Introduction of radiation damage calculation in PHITS for high-energy region

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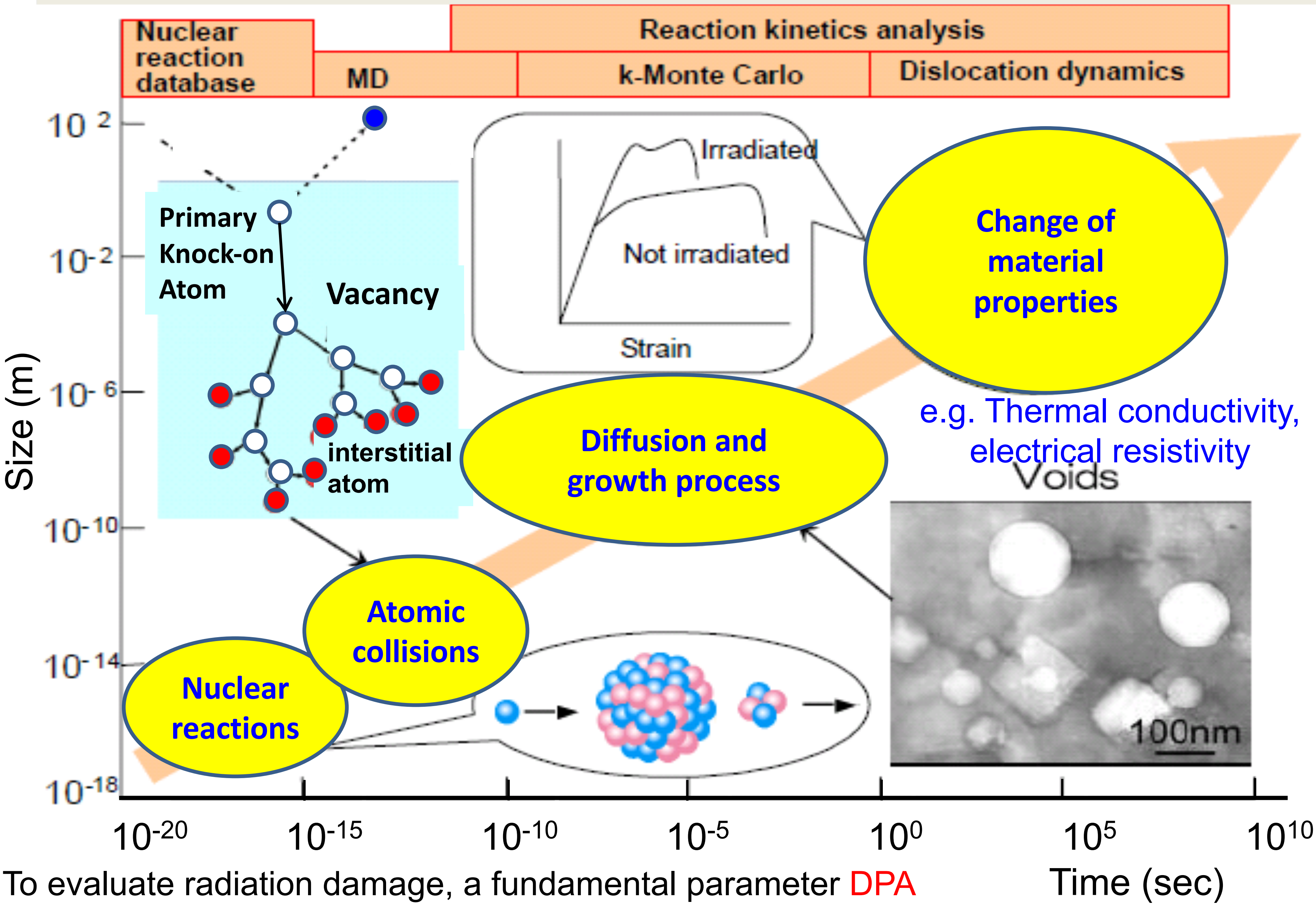
Outline
- Introduction
- Displacement per atom (DPA) calculation method
- Comparison between PHITS and other codes
- RaDIATE examples with PHITS
- Summary

Scale of irradiation effect



To evaluate radiation damage, a fundamental parameter DPA that characterizes lattice displacement events is required.

Microscopic effects on material

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

$$\textbf{DPA}=\int \sigma_{disp}(E)\phi(E)dE$$

σ_{disp} : **displacement cross-section**

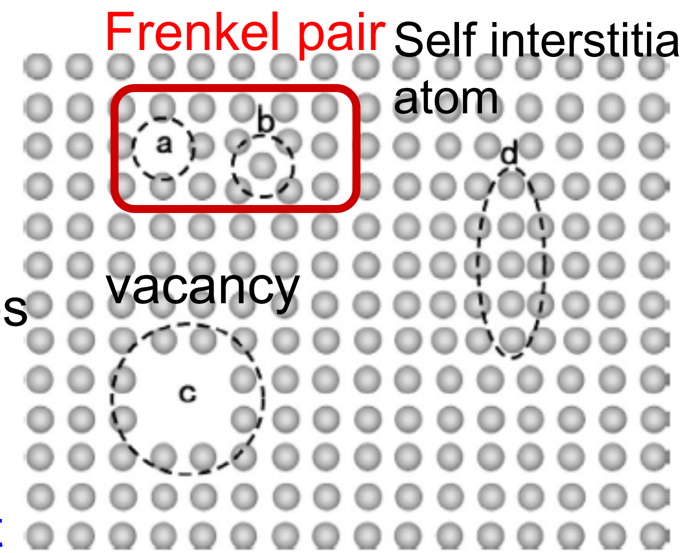
ϕ : irradiation fluence (particles/cm^2)

Related to the number of Frenkel pairs N_F:

$$\textbf{DPA}=\sum N_i N^i_F$$

N_i = number of particles

a scale of radiation damage intensity.



DPA is used as a damage-based exposure unit and used to compare radiation damage by different radiation sources.

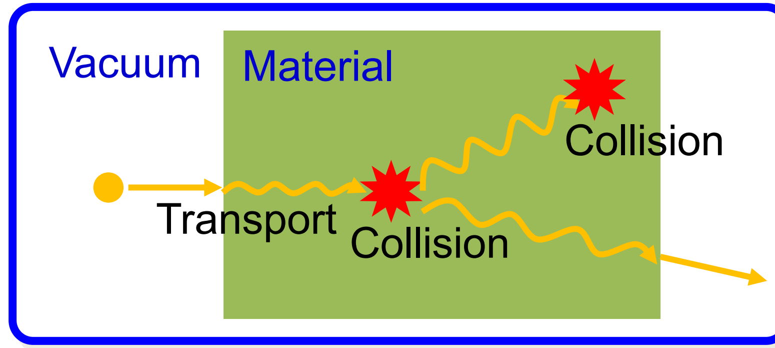
MC codes (PHITS, MARS, FLUKA, MCNP…) calculate DPA values:

1. Using database of σ_{disp} → limitation for kind of incident particles and materials.
2. Calculating σ_{disp} for all particles with physics models event by event

This presentation shows radiation damage calculation with physics models in PHITS

