INDC reporting - CRP Evaluation Primary Radiation Damage Cross Sections

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IAEA

International Atomic Energy Agency

CRP objectives

- To find ways to overcome the drawbacks, limitations of the Norgett-Robinson-Torrens displacement per atom NRT-dpa by relying on recent/modern research and development in primary radiation damage simulations
- Elaborate upgraded primary radiation defect metrics to better capture the annealing, evolution of defects in the recoil cascades but also thereafter
- Demonstrate better metrics to correlate experimental (ions based) to model parameters (neutron based) for microstructural material damage

CRP objectives

- Encourage, entice the nuclear data/processing and materials research communities to more efficiently work together,
- Engage the true multi-scale: atom/isotope-molecule/element-alloy/material aspects of characterising materials properties evolution under particles irradiation
- Provide, elaborate and engineer more robust methodologies able to cover all experimental and modelling aspects of study of materials under ions and neutron irradiations. Most experimental information are based on ions, while the next generation devices will endure high energy neutrons
- Develop the physics and metrics to bridge the gaps

Results achieved:

Results achieved based on the CRP objective

- Isotopic and Elemental numerical databases for defect production metrics as well as gas production and kerma kinetics energy per materials
- A much better understanding of the different physics at play, the high energy non-elastic and time dependent events
- The pivotal review published as a journal Article Eur. Phys. J. Plus (2019) 134: 350 written by the savant society members now fully integrates an even more concerted World effort in further developing our knowledge of radiation damage and exposure
- The specific objectives were met with some success as now a day more research communities are working in unison, whilst the multi-physics, multi-scale aspects of the field are truly emerging, taken into account in new material/plant design

14 Countries - 19 Contracting Institutes

BEL Centre d'etude de l'energie nucleaire (SCK.CEN)
CPR City University of Hong Kong
FIN University of Helsinki
FRA Commissariat à l'énergie atomique CEA Centre de Saclay
GFR Karlsruher Institut fuer Technologie KIT
JPN Japan Atomic Energy Agency (JAEA); Nuclear Science and Engineering Directorate
NET Nuclear Research and Consultancy Group NRG
ROK Korea Atomic Energy Research Institute KAERI
RUS Institute for Physics and Power Engineering IPPE; State Scientific Center of the Russian Federation
SPA Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas (CIEMAT)
SPA Universidad Politecnica Madrid
SPA University of Alicante
SWE Uppsala University
UK United Kingdom Atomic Energy Authority (UKAEA)
UKR National Science Center "Kharkov Institute of Physics and Technology"
USA Battelle Pacific Northwest Division (PNL)
USA Los Alamos National Laboratory (LANL)
USA Oak Ridge National Laboratory (ORNL)
USA Sandia National Laboratories (SNL)

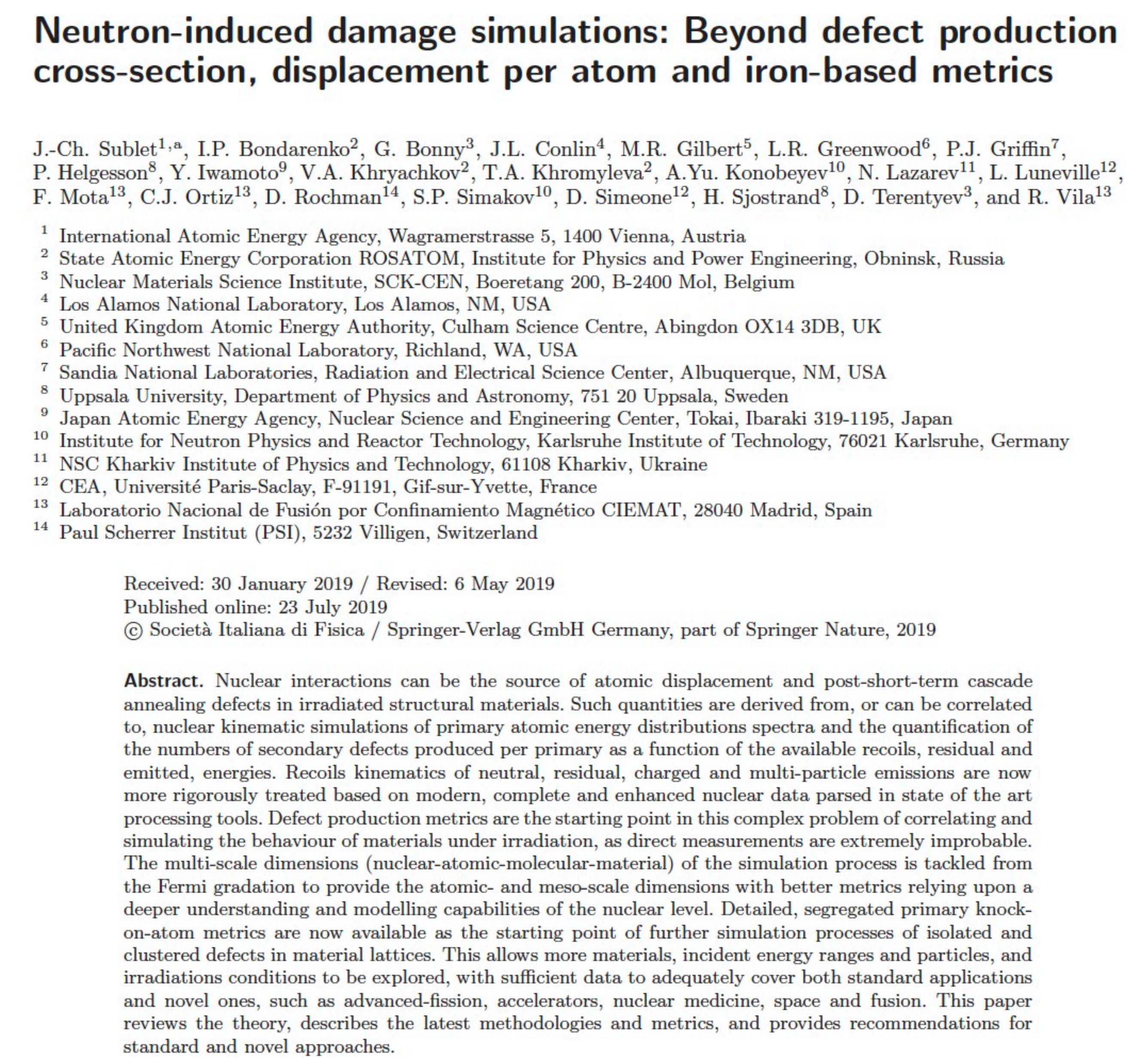
Publications

- Web site https://www-nds.iaea.org/CRPdpa/
- One additional TC in 2016 on processing issues
- Generated some 40 publications/articles
- A review “Neutron-induced damage simulations: Beyond defect production cross-section, displacement per atom and iron-based metrics” https://doi.org/10.1140/epjp/i2019-12758-y

Eur. Phys. J. Plus (2019) **134**: 350
DOI 10.1140/epjp/i2019-12758-y

THE EUROPEAN
PHYSICAL JOURNAL PLUS

Review



Neutron-induced damage simulations: Beyond defect production cross-section, displacement per atom and iron-based metrics

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Abstract. Nuclear interactions can be the source of atomic displacement and post-short-term cascade annealing defects in irradiated structural materials. Such quantities are derived from, or can be correlated to, nuclear kinematic simulations of primary atomic energy distributions spectra and the quantification of the numbers of secondary defects produced per primary as a function of the available recoils, residual and emitted, energies. Recoils kinematics of neutral, residual, charged and multi-particle emissions are now more rigorously treated based on modern, complete and enhanced nuclear data parsed in state of the art processing tools. Defect production metrics are the starting point in this complex problem of correlating and simulating the behaviour of materials under irradiation, as direct measurements are extremely improbable. The multi-scale dimensions (nuclear-atomic-molecular-material) of the simulation process is tackled from the Fermi gradation to provide the atomic- and meso-scale dimensions with better metrics relying upon a deeper understanding and modelling capabilities of the nuclear level. Detailed, segregated primary knock-on-atom metrics are now available as the starting point of further simulation processes of isolated and clustered defects in material lattices. This allows more materials, incident energy ranges and particles, and irradiations conditions to be explored, with sufficient data to adequately cover both standard applications and novel ones, such as advanced-fission, accelerators, nuclear medicine, space and fusion. This paper reviews the theory, describes the latest methodologies and metrics, and provides recommendations for standard and novel approaches.

