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Radiation Damages Bohr's Metrics: the Accelerator & Elemental Landscapes

J.-Ch. Sublet & Mark Gilbert

Nuclear Data Services Unit Head, IAEA

United Kingdom Atomic Energy Agency, UKAEA

Background

- Nuclear interactions can be the source of atomic displacement; post-short-term cascade annealing defects; atomic, lattice interstitial gas dislocation; atomic activation, transmutation and heating in irradiated structural materials and fuels

- Such quantities are derived from, or can be correlated to, nuclear kinematic simulations of the energy spectra of primary atomic recoil distributions, and the quantification of the numbers of secondary defects produced per primary as a function of the available recoils, residual or transmutant and emitted particles

Backgound

- The ostensible incident particle is the neutron, however important emitted secondaries are p and α
- While achievable experiments usually rely for convenience of production on accelerator and light ions

- In contrast to nuclear fuel (Uranium oxide UOX, Uranium-plutonium oxide MOX) nuclear component material are by nature composed of natural elements, usually a handful of them
- This emphasises the reason to use metrics for the element to characterise the alloys

Background

- Recoil kinematics of neutral (neutron), residual (the target), charged and multi-particle emissions (n, p, γ, H, D, T, α, He) are now more rigorously treated based on modern, complete and enhanced nuclear data parsed in state-of-the-art processing tools

- Novel data forms for 83 naturally occurring element that include total and partial neutron defect-energy production, gas production cross section and kinetic energy release in material KERMA factors, have been systematically derived from ENDF/B-VIII.0, JENDL-5.0, JEFF-3.3, TENDL-2021 and CENDL-3.2 libraries

Background

- Numerical instance of integral damage quantities for legacy and novel nuclear components material alloys in NPPs, piles, fusion and accelerator devices typical irradiation conditions are been simulated in order to applicably founds material damage metrics landscapes

- There has been significant progress at the nuclear scale whereby the basic nuclear data has improved considerably to better serve above and beyond the classic NPP’s criticality simulations where only the neutron balance matters

Locations of the products of various nuclear processes

Residual	Os	Mo	Ni	P
Residual	Re	Nb	Co	Si
Target	W	Zr	Fe	Al
Residual	Ta	Y	Mn	Mg
Residual	Hf	Sr	Cr	Na

residual Z+2 transmutation				(α,n)	α in
residual Z+1 transmutation	(p,2n)	(p,n) β-	(p,g) (d,n) p in	d in	
Z activation	(n,3n)	(n,2n)	Target (n,n’)	(n,g) n in	
residual Z-1 transmutation		(n,t) (n,nd)	(n,d) (n,np)	(n,p) β+	
residual Z-2 transmutation	α out	(n,α)			

(entrance,emitted)

Fe as target the “residuals” seems to be alloy constituent, this is unlikely to be always the case, particularly for non Iron based alloys in high neutron energy fields

Reactions and decays

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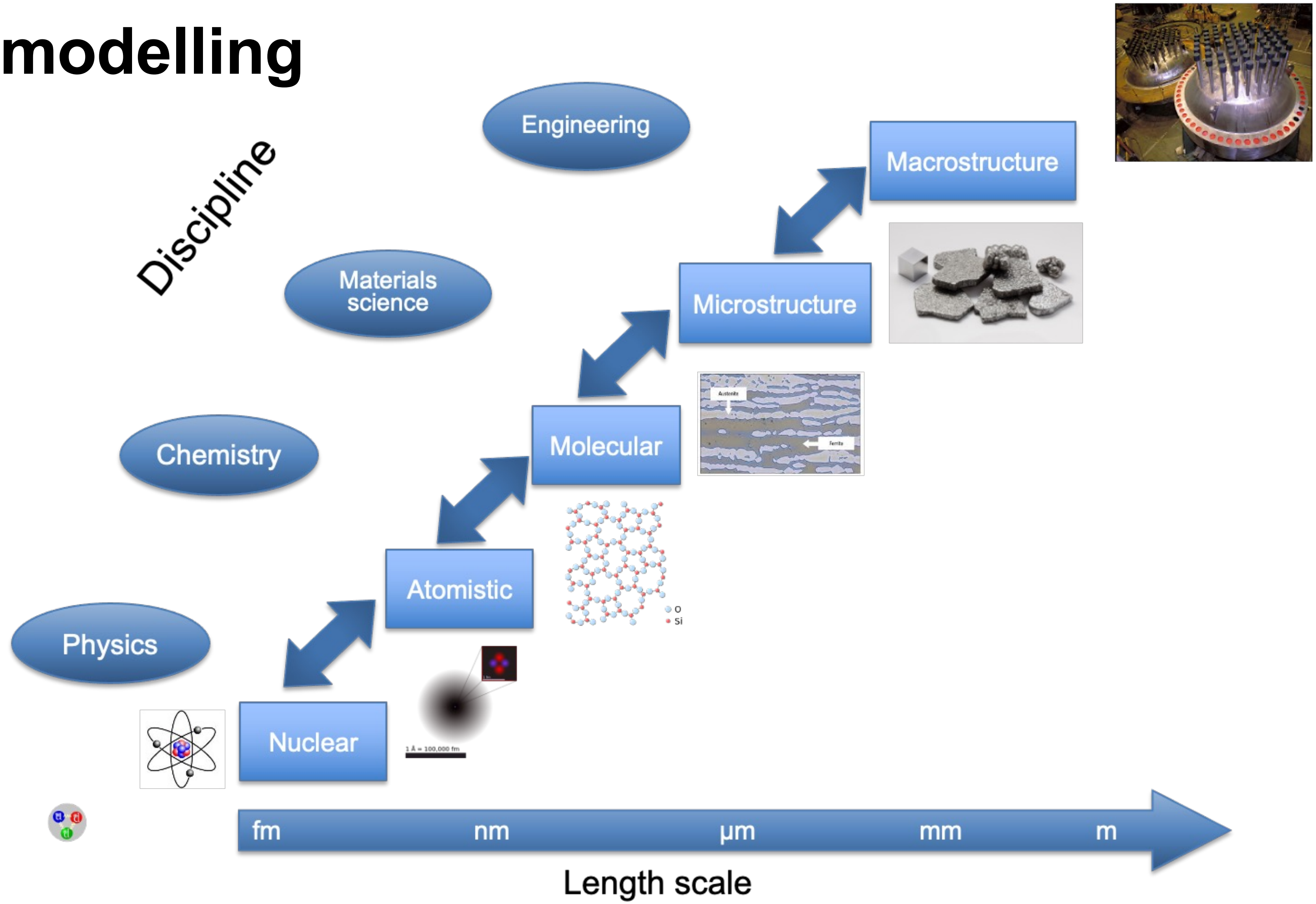
Multiscale modelling

