DPA modeling in the PHITS code

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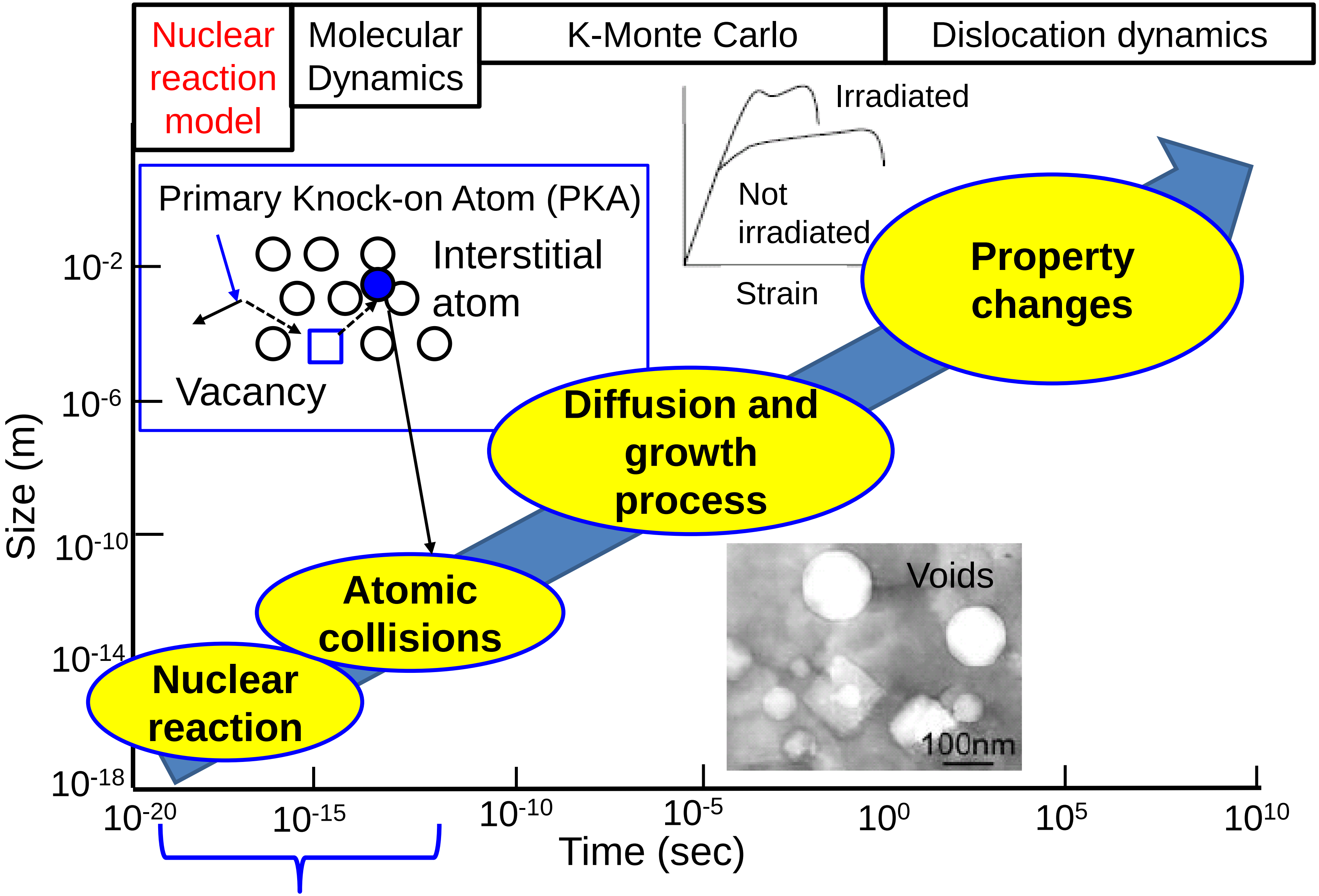
Scale on total irradiation effect



This work deals with the nuclear reaction and the approximation of displacement damage, which are the initial stages of damage.

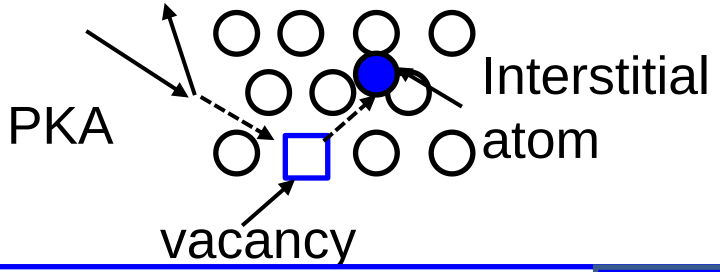
Microscopic effects on material

DPA: average number of displaced atoms per atom of a material

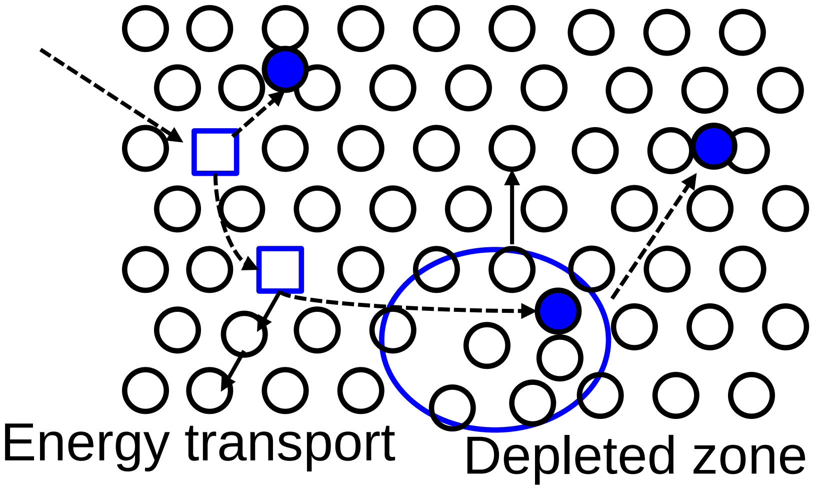
DPA= $\sigma_d \phi$

σ_d : **displacement cross-section (m^2)**

ϕ: irradiation fluence (particles/m^2)



Frenkel-pairs causes cascade damage.



"**Cascade damage**" due to subsequent, continuing damage effects

Cascade damage deals with primary damage state only,
i.e. damage produced during first few ps.

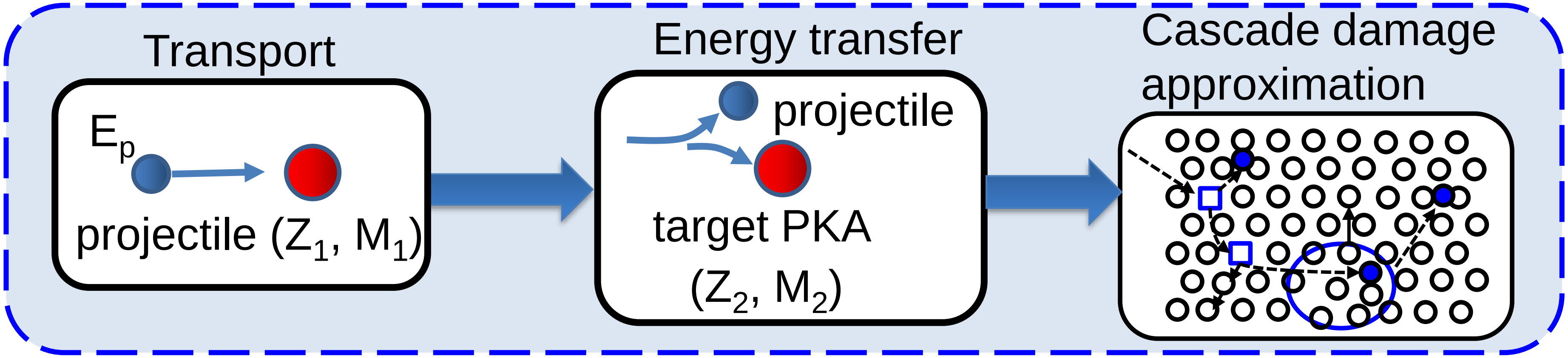
Long-range thermally activated defect motion is excluded.