Databases & Tools

- NJOY-2016 pointwise data forms of heating kerma (kinetic energy release in material), NRT-dpa damage energy and gas production metrics for up to 83 elements Hydrogen to Uranium from:
  - TENDL-2019
  - JENDL-4.0
  - ENDF/B-VIII.0

- Graphical comparison plots :
  - TENDL-2019 versus ENDF/B-VIII.0
  - TENDL-2019 versus JENDL-4.0
  - ENDF/B-VIII.0 versus JENDL-4

when the response exists in both sources

Databases & Tools

- NJOY-2016 groupwise isotopic (287stables) and elemental (83) recoils and emitted particles PKA spectra

- SPECTRA-PKA as a modern open-source command-line driven programme for calculating the expected primary knock-on atom (PKA) spectra for any given material under neutron or charged particle irradiation
  - open source on GitHub https://github.com/fispact/SPECTRA-PKA

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
  - transmutation, decaying effects (also happen after irradiation)
  - non-elastic events
  - Incident particle energy dependence

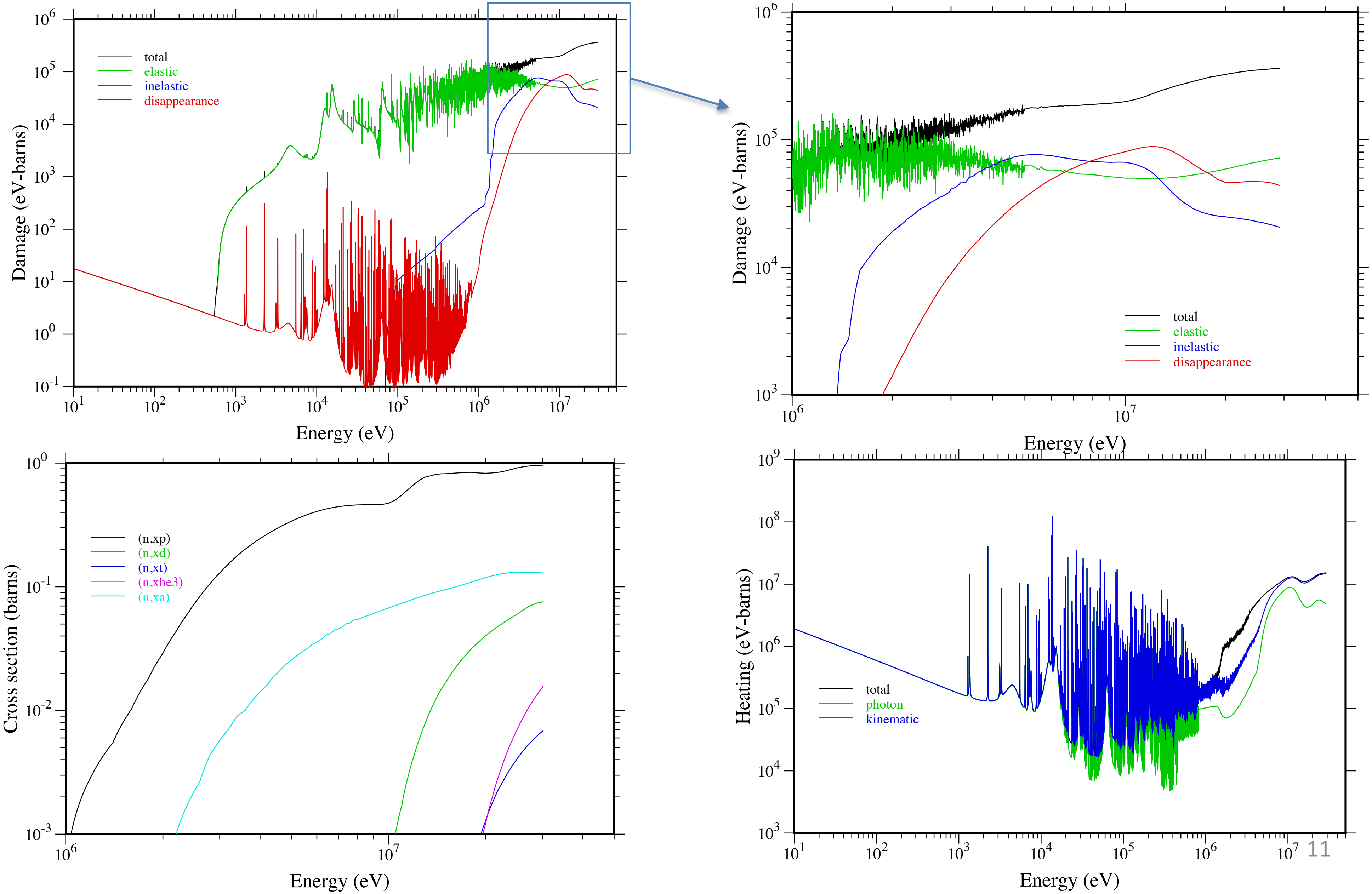
- A much better coverage of the high energy range
- Novel event per event, channel metrics: "Differential dpa calculations with SPECTRA-PKA Journal of Nuclear Materials 504 (2018) 101-108
- Uncertainty quantification and propagation UQP

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

IAEA

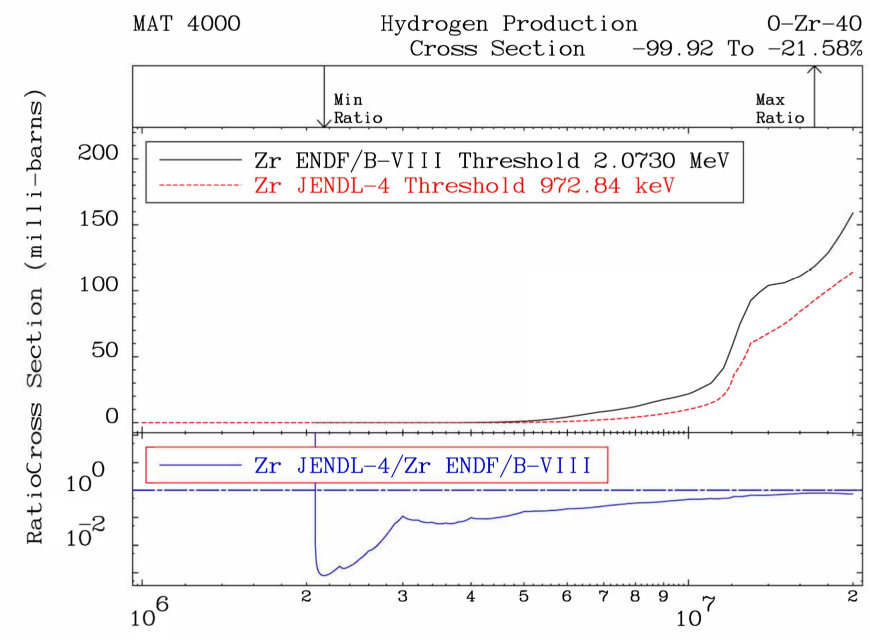
Processing protocols

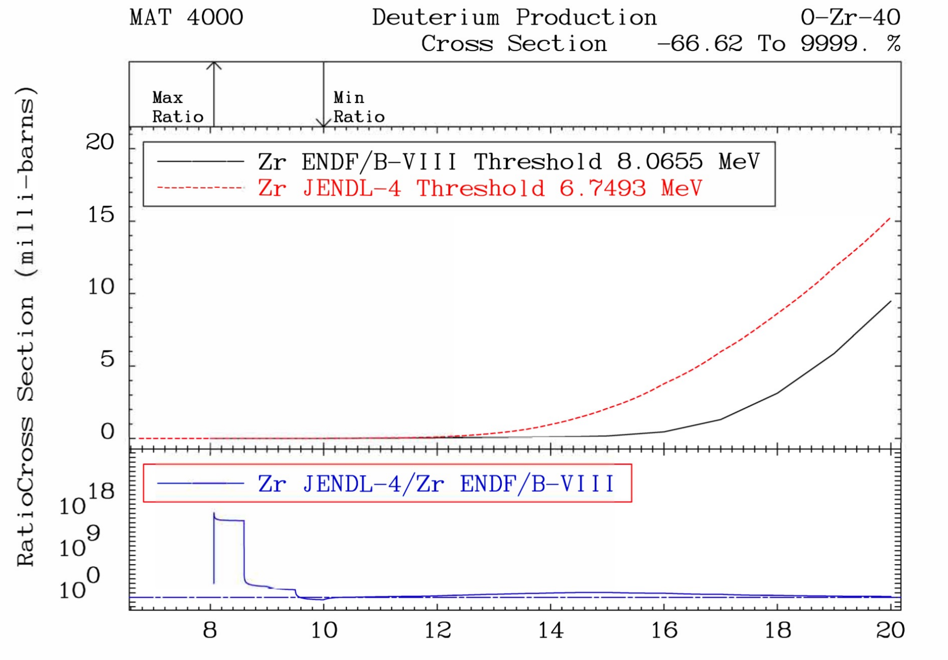
- Kerma, Damage Energy, Gas Production (Ni)

