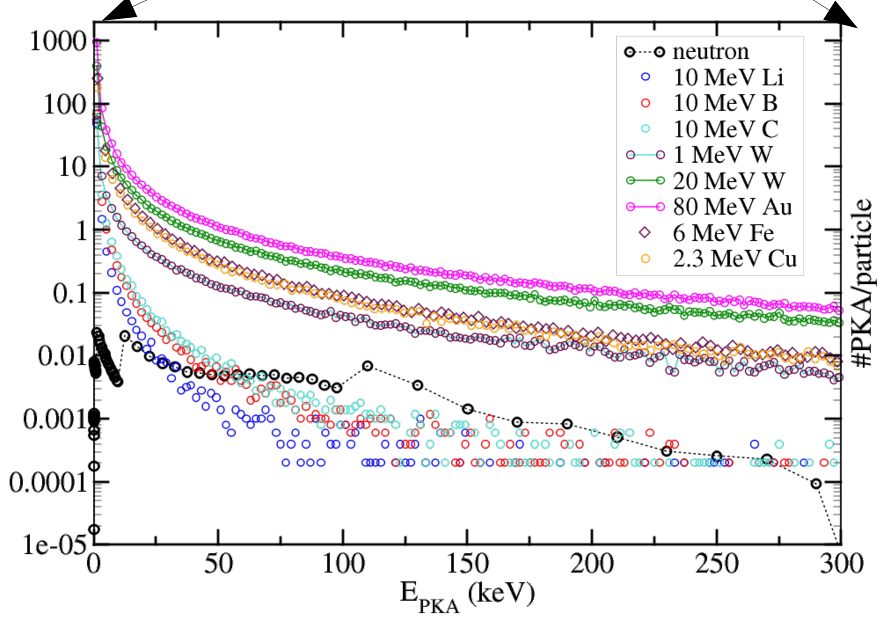
Sequential irradiation of Au + D, B+D, He+D, Au+He+D

Recoil spectra for ions & neutrons

Energy loss mechanisms, depth of penetration & heat

per projectile





PKA of low mass ions are closer to neutrons

Is the defect structure similar?

Recrystallized W-foil samples

- 0.8 x 0.8 x 0.1 mm^3
- 50 min at 1838 K in Ar+H

- Positron bulk-life time:

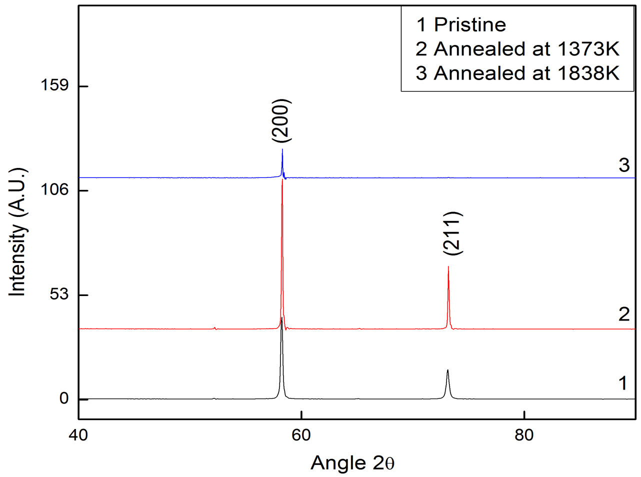
τ_1 = 107.3 ± 1.7 ps (70 %)

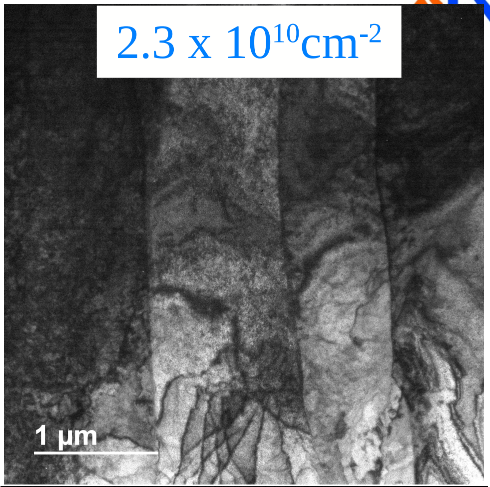
τ_2 = 237.3 ± 5.6 ps (30%)

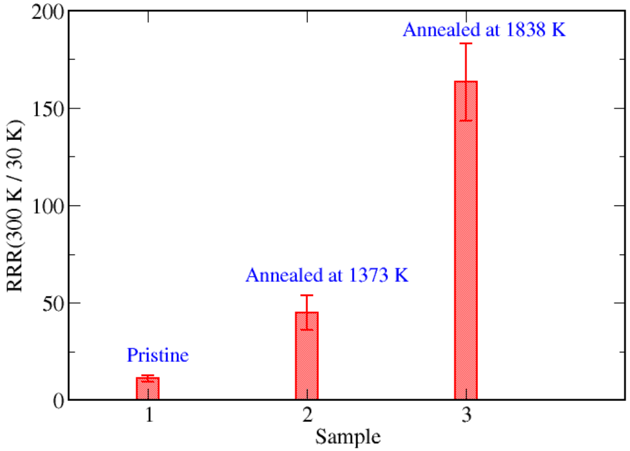
Multiple vacancies

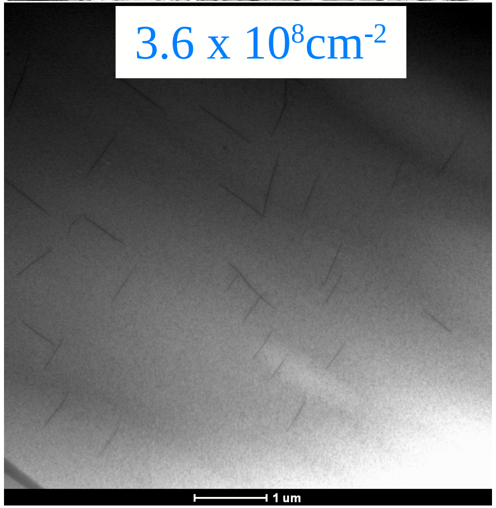
Defect-free W: 105 ± 3 ps

Troev et.al., JPCS, 207 (2010) 012033





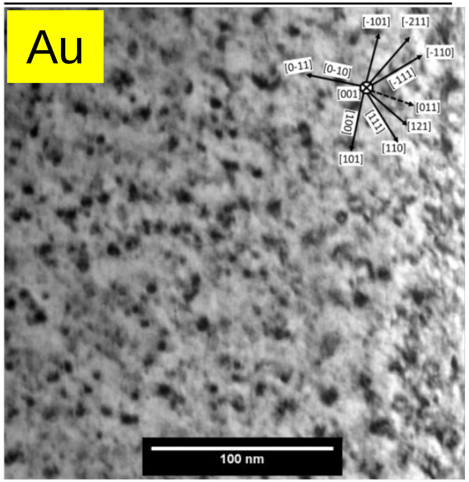


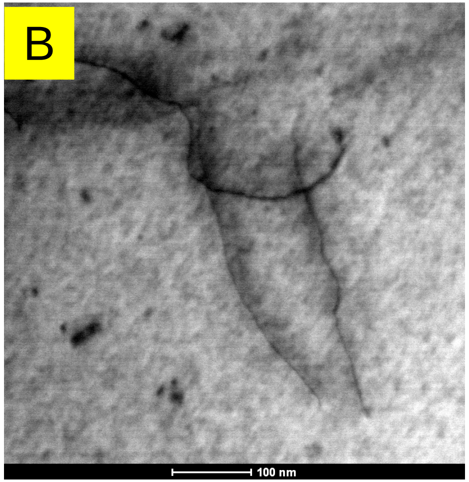


Annealing: S. Akkireddy et.al. ***EX/P4-12***

Defect clusters – TEM studies

Defect cluster size of Au-irradiated samples is similar to neutrons





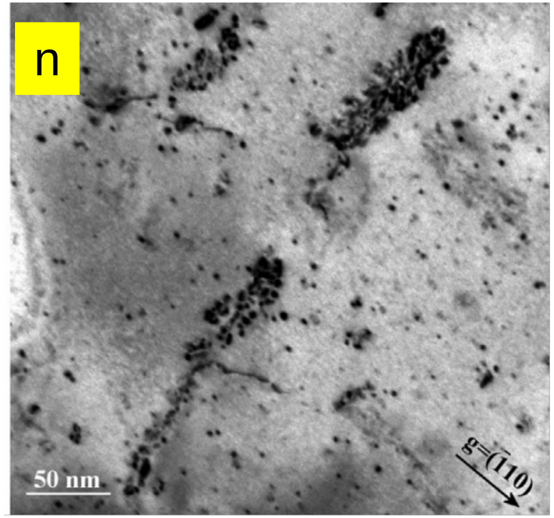
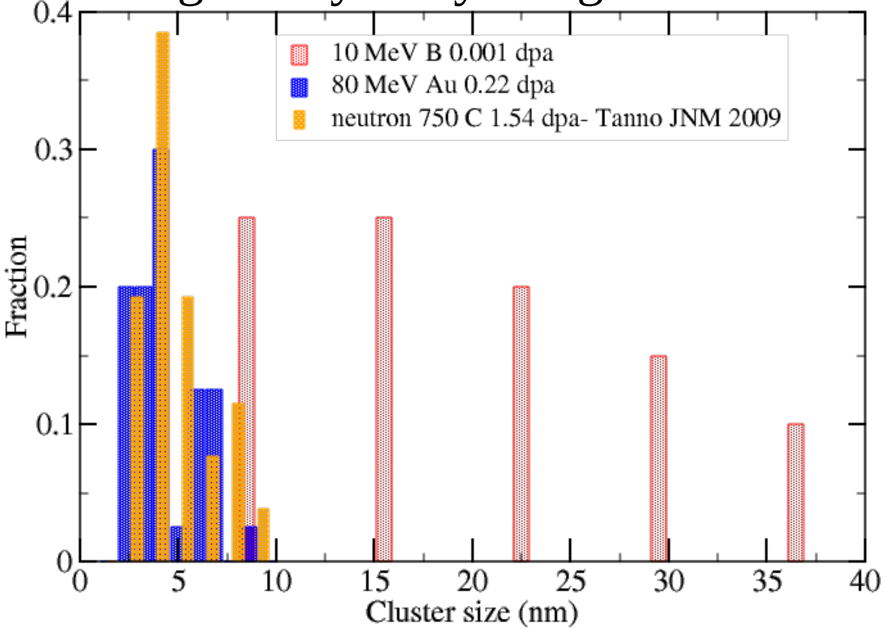


