Radiation damage calculation in PHITS

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- Radiation damage model in PHITS
- Radiation damage calculation
  - proton, heavy-ion, neutron incidences
- Example of heat calculations
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Introduction

As the power of proton and heavy-ion accelerators is increasing,
the prediction of the structural damage to materials under irradiation is essential.

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

$$\mathrm{DPA} = \phi t \sigma$$

σ : the **Displacement cross-section**.

ϕt : the irradiation fluence.

For example, 10 dpa means each atom in the material has been displaced from its site within the structural lattice of the material an average of 10 times.

The **Monte Carlo particle transport code systems** have been developed for the radiation shielding design, radiation damage calculation, and so on.

PHITS, MARS, FLUKA, MCNPX…

Introduction ~Overview of PHITS~

Particle and Heavy Ion Transport code System

Development

JAEA (Japan), RIST (Japan), KEK (Japan), Chalmers Univ. Tech. (Sweden)

Capability

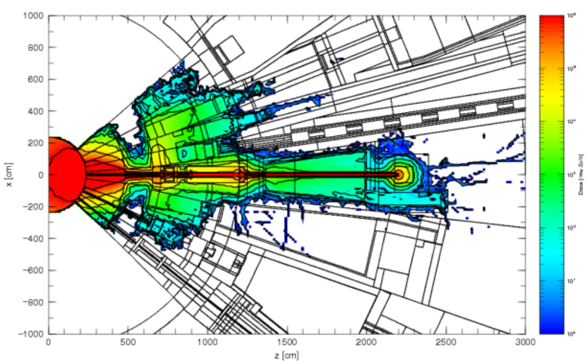
Transport and collision of various particles over wide energy range

in 3D phase space
with magnetic field & gravity

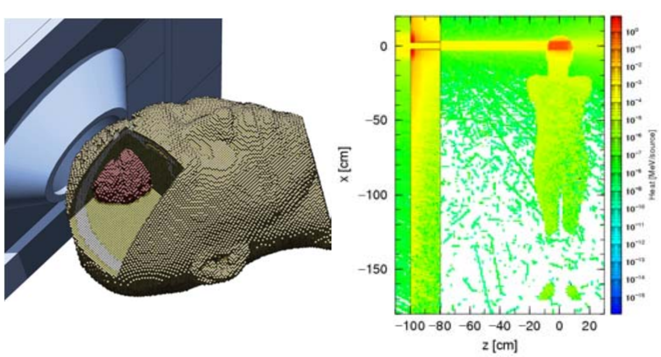
neutron, proton, meson, baryon
electron, photon, heavy ions

up to 100 GeV/n

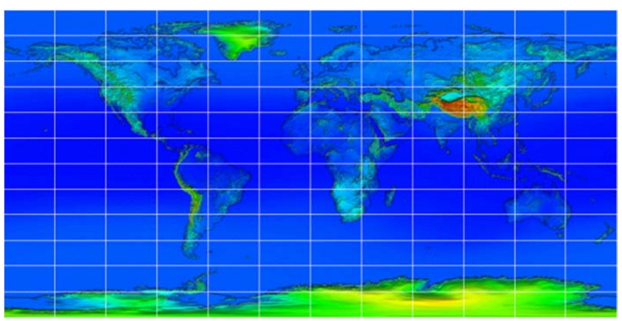
Application Fields



Accelerator Design



Radiation Therapy

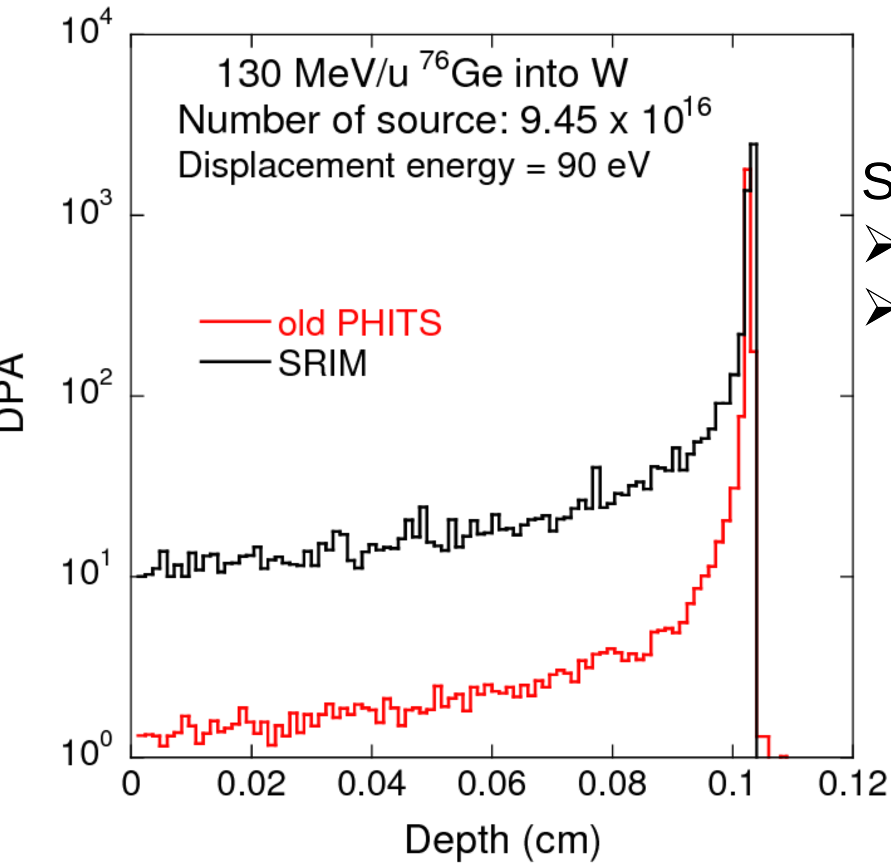


Space Application

http://phits.jaea.go.jp

available from NEA databank

Introduction



➢Comparison old PHITS with SRIM

SRIM is most famous code in radiation damage study.

- ➢ Coulomb scattering is implemented.
- ➢ No nuclear reactions in SRIM.

Coulomb scattering in PHITS was not correct.

Calculated results by old PHITS are much smaller than SRIM one.