- **The landscapes**



Defect Production Cross Sections (DPCS)

- The most common DPCS is for displacement of atoms. Displacement-Per-Atom irradiation exposure units are widely used for correlating neutron data and as partial basis for neutron-charge-particle inter-comparison
- Although not an actual defect, the total kinetic energy, T_{dam} imparted to recoils atoms as a function of PKA energy is used as a damage exposure index. The remaining PKA's is dissipated to electrons by excitation and ionization
- Norgett-Robinson-Torrens NRT-dpa assumes a threshold energy E_d, with a probability = 0 below E_d and 1 above
- Lindhard-Schraff electronic screening theory

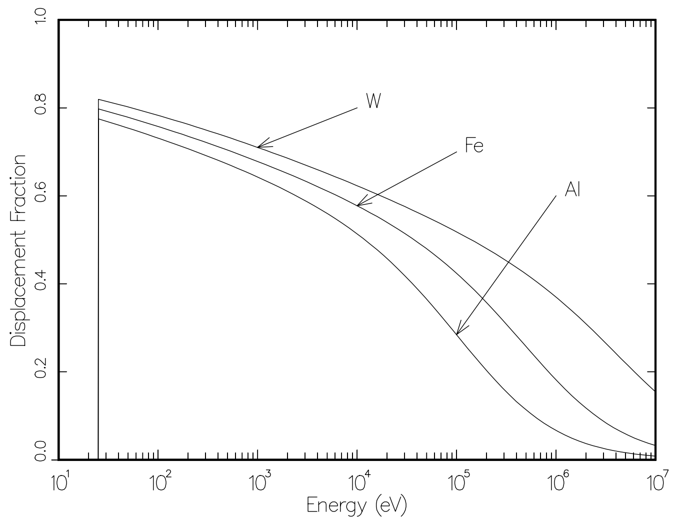
- Others ACR-dpa, or RPA metrics have been proposed
- Better recoils information/processing are been made available

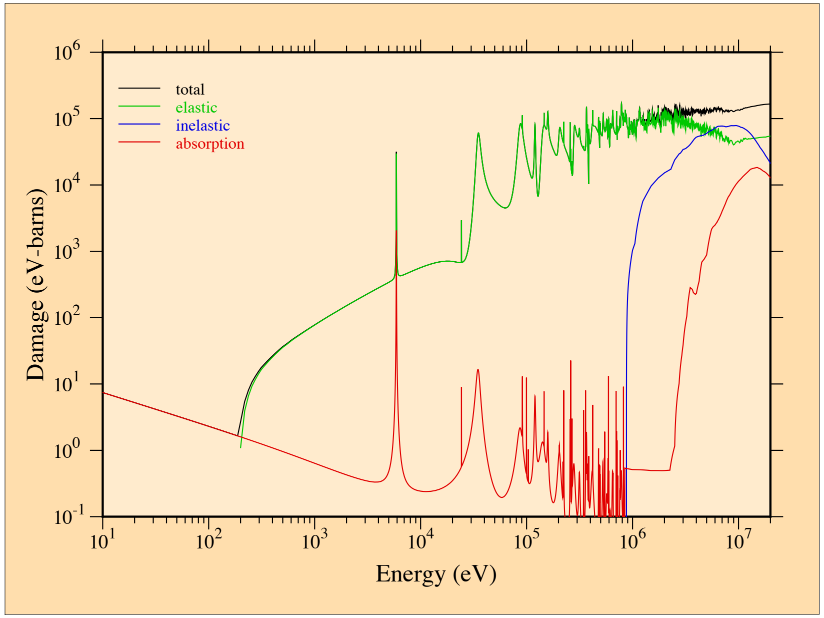
Processing protocols

- Using the HEATR, GASPR and GROUPR module protocols of the most recent NJOY2016 release **https://github.com/njoy/NJOY2016**
- Novel data forms for some 83 naturally occurring elements (assembled from their isotopic parts (287 stable targets) that in fine will compose the alloy) that include
  - total and partial neutron induced defect production metrics
  - gas production cross section
  - kerma factors
- Detailed residual nucleus (A > 4) and emitted particle matrices: energy-angle distribution
- Have been systematically and uniformly derived from the latest ENDF/B-VIII.0, JENDL-5.0, TENDL-2021 and CENDL-3.2 **https://www-nds.iaea.org/CRPdpa**