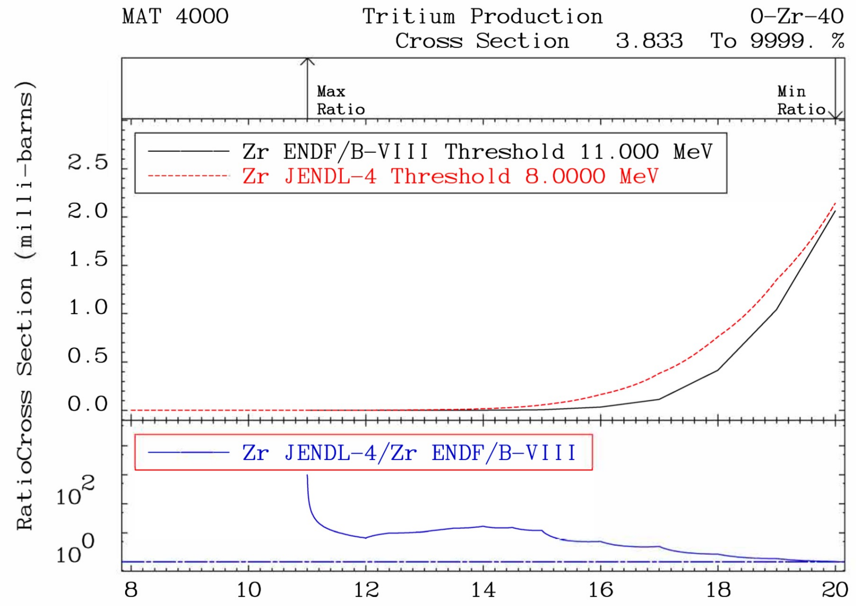


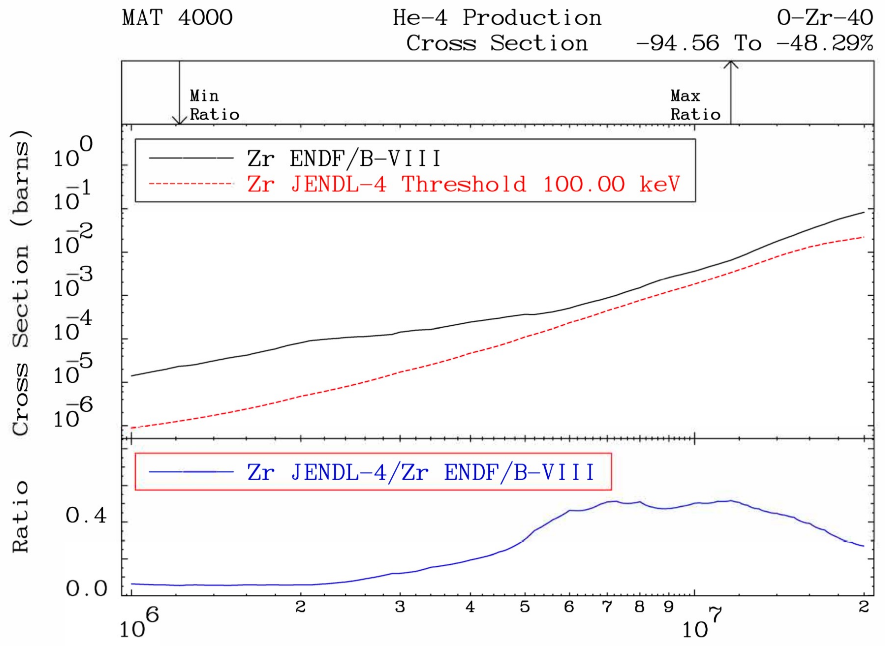
Processing : Gaz production comparison

- Library comparison (Zr), large differences



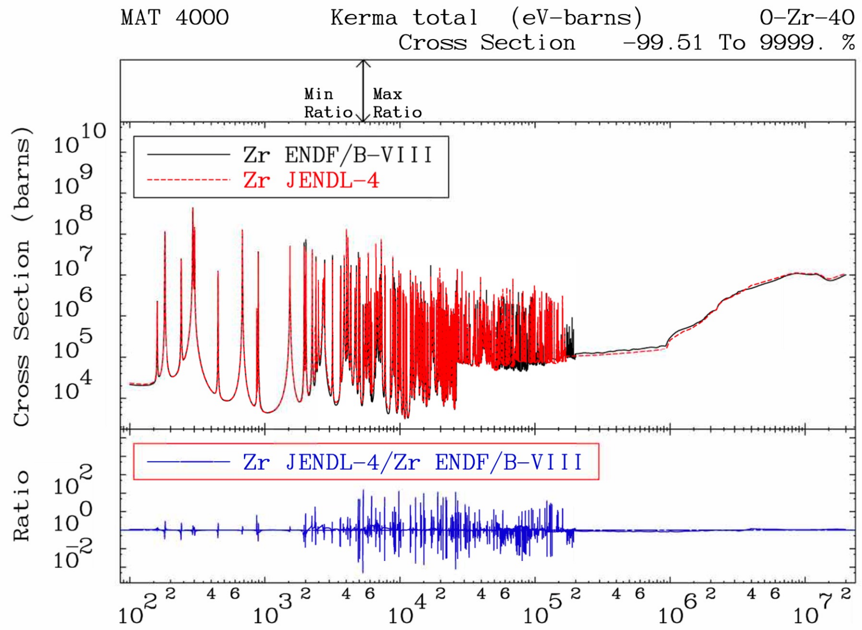


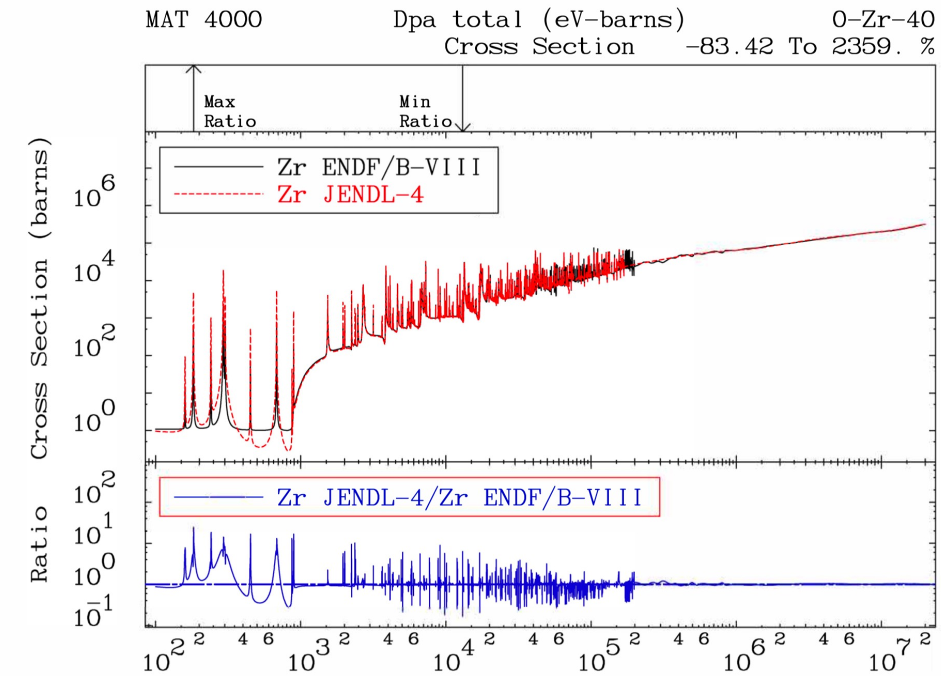


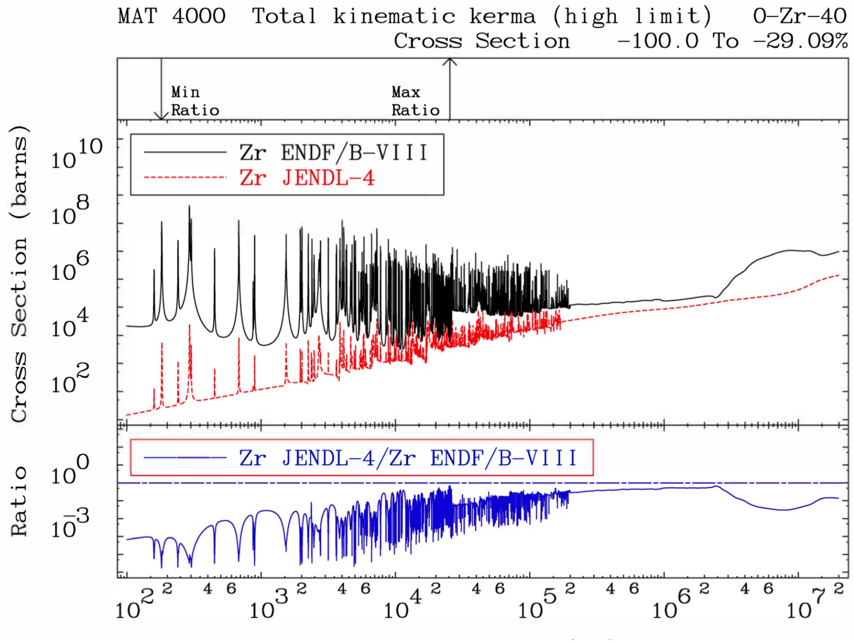


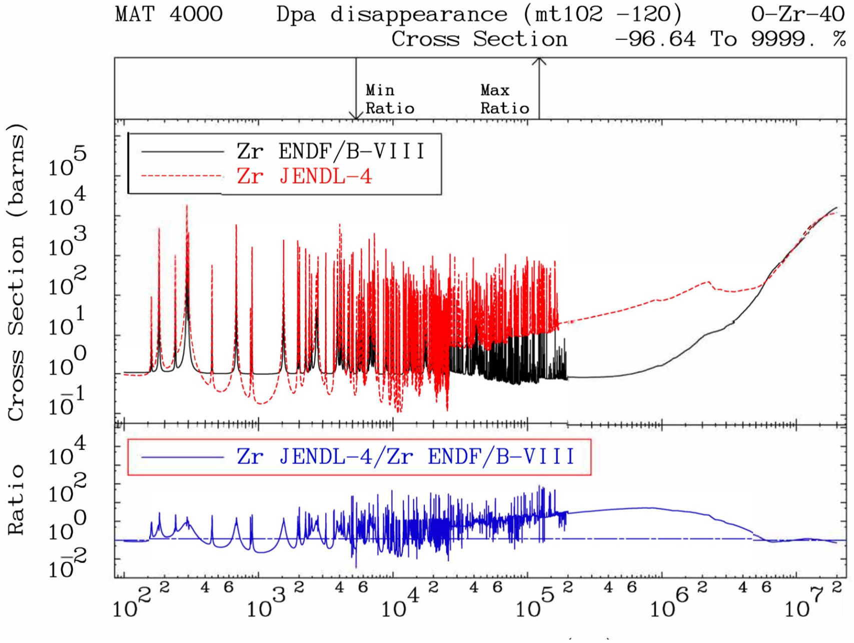
Processing: KERMA, DPA comparison

- Library comparison (Zr), good and bad





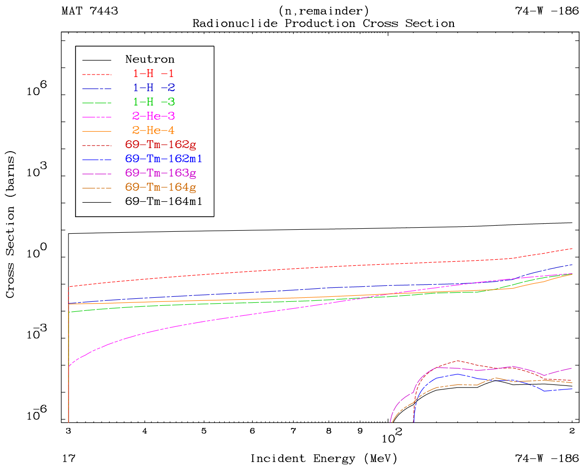


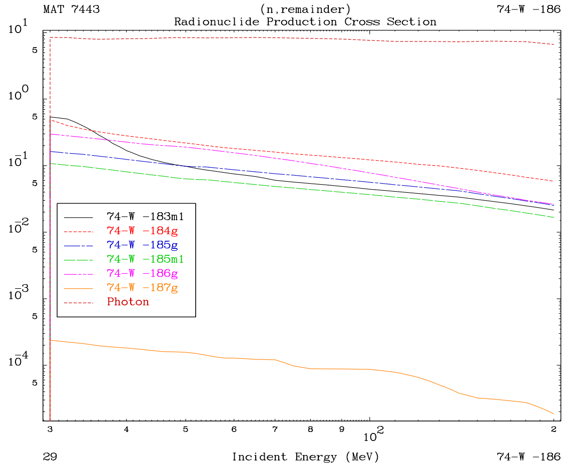


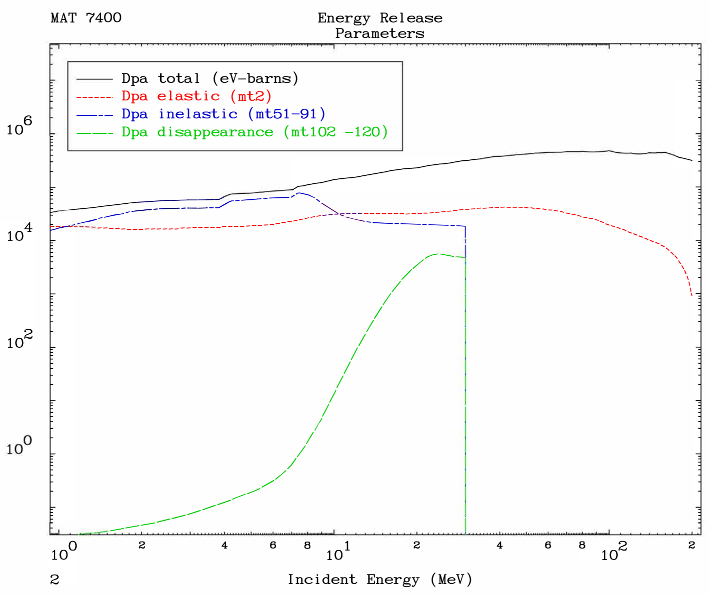
Progress @ nuclear scale

- Extension of DPCS simulation to high neutron energies (i.e. > few MeV) is uncertain 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 uncertain due to changes in nuclear data format structure (mf3-mt5*mf6; lumped A<4 + heavy residuals)







Locations of the products of various nuclear processes

	Os	Mo	Ni	P