G. S. Was, Fundamentals of Radiation Materials Science, New York, USA: Springer Press, 2017

Radiation damage model

SRIM (Transport of Ions in Material): Major code for radiation damage

J.F. Ziegler, et al, see www.srim.org



Transport

E_p

projectile (Z_1, M_1)

Energy transfer

projectile

target PKA (Z_2, M_2)

Cascade damage approximation

no treatment of nuclear reaction in high-energy region

no production of PKAs created by the secondary particles

extend to high-energy region

Radiation damage model in advanced Monte Carlo particle transport codes. e.g. PHITS, FLUKA, MARS, MCNP

Contents

Overview of PHITS

Particle and Heavy Ion Transport code System

Development

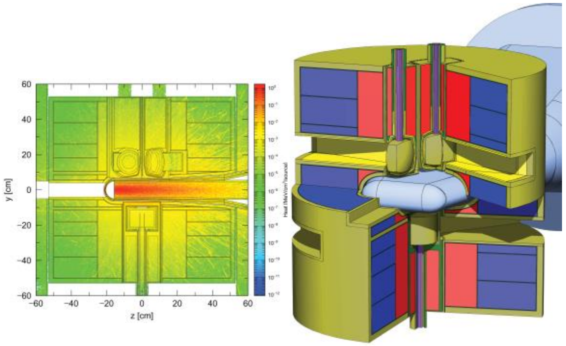
JAEA (Japan), RIST (Japan), KEK (Japan), Technische Universitat Wien(Austria)
RIKEN (Japan), CEA (France), Kyushu Univ. (Japan)

Capability

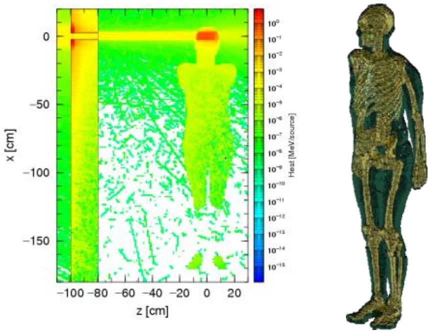
Transport and collision of various particles over wide energy range

in 3D phase space	neutron, proton, meson, baryon electron, photon, heavy ions	up to 100 GeV/u

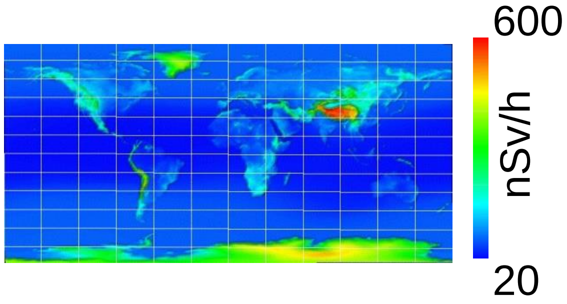
Application Fields



Accelerator Design



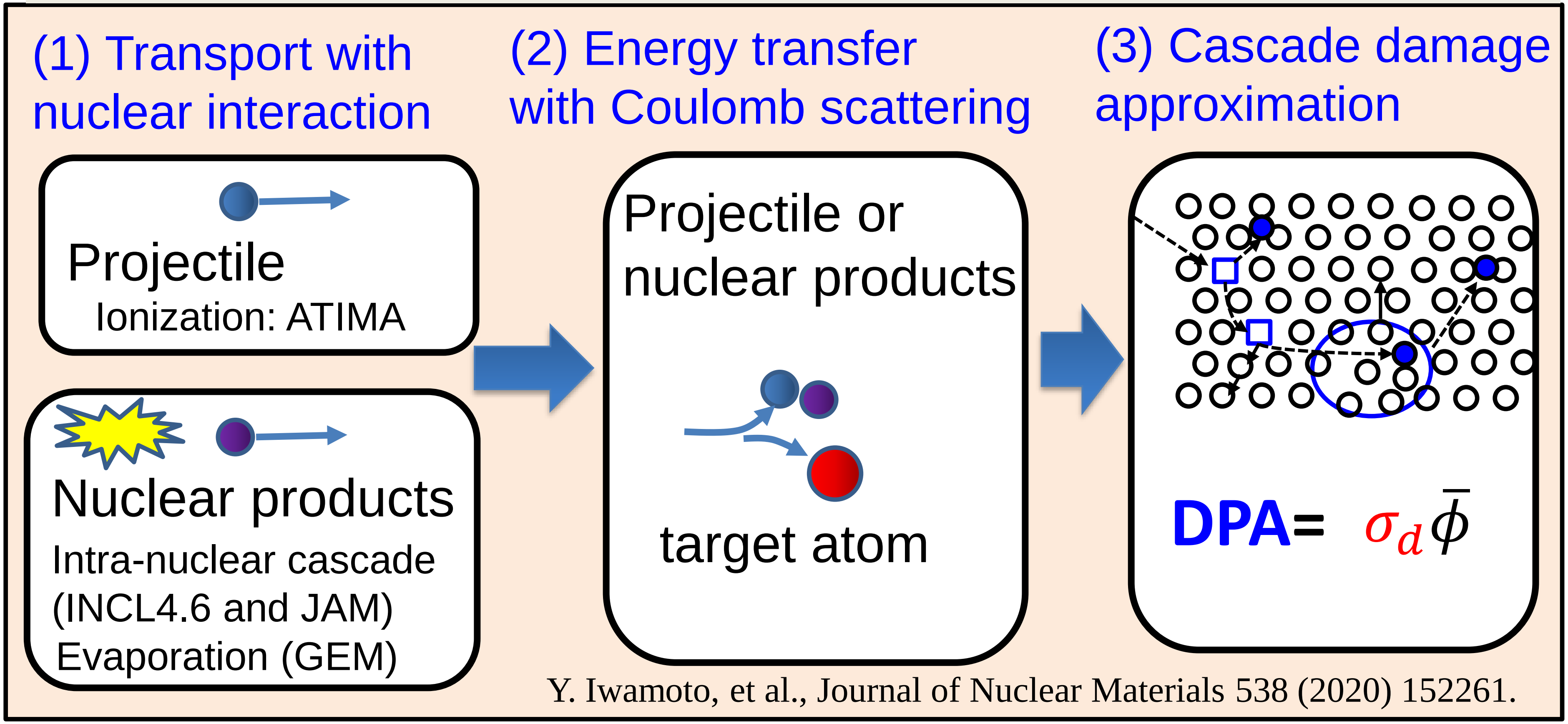
Radiation Therapy



Space Application

T. Sato et al., J. Nucl. Sci. Technol., 61, (2023) 127–135.

DPA calculation method in PHITS



(1) Transport with nuclear interaction

Projectile

Ionization: ATIMA

Nuclear products

Intra-nuclear cascade (INCL4.6 and JAM)

Evaporation (GEM)

(2) Energy transfer with Coulomb scattering

Projectile or nuclear products

target atom

(3) Cascade damage approximation

DPA= $\sigma_d \bar{\phi}$

Y. Iwamoto, et al., Journal of Nuclear Materials 538 (2020) 152261.

DPA cross section

t: dimensionless paramater

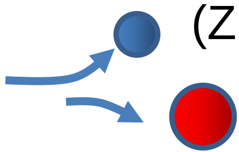
$$\sigma_d = \int_{t_d}^{t_{max}} \frac{d\sigma_{Coul}(t)}{dt} \cdot \frac{0.8T_d(t)}{2E_d} \cdot \zeta_{arc}(t)\, dt$$

Differential Coulomb scattering cross section

Number of displacement

Defect production efficiency

Differential Coulomb scattering cross section



(Z_1, M_1) E_p :kinetic energy of proton or nuclear products

(Z_2, M_2) T: transferred energy to target atom

Classical scattering theory

$$\frac{d\sigma_{Coul}(t)}{dt} = \frac{\pi a_{TF}^2}{2} \frac{f(t^{1/2})}{t^{3/2}}$$

t: dimensionless parameter

$$\equiv \varepsilon^2 \frac{T}{T_{max}}$$

It contains information about energy, emission angle, and distance between nuclei.