Purpose of this study

➢Improvement of radiation damage model

➢Radiation damage calculations using improved PHITS

- Charged particle incidence
- Reactor neutrons and 14 MeV neutrons incidence

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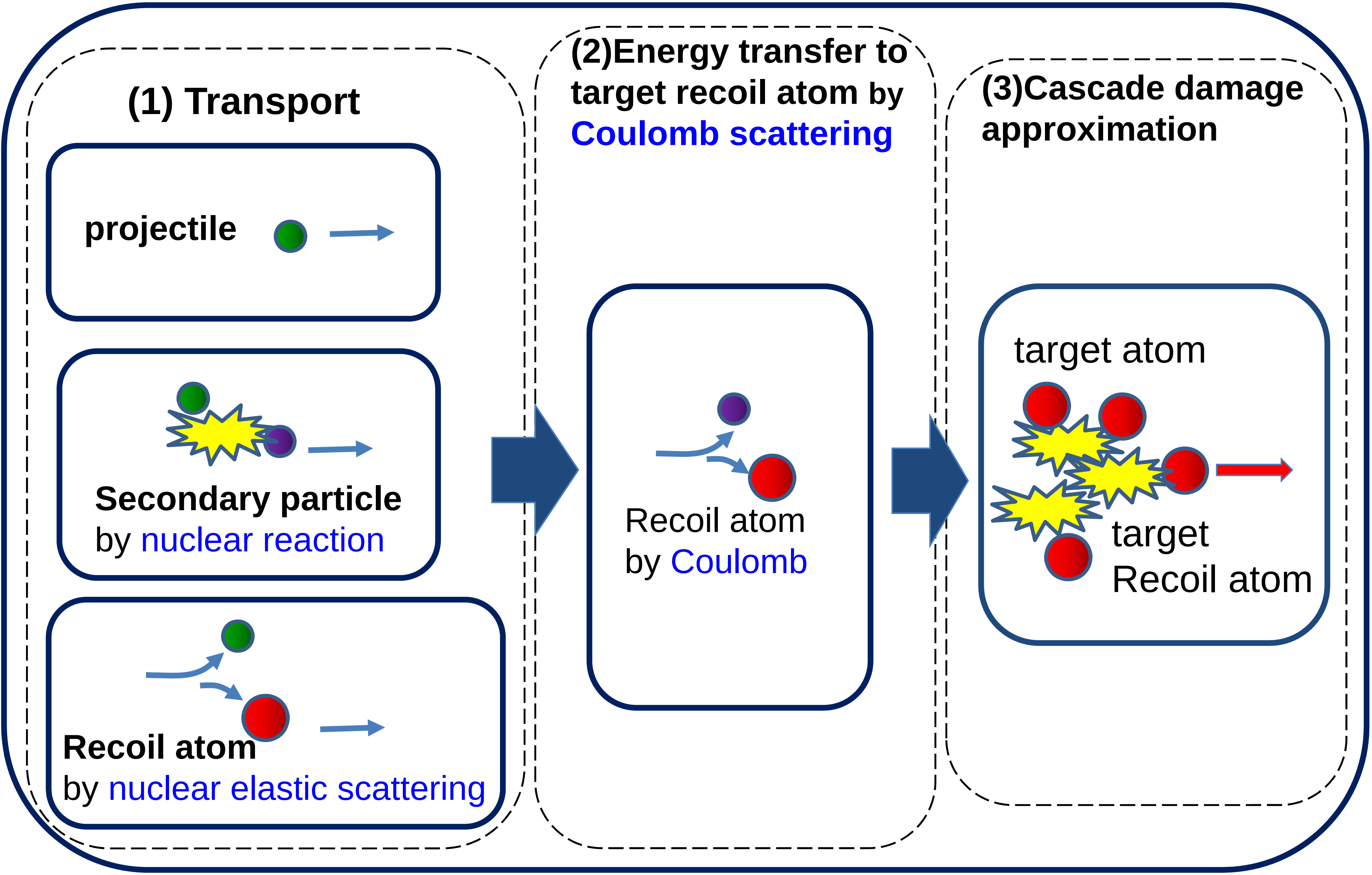
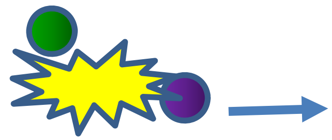
Overview of radiation damage model in PHITS



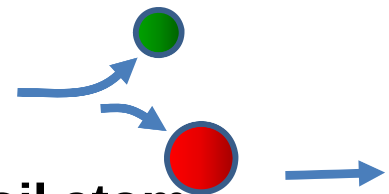
Radiation damage model in PHITS(1)

(1)Transport → (2) Energy transfer to target recoil atom with Coulomb scattering → (3)Cascade damage approximation

projectile



Secondary particle
by nuclear reaction



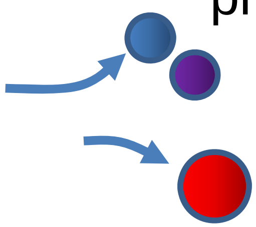
Recoil atom
by nuclear elastic scattering

	Models in PHITS
Collision distance between particles	Total reaction cross section produced by systematic formula
Stopping power dE/dx and ranges	SPAR based on Bethe formula
Nuclear reaction E>20MeV, all particles	Intra-nuclear cascade model
E<20MeV, low energy neutron	Nuclear data, event generator

Radiation damage model in PHITS(2)

(1)Transport → Improvement: **(2) Energy transfer to target recoil atom with Coulomb scattering** → (3)Cascade damage approximation

Coulomb elastic scattering



E_p :kinetic energy, (Z_1, M_1)

T: transferred energy, (Z_2, M_2)

The Coulomb scattering part, which alone leads to the deflection of the projectile and secondary, is described by classical scattering theory using the screening functions $f(t^{1/2})$.

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

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

Thomas-Fermi λ=1.309, *m*=1/3, *q*=2/3

- Dimensionless collision parameter *t*= $\varepsilon^2 \frac{T}{T_{\text{max}}} = \varepsilon^2 sin^2\left(\frac{\theta_c}{2}\right)$

Dimensionless energy *ε*= $E_p a_{TF} M_2 / Z_1 Z_2 e^2 (M_1 + M_2)$

- Transferred energy from projectile and secondary to target atom $T = T_{\text{max}} \times \frac{t}{\varepsilon_{\text{p}}^2}$

Radiation damage model in PHITS(3)

(1)Transport → (2) Energy transfer to target recoil atom with Coulomb scattering → **(3)Cascade damage approximation** (Improvement)

Damage energy

$$\sigma_{\mathrm{damage}} = \int_{t_{\mathrm{d}}}^{t_{\max}} \frac{d\sigma_{\mathrm{scat.}}}{dt} \cdot \frac{0.8}{2 \cdot T_{\mathrm{d}}} \frac{T}{1 + k_{\mathrm{cascade}} \cdot g(\varepsilon)} dt$$

Number of defects developed by NRT

M.J. Norgett, M.T. Robinson and I.M. Torrens: Nucl. Engineering and Design, 33, 50 (1975).

Integrating using dimensionless collision parameter *t*

→ Number of defects developed by NRT

T_d: the value of the threshold displacement energy. 30 eV for Cu and 90 eV for W