Image analysis by ImageJ software



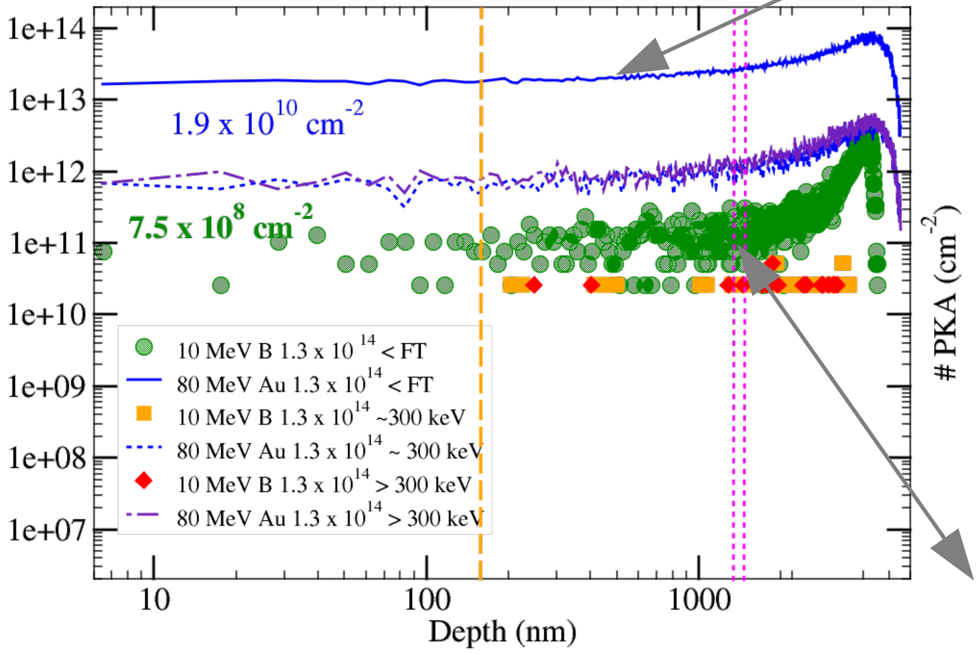
Note: larger clusters in B-irradiation

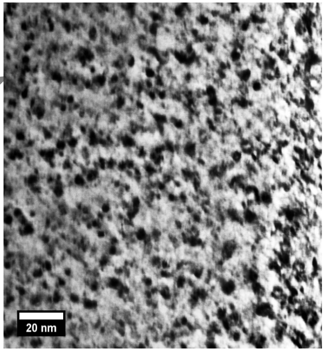
Cluster-size decreases with fluence

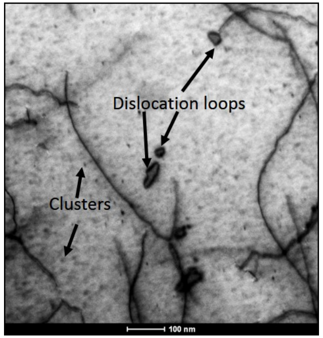
(Renterghem JNM 477 2016, p 80)

TEM Studies: P. Sharma et.al. ***EX/P2-10***

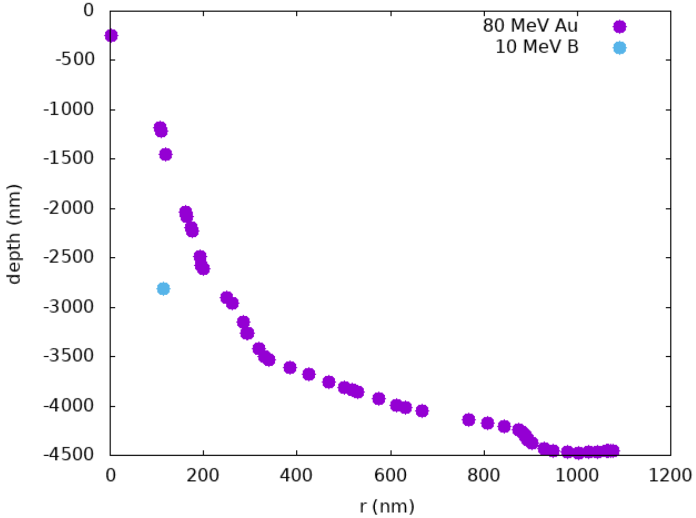
The reason for cluster size difference is related to spacing between recoils





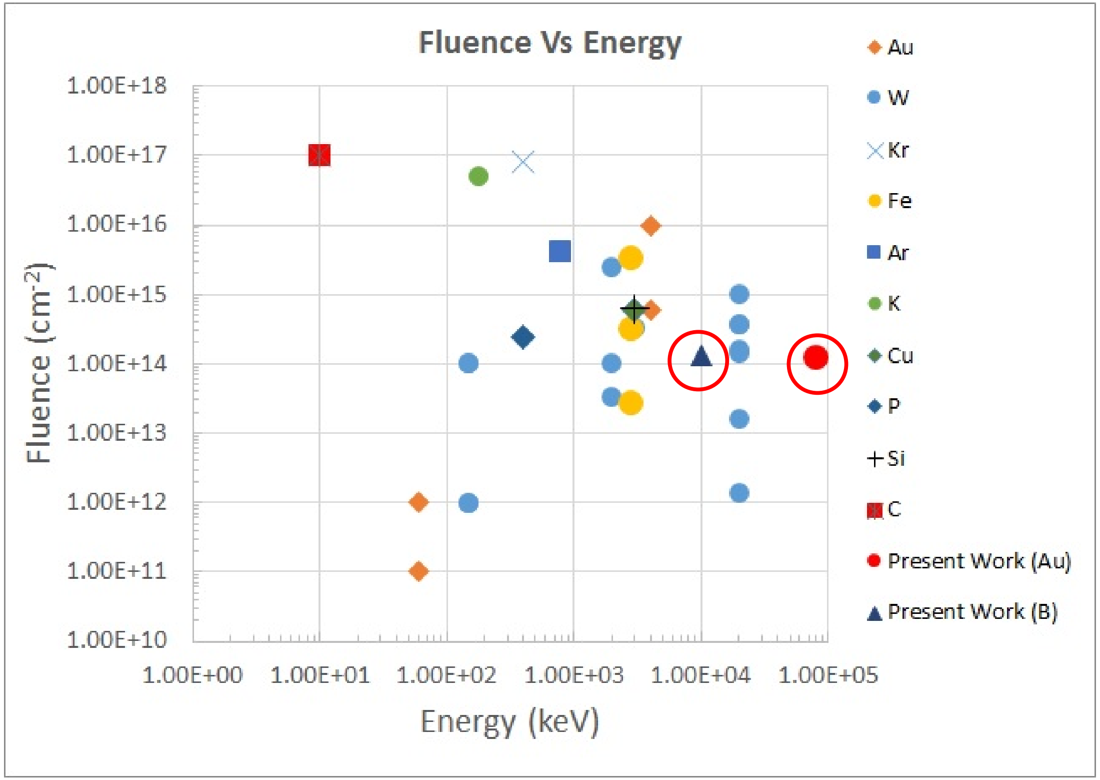


Spacing between recoils within a cascade (>50 keV)



B ~ 10 nm
Au ~ 0.2 nm

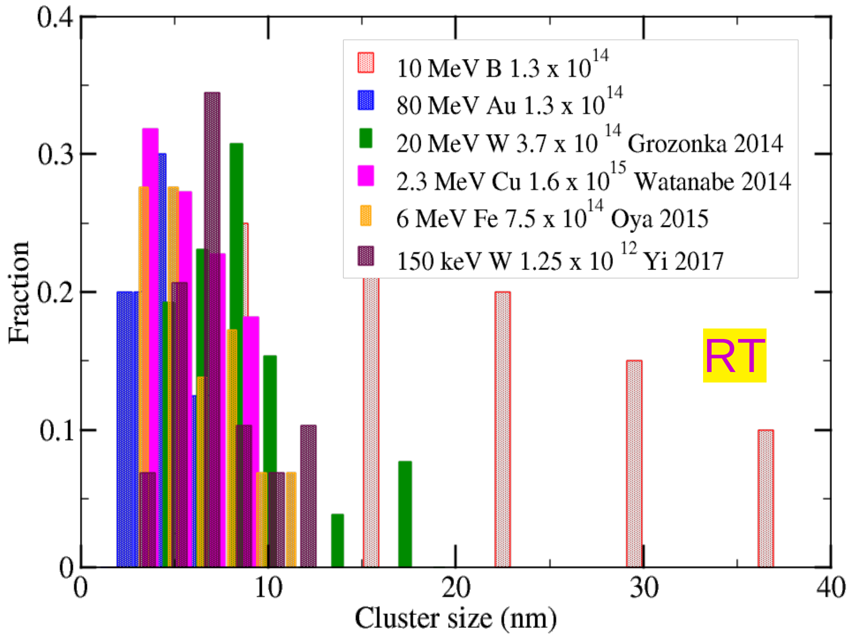
Did others observe similar effects?

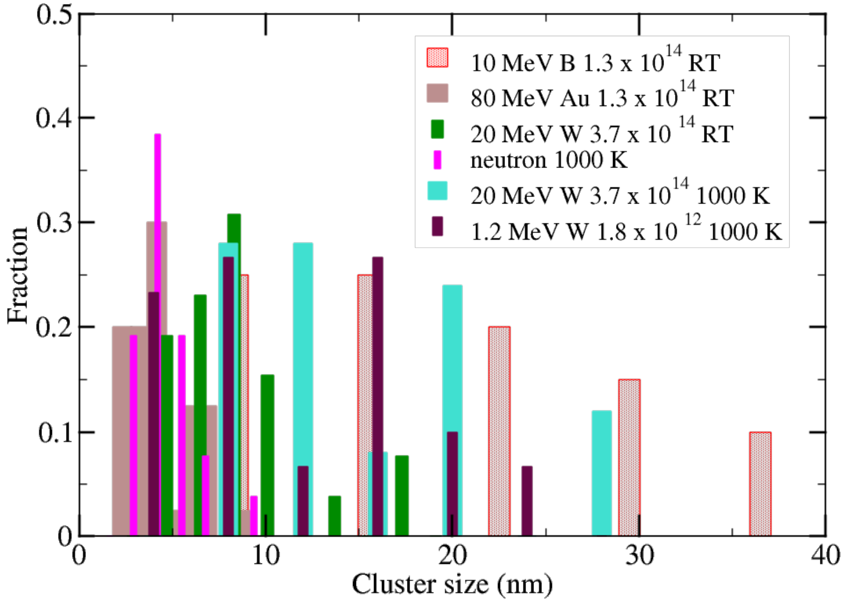


References of heavy ion irradiation

S. No.	Author	Year	Journal
1	Ciupinski Ł. et al.	2013	Nuclear Instruments and Methods in Phy. Research B, 317, (159–164)
2	El-Atwani O. et al.	2015	Materials Characterization, 99, (68–76)
3	Grzonka J. et al.	2014	Nuclear Instruments and Methods in Phy Research B, 340, (27–33)
4	Hwang T. et al.	2016	Nuclear Materials and Energy, 9, (430-435)
5	Jager W. et al.	1975	Phys. Stat. Sol. (a), 32, 89
6	Kim K.T. et al.	1990	Materials Letters, 9,9, (295-301)
7	Mason D.R. et al.	2014	Journal of Physics: Condensed Matter, 26, 37
8	Maya P.N. et al.	2018	
9	Ogorodnikova O.V. et al.	2014	Journal of Nuclear Materials, 451, (379–386)
10	Oya Y. et al	2011	Phys. Scr. T145, (014050)
11	Oya Y. et al.	2015	Journal of Nuclear Materials, 461, (336–340)
12	Ran G. et al.	2014	Journal of Nuclear Materials, 455, (320–324)
13	Sakamoto R. et al.	1995	Journal of Nuclear Materials, 220-222, (819-822)
14	Sakurada et al.	2017	Journal of Nuclear Materials, 490, (242-246)
15	Sakurada S. et al.	2016	Nuclear Materials and Energy, 9, (141-144)
16	Snoeks E. at al.	1997	Applied Physics Letters, 71, 267
17	Wang H. et al.	2013	Journal of Nuclear Materials, 442, (189–194)
18	Watanable H. et al.	2014	Journal of Nuclear Materials, 455, (51–55)
19	Xiaoou Yi et al.	2016	Acta Materialia, 112, (105-120)
20	Xiaoou Yi et al.	2015	Acta Materialia, 92, (163–177)
21	Zhang Z. et al.	2015	J. Plasma Fusion Res. SERIES, 11
22	Zhang Z. et al.	2016	Journal of Nuclear Materials, 480, (207-215)
23	Zhang Z.X. et al.	2016	Fusion Engineering and Design, 98–99 (2103–2107)