T_{max}: maximum T

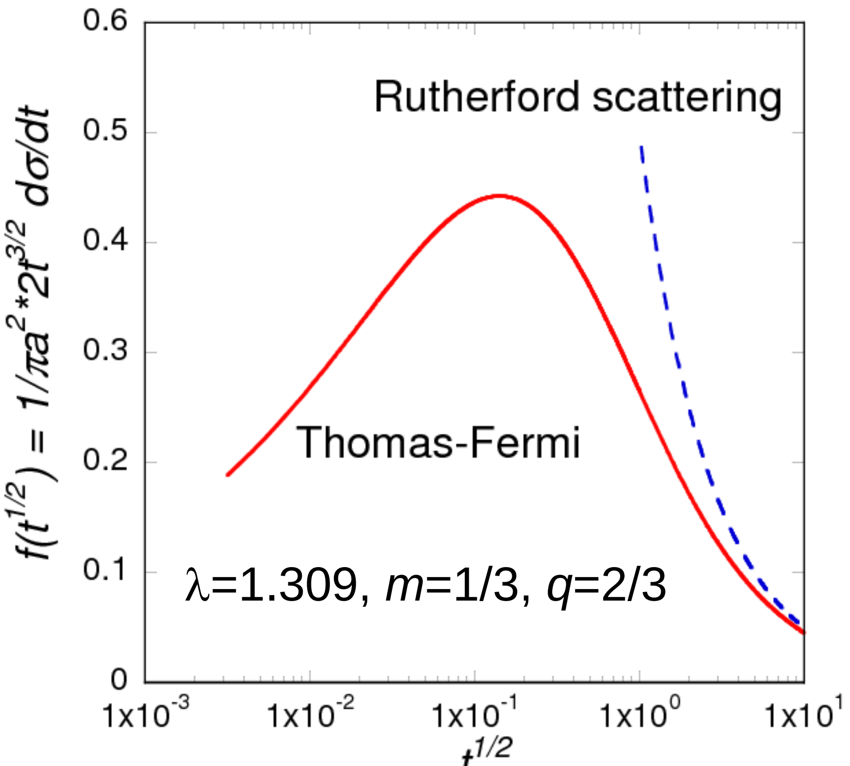
$$= \frac{4M_1M_2E_p}{(M_1+M_2)^2}$$

ε :dimensionless energy

$$= \frac{E_p a_{TF} M_2}{Z_1Z_2e^2(M_1+M_2)}$$

Screening functions:

$$f(t^{1/2}) = \lambda t^{1/2-m}\left[1+(2\lambda t^{1-m})^q\right]^{-1/q}$$



Large t → large T in close collisions

Small t → small T in distant collisions

Number of displaced atoms

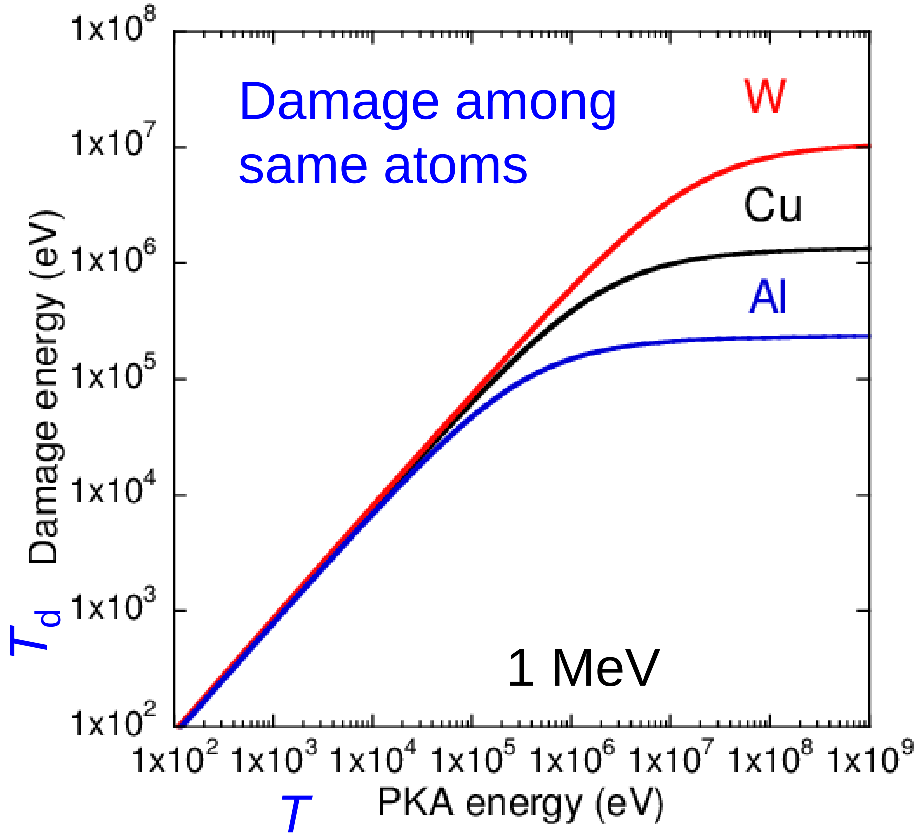
Number of displaced atoms is calculated using phenomenological approach.

$$N_{\mathrm{NRT}} = \frac{0.8T_{\mathrm{d}}}{2E_{\mathrm{d}}}$$

- E_{d} :threshold energy of displaced atom several eV to 100 eV

$$T_{\mathrm{d}} = \frac{1}{1+kg}T$$

- T_{d} :damage energy is the energy available to generate atomic displacements by elastic collisions
- The energy lost in the cascade by electron excitation is subtracted.
- Damage energies are saturated with PKA energy over 1 MeV.



Relationship between PKA energy and damage energy

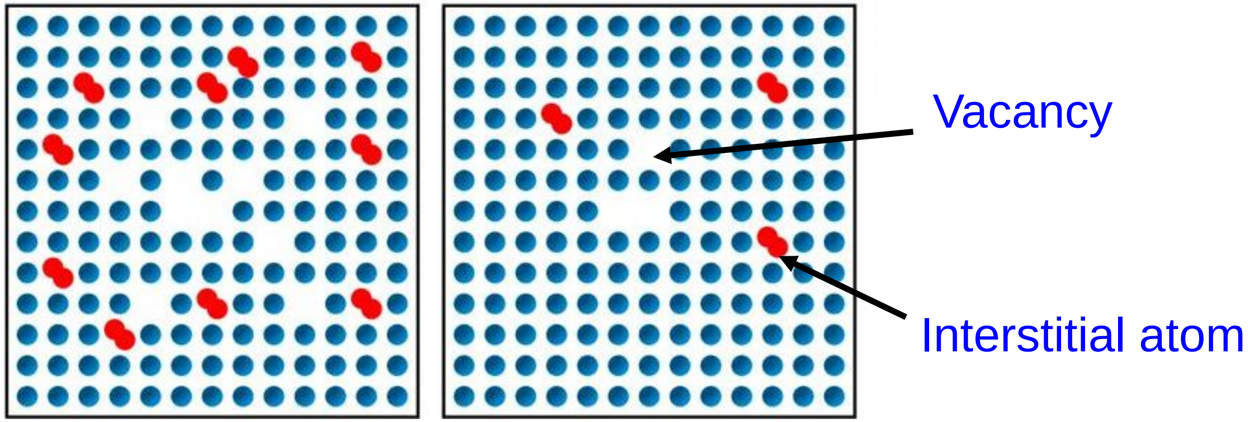
J. Lindhard et al., Dan Vidnsk Selsk Mat Fyf Medd 33:1 (1963).