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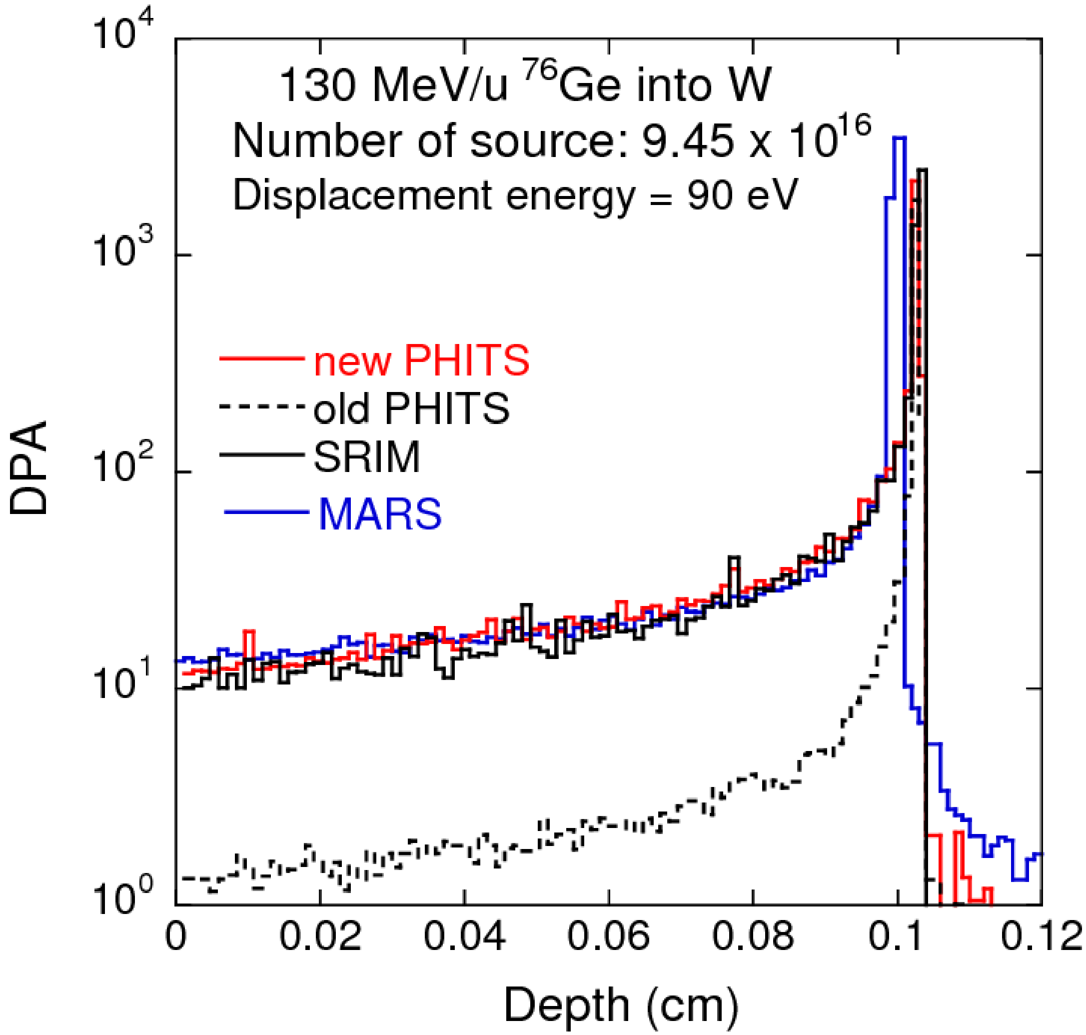
Comparison new PHITS with other code