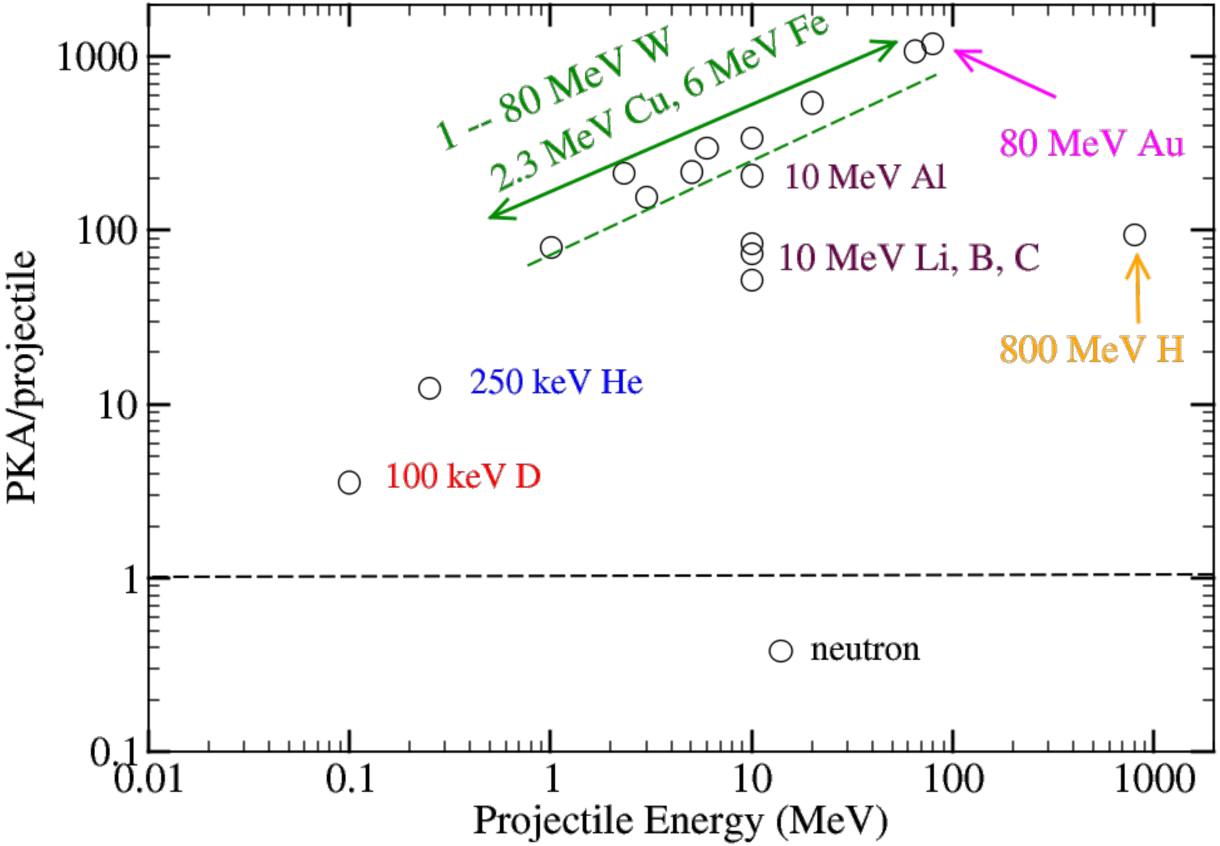
Heavy ion irradiation experiments show similar cluster size independent of energy and fluence



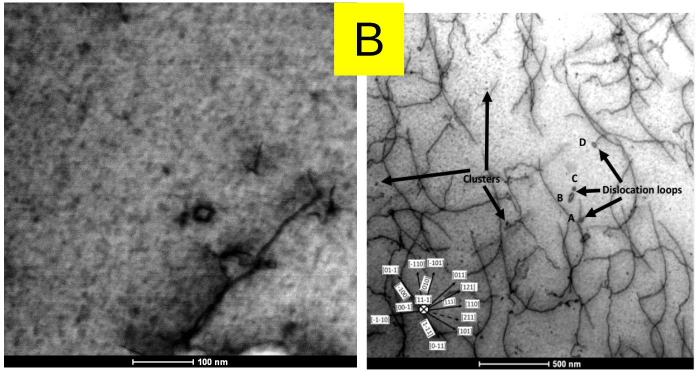


Cluster size increases with temperature

TRIM calculations were also carried out and found that heavy ions produce several PKA/particle close to each other over a *small depth range*

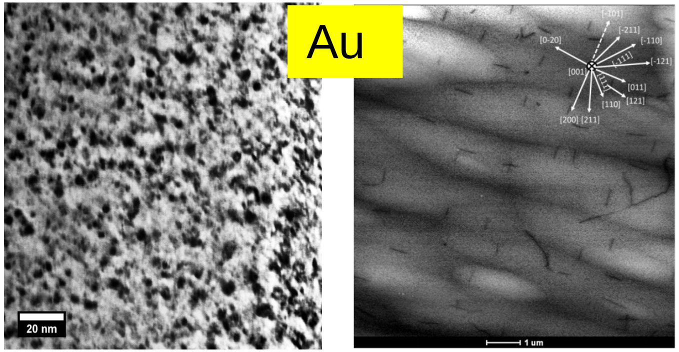

1 -- 80 MeV W
2.3 MeV Cu, 6 MeV Fe
80 MeV Au
10 MeV Al
10 MeV Li, B, C
800 MeV H
250 keV He
100 keV D
neutron
PKA/projectile
Projectile Energy (MeV)
1000
100
10
1
0.1
0.01
0.1
1
10
100
1000

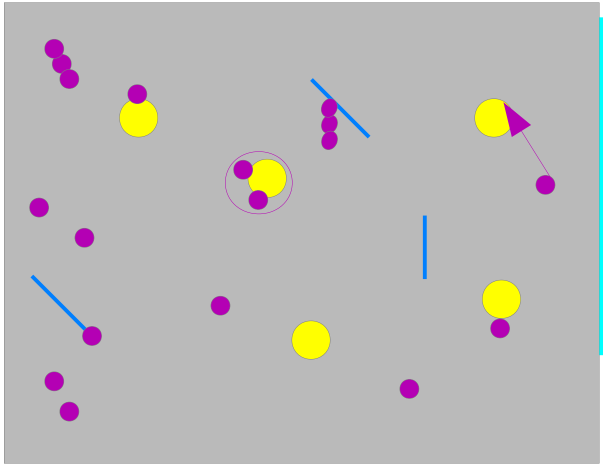
Competitive capture of mobile FP by seed clusters and dislocation lines?



Initial line density

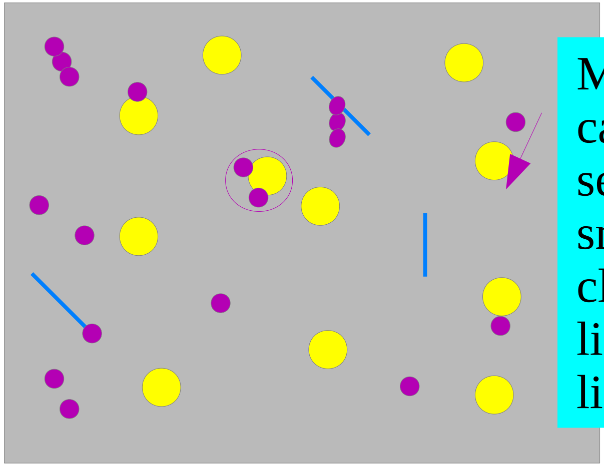
$3.6 \times 10^{8} cm^{-2}$





Mobile FP agglomerate and captured by fewer seeds large scale clusters & branching of lines

Shorter lines (80-1100 nm)
Higher density - $1.9 \times 10^{10} cm^{-2}$
Sparse clusters - $9.3 \times 10^{9} cm^{-2}$

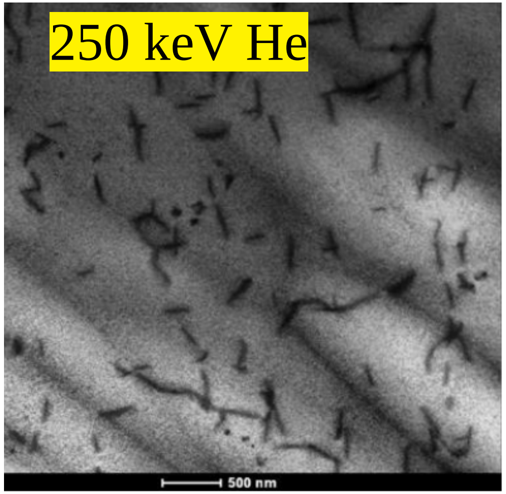


Mobile FP – captured by several seeds small scale clusters and lines & Long lines

Long lines (400-3000 nm)
Lower density - $6.1 \times 10^{8} cm^{-2}$
Dense clusters - $1.3 \times 10^{12} cm^{-2}$

Irradiation with He (250 keV) & D (100 keV) ions

Cluster size of He irradiated samples is similar to Au-irradiation



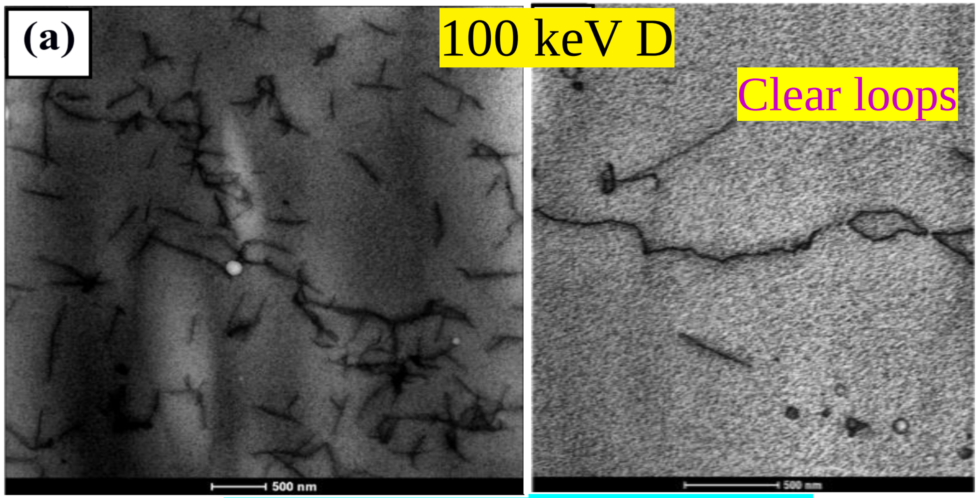
5×10^{15} cm^{-2} (0.02 dpa)