Next: Defect production efficiency

Athermal recombination correction

Molecular dynamic simulation study

K. Nordlund et al., Nature Comm. 9 (2018) 1084.



NRT damage model

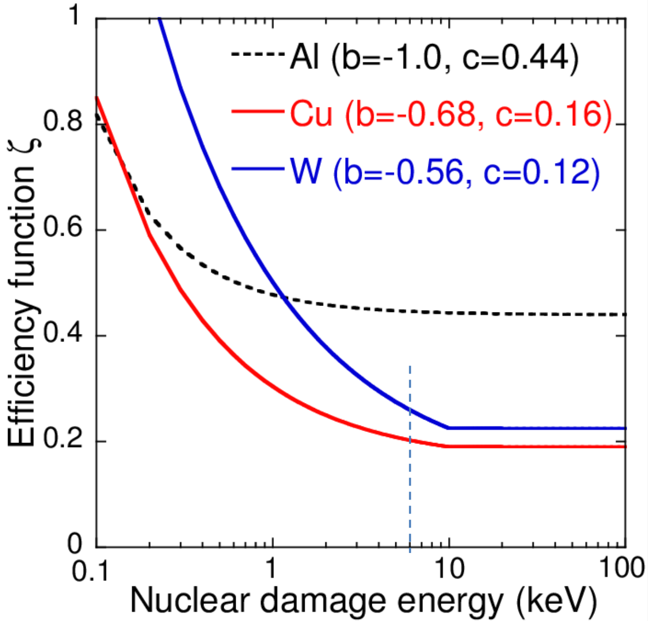
Actual damage production

Schematic illustration of the damage for the case of ~1 keV damage energy in a metal

Actual damage production is addressed by new athermal recombination correction (arc-dpa) using efficiency function based on tabulated parameters.

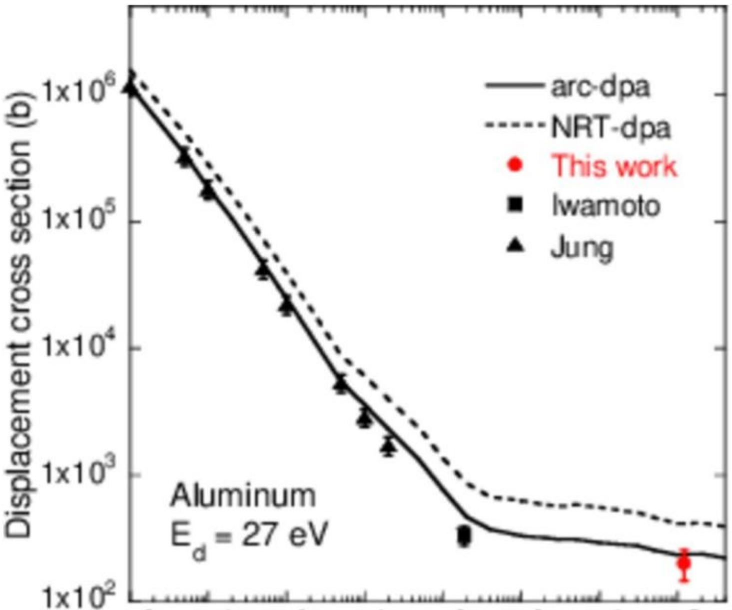
$$N_{\mathrm{arc}}(\varepsilon_{\mathrm{p}}) = \frac{0.8}{2E_{\mathrm{d}}} T_{\mathrm{d}}(\varepsilon_{\mathrm{p}}) \zeta_{arc}(E_{\mathrm{d}})$$

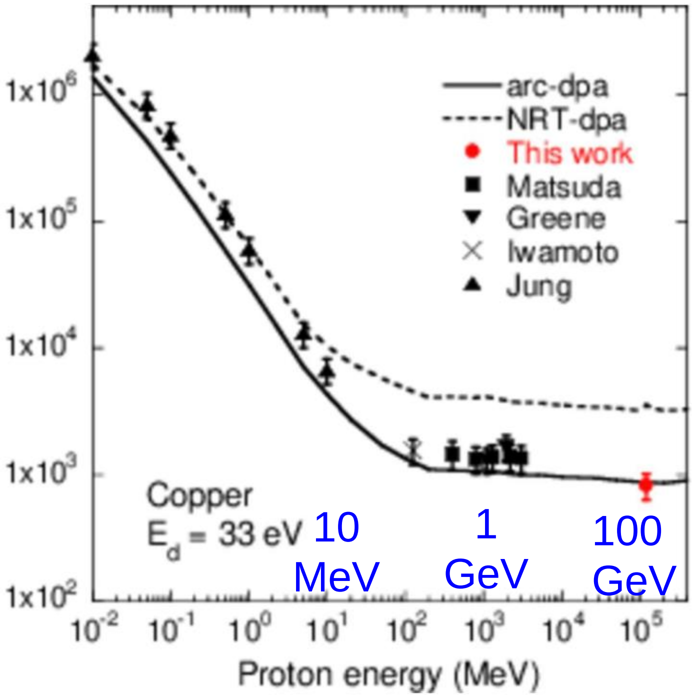
$$\zeta_{arc} = \frac{1-c}{(2\,E_{\mathrm{d}}/0.8)^{b}} E_{\mathrm{d}}^{b} \quad + c$$

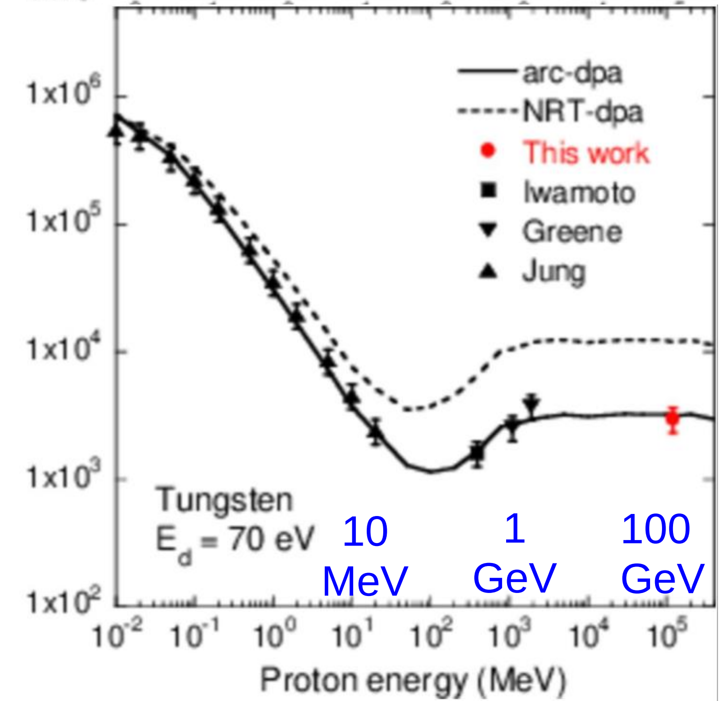


Defect production efficiency

Displacement cross sections for Al, Cu, and W







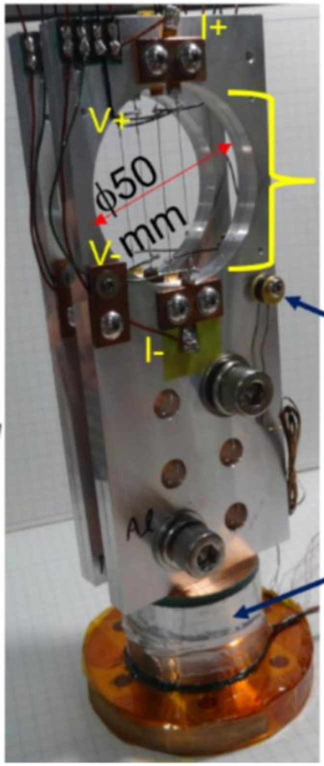
0.1 GeV or more: Contribution of nuclear reaction products. Nuclear damage energy is constant

NRT(standard) is larger than arc-dpa by roughly a factor of 3.

Red points: 120 GeV proton irradiation on metals at cryogenic temperature

Y. Iwamoto et al., Nucl. Instrum. Meth. B, 557 (2024) 165543.

120 GeV proton expt. at FNAL



Al, Cu, Nb, and W wire samples with 0.25 mm diameter

Cernox resistance thermometer

Electrical heater with 24 Ω resistance

Experimental data: **Damage rate at cryogenic temperature**.