DPCS and NRT-dpa Ed

Element	E_d (eV)	Element	E_d (eV)
Be	31	Co	40
C	31	Ni	40
Mg	25	Cu	40
Al	27	Zr	40
Si	25	Nb	40
Ca	40	Mo	60
Ti	40	Ag	60
V	40	Ta	90
Cr	40	W	55
Mn	40	Au	30
Fe	40	Pb	25





$$DPA / s = \frac{E_{dam}}{2E_d} N\phi$$

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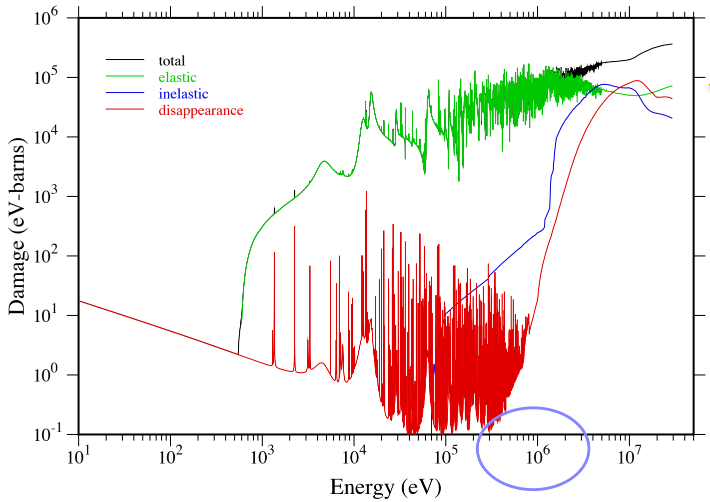
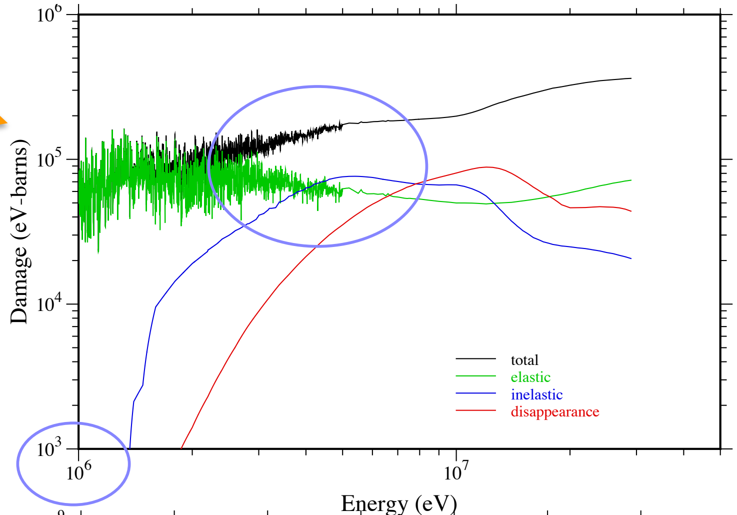
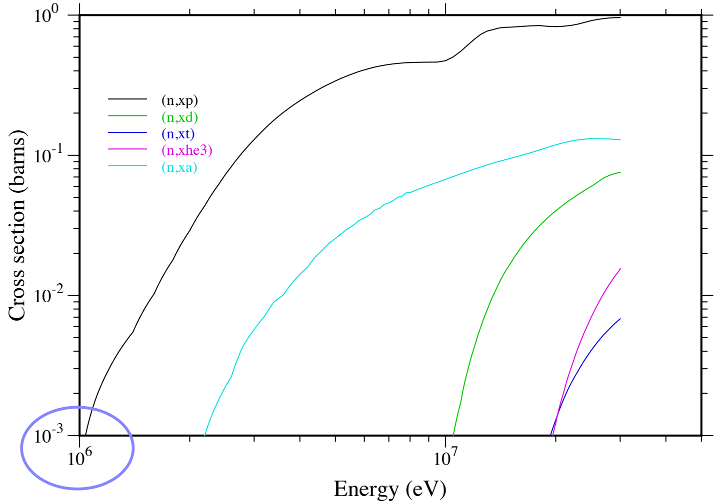
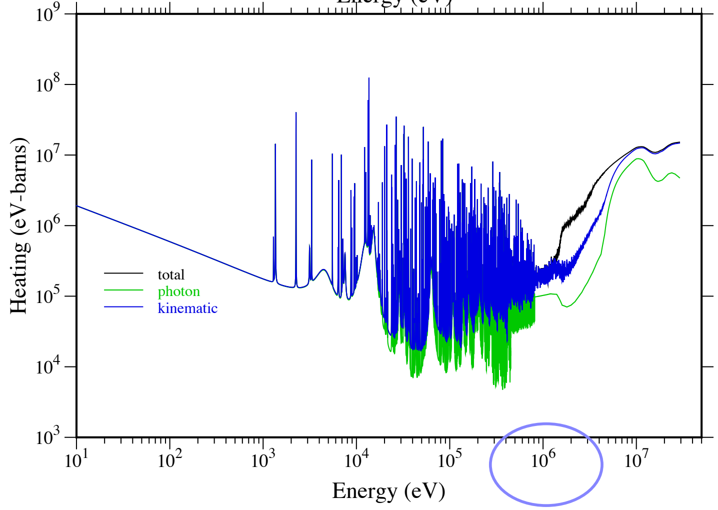
Processing protocols









- **Kerma**
- **Damage Energy**
- **Gas Production**
- **(Ni)**
  - **Ni58 68%**
  - **Ni60 26%**
  - **Ni61 1%**
  - **Ni62 4%**
  - **Ni64 1%**
- **Above the MeV's…**