	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,γ) (d,n) p in	d in	
Z activation	(n,3n)	(n,2n)	Target (n,n’)	(n,γ) 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)			

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

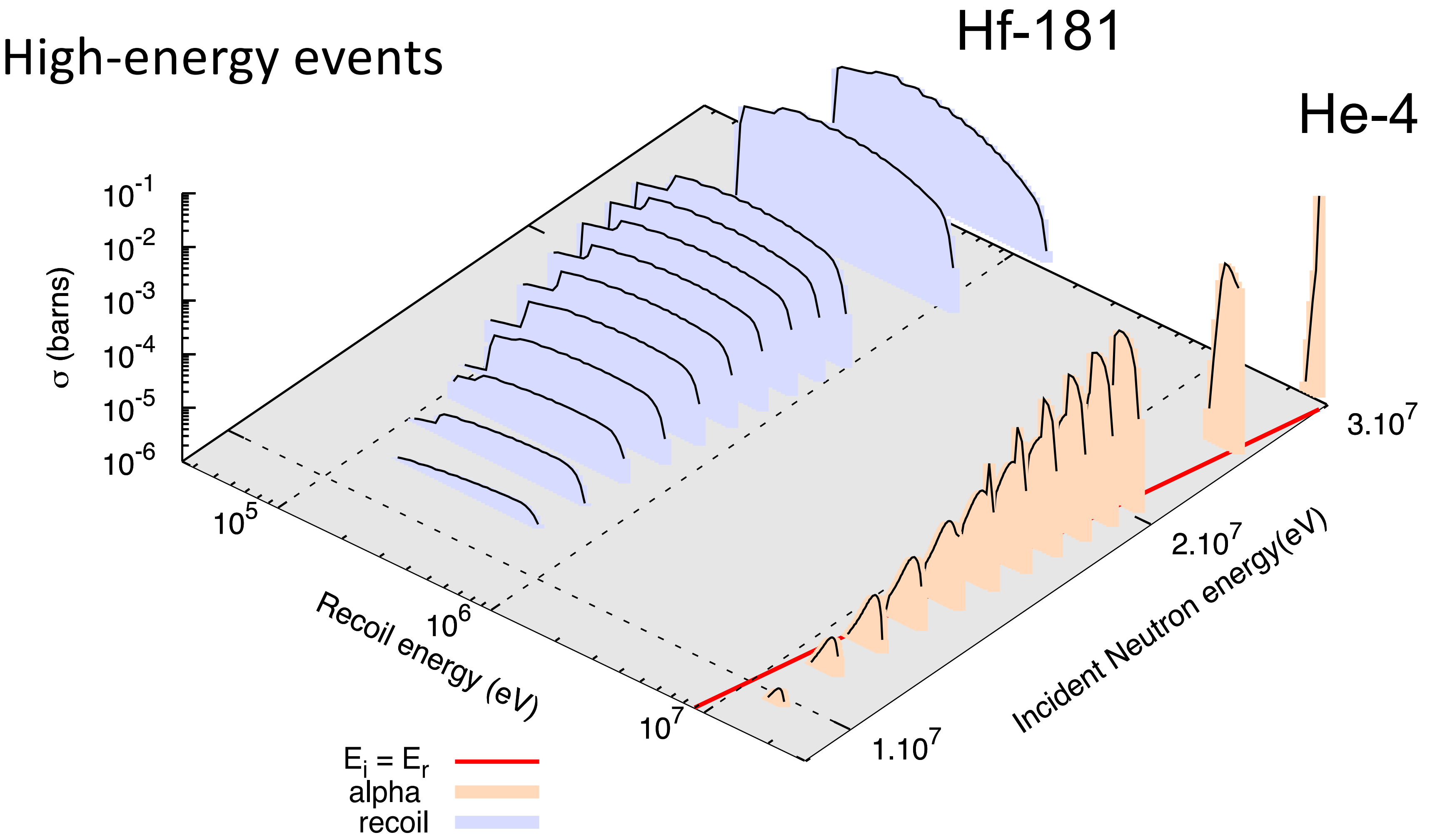
Progress @ nuclear scale

Nature 565, pages 328–330 (2019) The surprisingly large neutron capture cross-section of ^{88}Zr
^{88}Zr thermal capture: **861000 barns**, third largest after ^{135}Xe, ^{157}Gd !! Theory predicted 10 barns
Production ^{89}Y(p,2n)^{88}Zr - ^{89}Zr thermal capture < 12000 barns

- Yttrium and Niobium have only one stable isotope
- Strontium: 4 stables

W-184 example of matrices

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

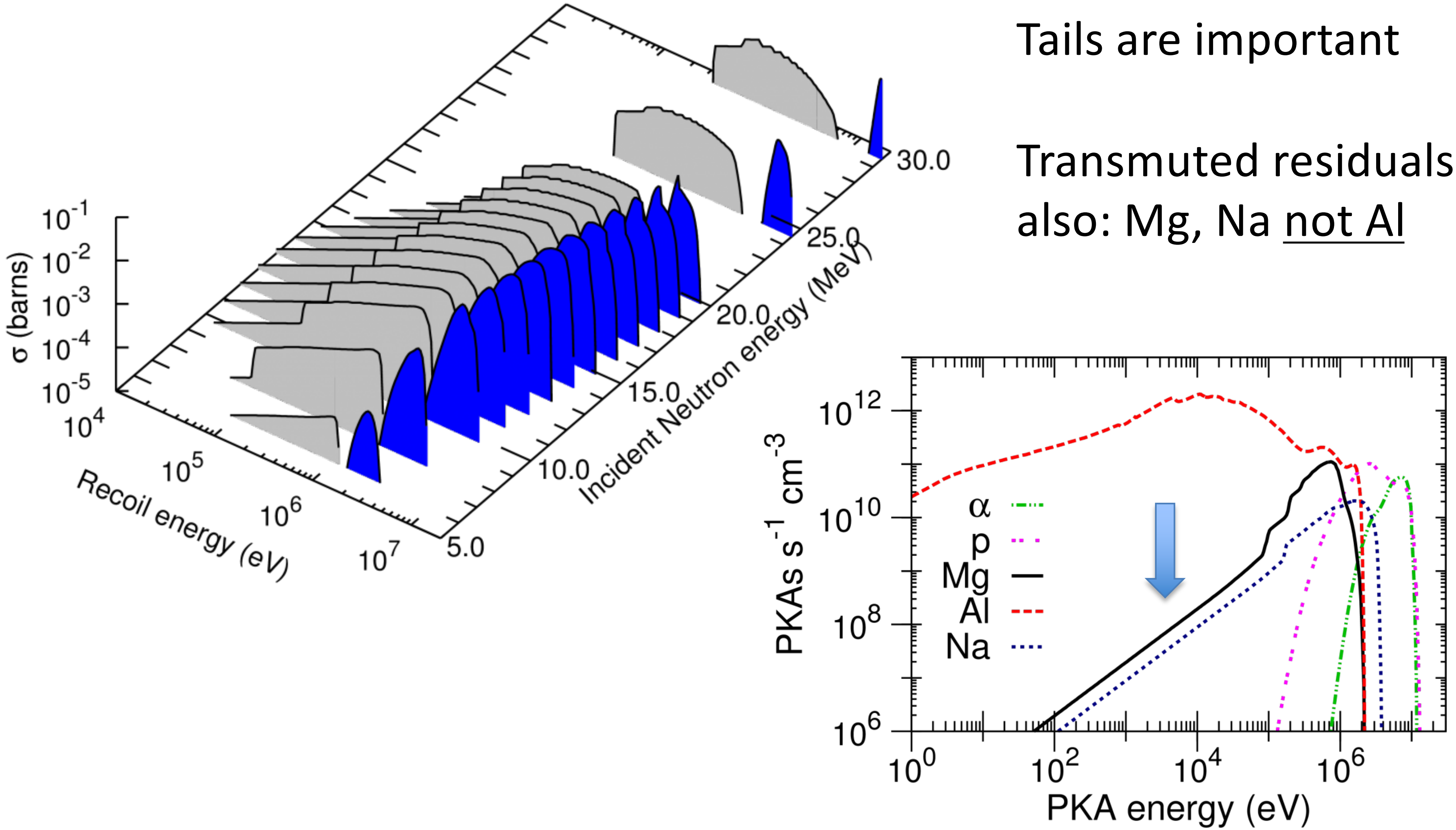


Q positive (7.3 MeV) means that the alpha energy can be much higher than the energy of the n-incident !!! At 22.7 MeV and above the secondary energy grid is truncated !!!