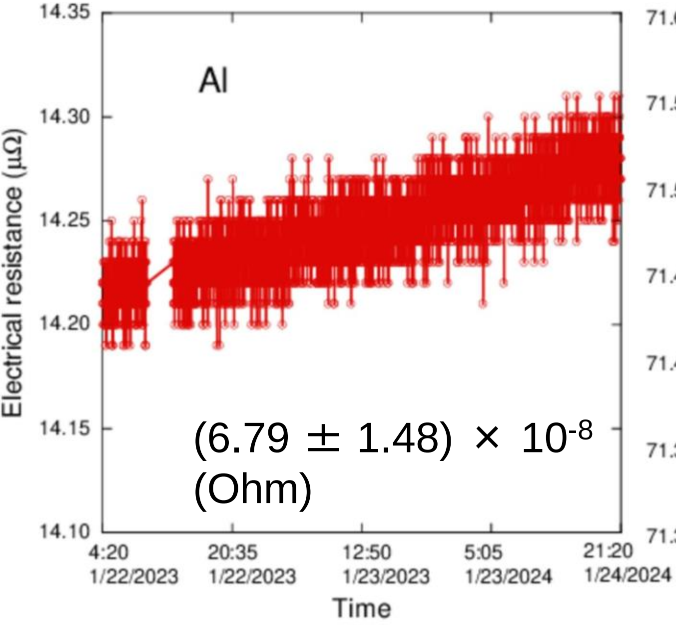
$$\sigma_{\exp} = \frac{1}{\rho_{FP}} \boxed{\frac{\Delta\rho_{metal}}{\phi}}$$

$\Delta\rho_{metal}$: Resistivity increase due to defect (Ωm)

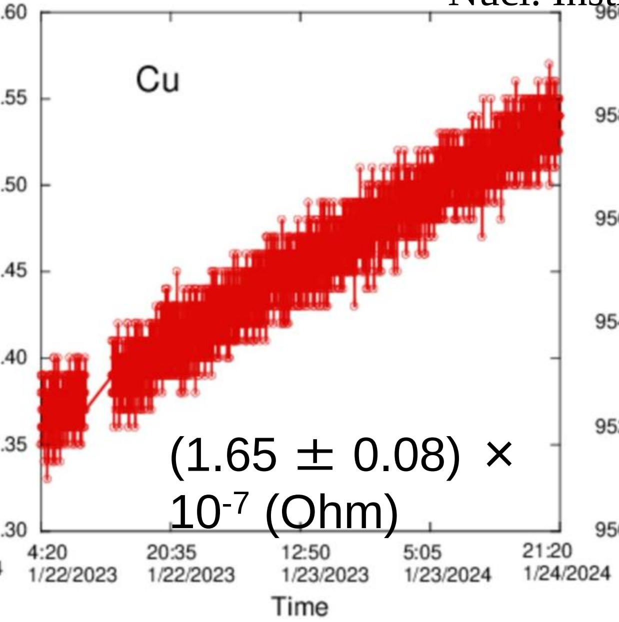
Φ: Beam fluence ($1/m^2$)

ρ_{FP}: Electrical resistivity per Frenkel-pair (Ωm)

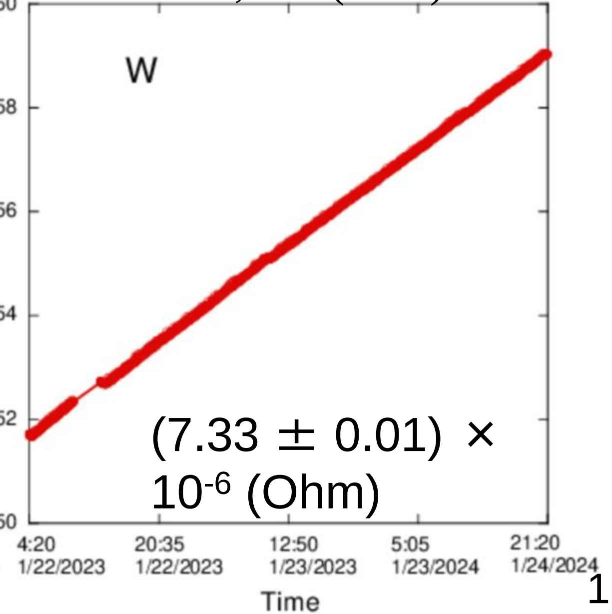
Nucl. Instrum. Meth. B, 557 (2024) 165543.



$(6.79 \pm 1.48) \times 10^{-8}$ (Ohm)



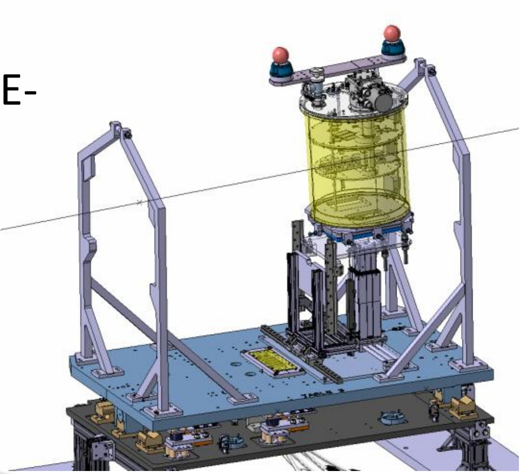
$(1.65 \pm 0.08) \times 10^{-7}$ (Ohm)



$(7.33 \pm 0.01) \times 10^{-6}$ (Ohm)

Ep 440 GeV at HiRadMat CERN (plan)

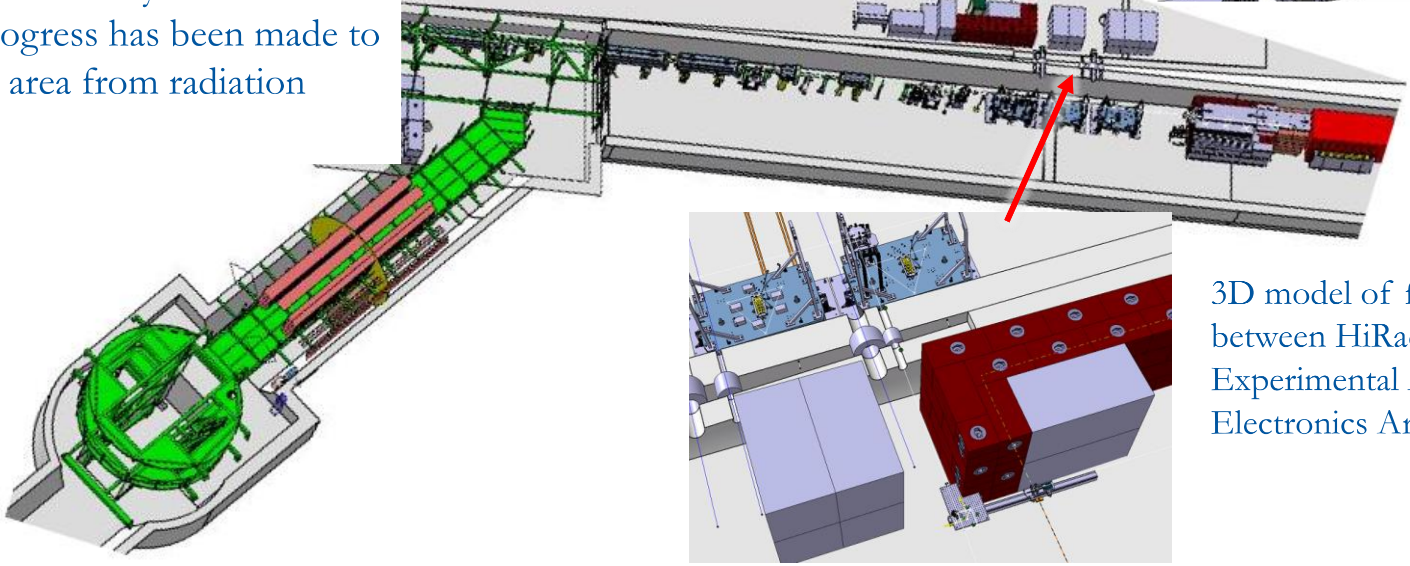
Borrowing vac. chamber and cryocooler from MPE-CB group, using at HiRadMat



Irradiation Area

TT61

HiRadMat has dedicated feed-throughs into an adjacent tunnel (TT61) where additional electronic and measurement systems can be added. Progress has been made to shield this area from radiation effects.