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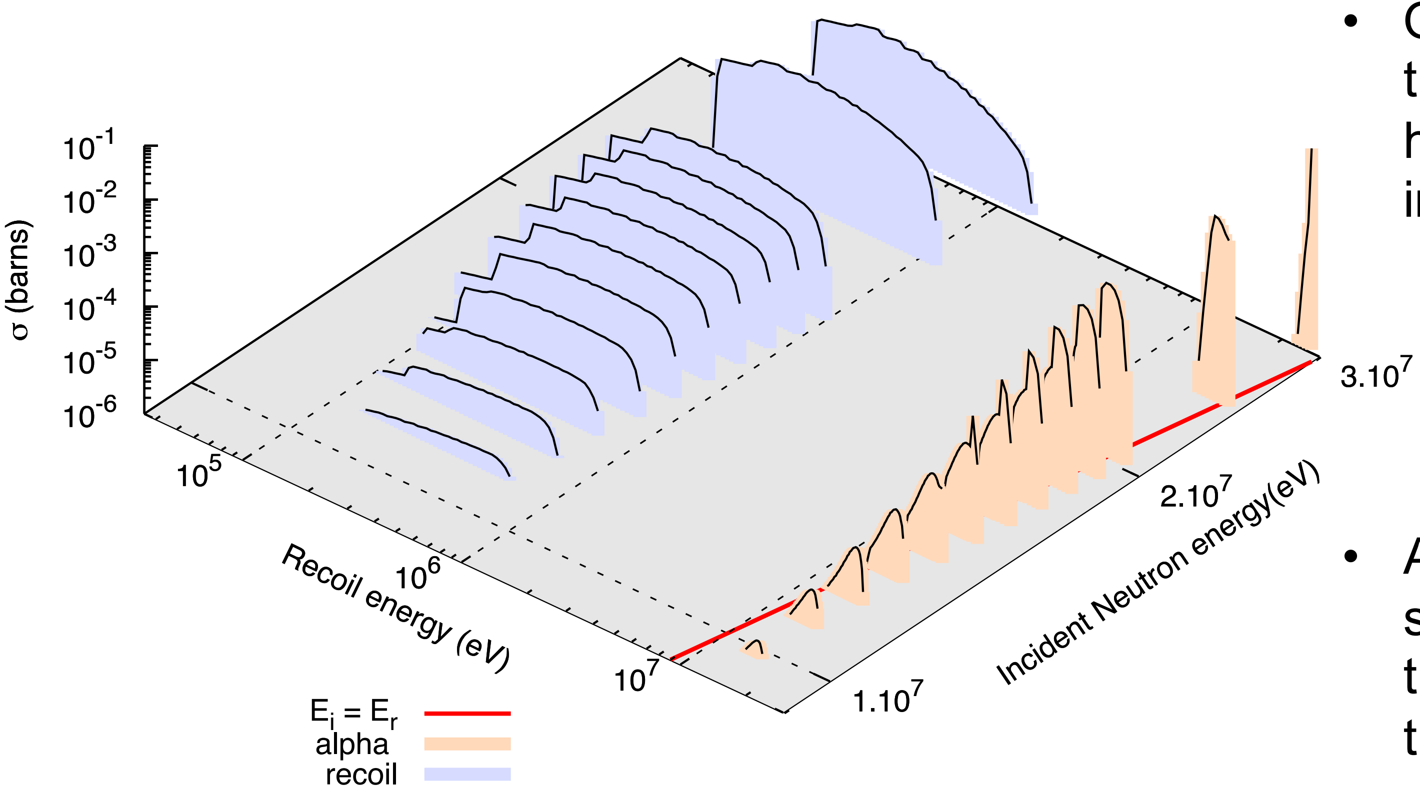
Example of matrices (n,α)

Target was W-184 - Residual was Hf-181 - $T_{1/2}$= 42 days, Beta- to Ta-181 (stable)



- Q positive (7.3 MeV) means that the alpha energy can be much higher than the energy of the n-incident !!!

- At 22.7 MeV and above the secondary energy grid is truncated !!! because if the transition energy at 30 MeV

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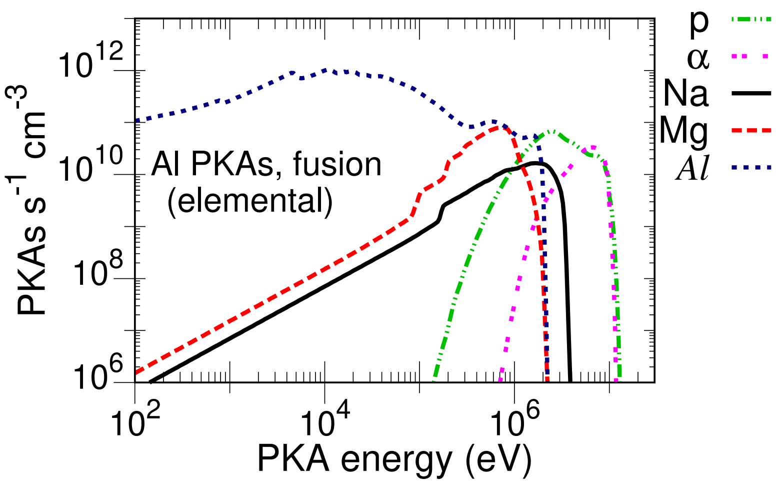
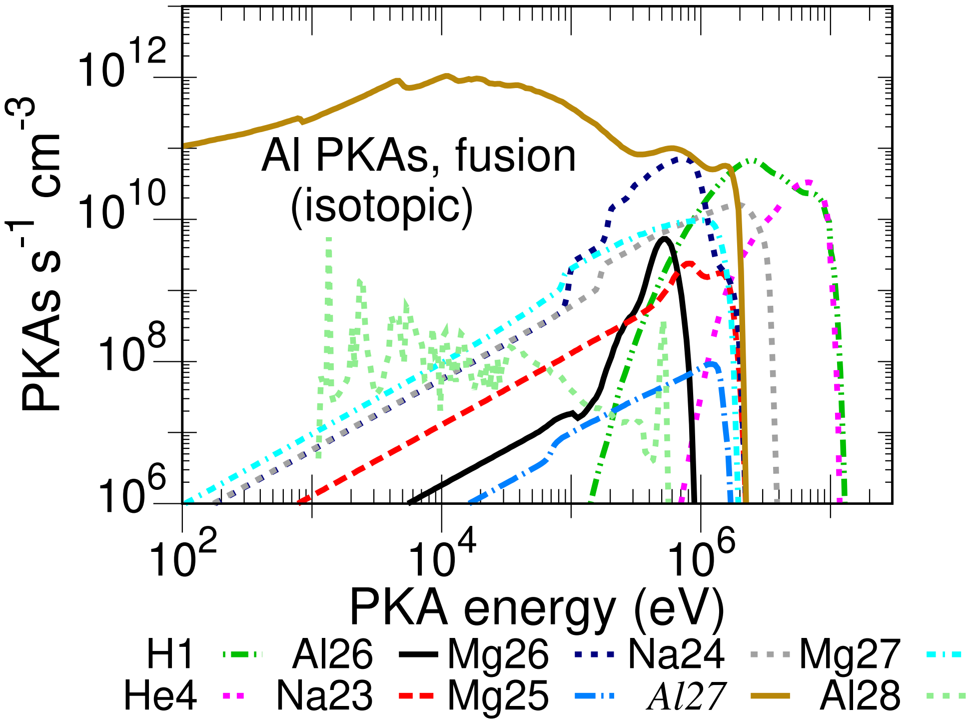
Damage metrics