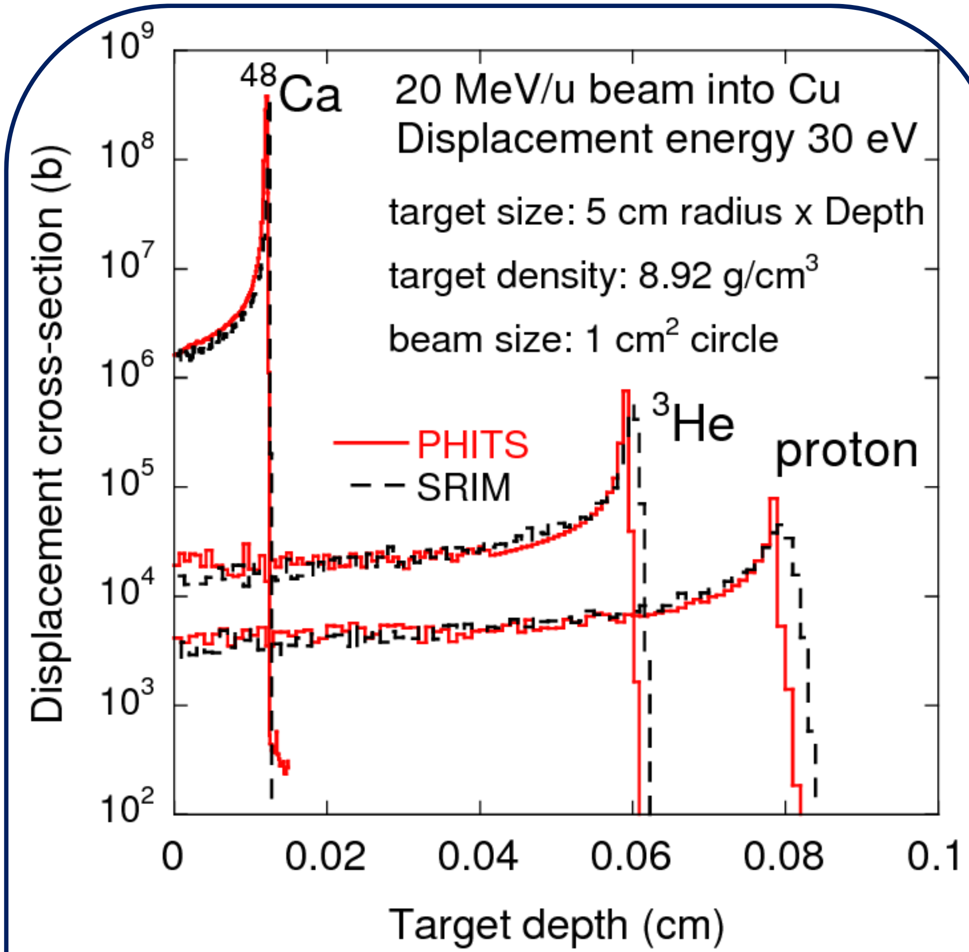
DPA=$\phi\, t\, \sigma_{damage}$

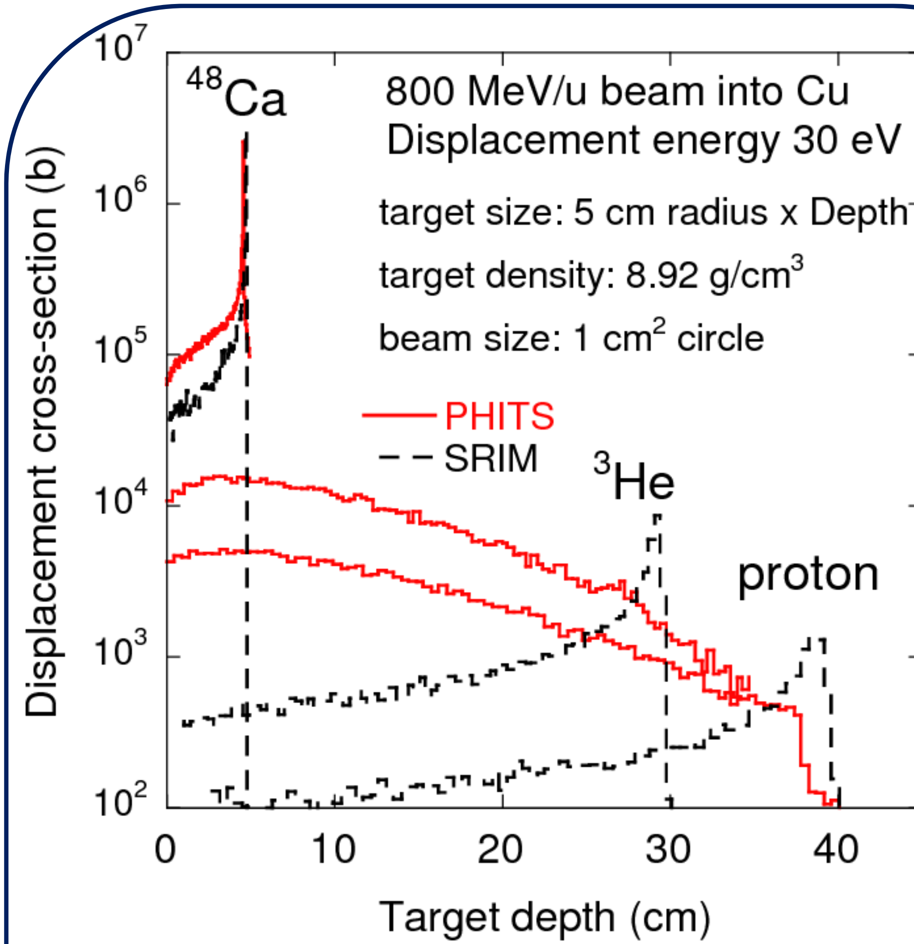
MARS result:
Courtesy Nikolai Mokhov

MARS also folds with Coulomb scattering and nuclear reaction.

➢Agreement is very good except for old PHITS.

Displacement cross section to target depth



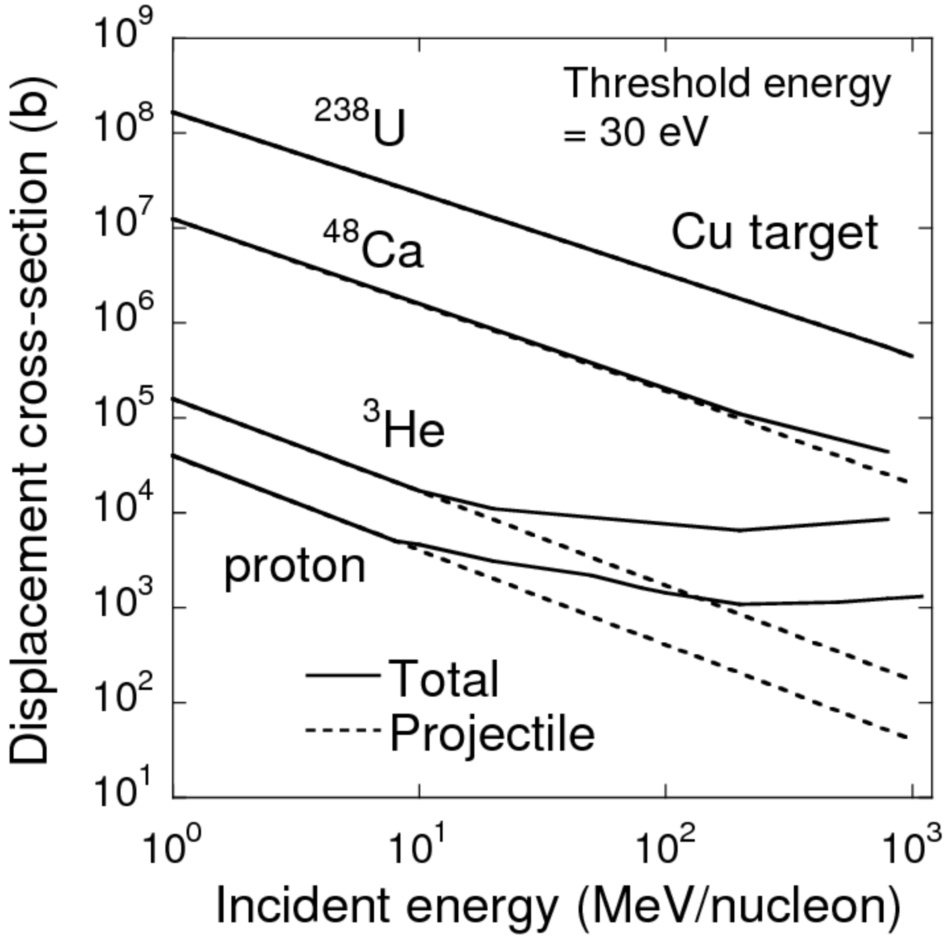


- The beam range in materials is less than the mean free path for nuclear reactions.

- Nuclear reactions occur before stopping range is reached.
- The curves show the characteristics of well-developed hadronic cascades.

◆Damage calculations without nuclear reaction lead to sever underestimation where projectile energy is high enough to create nuclear reactions.

Displacement cross section using PHITS for proton, ^{3}He, ^{48}Ca and ^{238}U



Dash line:
Radiation damage produced by recoil target atom created by projectile.

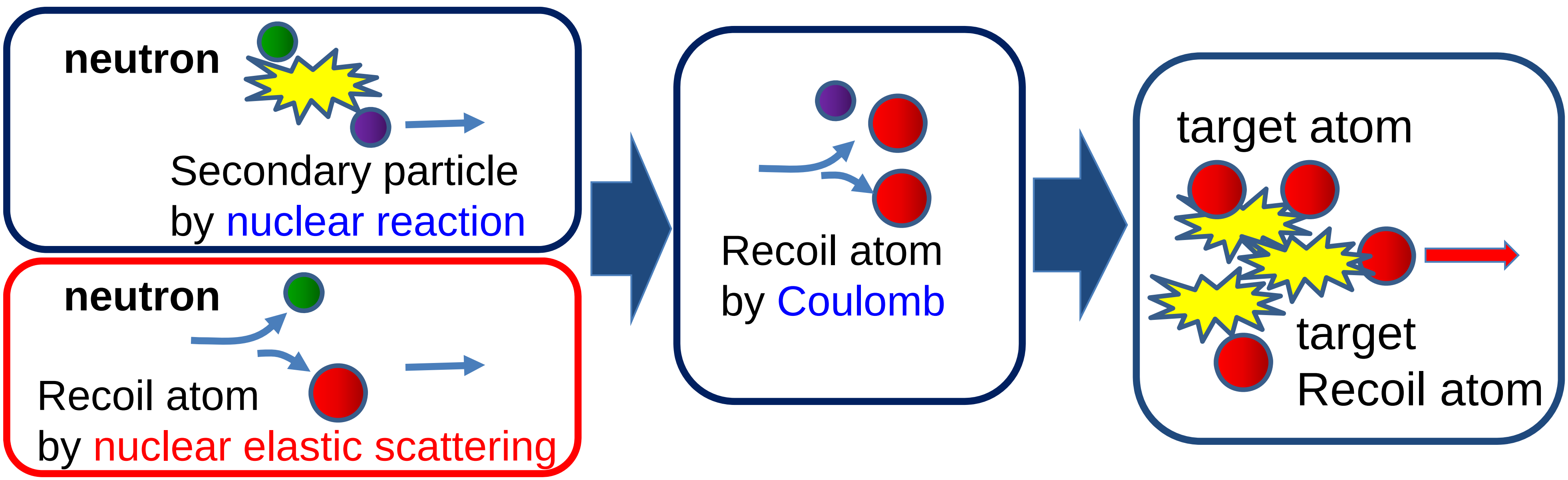
- For proton and ^{3}He beams, contribution of Coulomb scattering by recoil atom created by the secondary particles increases with energies.
- For ^{48}Ca and ^{238}U, the contribution of recoil atom created by the secondary is small.
- Displacement cross section of heavy ion is much higher than that of light ion.