3D model of feed-through between HiRadMat Experimental Area and Electronics Area.

12 ARIES 20-Dec-18 5th RaDIATE Collaboration Meeting F. Harden EN Engineering Department CERN

Experiment planned in May 2025

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Intercomparison of DPA calculations in target materials

Benchmarking against dpa value in the target is not the case for not directly observable value.

Intercomparison of radiation damage calculations in target materials at proton accelerator facilities using various Monte Carlo particle transport codes

Proceedings of 15th Workshop on Shielding aspects of Accelerators, Targets, and Irradiation Facilities (SATIF-15) (Internet), p.25 - 34, 2022/09

PHITS: Yosuke Iwamoto, Lan Yao (JAEA)

FLUKA: Francesco Cerutti, Robert Froeschl, Tommaso Lorenzon, Francesc Salvat Pujol, and Vasilis Vlachoudis (CERN)

MCNP: Çelik Yurdunaz (SCK/CEN)

Calculation condition

Output: depth distribution of DPA in the target.

1) Neutron source with the ^{9}Be(p,n) reaction

Beam: 30 MeV proton with a radius of 6 cm.
Target: ^{9}Be with a thickness of 5.5 mm, a radius of 6 cm, and 1.85 g/cm^{3}

2) Spallation neutron source in WNR, LANCE

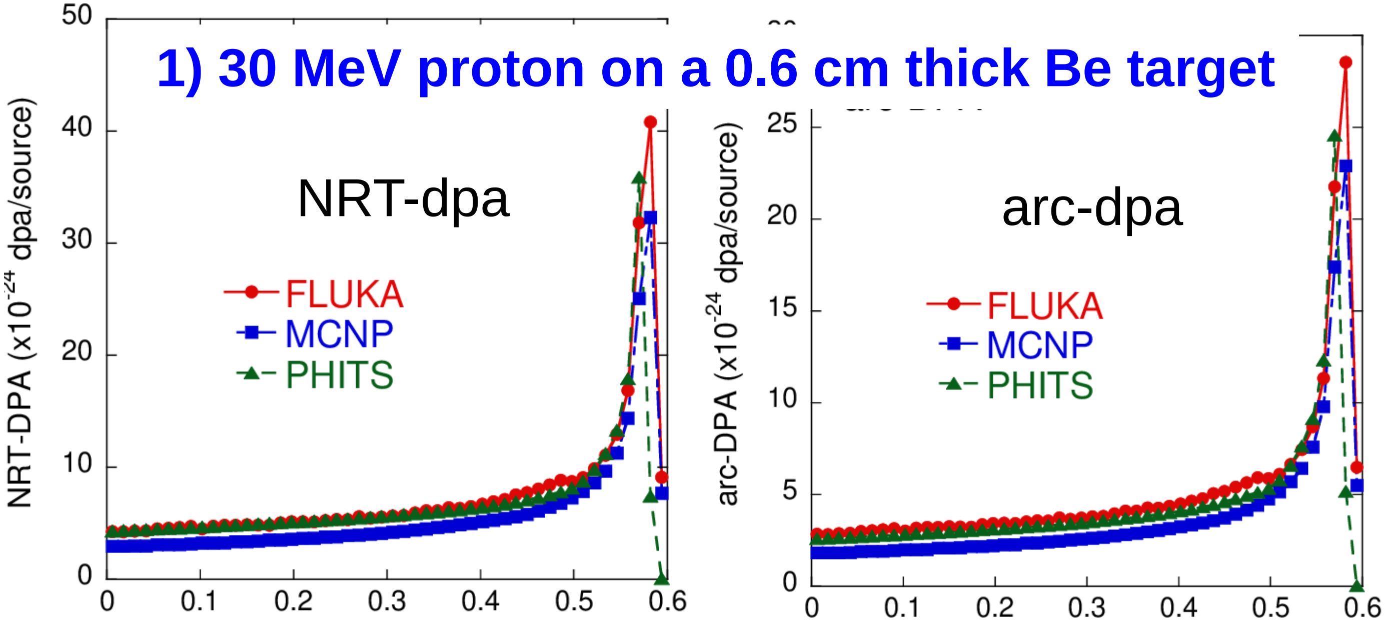
Beam: 800 MeV proton with a radius of 1 cm.
Target: Tungsten with a thickness of 20 cm, a radius of 1 cm, and 19.3 g/cm^{3}

3) Neutrino source target in J-PARC

Beam: 30 GeV proton with 1 cm radius
Target: Carbon with a 90 cm thickness, 1 cm radius, and 2.2 g/cm^{3}

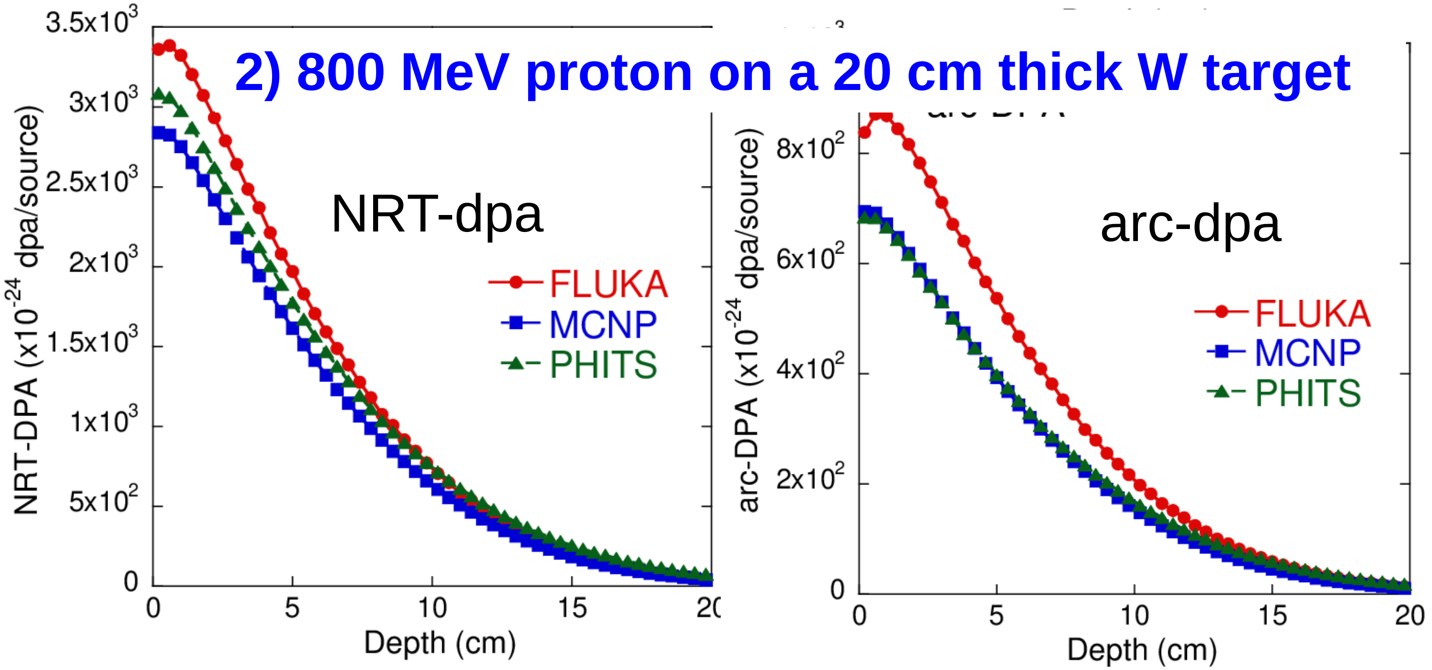
Results: case 1) and case 2)

1) 30 MeV proton on a 0.6 cm thick Be target



Equivalent to Bragg's peak.