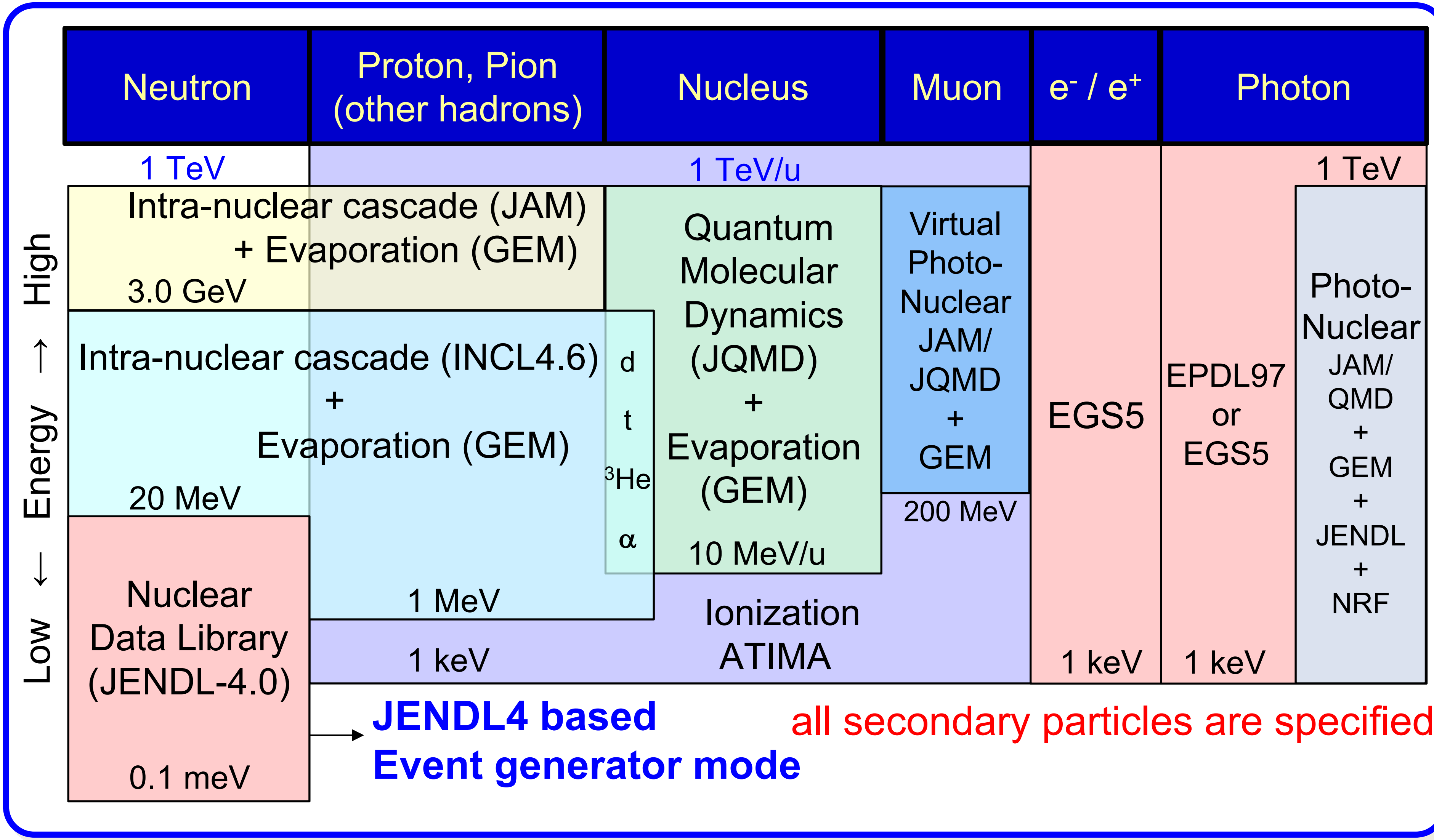
Physical Processes included in PHITS

T. Sato et al., JNST 50 (2013) 913.



- **Transport between collisions**
  - **External Field and Optical devices**
    - Magnetic Field
    - Gravity
    - Super mirror (reflection)
    - Mechanical devices, T0 chopper
  - **Ionization process for charge particle**
    - dE/dx : SPAR, ATIMA code
      Continuous-slowing-down Approximation (CSDA)
    - δ-ray generation
    - Microdosimetric function
    - Track-structure simulation
- **Collision with nucleus**
  - **Low-energy Neutrons** — Nuclear Data based (JENDL-4.0 etc.)
    Event Generator Mode
  - **Photons, Electrons** — Electromagnetic cascade with EGS5
  - **High-energy nucleons** — Intra-Nuclear Cascade → Evaporation
  - **Heavy Ions** — Quantum Molecular Dynamics → Evaporation

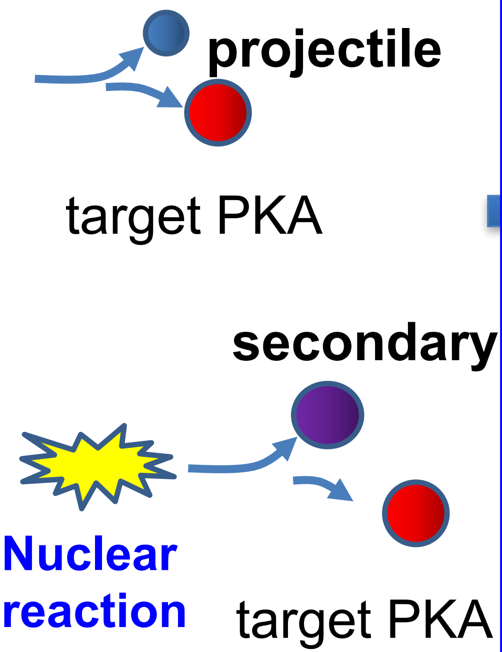
Map of Models in PHITS



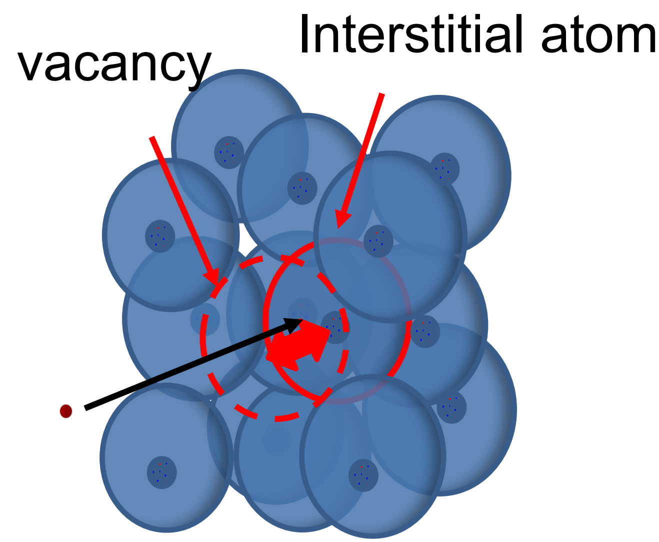
Next slide: DPA calculation method

DPA calculation method in PHITS

(1)Energy transfer with Coulomb scat.



(2)Cascade damage approximation



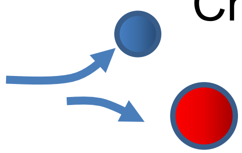
$$\sigma_{disp} = \underbrace{\int_{t_d}^{t_{\max}} \frac{d\sigma_{Coul}(t)}{dt}}_{\text{Coulomb scattering}} \underbrace{\eta \frac{0.8}{2 \cdot T_d} T_{dam}}_{\text{Number of displacement atoms}} dt$$

Coulomb scattering *Number of displacement atoms*

Y. Iwamoto et al., NIMB 274 (2012) 57.

(1)Energy transfer with Coulomb scattering

M. Nastasi et al., "Ion-Solid Interaction: Fundamentals and Applications "



Charged particle E_p *:kinetic energy*, (Z_1, M_1)

leads to the deflection of the particles

target PKA T*: transferred energy*, (Z_2, M_2)

Coulomb scat. cross section: one parameter

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

dimensionless collision parameter:

$$t \equiv \varepsilon^2 \frac{T}{T_{\max}} = \varepsilon^2 \sin^2(\frac{\theta}{2})$$

T : Transferred energy to target atom

T_{max} :maximum transferred energy

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

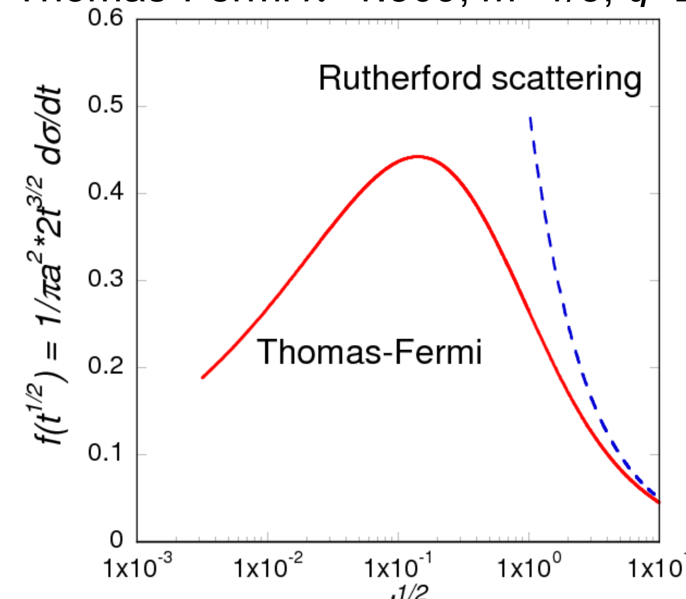
ε :dimensionless energy

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

Screening functions:

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

Thomas-Fermi λ=1.309, m=1/3, q=2/3



Large t → large T in close collisions

Small t → small T in distance collisions

Next slide: cascade damage approximation

(2) Cascade damage approximation

$$\sigma_{disp} = \int_{t_d}^{t_{\max}} \frac{d\sigma_{Coul}(t)}{dt} \eta \frac{0.8}{2 \cdot T_d} T_{dam} dt$$

Defect production efficiency

$$T_{dam} = \xi(\varepsilon) T(\varepsilon) = \frac{1}{1 + k_{cas} \cdot g(\varepsilon)} T(\varepsilon)$$

Damage energy: transferred to lattice atoms reduced by the losses for electronic stopping atoms in the displacement cascade

$$g(\varepsilon) = \varepsilon + 0.40244 \cdot \varepsilon^{3/4} + 3.4008 \cdot \varepsilon^{1/6}$$

$$k_{\mathrm{cascade}} = 0.1337 Z_{\mathrm{target}}^{\frac{1}{6}} (Z_{\mathrm{target}} / A_{\mathrm{target}})^{1/2}$$

number of displaced atoms using phenomenological approach: N_{NRT}

NRT(Norgett, Robinson, Torrens: 1975)

- 0.8: displacement efficiency derived from MD simulation of Robinson, Torrens 1972
- T_d: threshold displacement energy. Bonds should be broken to displace an atom.