- The SPECTRA-PKA code reads-in the recoil matrices and combines these with an incident neutron energy spectrum to define PKA event and energy distributions **https://github.com/fispact/SPECTRA-PKA**
- The code has the advantage of being fully compatible with the latest modern nuclear data libraries, for both neutron and charge particles, and can handle fine group structures
- The code can also consider any complex material composition containing an arbitrary distribution of target nuclide species.
- Even more significantly, it treats every nuclear reaction channel (on every target nuclide considered), and its associated recoil matrix, separately, which allows a deeper interrogation of the underlying nuclear data

Detailed metrics

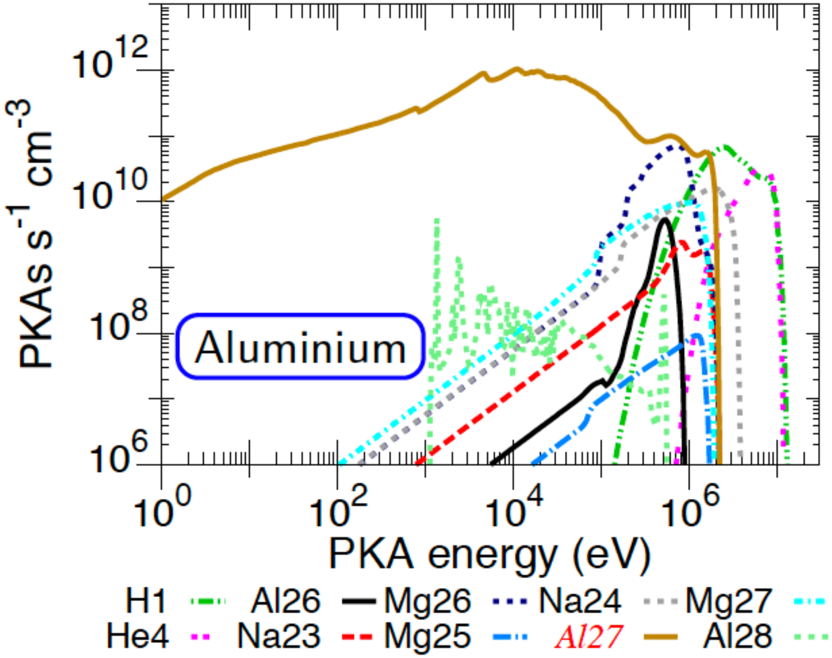
- Pure aluminum (100% ^{27}Al) transmuted residual elements and emitted particle PKA distributions under fusion neutron conditions, right elemental, left isotopic

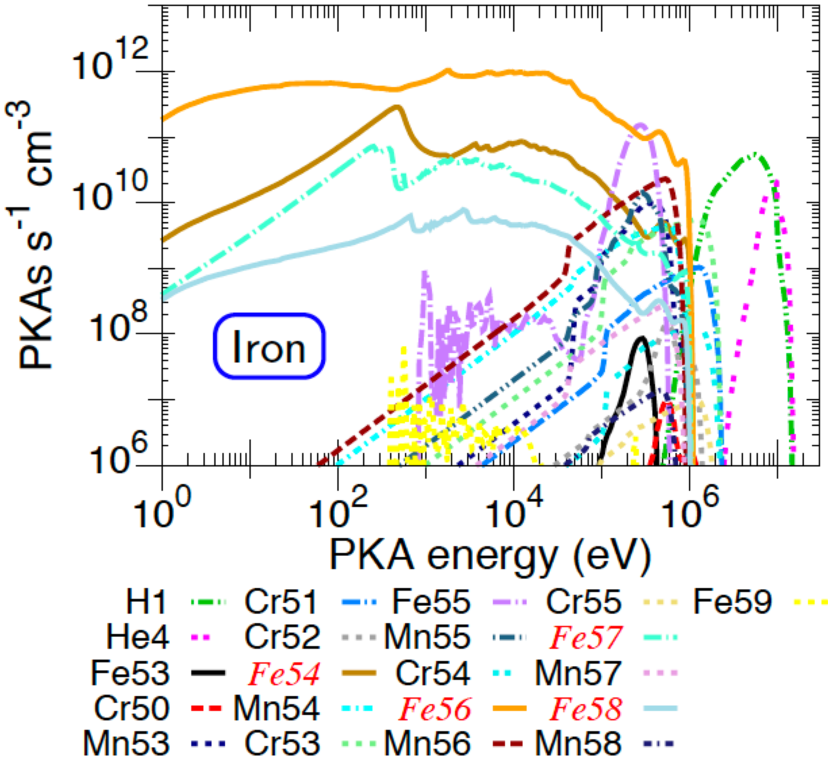




After a cascade what will be the impact of radioactive Na and Mg on the lattice?