Radiation damage for neutron

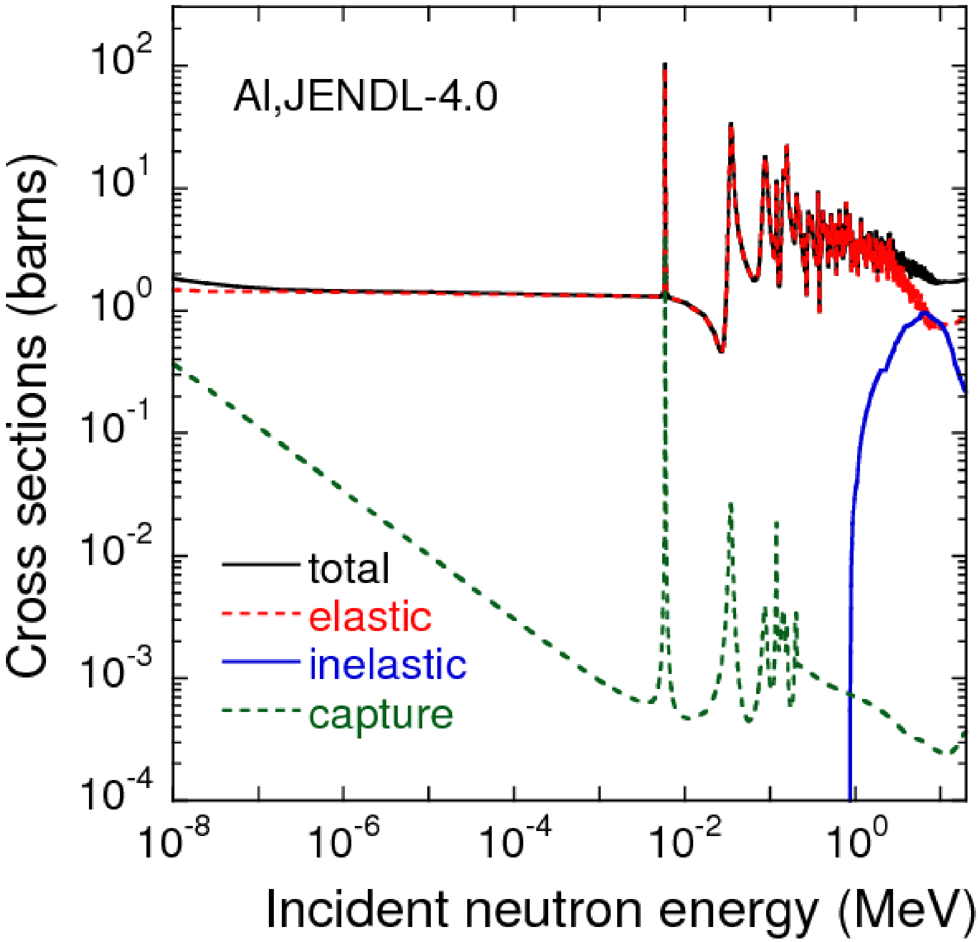
(1) Transport

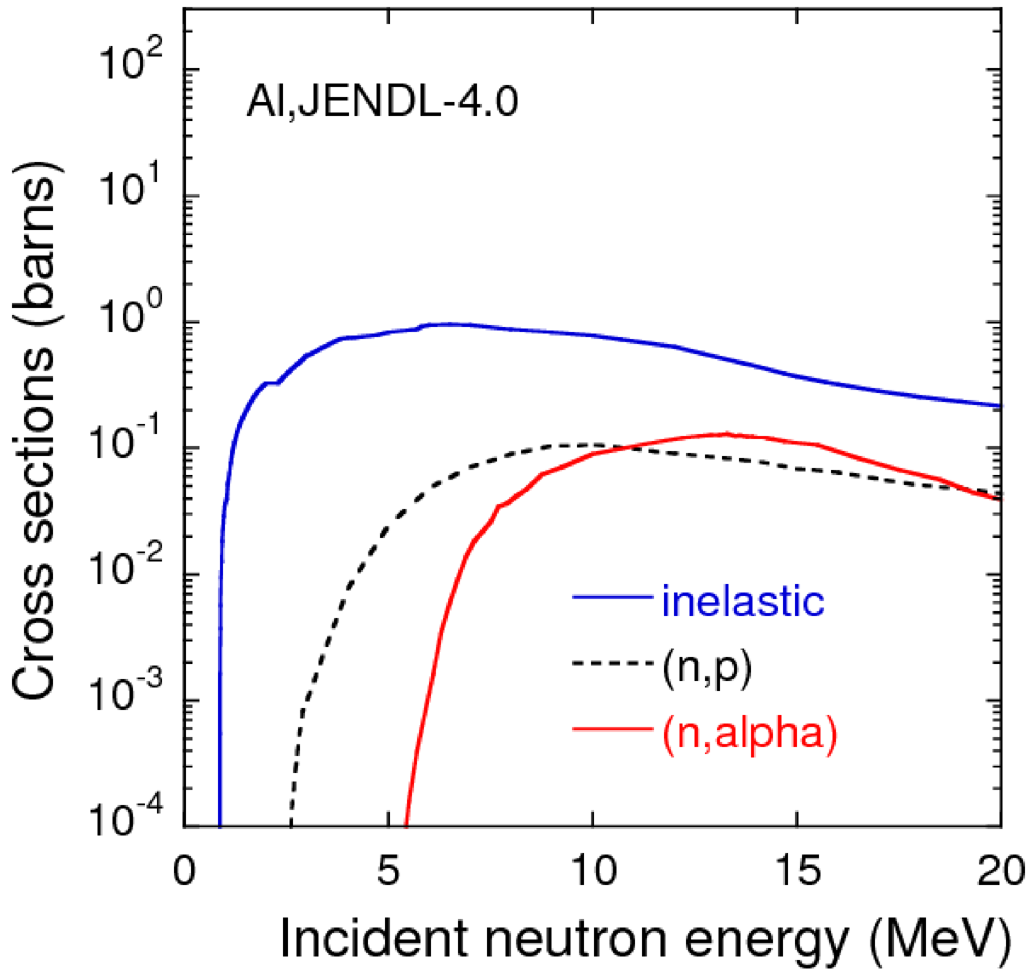
(2)Energy transfer to recoil atom
with Coulomb scattering

(3)Cascade damage
approximation



Cross sections for neutron incidence on Al



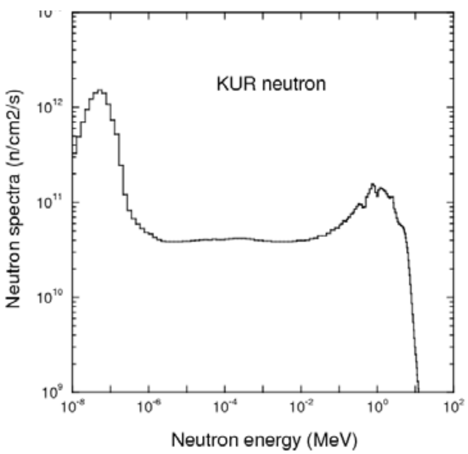


- ➢Elastic scattering is dominant below 1 MeV.
- ➢Nuclear reaction is dominant above 10 MeV.