NJOY processing ismooth = 1

Tails are important

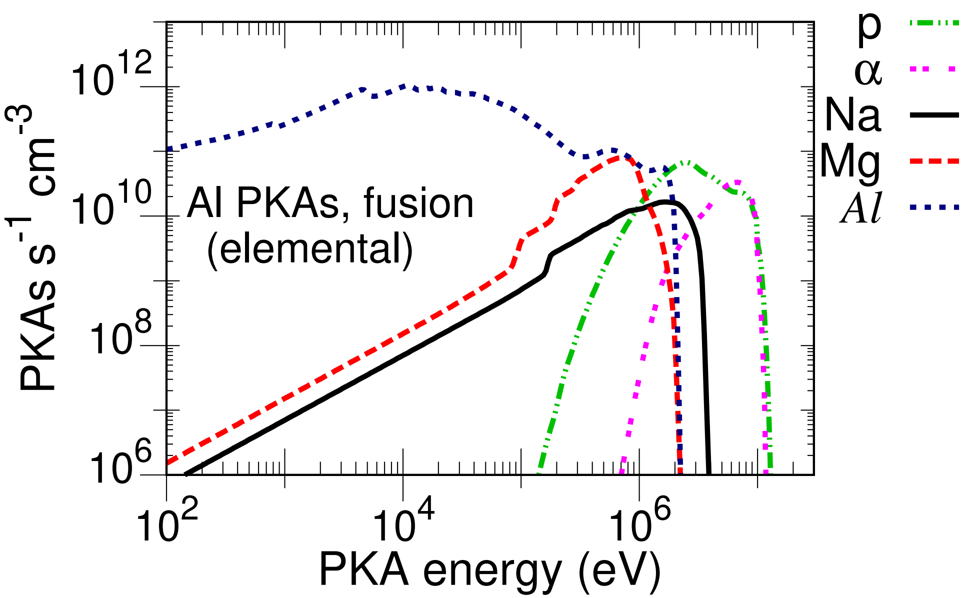
Transmuted residuals also: Mg, Na not Al

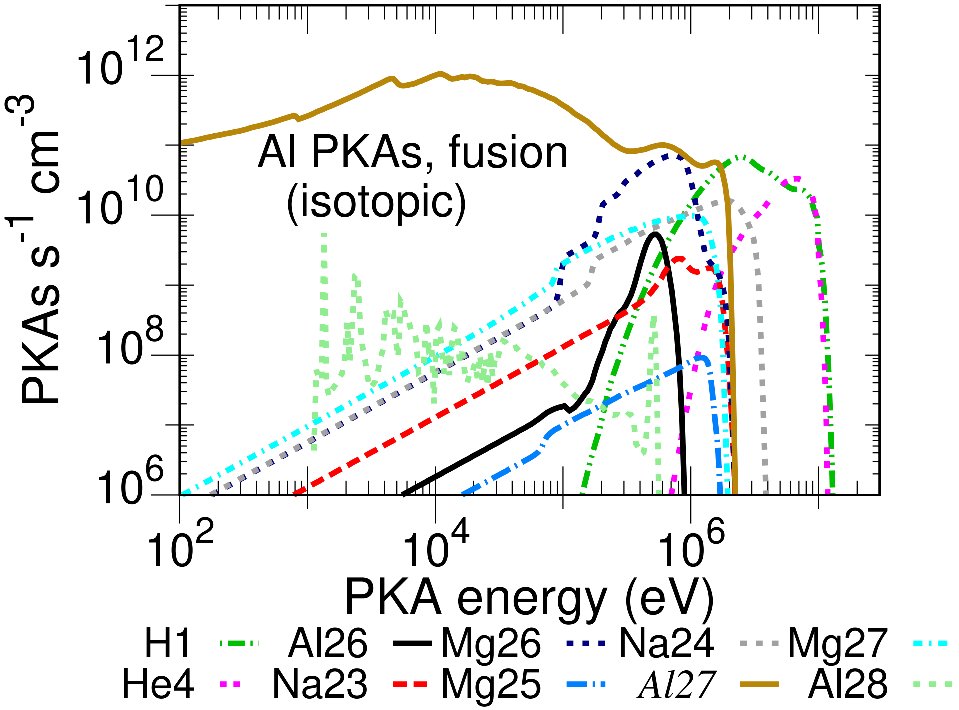


Q negative this time, but NJOY ismooth =1 ($\sqrt{E}$ shape) for when the evaluator decided to cut short the secondary energy grid of the recoil!

Detailed metrics

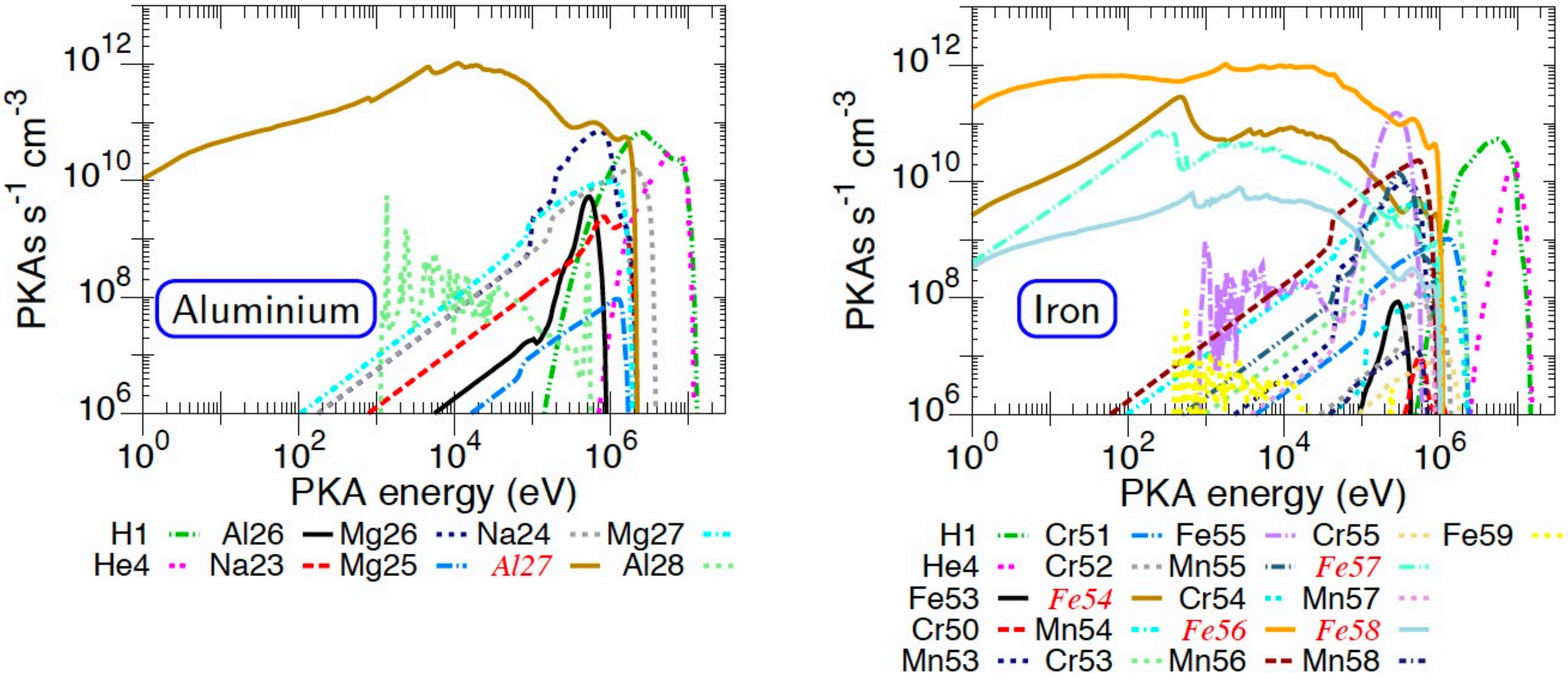
- Pure aluminum (100% ^{27}Al) transmuted residual elements and emitted particle PKA distributions under fusion neutron conditions, right elemental, left isotopic