Diffusion & agglomeration of FP to form clusters

Line density 1.05×10^{9} cm^{-2}
Length 40 – 1000 nm

Cluster density 5.6×10^{10} cm^{-2}
Size 5 – 15 nm

Loops and network of dislocations clearly visible in D-irradiation



5×10^{17} cm^{-2} (0.85 dpa)

Line density 9.7×10^{8} cm^{-2}
Length 120 – 1900 nm

Loop density 1.4×10^{8} cm^{-2}
Size 50 – 100 nm

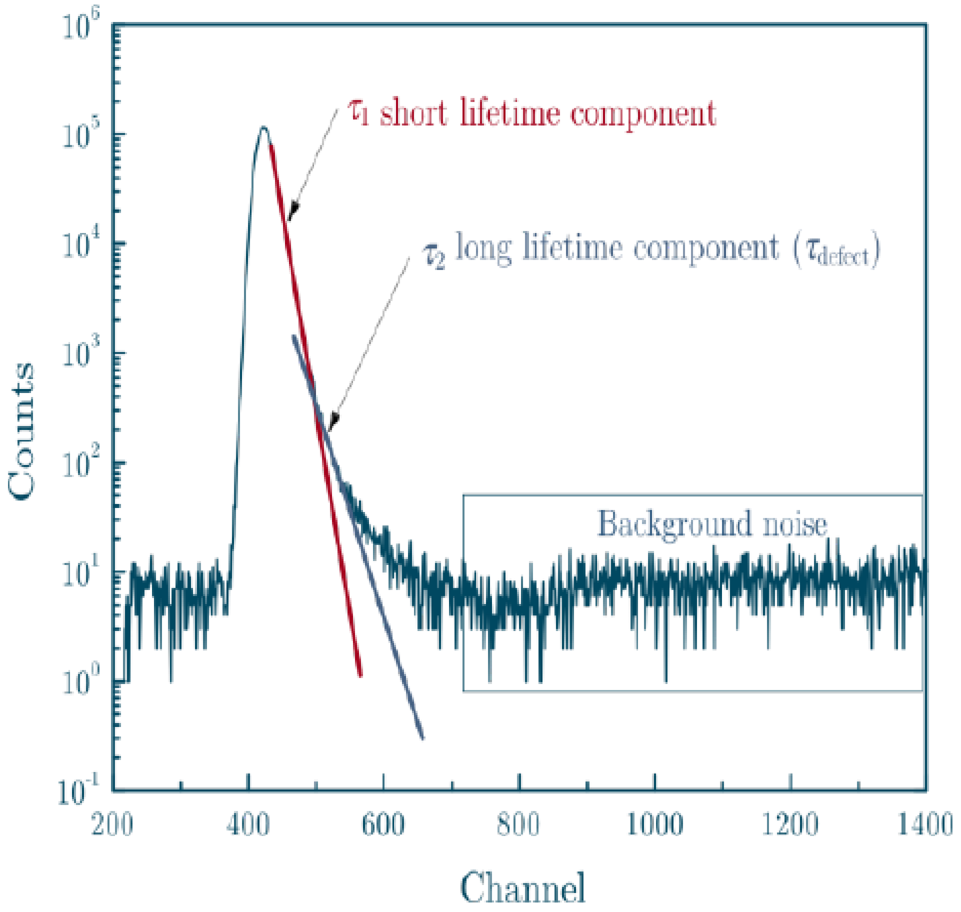
So far:

Correlation between PKA and defect needs to be studied for estimating T-trapping
Simulations show interstitials are mobile and show clustering at the end of the cascade
Vacancies are immobile at room temperature – leave the imprint of cascade

Interstitial cluster-size seem to depend only on the inter-PKA separation and hence on fluence
The capture of mobile FP by existing dislocation lines and existing clusters seem to explain the observed cluster sizes

Vacancy Defects – Positron Annihilation Spectroscopy Studies

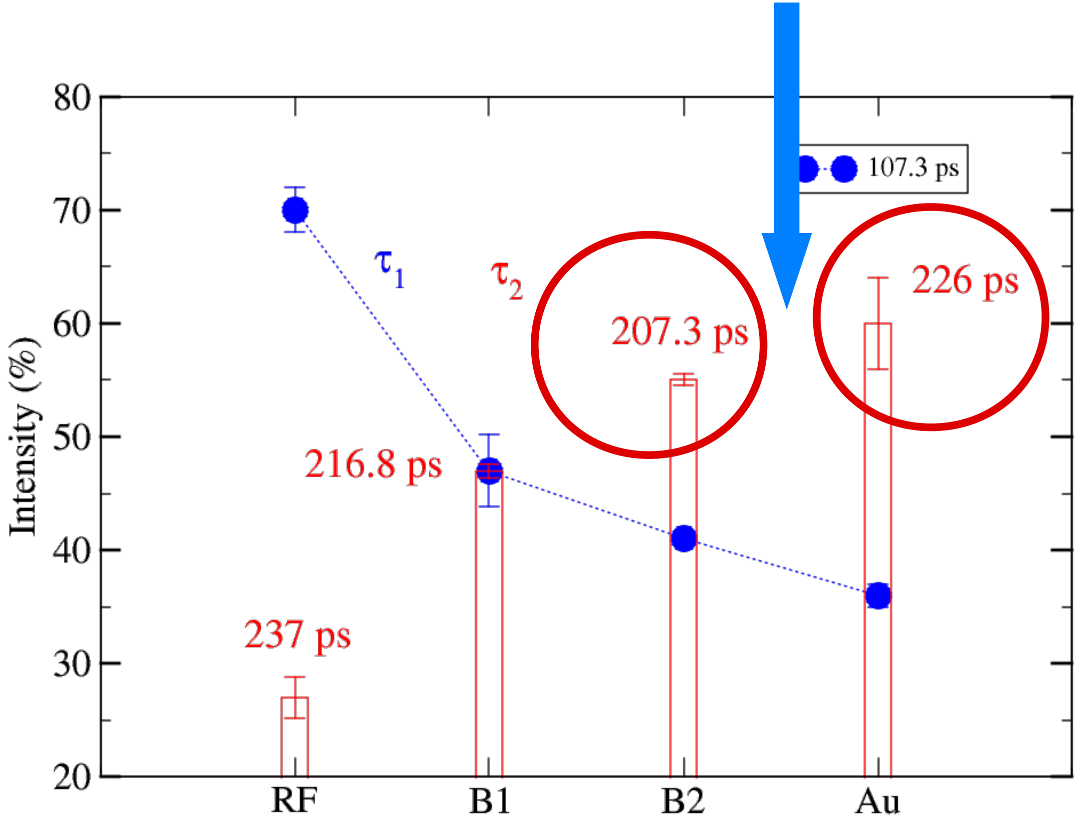
Positron life-time in the lattice $\tau = 1/(\pi r_e^2 n_e c)$