Example of dpa calculation

Calculation condition

Reactor neutrons in Kyoto U.

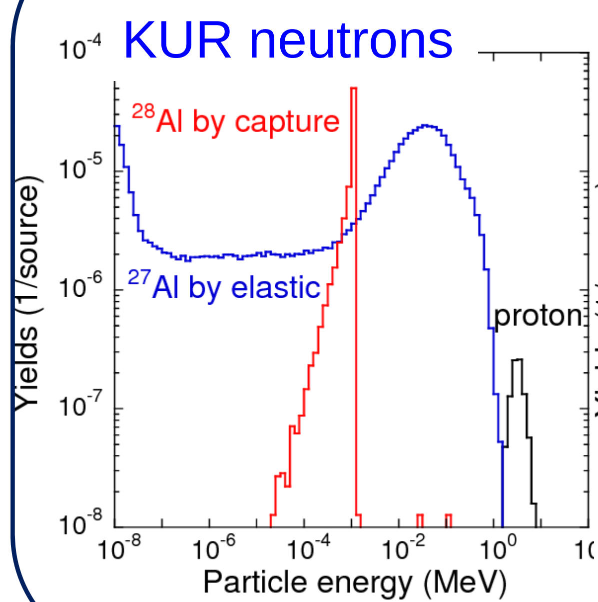


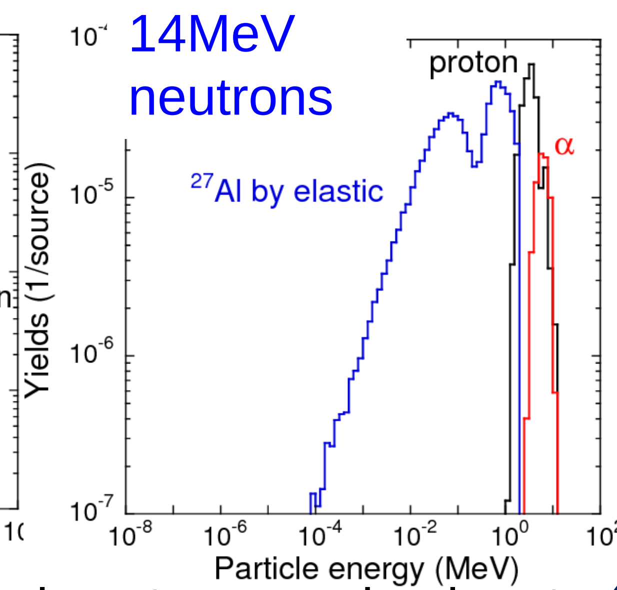
target

Al: 1mmx1mm
x50mm

14MeV neutrons

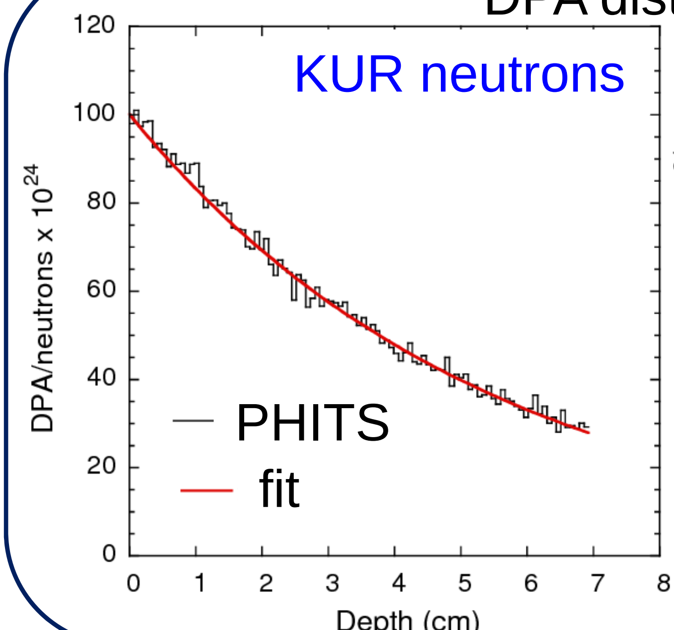
Particle production in target by PHITS

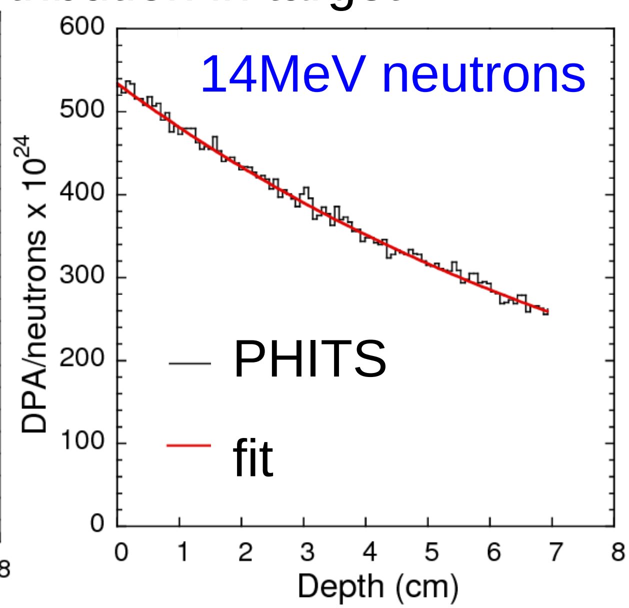




- Elastic scattering and capture are dominant.

DPA distribution in target





- PHITS can calculate detail dpa distribution in a target.
- SRIM code cannot calculate dpa for neutrons.
- DPA value decrease with depth, exponentially.