e.g. set to 40 eV in Ti but varies 15 – 90 eV in other atom

Efficiency of the defect production in material

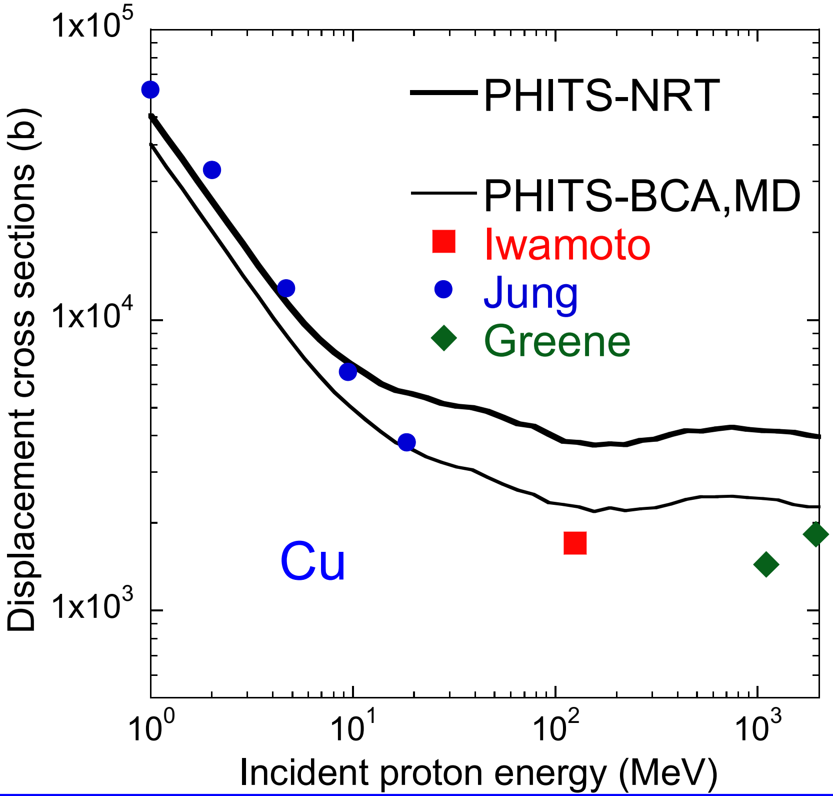
$$\eta = \frac{N_D}{N_{NRT}} = 0.7066 T_{dam}^{-0.437} + 2.28 \times 10^{-3} T_{dam}$$ for Cu

M.J. Caturla et al., J. Nucl. Mater. 296 (2001) 90.

N_D: number of stable displacements at the end of collision cascade ⟸ MD

N_{NRT}: number of defects calculated by NRT model

Account for atom recombination in elastic cascading



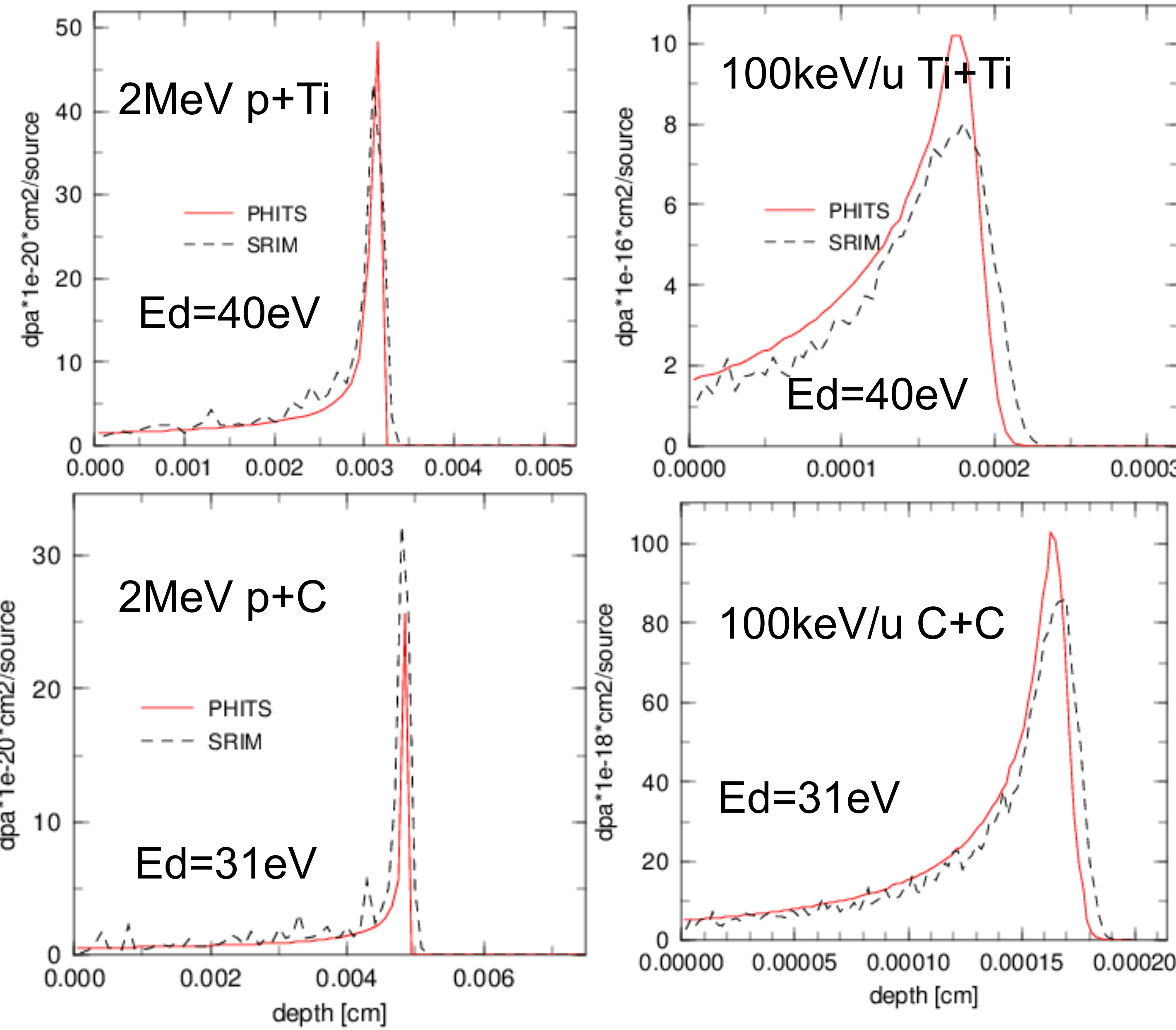
σ_{disp} with η reproduces experimental data in the high-energy region up to GeV for Cu.

Y. Iwamoto et al., JNM 458 (2015) 369.
P. Jung, JNM 117 (1983) 70.
G.A. Greene et al., Proc. of AccApp'03 (2004) 881.

Note: there are new efficiencies proposed by Stoller and Nordlund.
PHITS will include them soon.

In this presentation, NRT-DPAs are reported.