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

Underlying complexity shown with SPECTRA-PKA

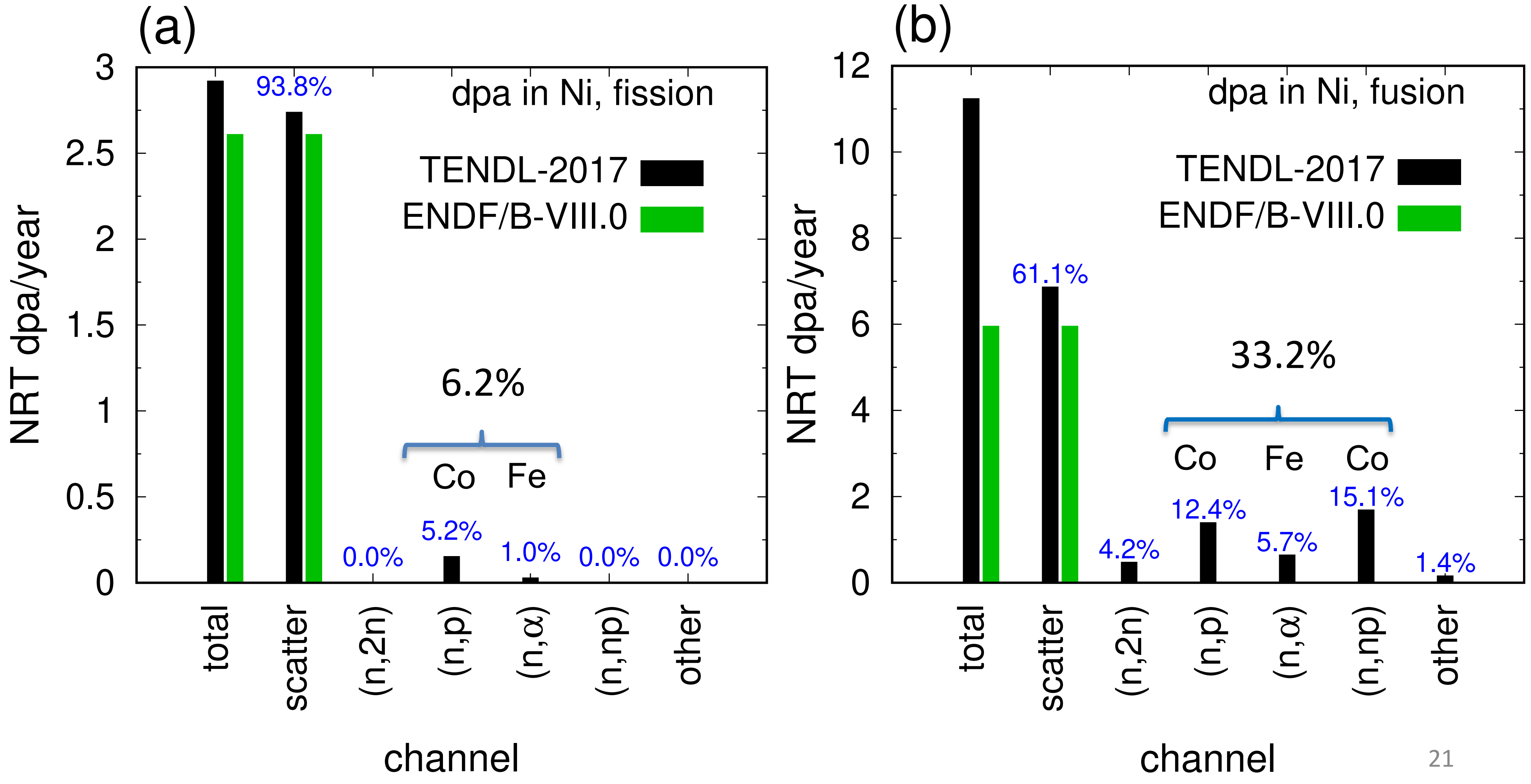


- very complex results with numerous recoils species (isotopes & elements, many radioactive)
- but already hiding some of the per-channel information that is available from the output

https://github.com/fispact/SPECTRA-PKA

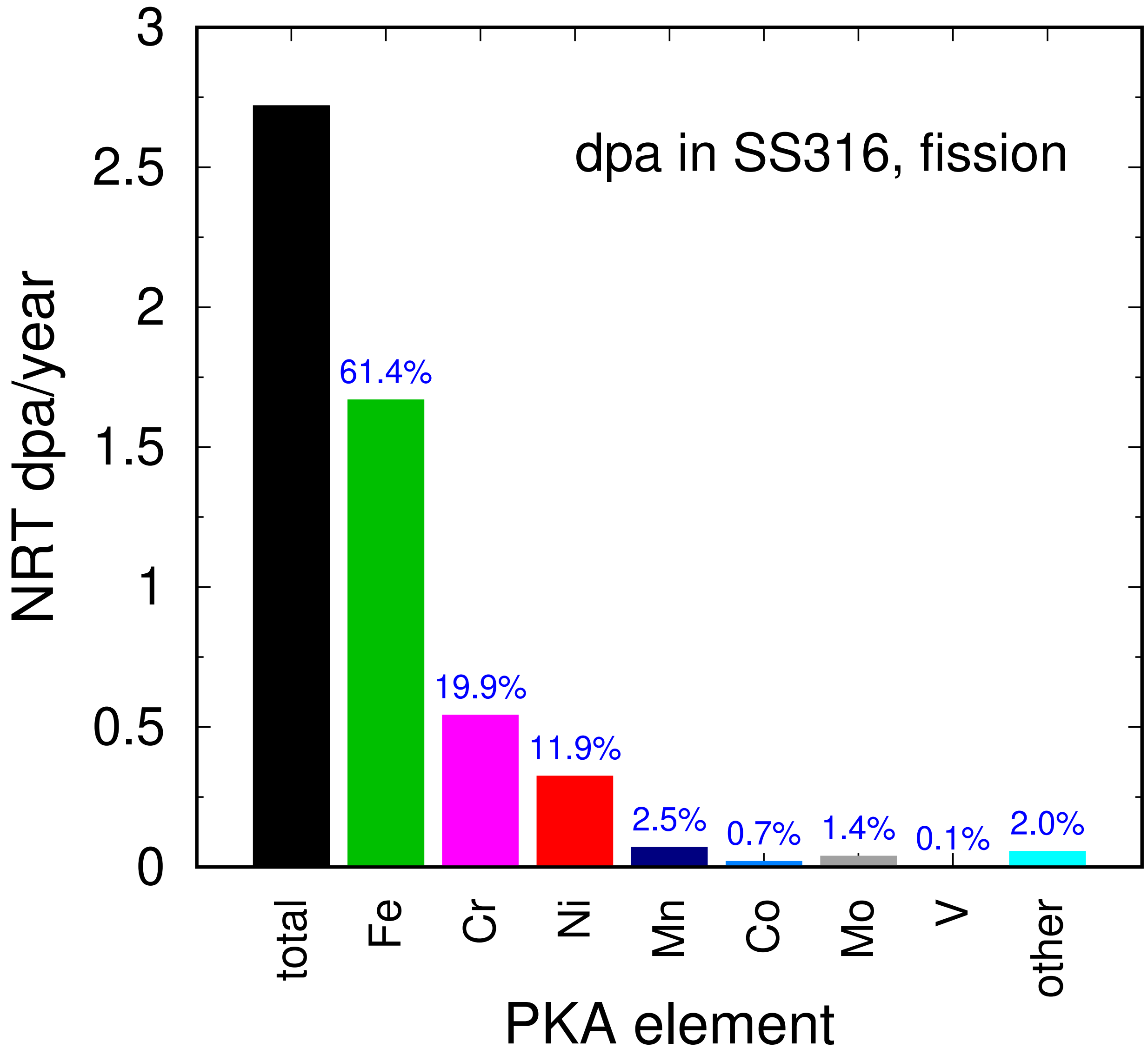
Novel metrics

- 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



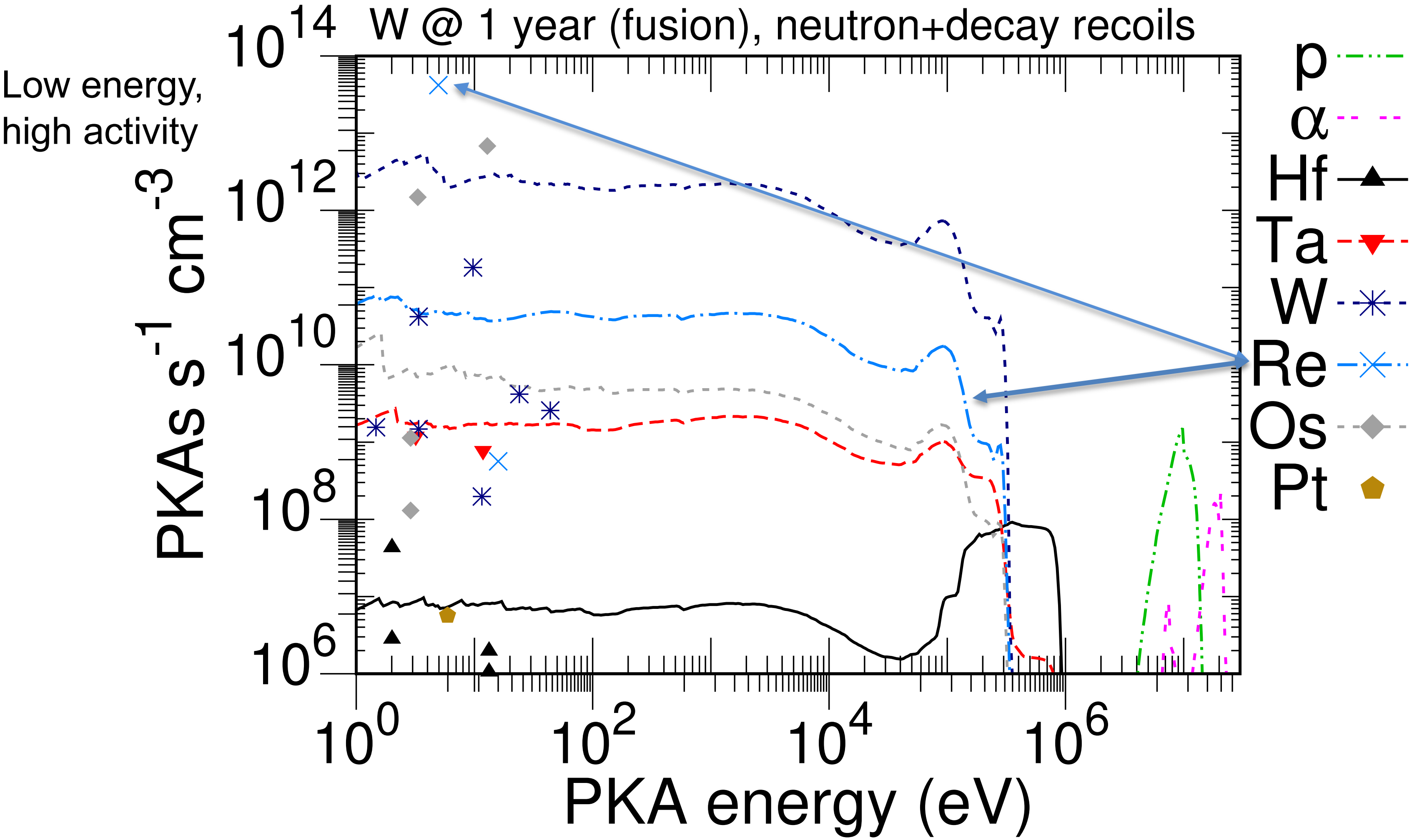
Novel metrics

- Dpa contributions to the total damage rate in SS316 steel under PWR conditions



Novel metrics

- PKA contributions from both transmutant/descendant elements (curves) and decaying species (points) to the PKA distributions in pure tungsten after a 1-year irradiation in a typical fusion neutron field