MF Barthe et.al, PFMC 2015

Multiple vacancy for Au, Single for B

The difference is good enough to distinguish between single & multiple vacancies



Fast e^+– ^{22}Na source

270 keV

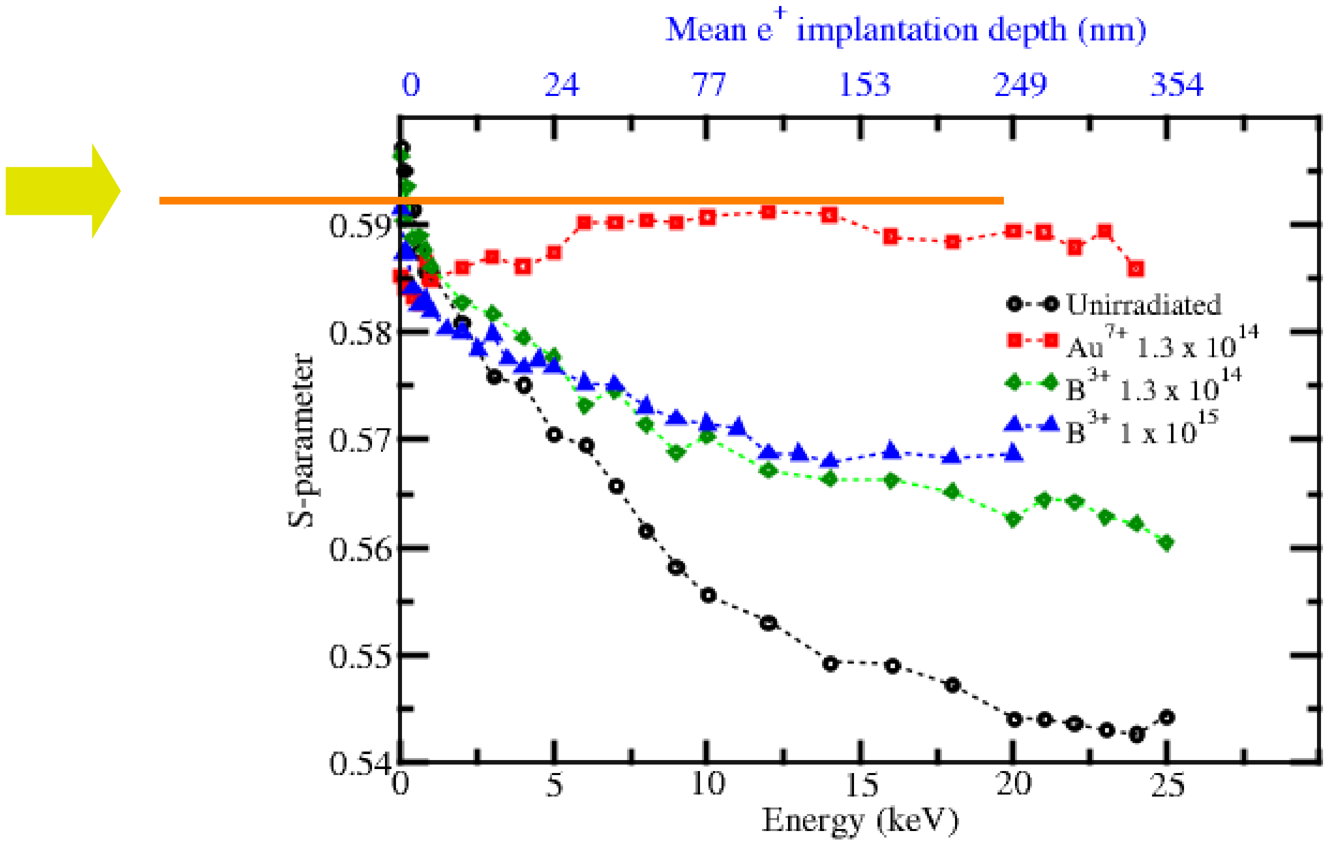
Penetration depth ~ 16 μm

Defect range ~ 5 μm

Defect-freeW: 105 ± 3 ps

Troev et.al., JPCS, 207 (2010) 012033

Saturation indicates dense vacancy clusters in Au-irradiation



Slow e^+ beam - 0.1 to 30 keV

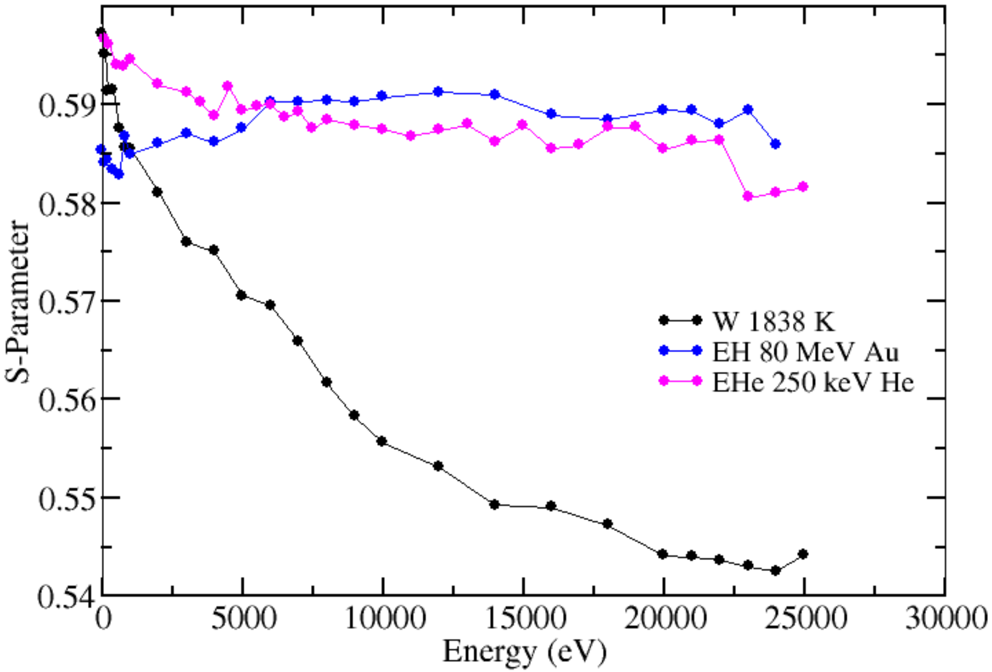
Doppler broadening of 511 keV γ

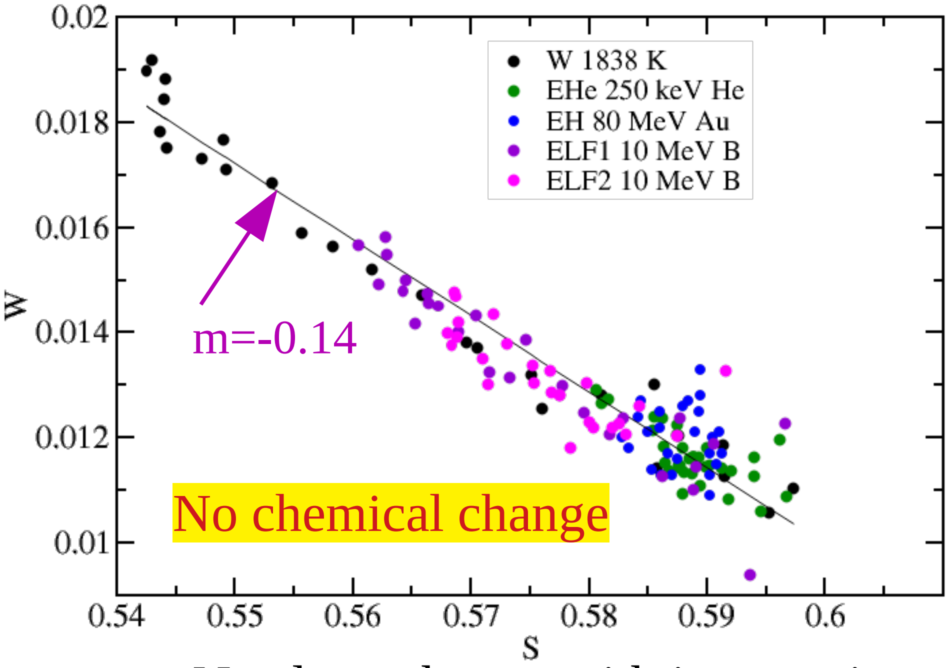
S – e^+-e^- from valance electrons

W – e^+- e^- from core electrons

similar effects: ***20 MeV W,*** *MF Barthe et.al*

He & Au shows saturation of S-parameter, indicating saturation of vacancies in the e$^+$ penetration range

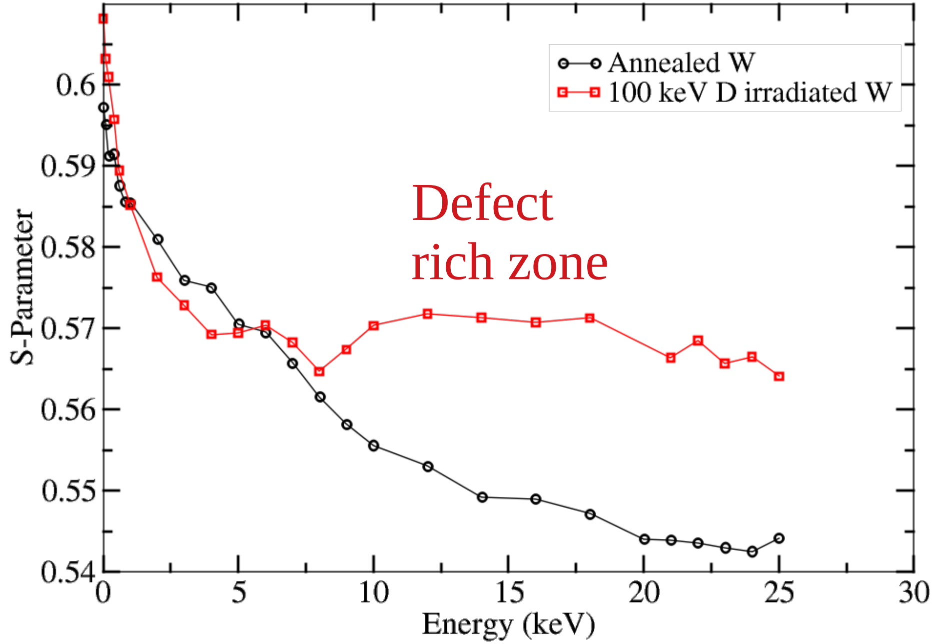




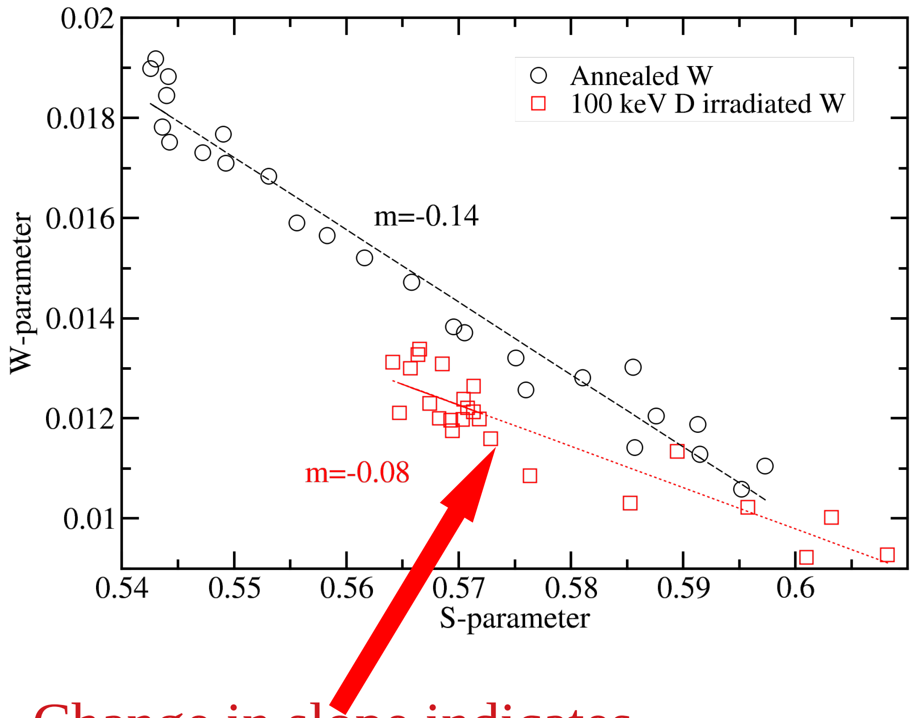
No slope change with ion species

Similar observations: P.E. Lhuiller et.al, JNM 433 (2013), Troev et.al.,NIMB 267 (2009)

Deuterium creates defects within 400 nm and D atoms are trapped in these defects(?)