Comparison between PHITS and SRIM codes

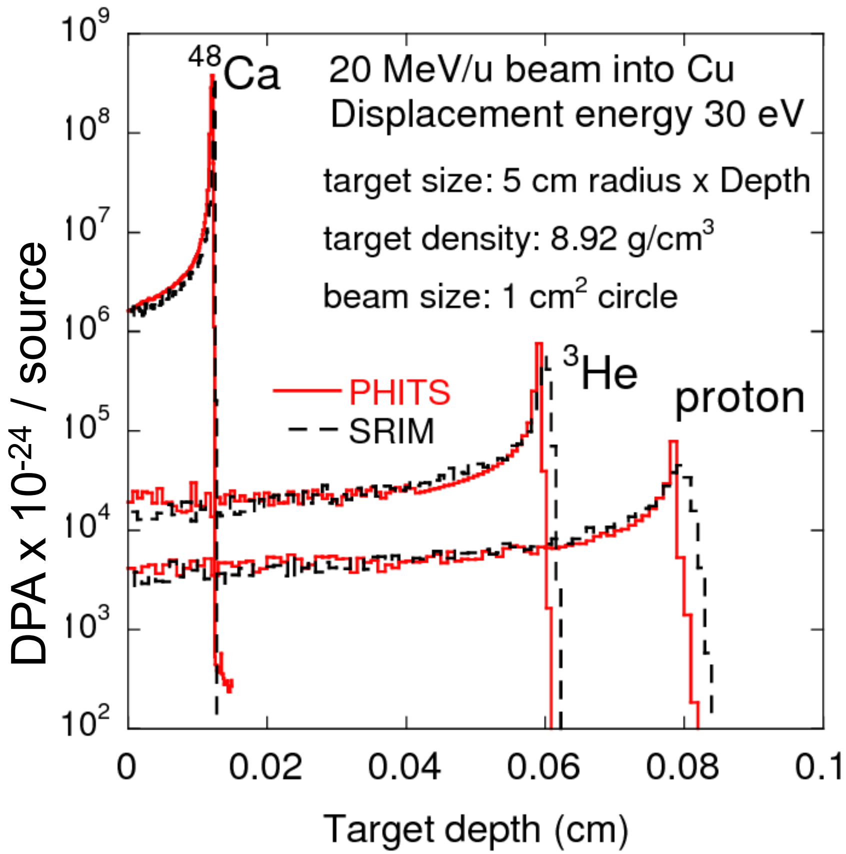


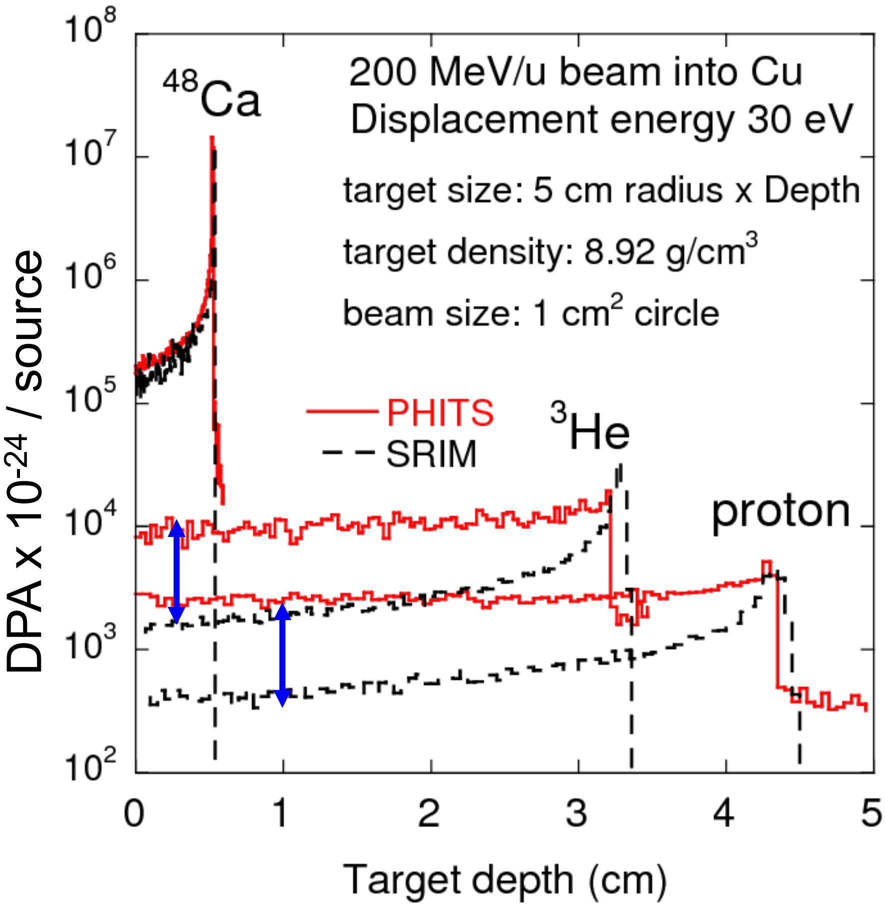
SRIM can simulate the transport of ions in matter without nuclear reaction.

http://www.srim.org/

Good agreement.

Comparison between PHITS and SRIM codes



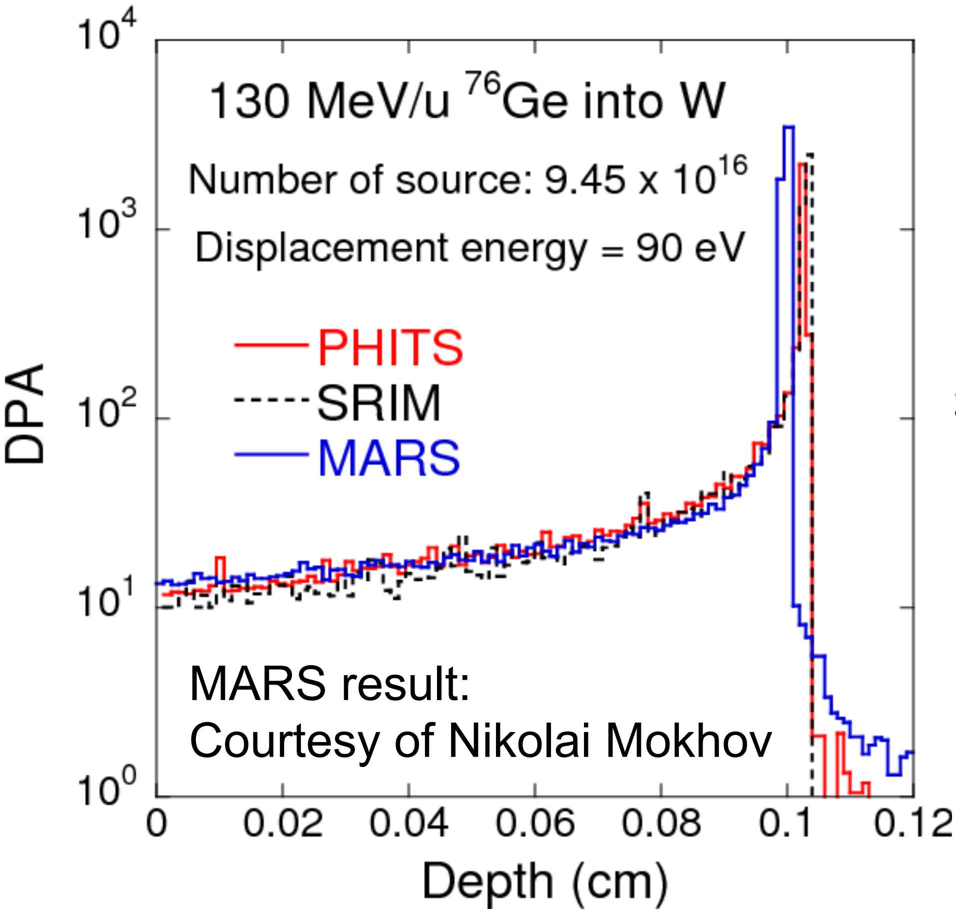


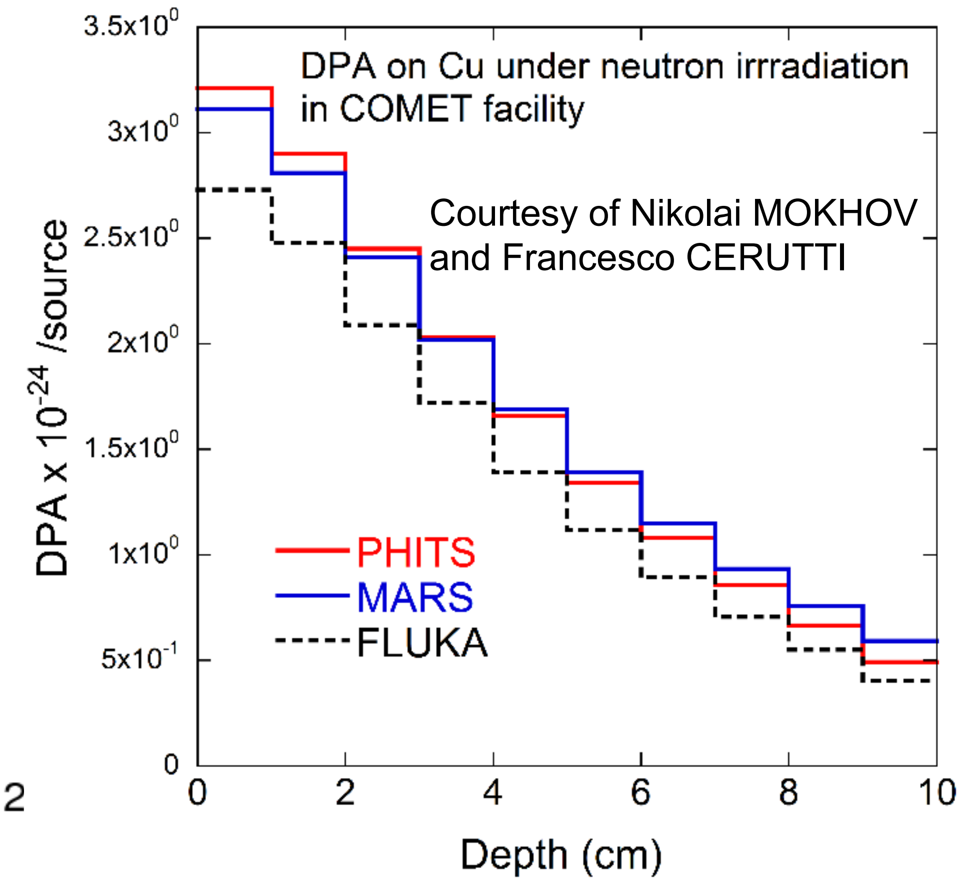
✓PHITS results are in good agreement with SRIM results.

✓ differences between two results:

⟶ Secondary particles created from sequential nuclear reactions

Comparison between PHITS, SRIM and MARS codes



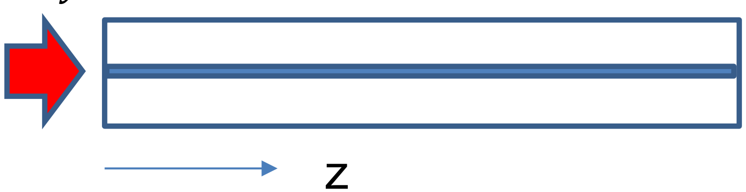


Good agreement.

RaDIATE example with PHITS

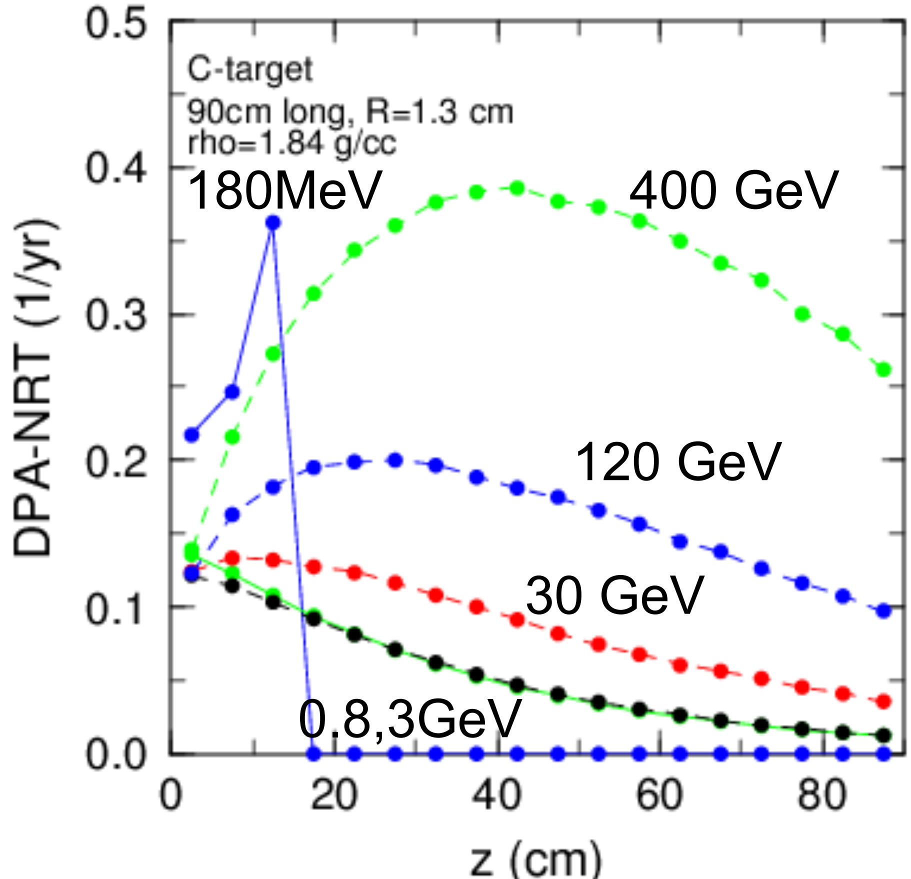
Proton gaussian beam
Energy: 0.18, 0.8, 3, 30, 120, 400GeV
(PHITS is not available at 7 TeV.)