Key Performance Indicators

- Good interaction with the Accelerator Simulation and Theoretical Modelling of Radiation Effects SMoRE-II CRP from NAPC physics section
- MiMES 2019 - Materials in Nuclear Energy system October 6-10, new conference created to serve the fission reactor materials community that grew out of, and supplants, biennial symposia held at the TMS meeting (Microstructure Processes in Irradiated Materials – MPIM) and the ANS meeting (Nuclear Fuel and Structural Materials – NFSM)
- M&C - August 25-29 2019, International Conference on Mathematics and Computational Methods Applied to Nuclear Sciences and Engineering

Key Performance Indicators

- Results that could not be achieved
  - ICTP-IAEA Workshop, Trieste, Spring 2022

  "Radiation Damage in Nuclear Systems: from Bohr to Young", the postponed 2020 event had 175 applicants, selected 54

  - Consensus across the physical societies: Nuclear, Atomic-molecular, Material sciences and Engineering

Impact/Relevance and Recommendations

- Impact:

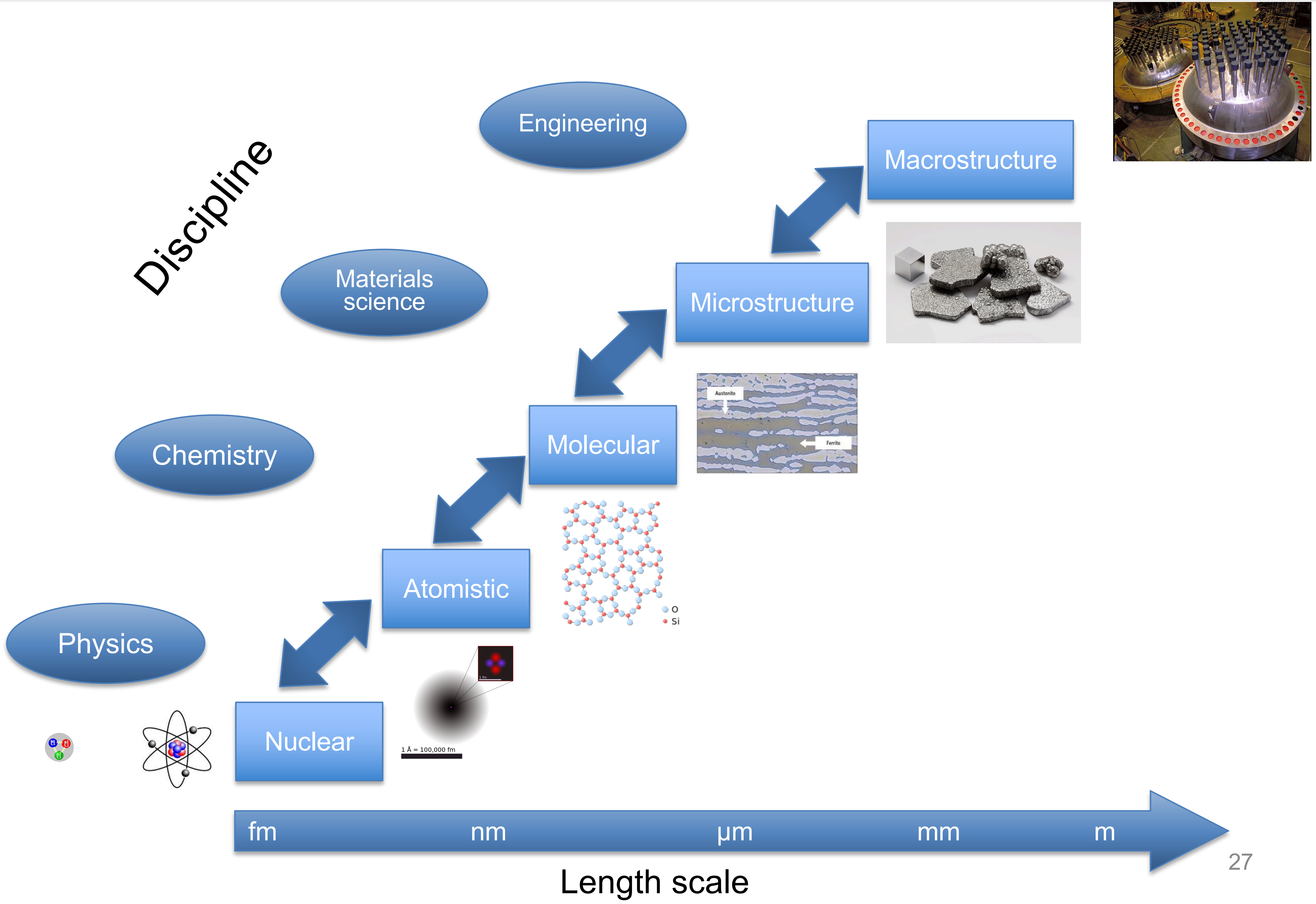
Significant impact on our understanding of radiation damage beyond the traditional iron-based-fission applications

- Relevance

The CRP allowed to clean-up the R&D, established new, better practices able to serve novel applications; advanced fission, accelerator, space, fusion, etc.

- Recommendation
    - Worth planning ahead for the multi scale-physic developments; workshop organised with the Physics section; Virtual event 12-16 July 2021, ICTP Trieste in 2022
    - CM on on nuclear radiation heat and particle's energy productions; Autumn 2021