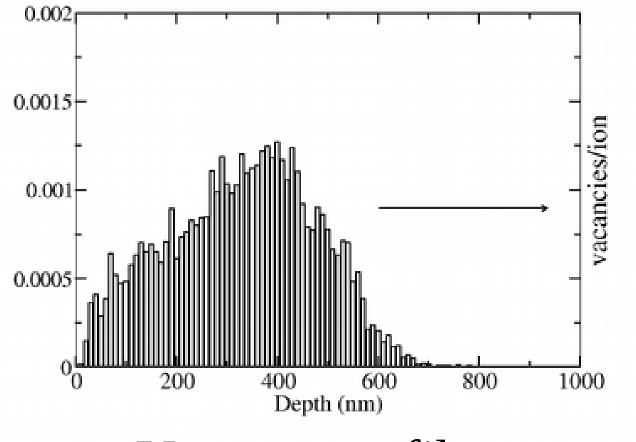


No saturation is seen unlike Helium

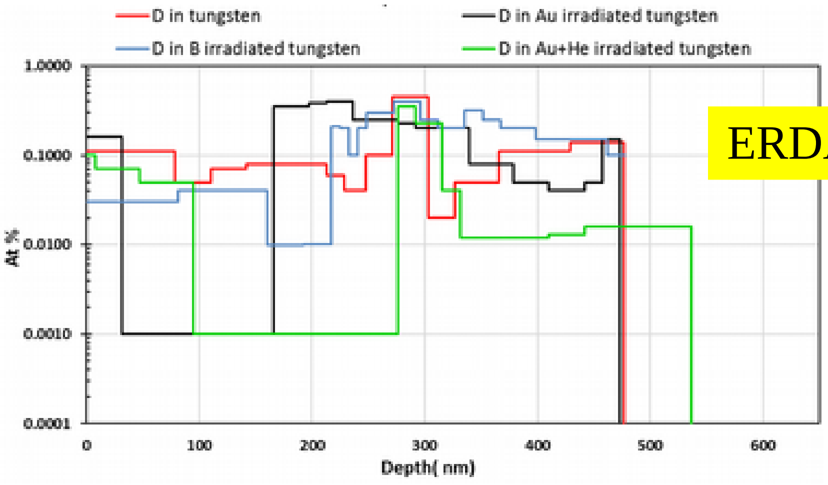


Change in slope indicates annihilation from different core electrons than W

Most of the deuterium found to be less than 500 nm

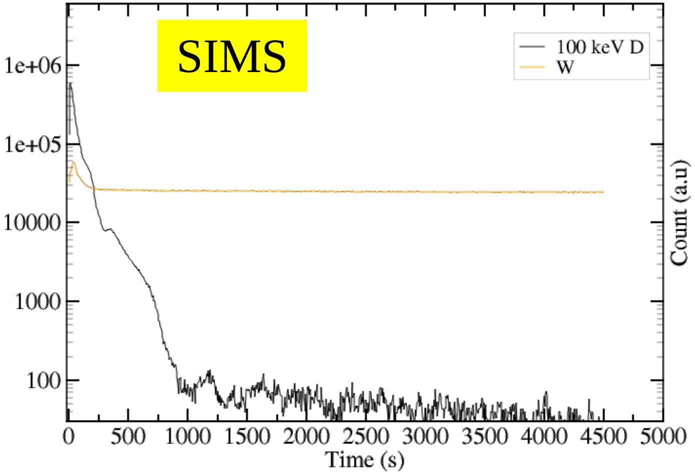


Vacancy profile



ERDA

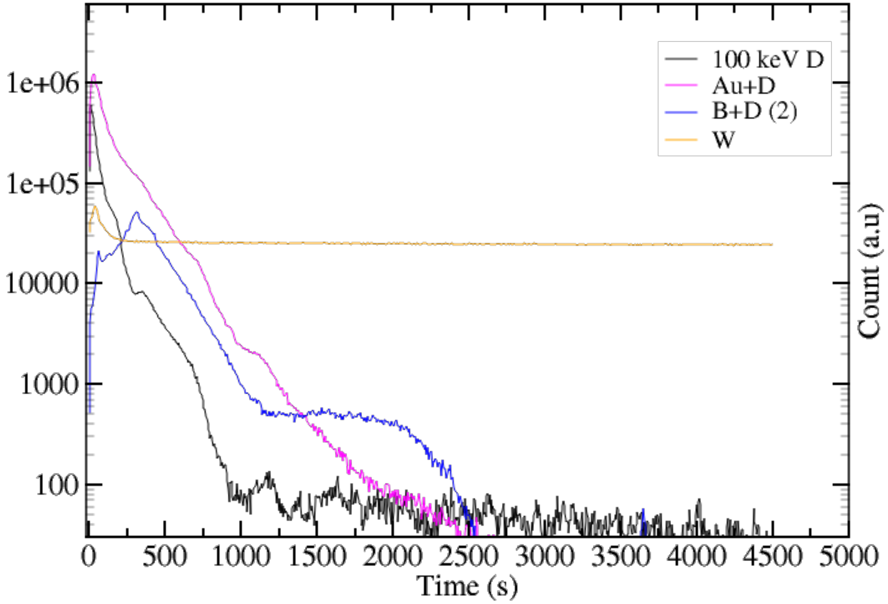
7.3 MeV C^{6+}



15 keV Cs^{+} ions; 23^{o} to normal

1 s = 0.5 nm

Deuterium depth profile in pre-irradiated tungsten



B-irradiated sample seem to trap more D than Au-irradiated sample.

Single vacancy traps more D than multiple vacancies *(Ahlgrene et.al, JNM 2012)*

It seems from PAS that B-irradiation creates more single vacancies as opposed to Au.

Ongoing investigations

So far:

Correlation between PKA and defect needs to be studied for estimating T-trapping
Simulations show interstitials are mobile and show clustering at the end of the cascade
Vacancies are immobile at room temperature – leave the imprint of cascade

Interstitial clustering seem to depend only on the inter-PKA separation and hence fluence
The capture of mobile FP by existing dislocation lines and existing clusters seem to explain the observed cluster sizes

Vacancy show the imprint of cascade and hence related to the PKA energy and their spectrum
T-trapping takes place predominantly at vacancies

Conclusions & Outlook

Correlation between PKA and defect needs to be studied for estimating T-trapping
Simulations show interstitials are mobile and show clustering at the end of the cascade
Vacancies are immobile at room temperature – leave the imprint of cascade

Interstitial clustering seem to depend only on the inter-PKA separation and hence on fluence
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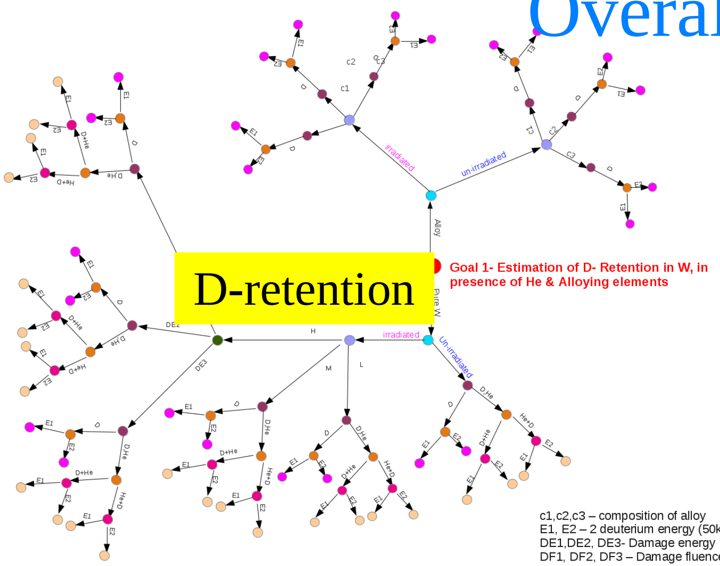
Vacancies show the imprint of cascade and hence related to the PKA energy and their spectrum
T-trapping takes place predominantly at vacancies

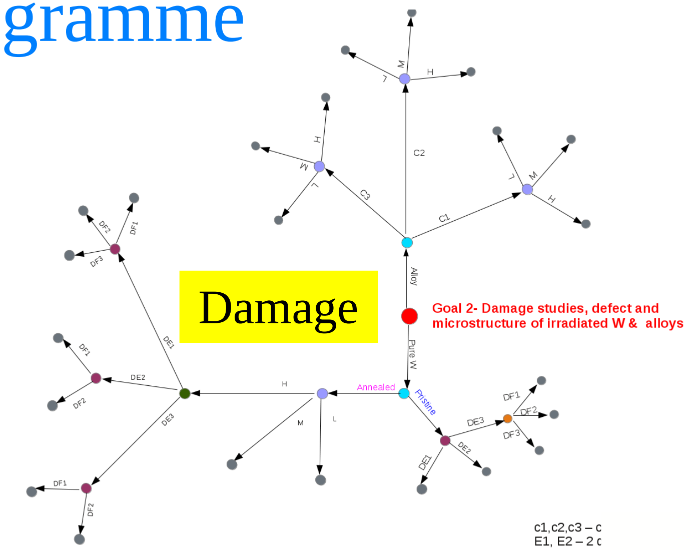
Accurate quantification of T-retention requires precise estimation of vacancies – using a combination of surrogate ions with controlled fluence of different mass, energy and temperature is urgently needed.

Overall Programme

Experiments

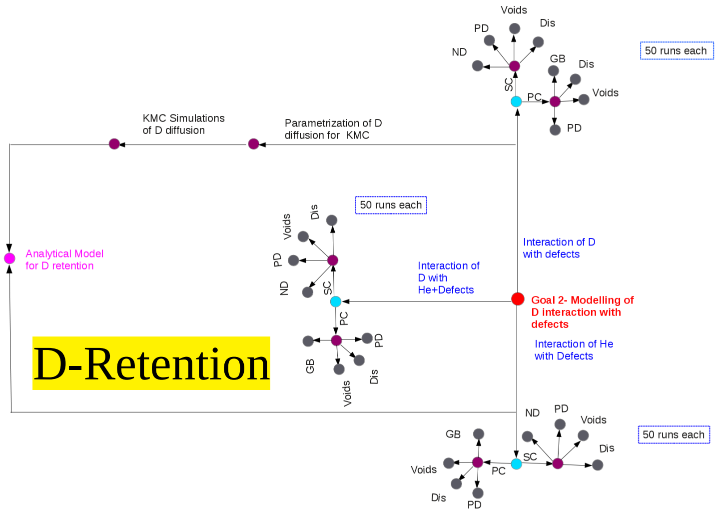


c1,c2,c3 – composition of alloy
E1, E2 – 2 deuterium energy (50keV, 100keV)
DE1,DE2, DE3- Damage energy
DF1, DF2, DF3 – Damage fluence