proton
$\sigma_x = \sigma_y = 0.43cm$



90 cm long, R=1.3 cm
C-target, density=1.84g/cm^3

Tally region: 90 cm long, r=0.2cm



DPA depth distribution in C-target

180 MeV: Bragg peak of protons contributes DPA.
0.8-30 GeV: Damage may occur at surface.
120GeV, 400 GeV: DPA increases with depth.

Other outputs (energy deposition, gas production) will be reported by Nikolai.

Summary

The displacement calculation method in PHITS is available for all incident particles, wide energy range (eV-TeV), and all materials.

Agreements between PHITS and other codes are good.

In the high energy region (> ~20 MeV) for proton and neutron, DPA created by secondaries increase due to nuclear reactions.

Future works

New defect production efficiency (Nordlund) will be implemented. (just implemented!)

Benchmark experiments will be performed at RCNP (100-400MeV) and J-PARC (400MeV-30GeV, see Meigo-san's talk).

This work has been supported by JSPS KAKENHI Grant Number 16H04638.

Experimental displacement cross section

Displacement cross section could be experimentally validated in Irradiation on metal at cryogenic temperature.

Recombination of Frenkel pairs by thermal motion is well suppressed.

Experimental displacement cross section

Damage rate

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

J. Nucl. Mater. 49 (1973/74) 161.

$\Delta\rho_{metal}$: Electrical resistivity change(Ωm)

Φ: Beam fluence($1/m^2$)

ρ_{FP}: Frenkel-pair resistivity (Ωm)

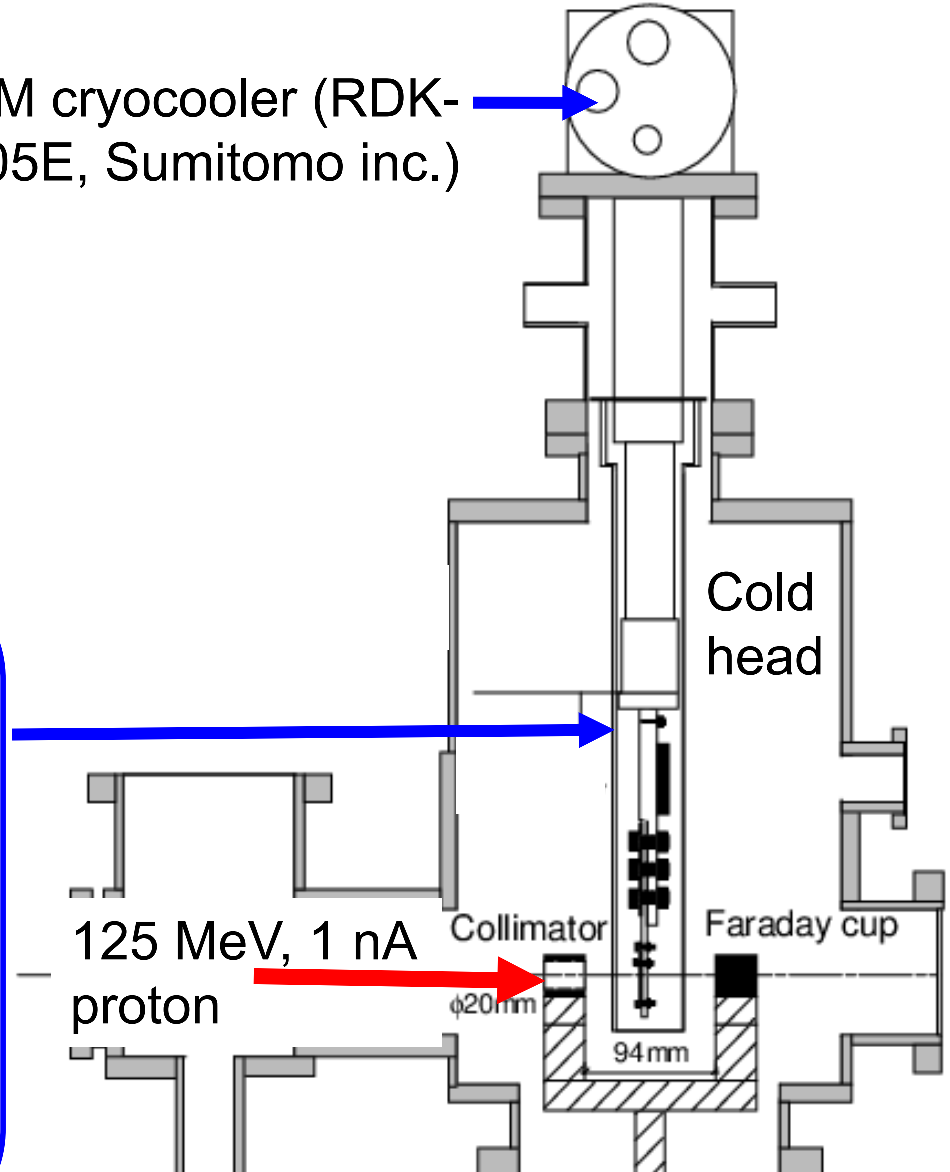
Resistivity increase is the sum of resistivity per Frenkel pair

Development of cryogen-free cooling system at FFAG/KURRI

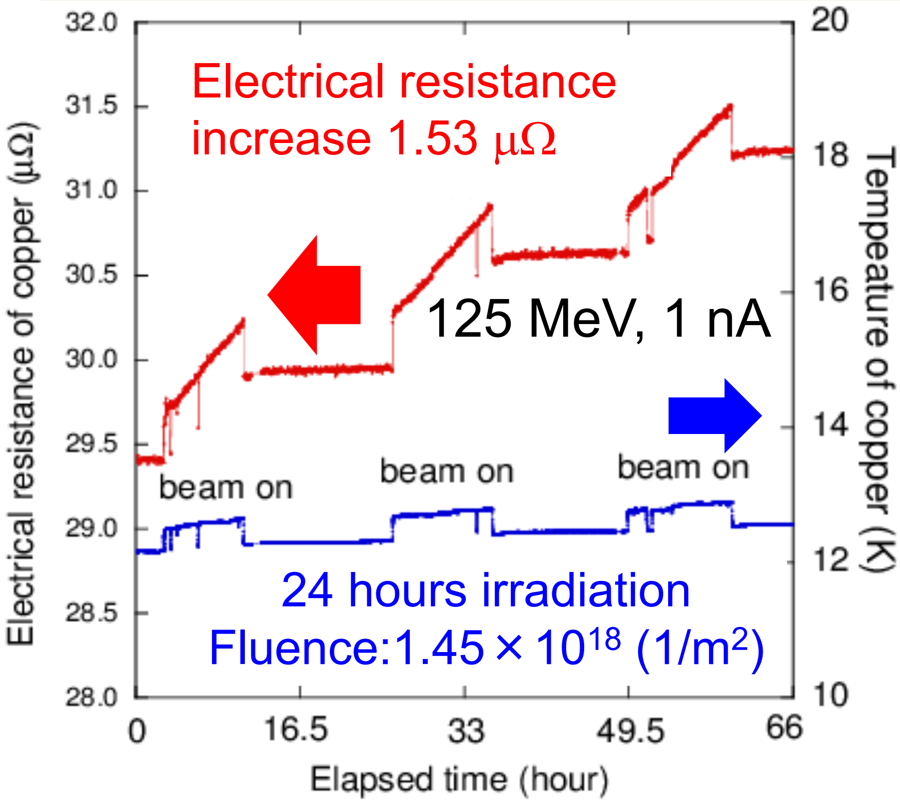
GM cryocooler (RDK-205E, Sumitomo inc.)