Underlying complexity shown with SPECTRA-PKA





- very complex results with numerous recoils species (isotopes & elements, many radioactive)
- but already hiding some of the per-channel information that is available from the output

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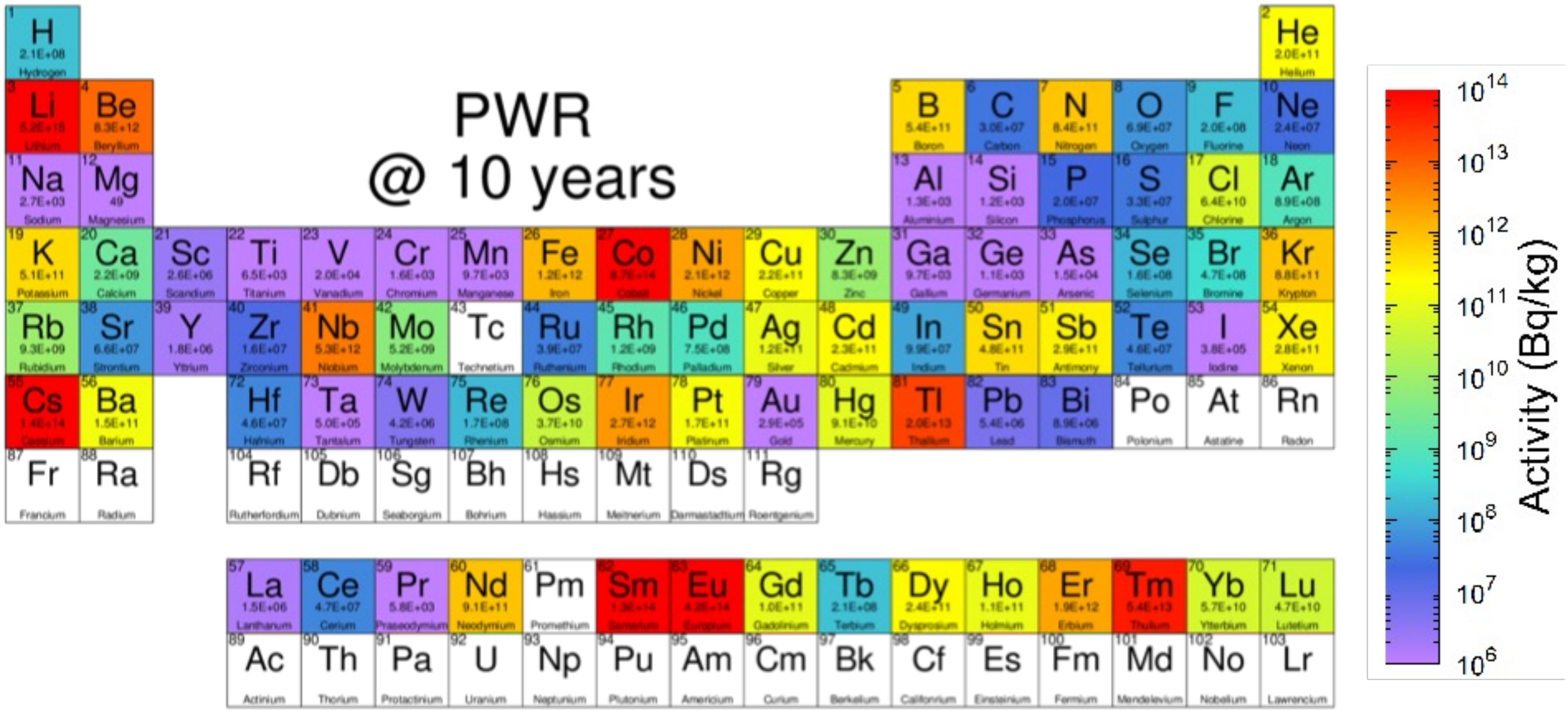
Quick and reproducible:
rapid scoping of materials under identical PWR conditions
(2 years operation and then cooling)