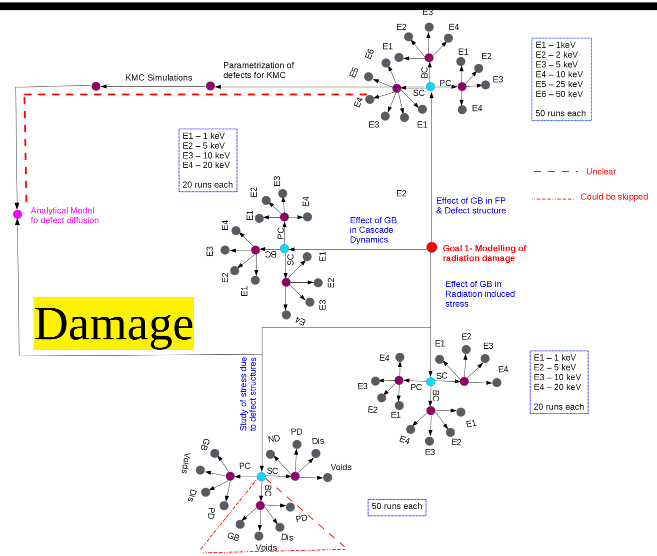


c1,c2,c3 – c
E1, E2 – 2 c
DE1,DE2, D
DF1, DF2, D

Multi-Scale Modelling

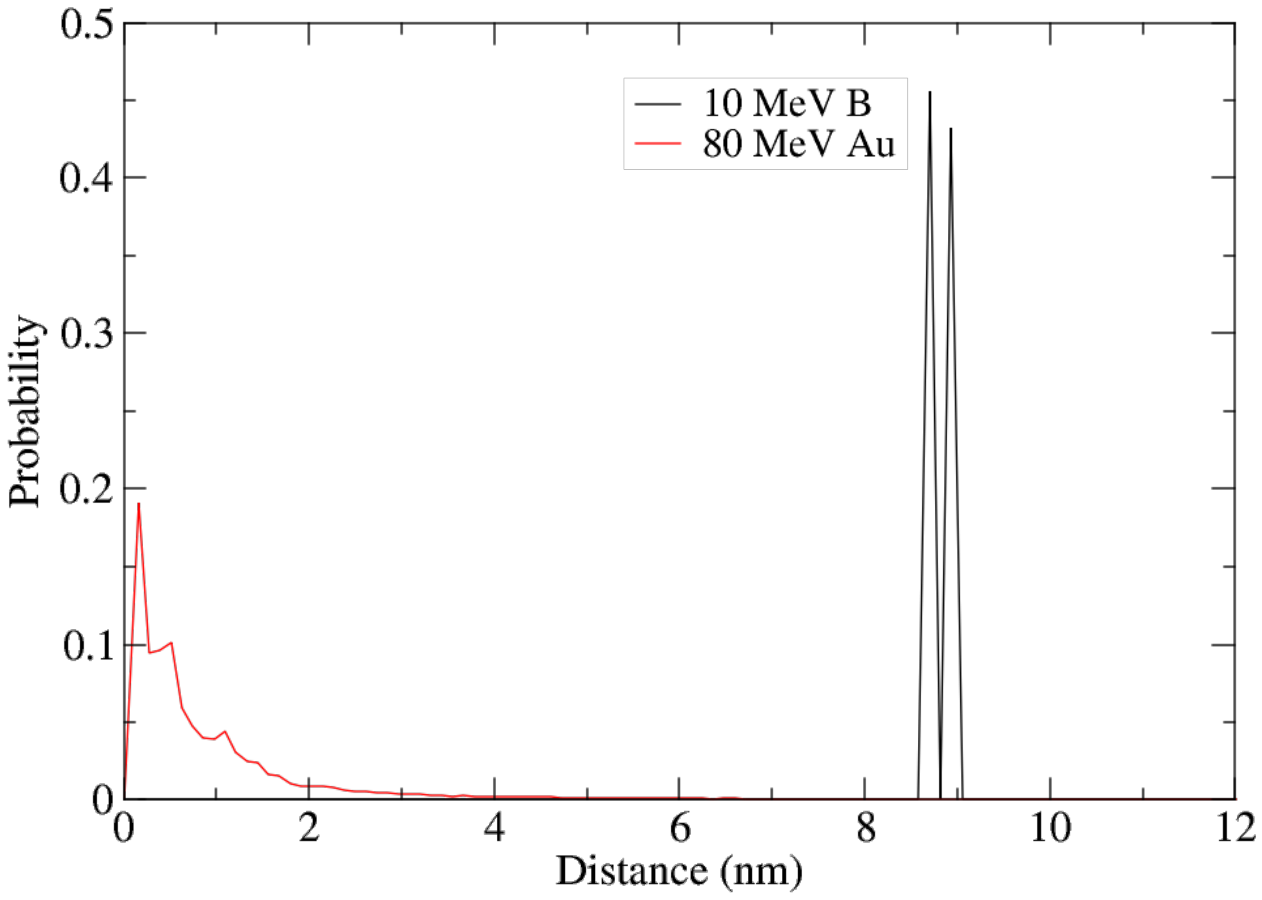


Thank you!



Backup slides

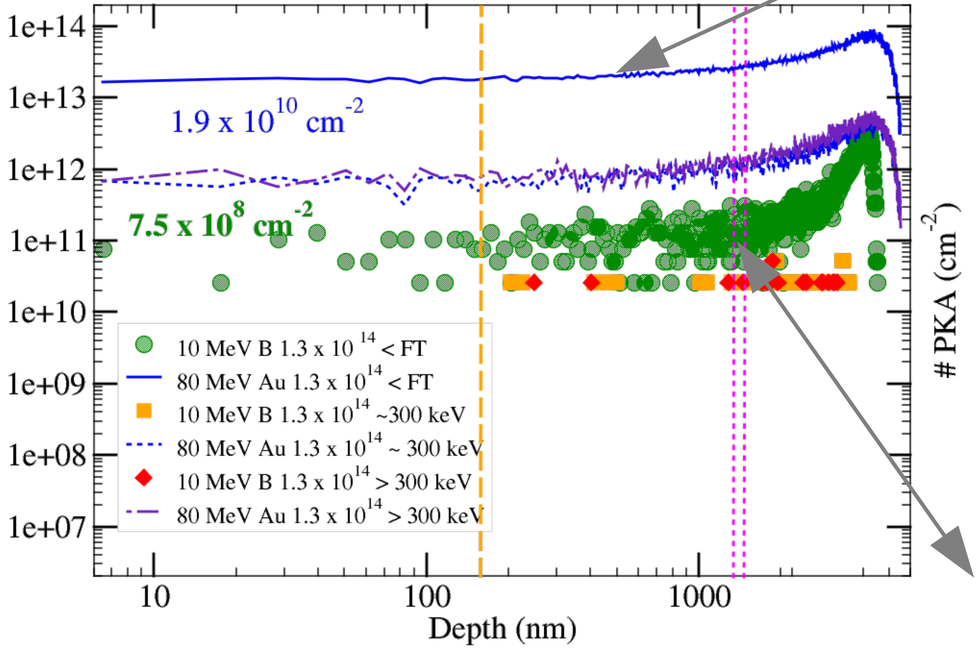
In a given cascade

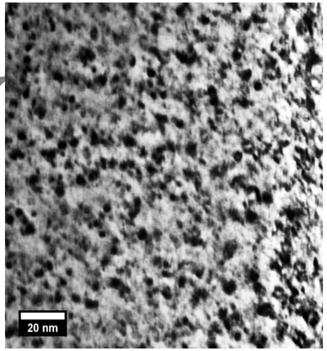


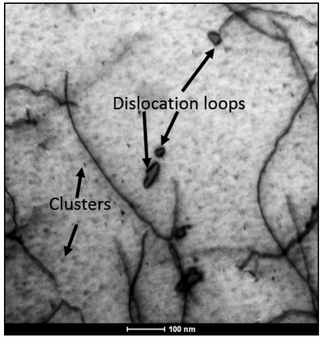
Crowdions have the highest mobility and formation energy

Mobility of interstitial clusters are limited

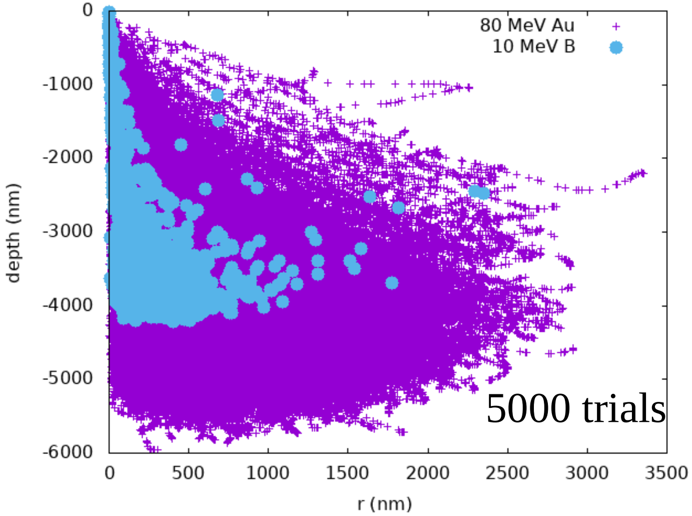
The reason for difference lies in the PKA spectra





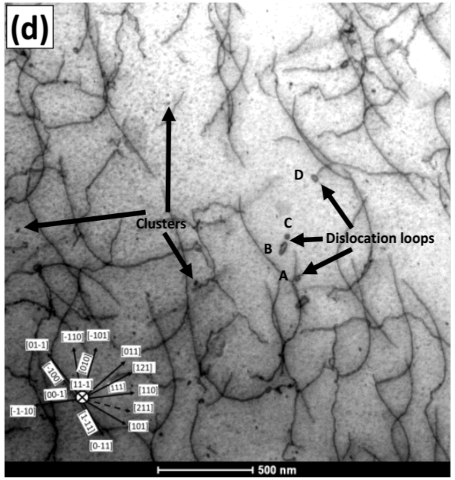


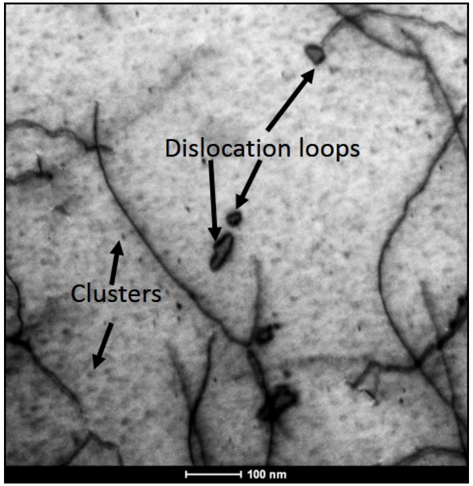
Spacing between recoils within a cascade (>50 keV)