Target assembly

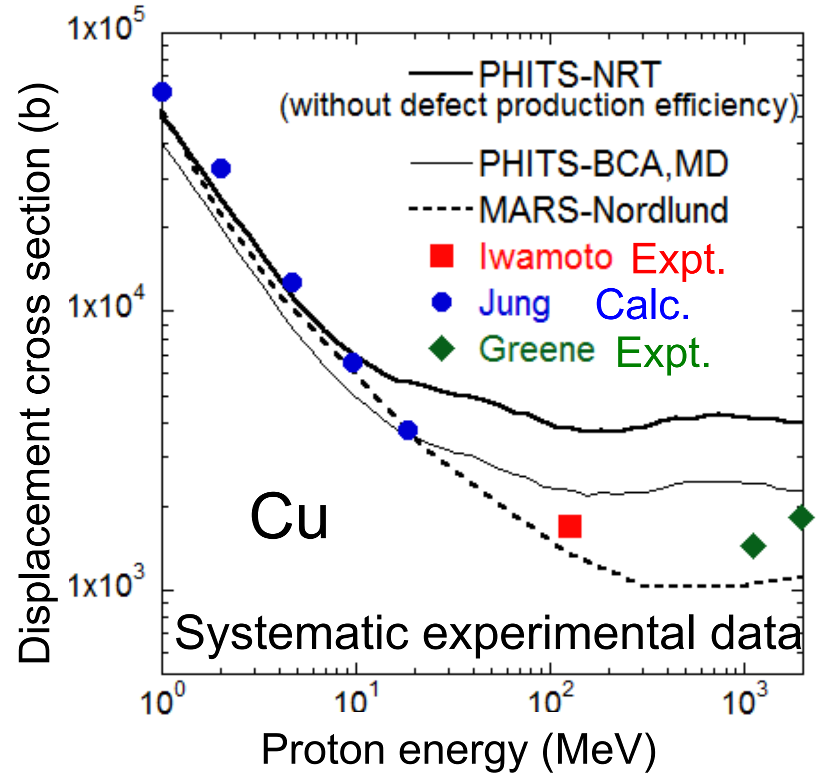
Sample was cooled by conduction coolant via Al and oxygen-free high-conductivity copper (OFHC).



Experimental results of copper



Electrical resistivity changes of copper



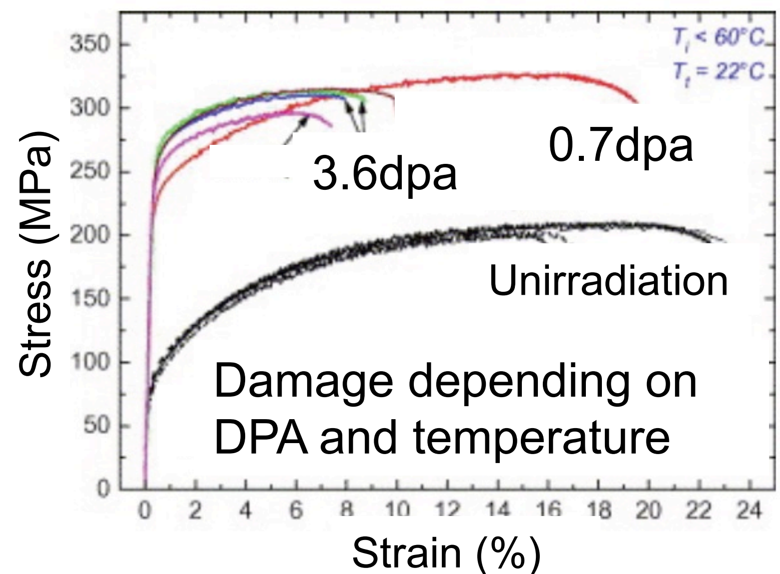
Displacement cross section of copper

Evaluation of radiation damage

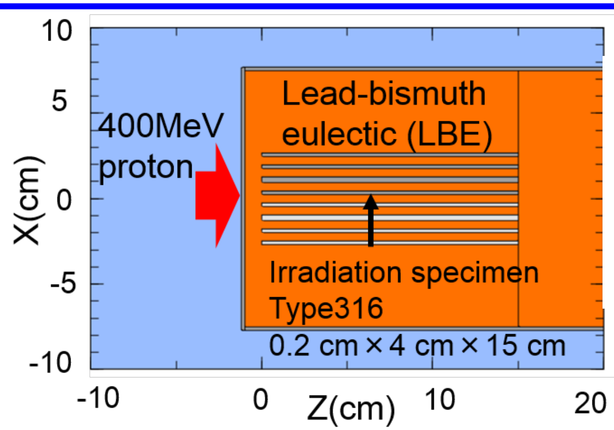
The average number of Displaced atoms Per Atom of a material (DPA) is used in evaluation of reactor and accelerator as a damage-based exposure unit.

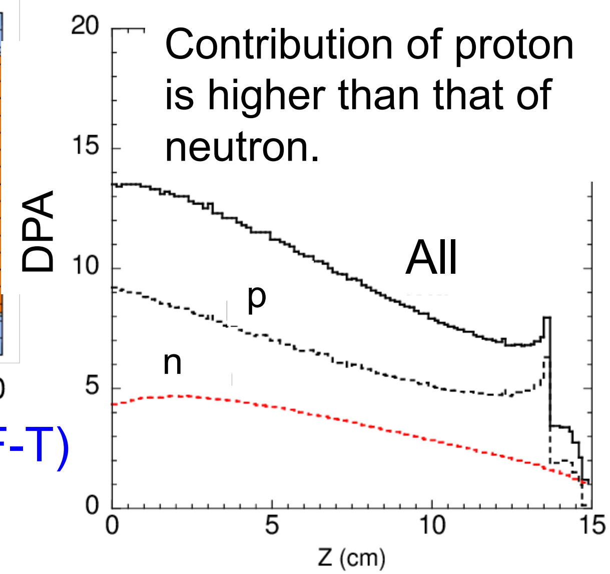
$$\textbf{DPA} = \int \sigma_{\mathrm{disp.}}(E)\phi(E)dE$$

Displacement cross section — Fluence



Irradiation effect on AlMg3 for 600 MeV proton irradiation

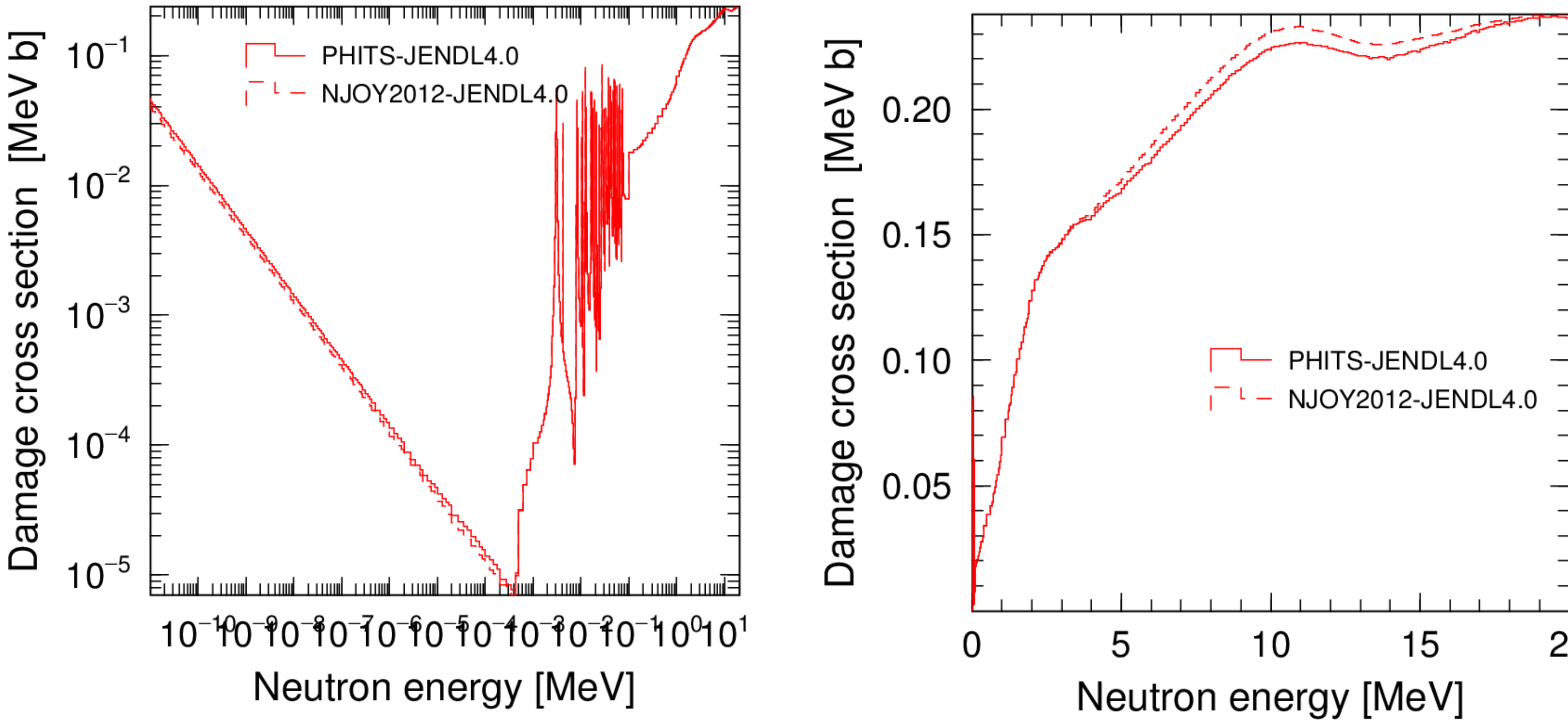




DPA for target at J-PARC ADS Target Test Facility (TEF-T) using Monte Carlo particle transport code PHITS