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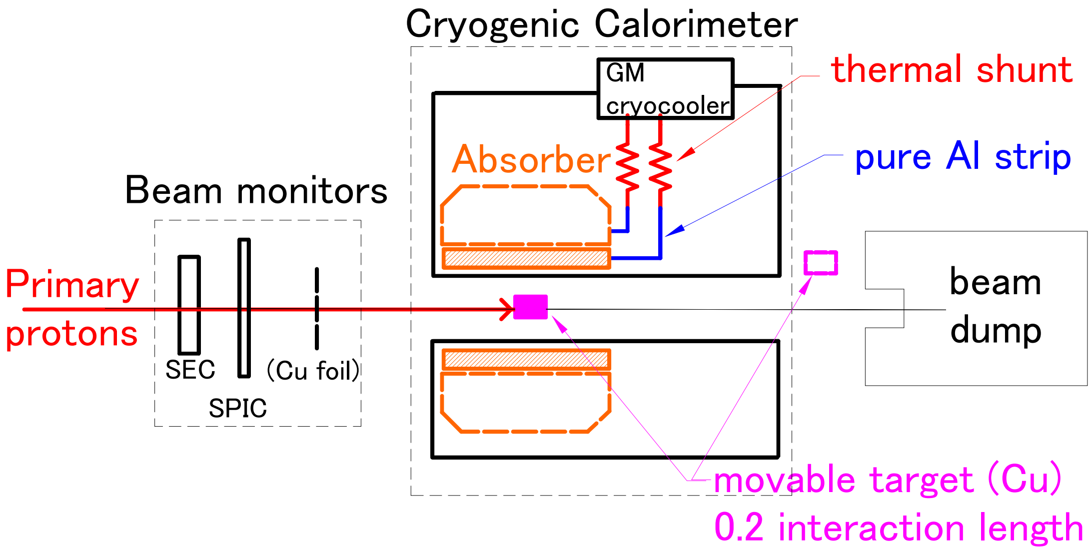
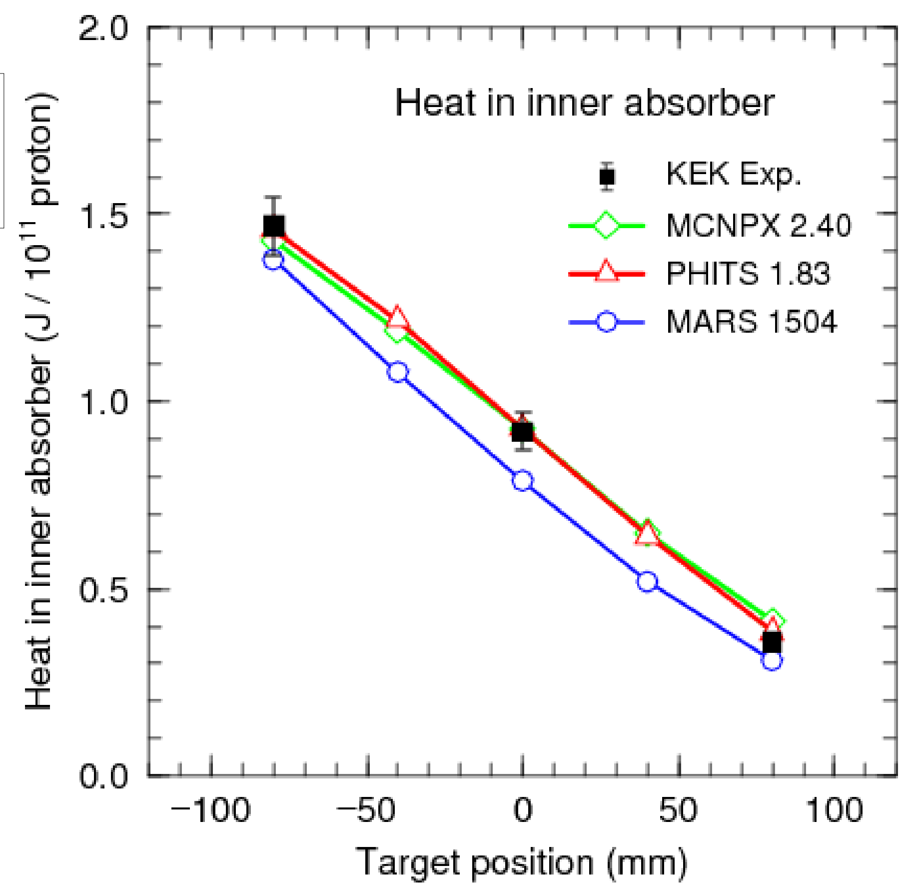
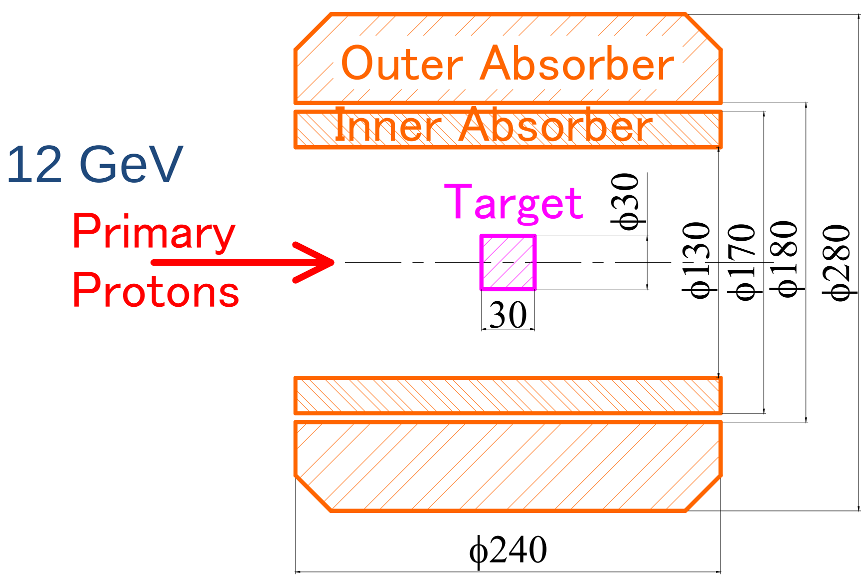
Benchmark test of HEAT(1) : compared with KEK experiment

Proton beam at 12 GeV



Exp. and Cal. by H. Ohnishi et al.
Nucl. Instr. and Meth. A545 (2005) 88.





MCNPX: calculated by N. Matsuda

PHITS results give good agreement with the experimental data.

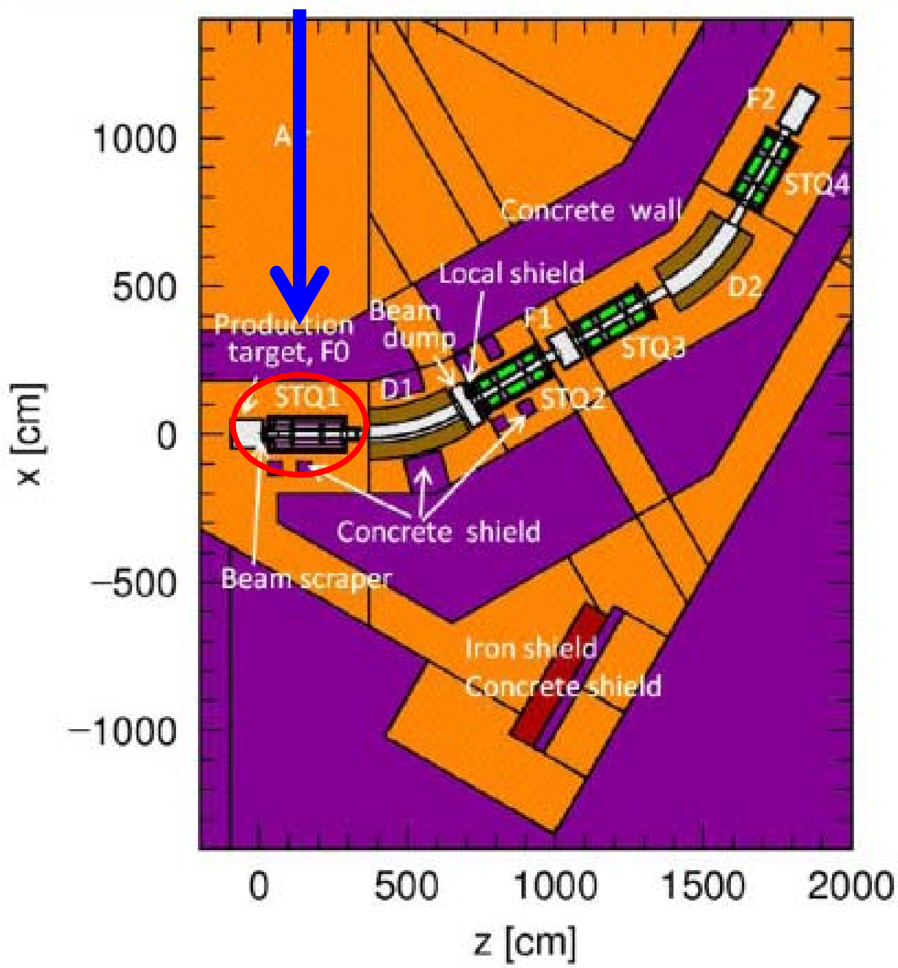
Benchmark test of HEAT(2) : compared with RIKEN experiment