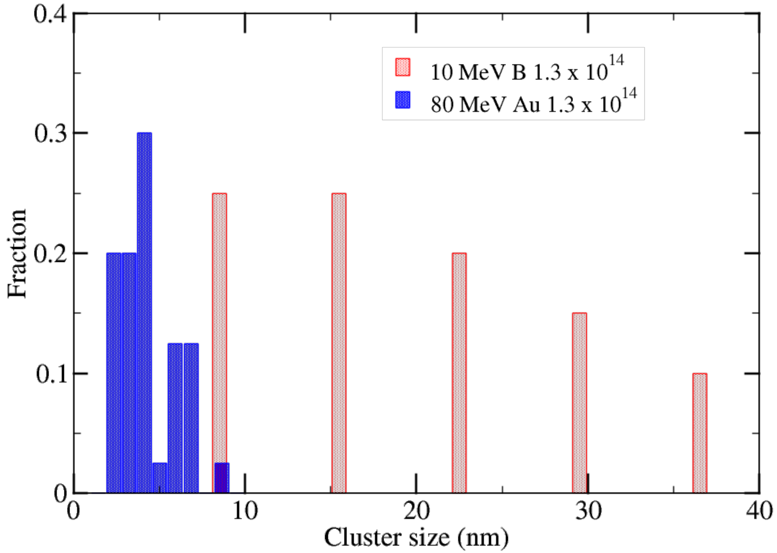


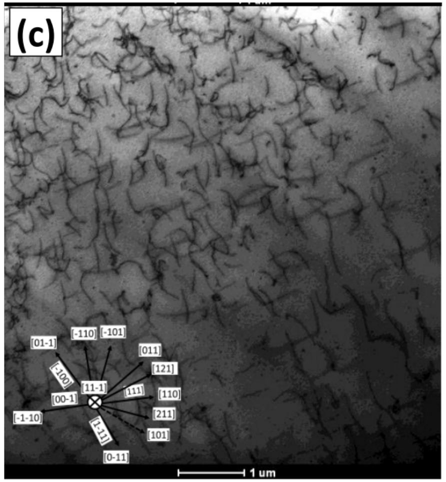
B ~ 10 nm
Au ~ 0.2 nm

Larger Sparse Loops in B-Irradiation



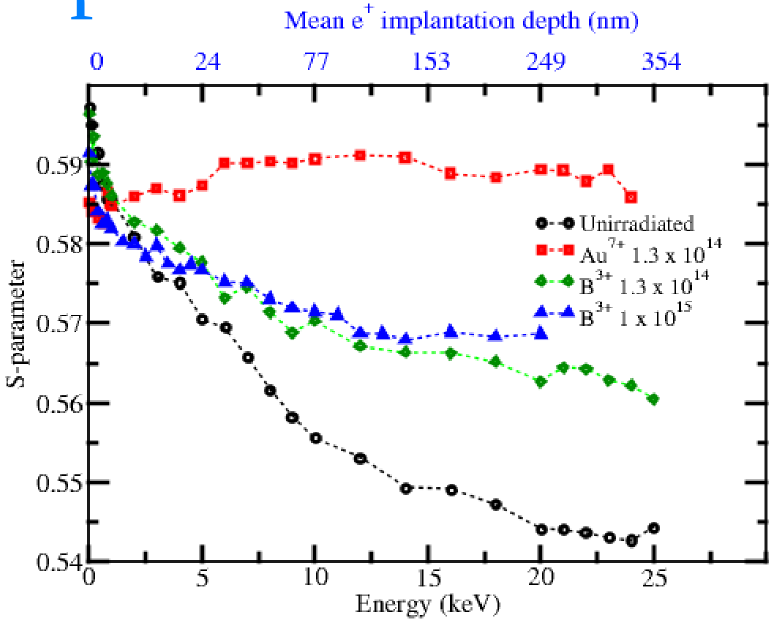


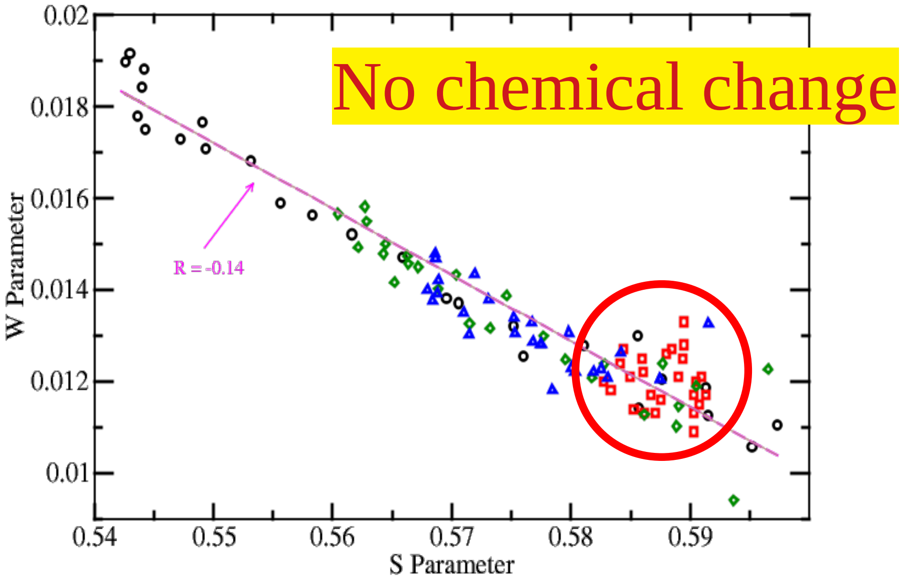




- Line density - 1.9 x 10^{10} cm^{-2}
  - Line length – 80 – 1100 nm
- Cluster density - 9.3 x $10^{9}$$cm^{-2}$
- Loop density – 6.9 x 10^{8} cm^{-2}

Depth Profile of Point Defects



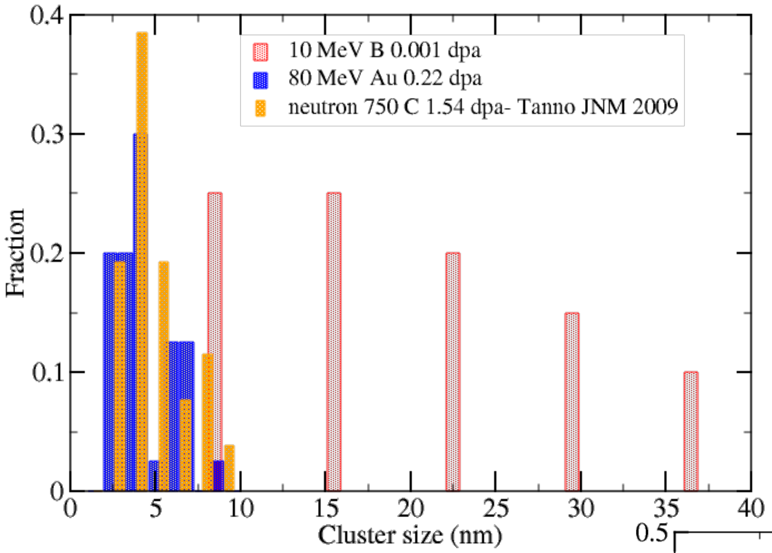


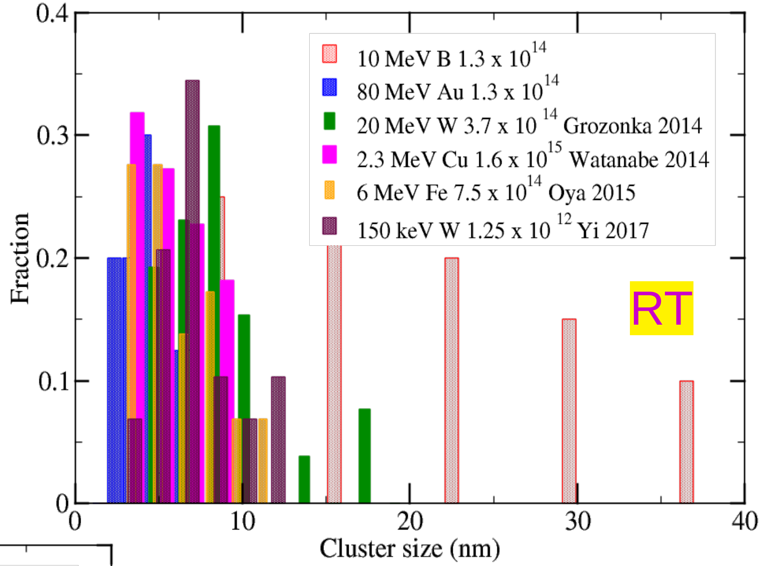
- Saturation of S - Au irradiation

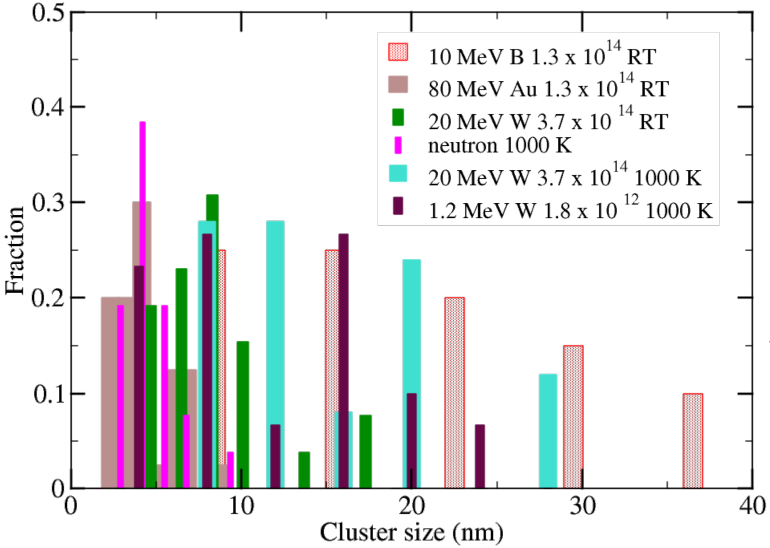
  similar effects: ***20 MeV W,*** *MF Barthe et.al*

- Fewer defects in Boron
- Vacancy clusters/loops

Au & N-irradiation Produce Small Clusters

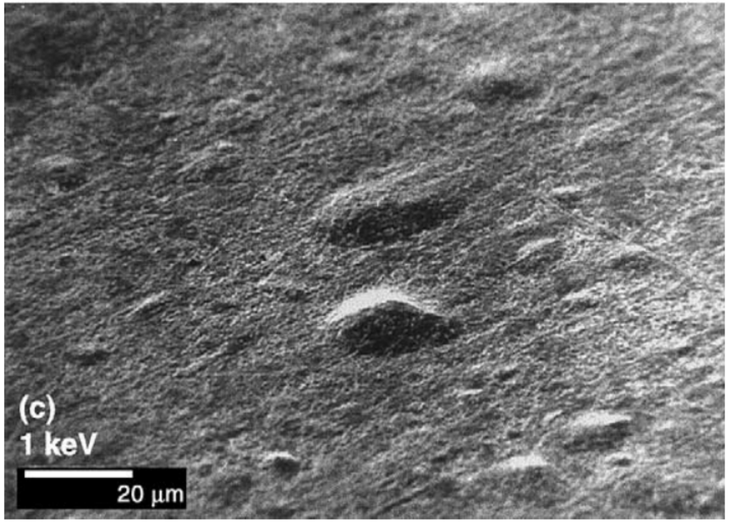


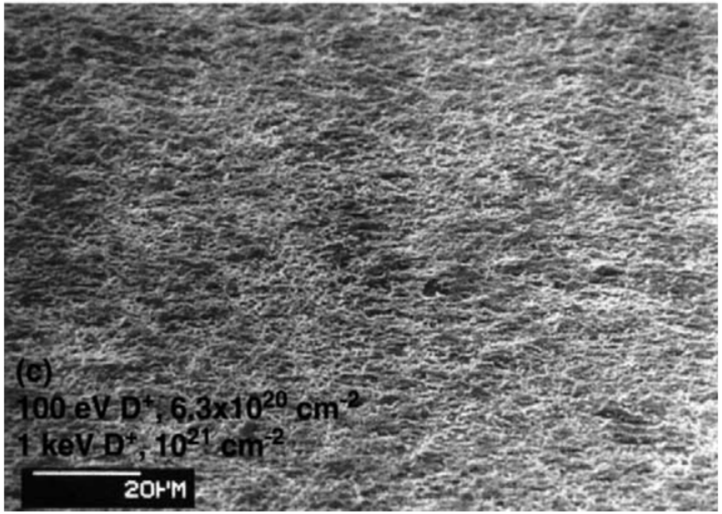


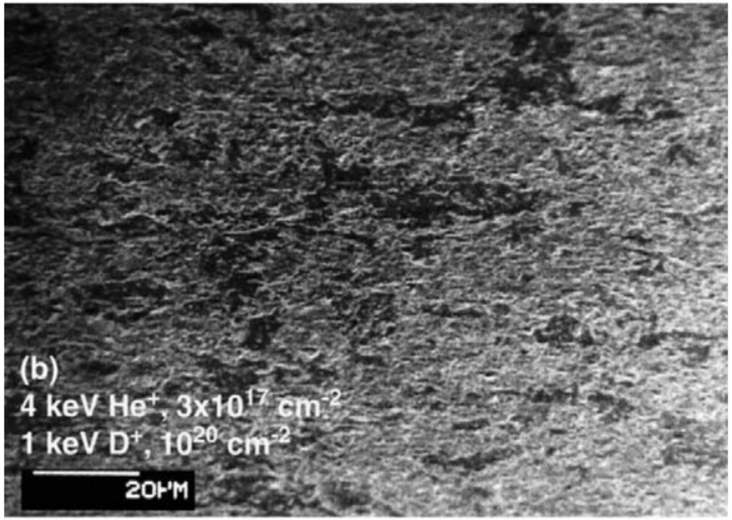


Similar defect size distribution for heavy ions at 300 K and neutrons at 1000 K

At high temperature heavy ions produce clusters similar to 300 K boron irradiation


(c)
1 keV
20 μm


(c)
100 eV D^+, $6.3x10^{20}$ cm^{-2}
1 keV D^+, 10^{21} cm^{-2}
20μM


(b)
4 keV He^+, $3x10^{17}$ cm^{-2}
1 keV D^+, 10^{20} cm^{-2}
20μM