Y. Iwamoto, et al., J. Nucl. Sci. Technol 51 (2014) 98-107.

① JENDL-4.0を用いたPHITSとNJOY2012 の損傷エネルギー断面積の比較

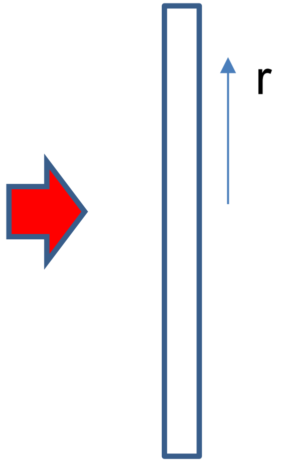


^{47}Ti

RaDIATE example with PHITS

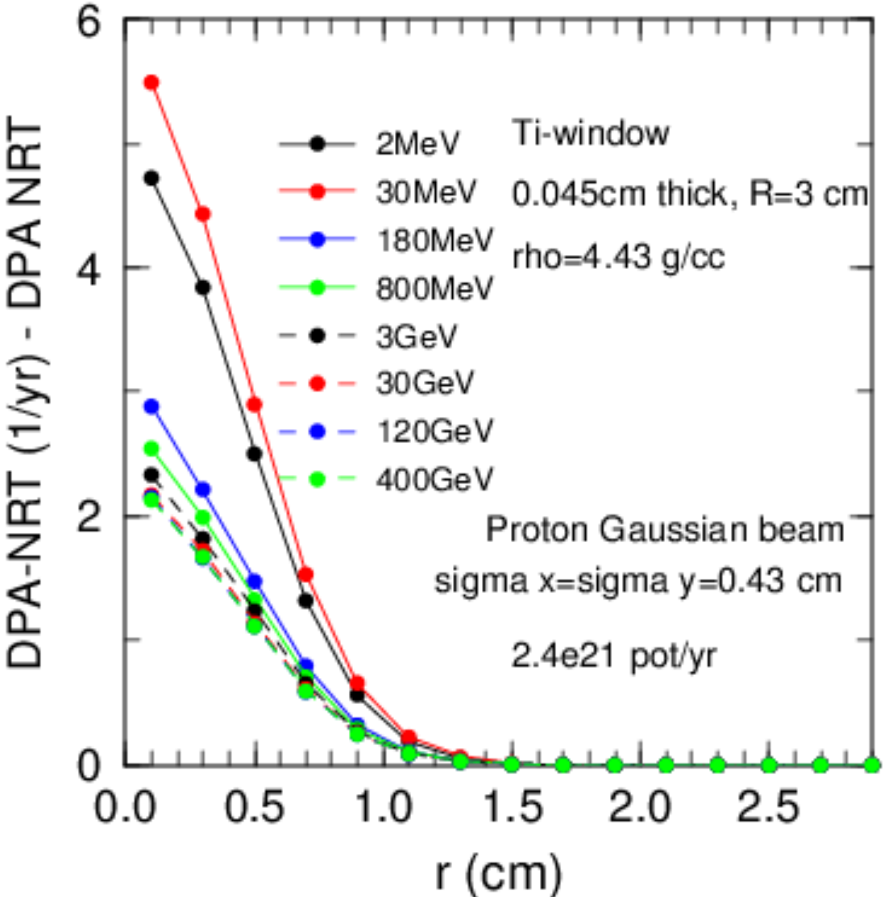
Proton gaussian beam
Energy: 2, 30 MeV
0.18, 0.8, 3, 30, 120, 400GeV

$\sigma_x = \sigma_y = 0.43cm$



0.045cm thick, R=1.3 cm
C-target, density=1.84g/cm^3

Tally region: r=0 – 1.3 divided by 10

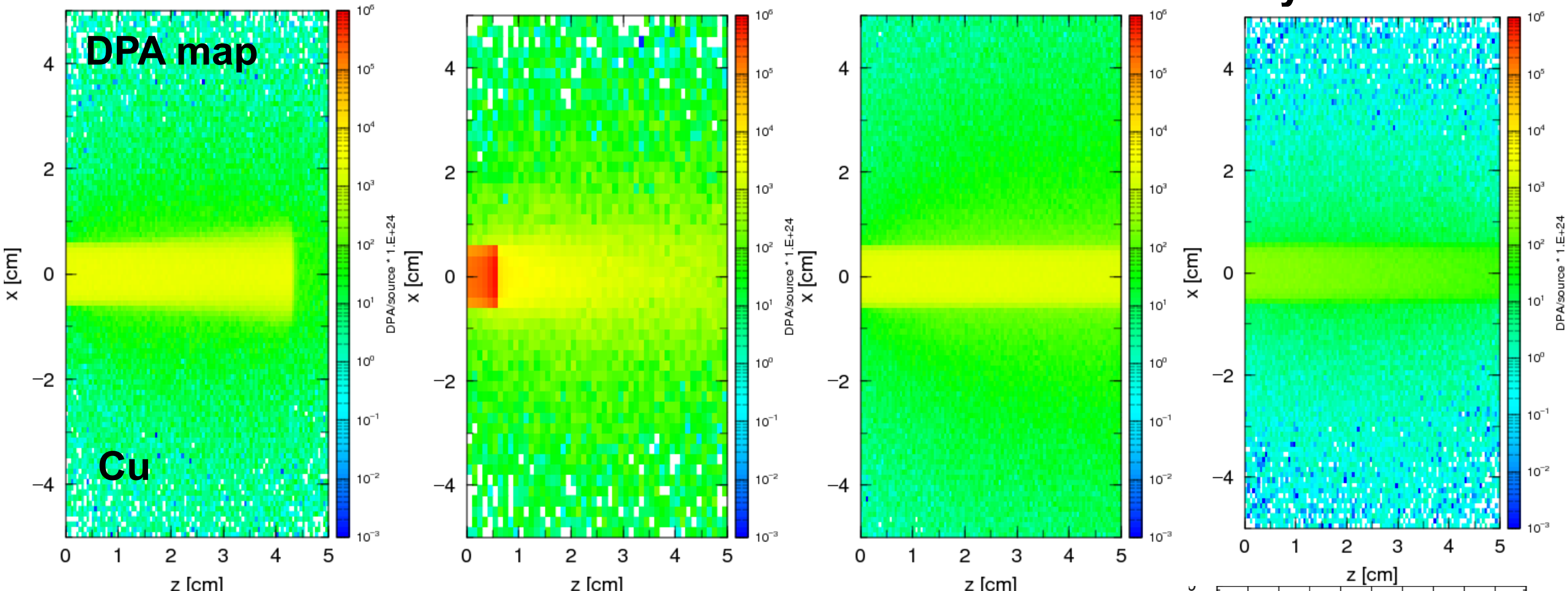


DPA radial distribution in Ti-target

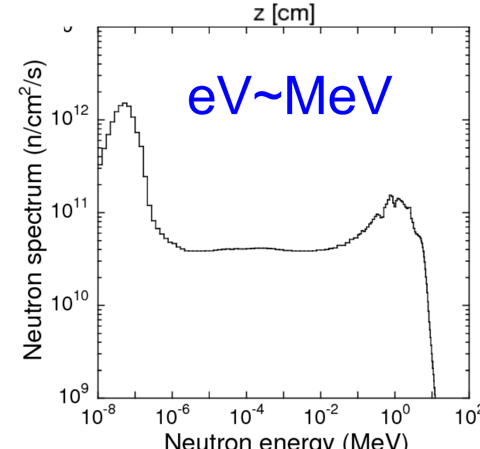
Two dimensional DPA distribution

Calculation condition

(1)200 MeV proton **(2)200 MeV/u ^{48}Ca** **(3)200 MeV neutron** **(4)Reactor neutron in Kyoto U.**



✓Beam size: 1cm^2
✓Target: 5 cm radius x depth Cu
✓Displacement energy: 30 eV



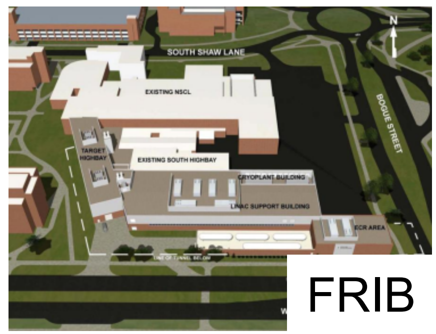
Introduction

Prediction of structural damage to materials under irradiation is essential for the design.

Spallation source J-PARC,SNS, ESS	Heavy ion facility FRIB,RIBF,GSI	International Fusion Materials Irradiation Facility

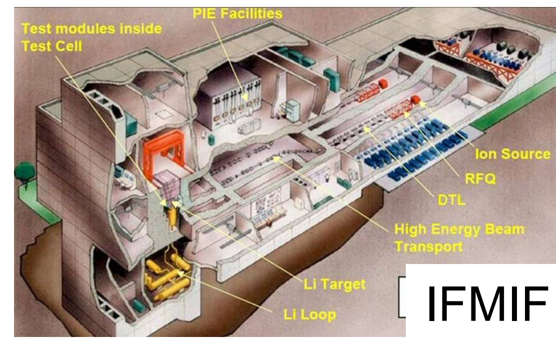
J-PARC

proton, neutron
thermal-TeV



FRIB

heavy-ion
MeV-GeV/nucleon



IFMIF

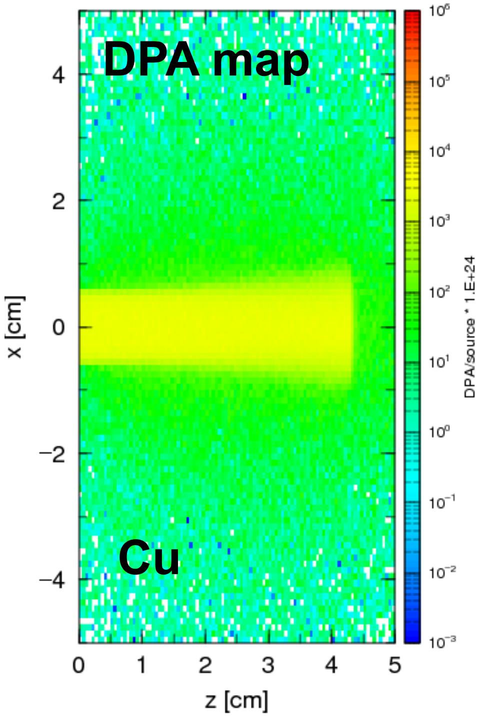
neutron, deuteron
~14MeV

To evaluate radiation damage, a fundamental parameter that characterizes lattice displacement events is required.