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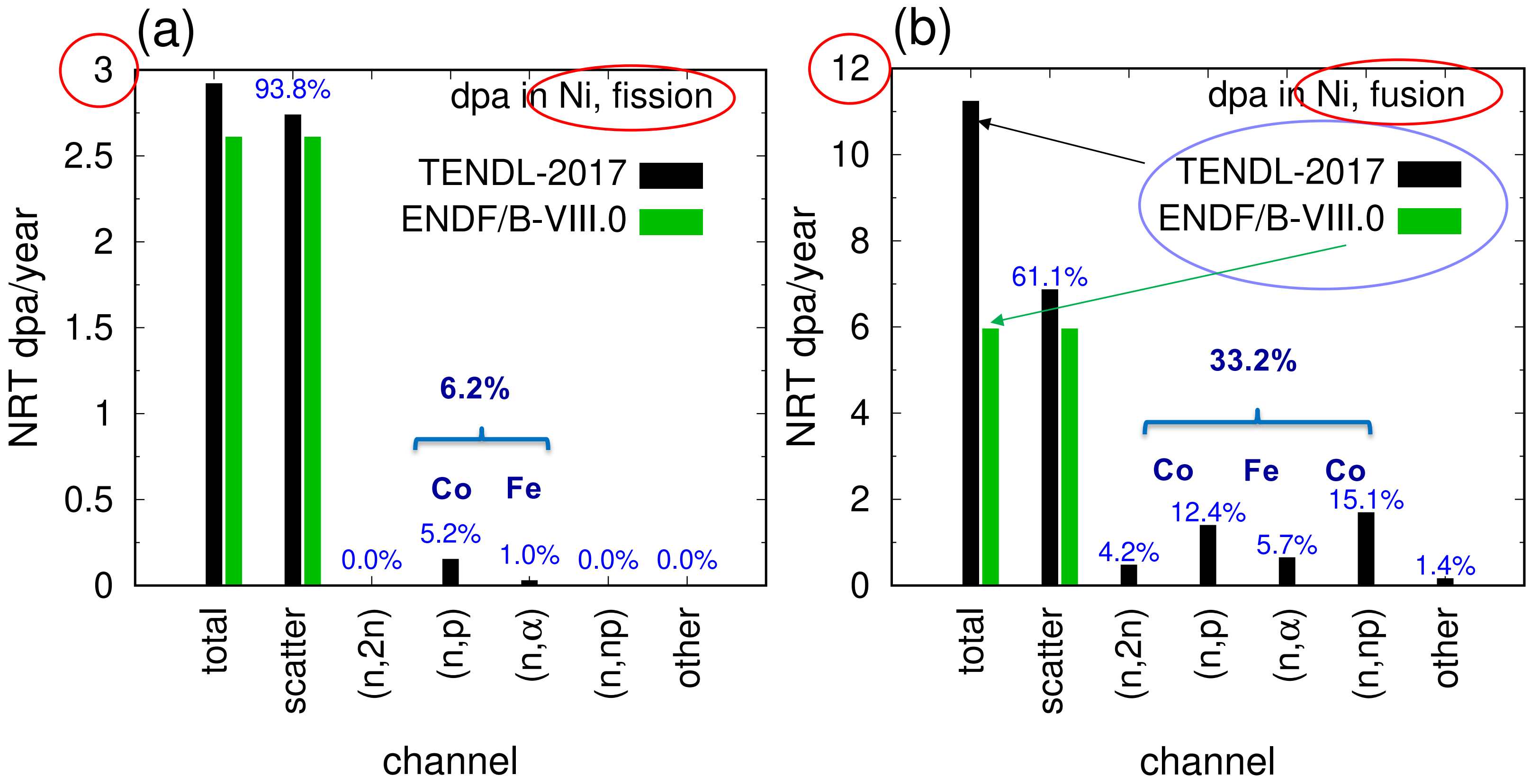
Novel metrics comparison

- New capabilities of SPECTRA-PKA have been exploited to analyze the relative significance of different nuclide channels to DPA damage production rates: (a) PWR - (b) Fusion FW
- Fusion spectral average DPCS are 2-4 times higher than Fission average



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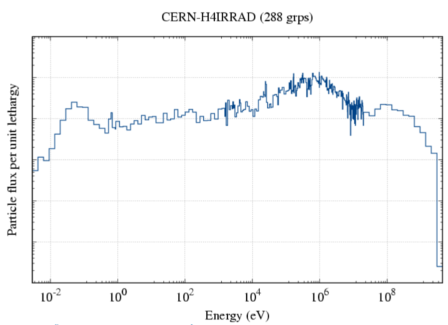
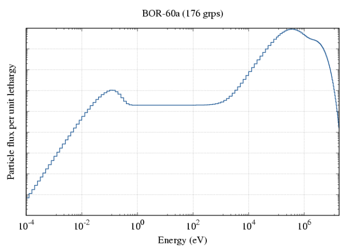
Novel metrics simulation results

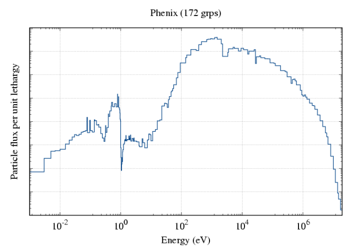
- Damages metrics in spectrum typical of the sodium cooled NPP prototype BOR-60 and a Fast Breeder Reactor assembly, Phoenix, mid-core

Flux	**2,27E+15**	n/cm2.s			**BOR-60**				
Fluence	**7,17E+22**	n/cm2							
	DPA/year	**He appm**	**H appm**	**He4**	**He3**	**H3**	**H2**	**H1**	**He /dpa**
Li	17	7106	6769	6929	177	6746	0	24	425
Be	35	4370	30	4369	1	29	0	0	126
SiC	56	34	35	34	0	0	0	35	1
V	45	0	8	0	0	0	0	8	0
Cr	31	5	263	5	0	0	0	262	0
Fe	30	2	86	2	0	0	0	86	0
Ni	34	52	1429	52	0	0	0	1429	2
Cu	31	5	263	5	0	0	0	262	0
Zr	36	1	2	1	0	0	0	2	0
W	12	0	0	0	0	0	0	0	0
WC	29	7	0	7	0	0	0	0	0
T91	31	6	85	6	0	0	0	85	0
Eurofer	31	2	80	2	0	0	0	80	0
SS316	32	9	220	9	0	0	0	220	0

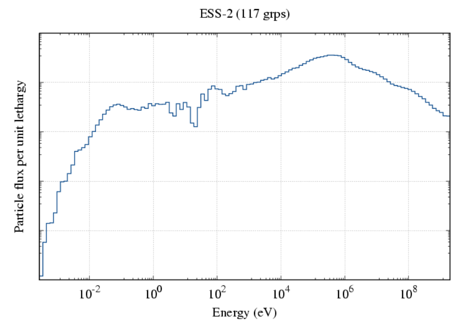
Flux	**2,38E+15**	n/cm2.s			**FBR**				
Fluence	**7,50E+22**	n/cm2							
	DPA/year	**He appm**	**H appm**	**He4**	**He3**	**H3**	**H2**	**H1**	**He /dpa**
Li	4	21614	21118	21251	363	20859	0	259	5842
Be	5	10	0	10	0	0	0	0	2
SiC	3	0	0	0	0	0	0	0	0
V	6	0	0	0	0	0	0	0	0
Cr	2	0	13	0	0	0	0	13	0
Fe	1	0	0	0	0	0	0	0	0
Ni	3	3	5	3	0	0	0	5	1
Cu	2	0	13	0	0	0	0	13	0
Zr	2	0	0	0	0	0	0	0	0
W	1	0	0	0	0	0	0	0	0
WC	2	0	0	0	0	0	0	0	0
T91	1	0	0	0	0	0	0	0	0
Eurofer	1	0	0	0	0	0	0	0	0
SS316	2	0	1	0	0	0	0	1	0







Same metrics for accelerator's environment: CERN, ESS, etc.