PHITS calculation and experiments for Heat load to the STQ1 cryostat

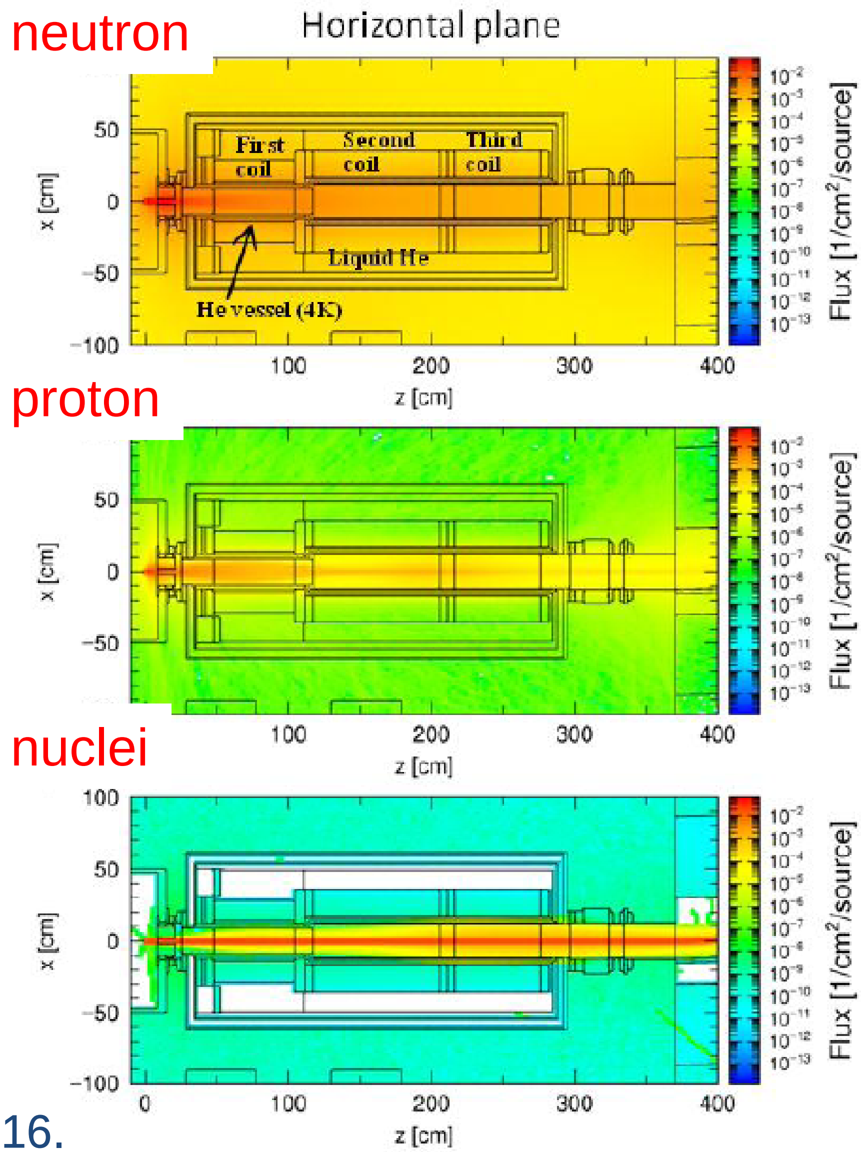
◆Calculation model of the BigRIPS separator

^{48}Ca beam at 345 MeV/nucleon

STQ1:Superconducting triplet pole



◆Calculated flux intensity of particle around STQ1



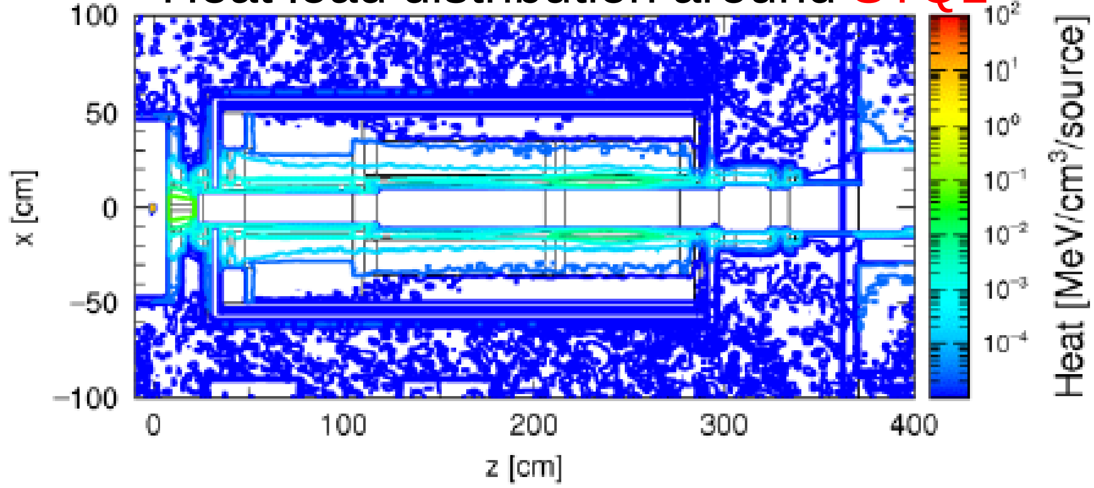
Exp. and Cal. by T. Ohnishi et al.

Progress in Nuclear Science and Technology (2011) 416.

Neutrons are produced at the target,and pass through STQ1.

Benchmark test of HEAT(2) : compared with RIKEN experiment

Heat load distribution around STQ1



Heat load mainly distributes at the inner duct.

◆Experimental condition and measured heat load to the STQ1 cryostat

Setting	Target isotope	Bρ* [Tm]	Be target thickness [mm]	Average current [μA]	Heat load [W]	Heat load(PHITS) [W]
I	^{31}Ne	8.2	15	0.53	11.9	12.0
II	^{32}Ne	8.4	20	2.25	42.6	63.8
III†	^{24}O	8.1	15	3.5	32.7	45.9
IV†	^{33}Al	7.0	10	3.7	26.8	34.4

Estimated results are about 1.3 - 1.5 times larger than the measured heat loads.

Summary

- The radiation damage model using Coulomb scattering in PHITS has been improved.

- Damage calculation only by recoil target atom directly created by the projectile lead to sever underestimation where projectile energy is high enough to create nuclear reactions.

- Energy distributions of particles produced by elastic scattering and nuclear reactions are important to determine the DPA values.

- PHITS is a powerful code to calculate DPA value and heat load to the material.