Multi-scales modelling



Discipline

Engineering

Materials science

Chemistry

Physics

Macrostructure

Microstructure

Molecular

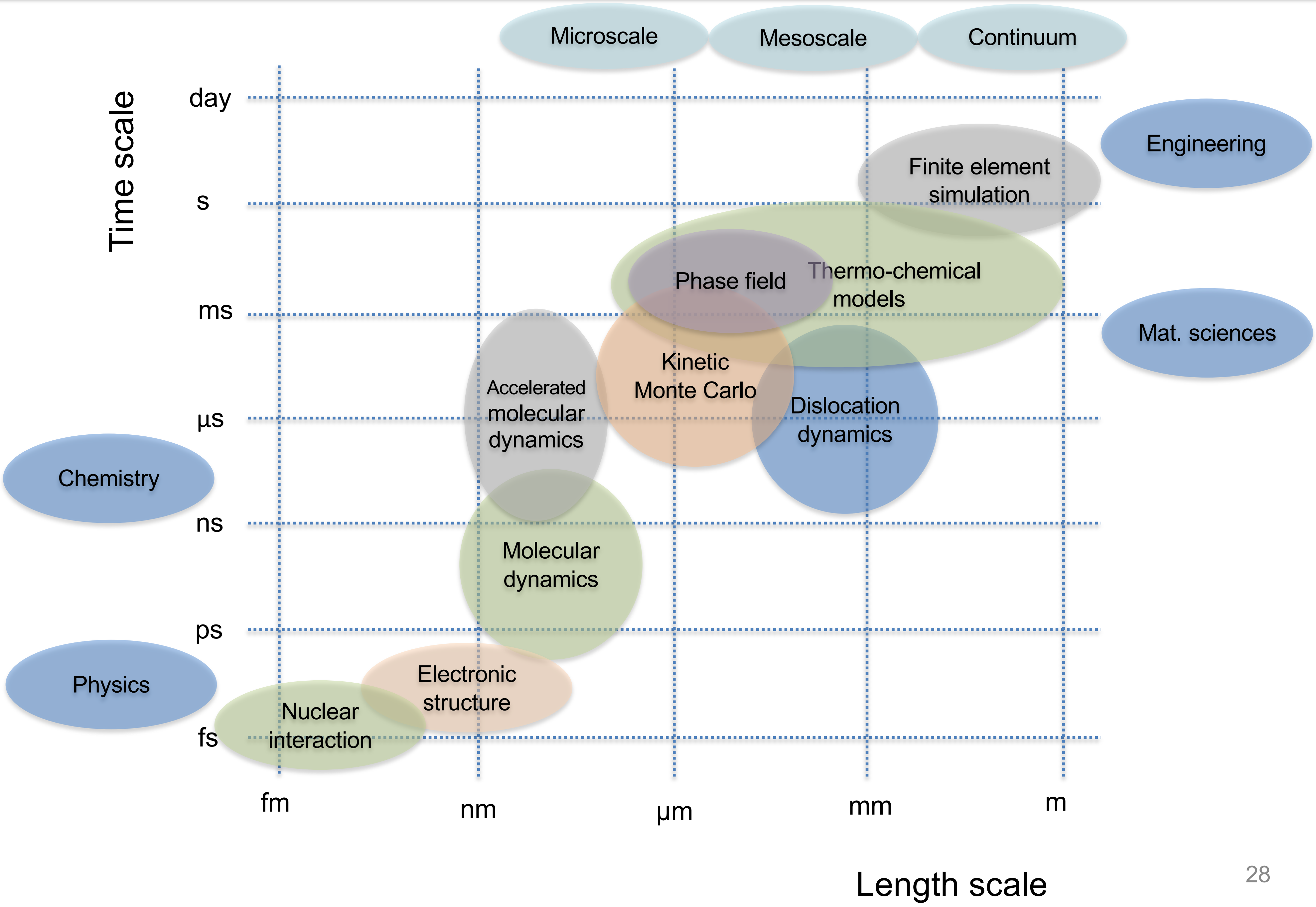
Atomistic

Nuclear

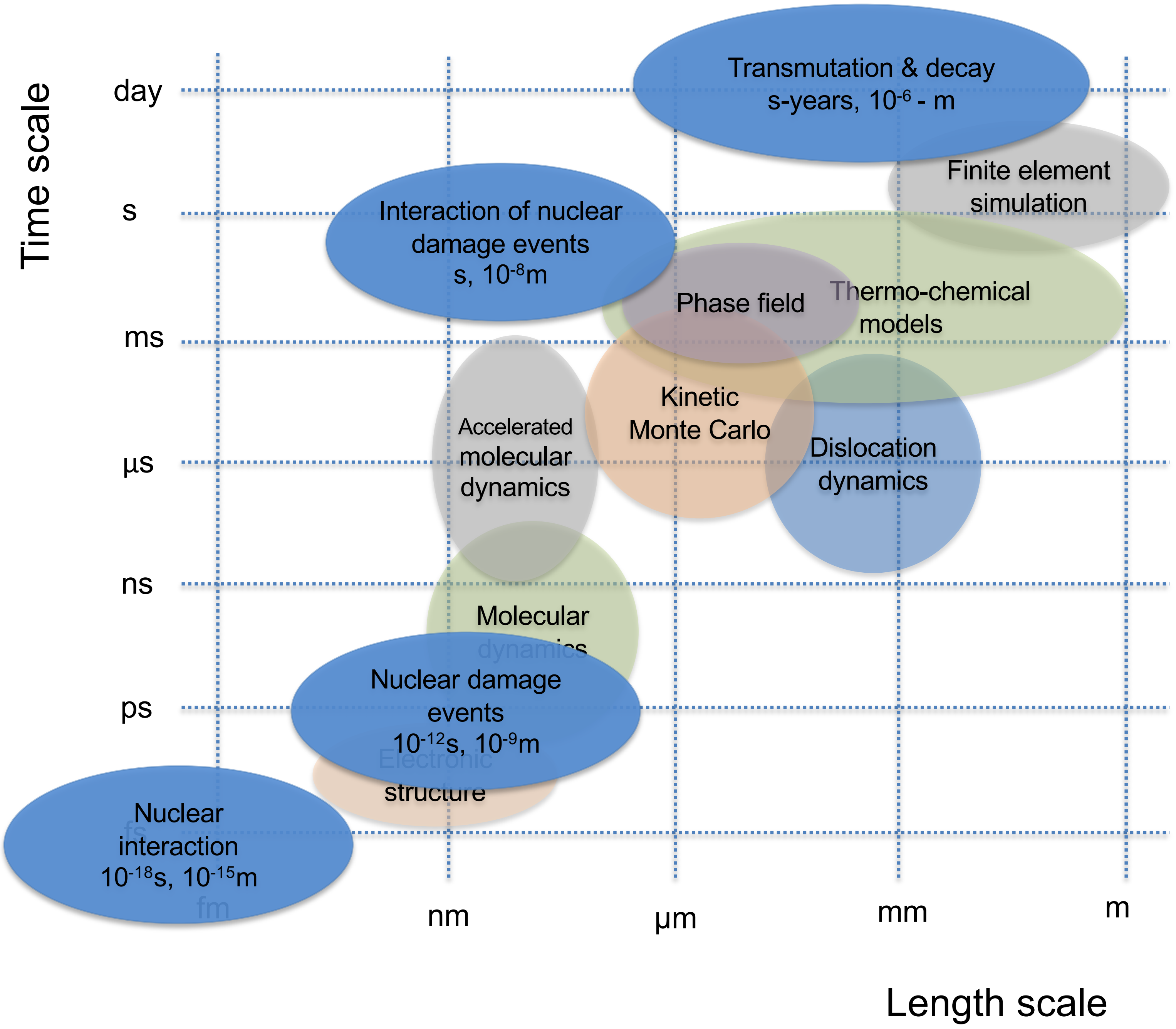
fm nm µm mm m

Length scale

Multi-scales modelling



Nuclear inputs to multi-scales modelling



Conclusions

- Multiscale modelling of materials across the length and times scales requires overcoming the borders between the disciplines for a seamless integration of the models on different length scales into one coherent multi-scale modelling framework (After D.G. Pettifor, 1991)
- A third scale exist: matter state, temperature scale
- Modelling difficulties are not so much with components or atoms but in-between

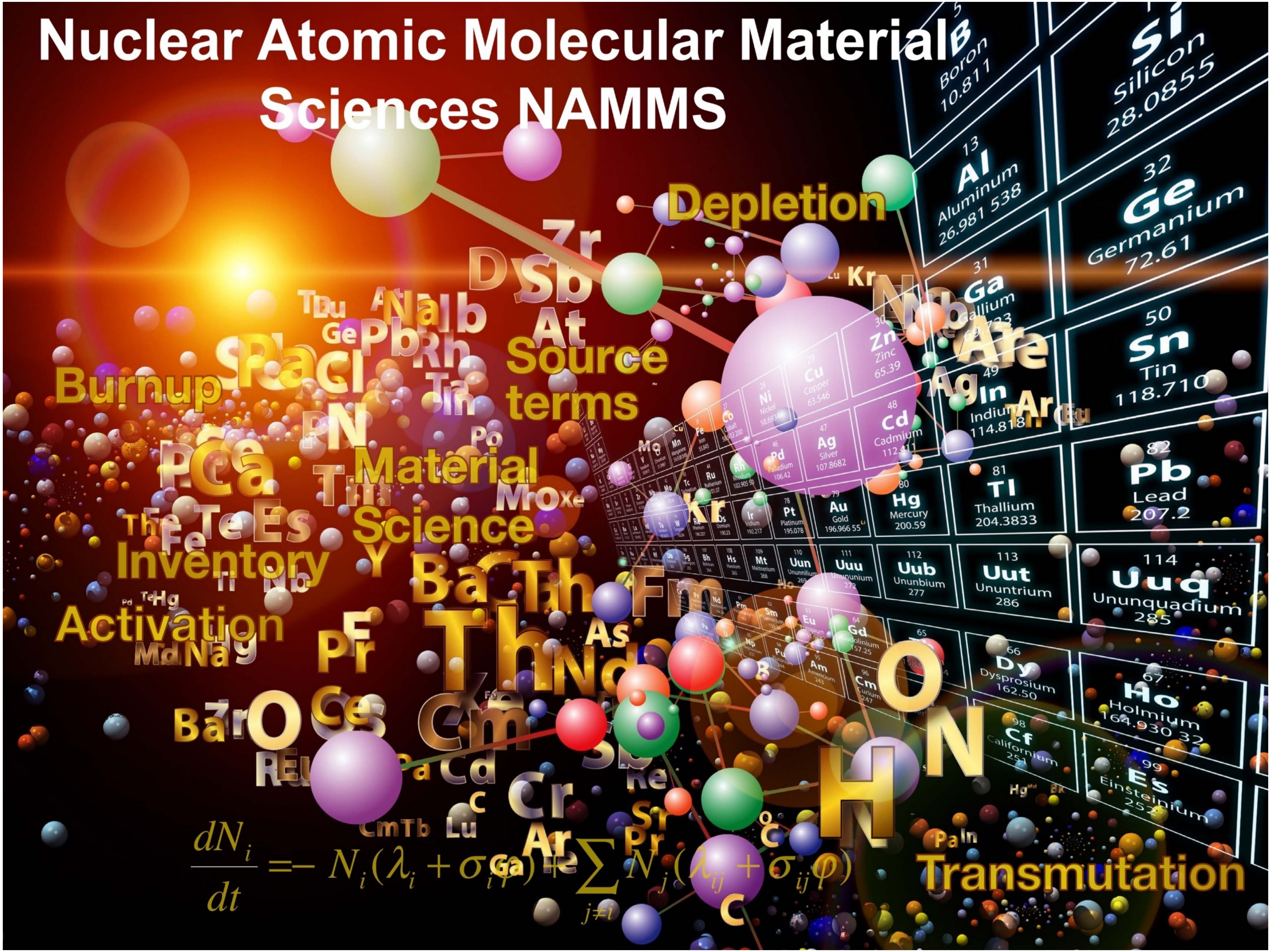
Conclusions

- Progress in data provision at the nuclear scale, assuming that the general purpose nuclear data file are fit to the tasks (of sufficient completeness to capture all relevant processes particularly at high energy), is a step forward in the proper understanding of material defect metrics induced by radiation but this is very small step with regard to the seamless integration of the models across the length (nm - µm - mm - m) and time (ps - µs - ms - s) scales into one coherent modelling framework.

Conclusions

- Fundamentally, the CRP leads to the conclusion that a simple integral measure such as dpa (NRT, arc, or other) is not sufficient, even though it may be a good first order estimate, to fully capture the damage metrics from complex irradiation.
- More substantial methodologies and algorithms from the nuclear-reaction space to the molecular-material ones must be included in complete plant and material modelling.

Nuclear Atomic Molecular Material Sciences NAMMS



$$\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_i\varphi) + \sum_{j\neq i} N_j(\lambda_{ij} + \sigma_{ij}\varphi)$$