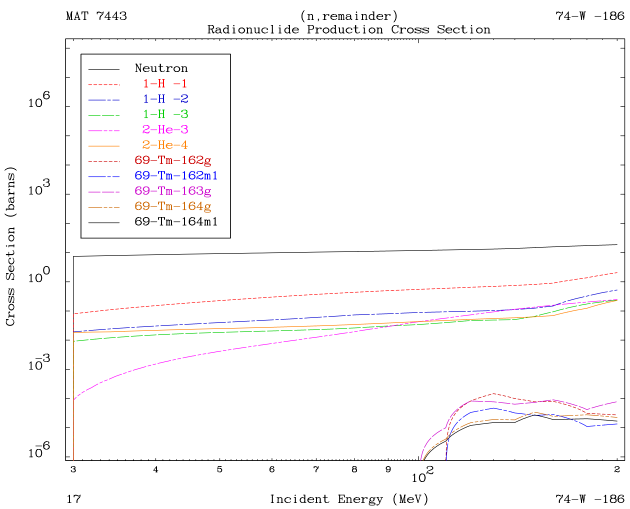
Progress @ nuclear scale

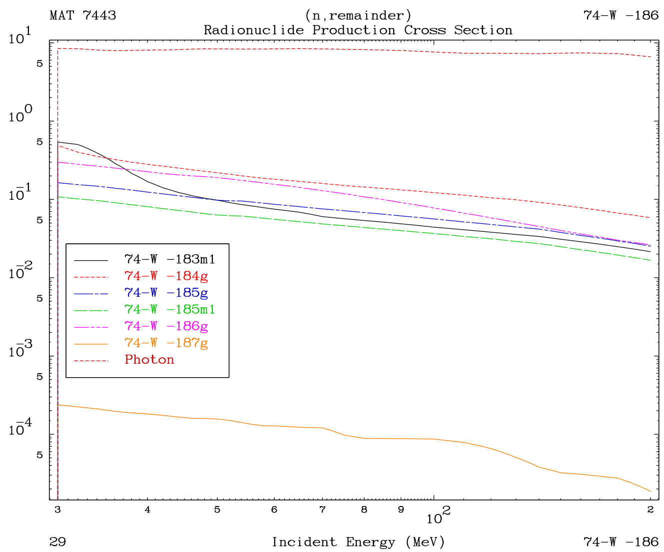
- Definitely, a step forward in the proper understanding of materials defect metrics induced by radiations
  - much better nuclear data (with uncertainty)
  - more complete data forms; recoil, emitted particles spectra
  - transmutation, decaying effects (also happens after irradiation)
  - non-elastic events: (n,2n), (n,p), (n,a)
  - incident particle(s) energy dependence
  - multiplicity of sources, ➔ complementarity and difference
  - a much better coverage of the high (> MeV) energy range
- Novel event per event, channel metrics: "Differential dpa calculations with SPECTRA-PKA" Journal of Nuclear Materials 504 (2018) 101-108
- Uncertainty quantification and propagation UQP can be envisaged

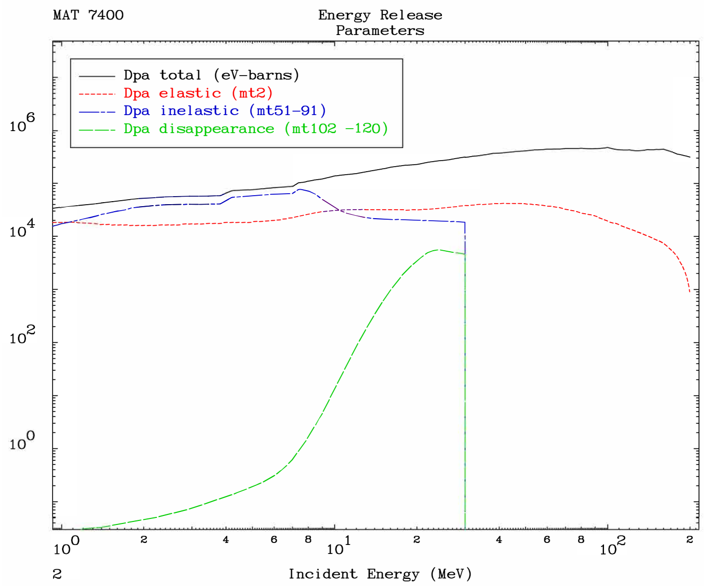
==> to better serve multi-scale, -physics simulations system

Progress @ nuclear scale

- Extension of DPCS simulation to high neutron energies (i.e. > 2 MeV) is incorrect due to model errors (single neutron, particle emission frame, non-elastic events predominance, transmutation, radioactive residual,..)
- Extension of DPCS simulation above the transition energy (i.e. > 20, 30 MeV) is incorrect due to changes in nuclear data format structure (mf3-mt5*mf6; lumped A<4 + heavy residual)







30 MeV cutoff !!

Conclusions

- Multiscale modelling of materials damages across the length and times scales requires overcoming the borders between the disciplines for a seamless integration of the models on the different scales
- Other scale exist: state (plasma, density), temperature scale (KERMA), time,..
- Modelling difficulties are not so much with components or atoms but in-between
- Progress are been made, accelerator are marvelous tools

ICTP-IAEA Workshop, Trieste, Q2 2023 !!
Radiation Damage in Nuclear Systems: from Bohr to Young