2) 800 MeV proton on a 20 cm thick W target

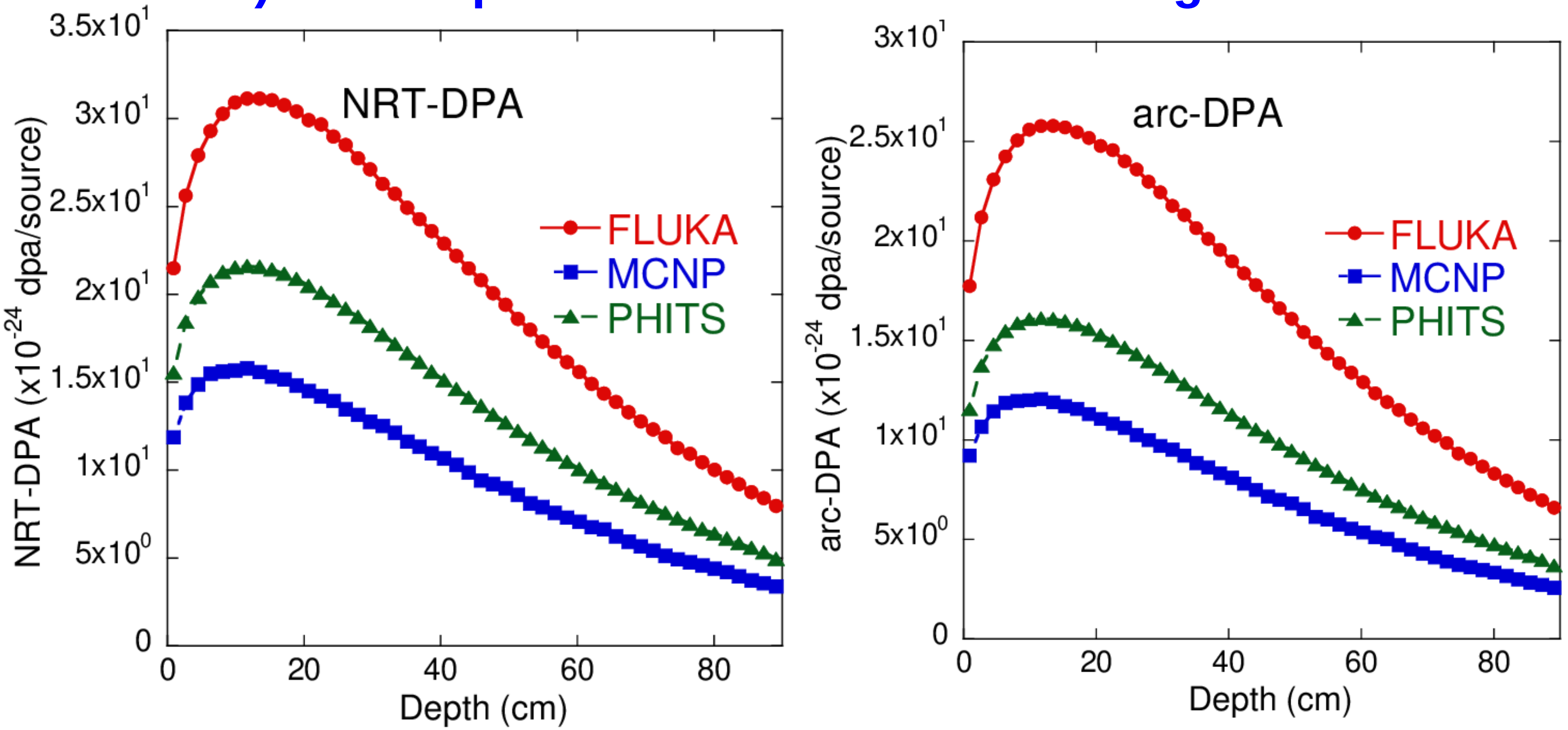


The contribution of secondary particles becomes larger with the incident proton energy above around 100 MeV.

All codes agree within a factor of 2.

Results: Case 3)

3) 30 GeV proton on a 90 cm thick C target



With increasing the energy of the incident protons, the contribution of secondary particles becomes larger at a deeper position.

FLUKA is larger than PHITS by a factor of around 1.5 and MCNP by a factor of around 2.

The possible reasons for this are as follows

- Differences in the σ_{disp} of protons, neutrons, and pions
- Lack of σ_{disp} for electrons and photons due to electromagnetic showers (MCNP, PHITS)

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Summary

- DPA modeling has been developed in the PHITS code.

- In the high energy region (> ~100 MeV) for proton beams,
  DPA created by secondaries increase due to nuclear reactions.

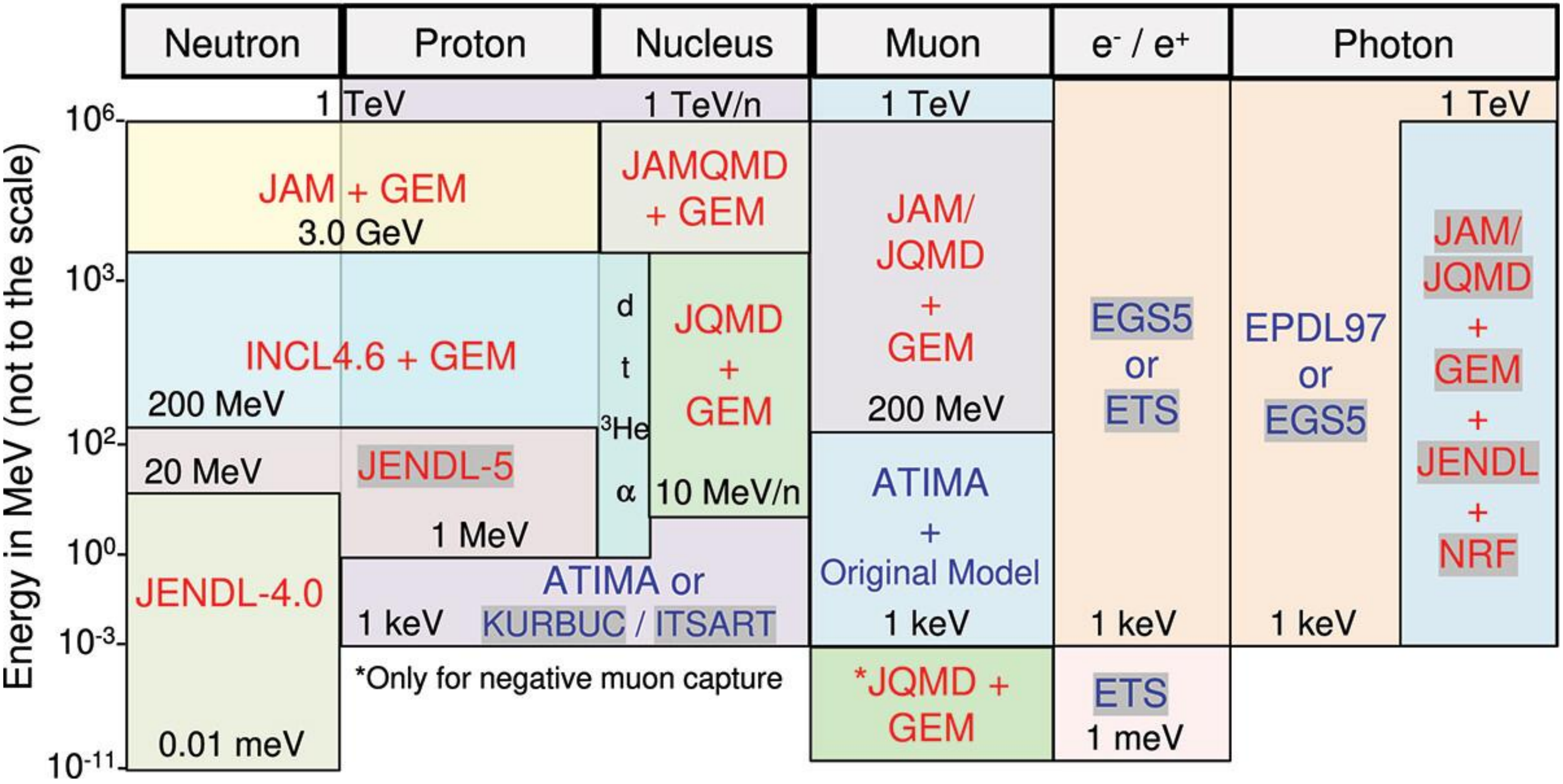
- In comparing the calculated and experimental results for $\sigma_{dpa.}$,
  - ･NRT-dpa (standard) is approximately three times greater than arc dpa.
  - ･Arc dpa reproduces the experimental data well.

- For the comparison of the depth distribution of DPA in thick targets between codes,
  - ･ The difference in the results becomes larger
    at proton energies of 30 GeV or higher.
  - ･ The displacement cross section of all particles
    in the high-energy region needs to be confirmed in the future.

Backup

Red: Nuclear reaction model or library Blue: Atomic interaction model or library

Models and libraries highlighted in gray are not used in the default setting



Displacement cross sections in this work

DPA is calculated by folding displacement cross section with particle spectrum

$$\mathbf{DPA} = \int \sigma_{\mathrm{disp}}(E)\,\emptyset(E)\,dE$$

$\sigma_{\mathrm{disp}}(E)$: **displacement cross section** (barns)

$\emptyset(E)$: Fluence (1/cm^2/source particle)

PHITS3.26 σ_{disp} for neutrons, protons, pion+, and pion- up to 120 GeV were calculated by PHITS.

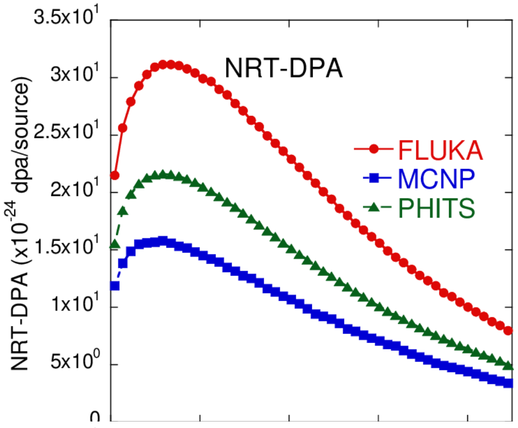
FLUKA4-3.0 σ_{disp} for neutrons, protons, pion+, pion-, others were calculated by FLUKA.

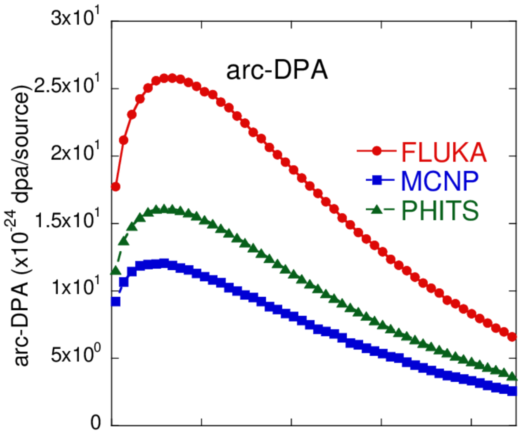
MCNP6 σ_{disp} for neutrons and protons up to 10 GeV were obtained from the following the IAEA database.

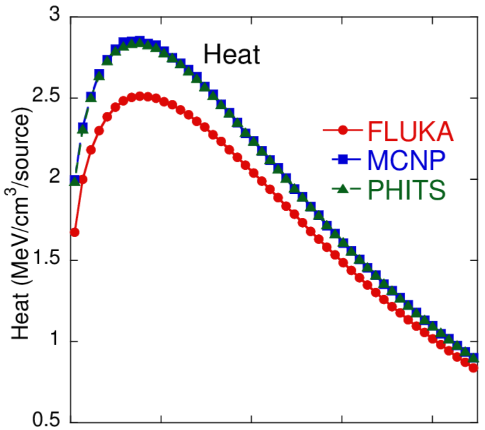
https://www-nds.iaea.org/public/download-endf/DXS/ A.Yu.Konobeyev,et al.

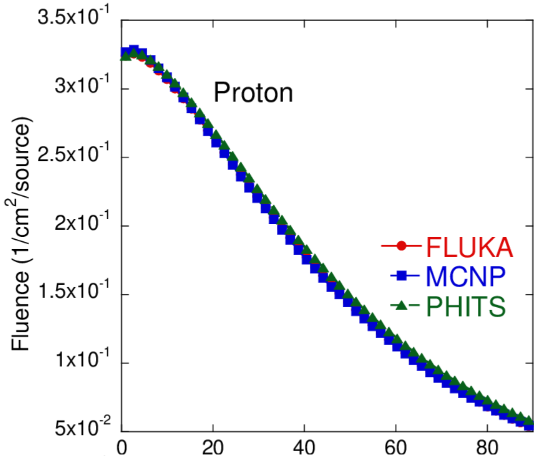
In energies above 10 GeV, σ_{disp} of 10 GeV were adopted.

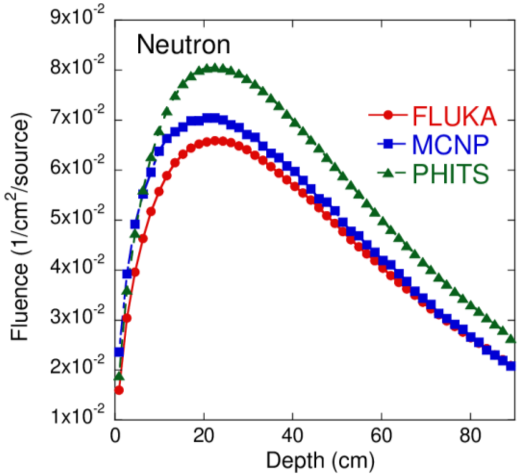
Results 3) 30 GeV proton on a 90 cm thick Graphite

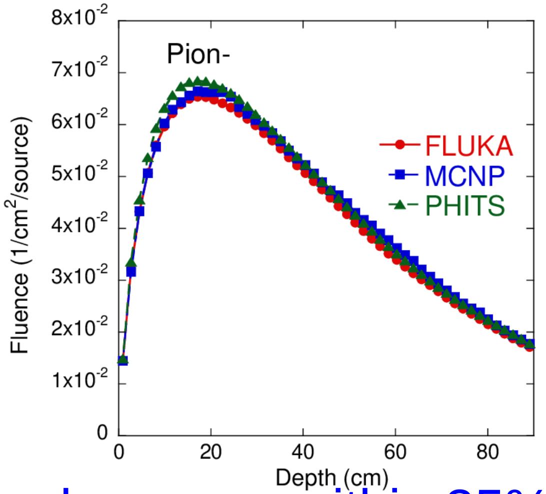


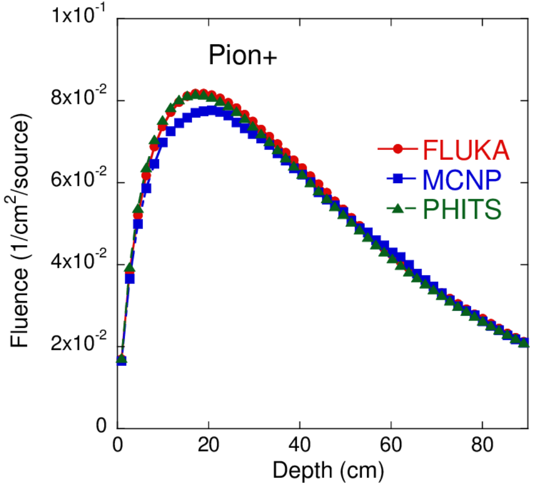












Fluence and heat: All codes agree within 35%.

DPA: FLUKA > PHITS > MCNP.

The possible reasons for this are as follows

1. Differences in the σ_{disp} of protons, neutrons, and pions
2. Lack of pion σ_{disp} (MCNP)
3. Lack of σ_{disp} for electrons and photons due to electromagnetic showers (MCNP, PHITS)