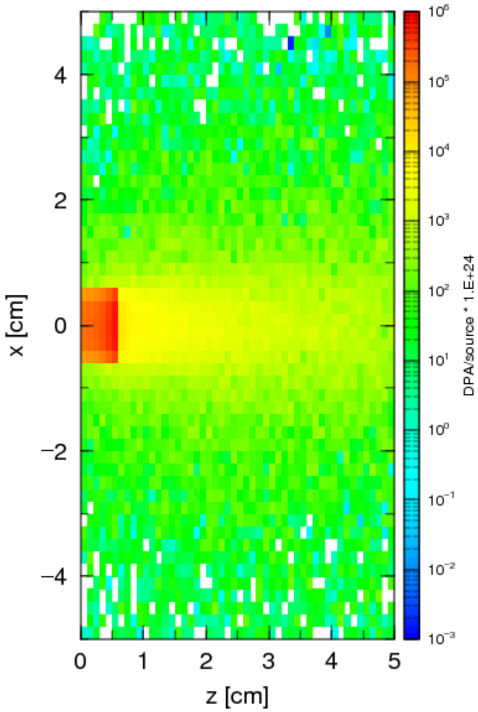
Effect of nuclear reaction and elastic scattering

Calculation condition

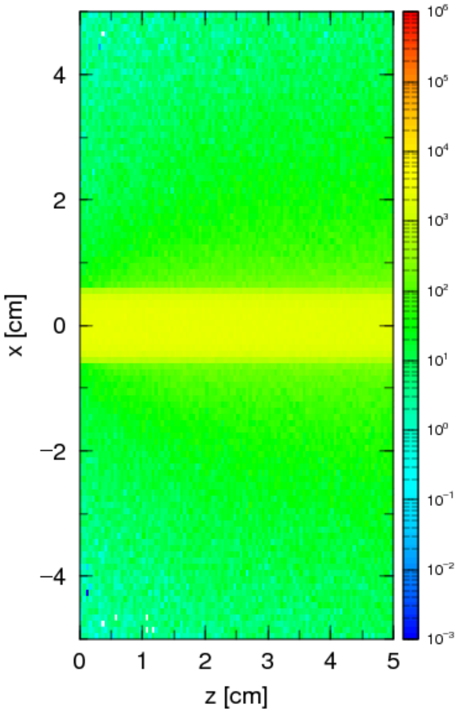
(1)200 MeV proton



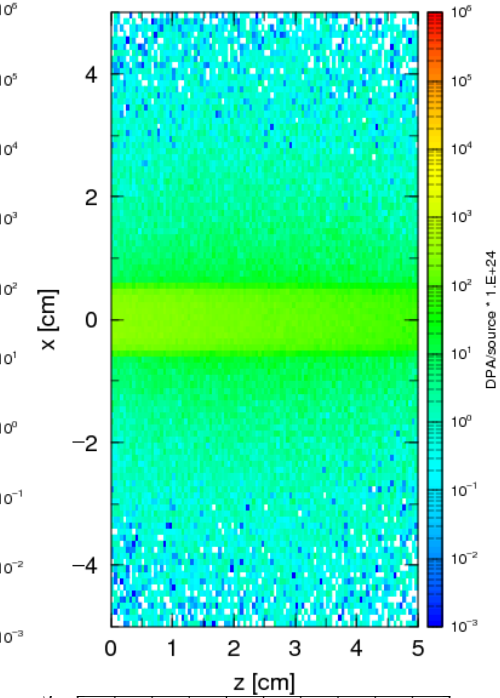
(2)200 MeV/u ^{48}Ca

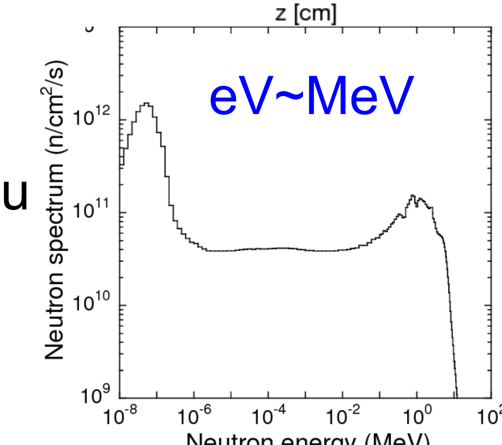


(3)200 MeV neutron



(4)Reactor neutron in Kyoto U.





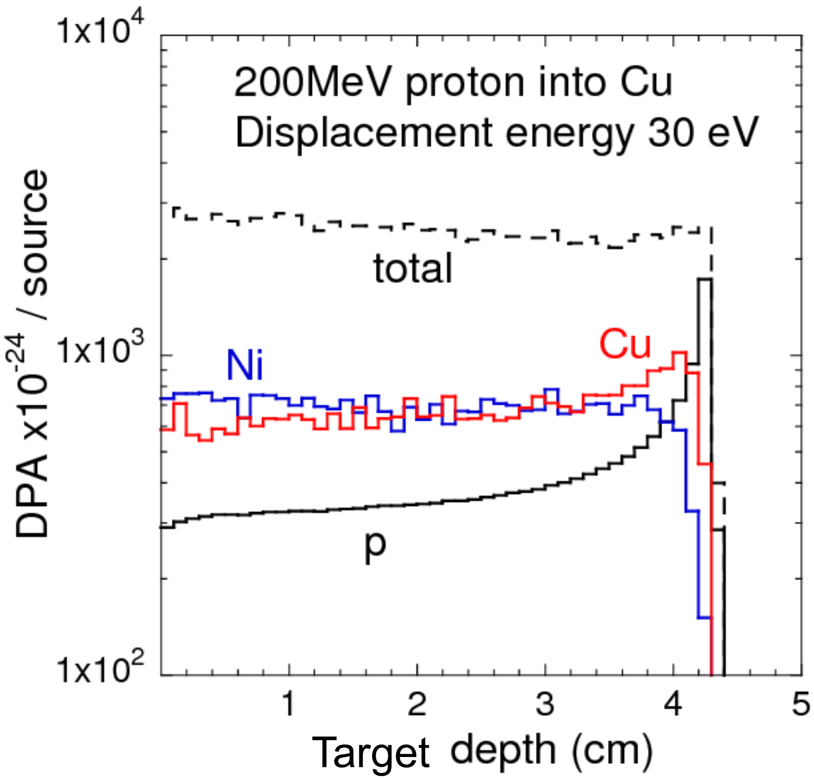
(5)14 MeV proton

(6)14 MeV neutron

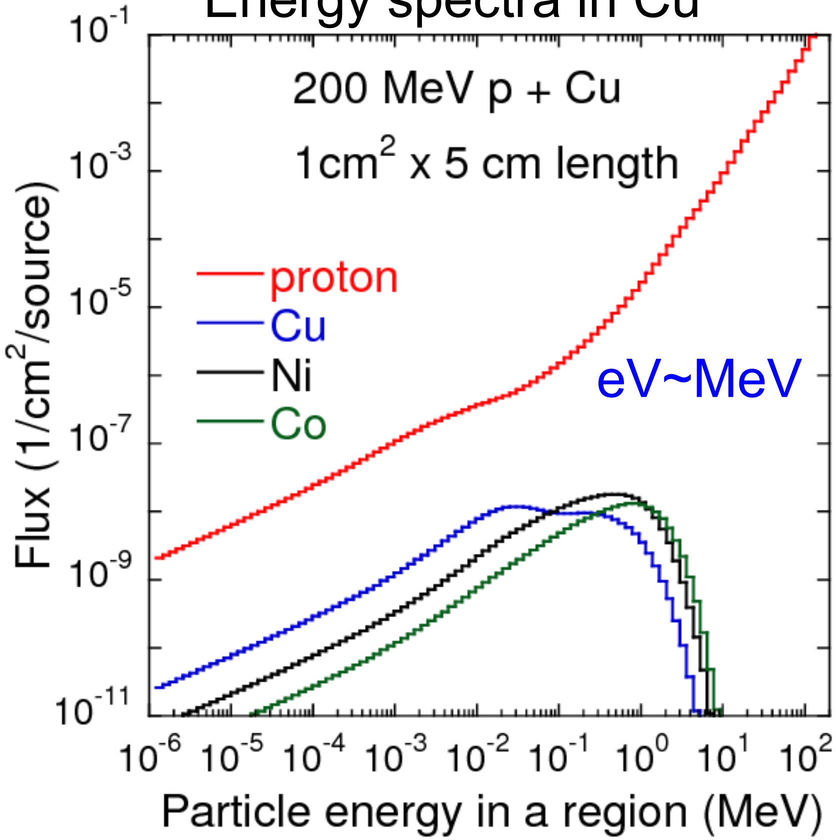
- ✓Beam size: 1cm^2
- ✓Target: 5 cm radius x depth Cu
- ✓Displacement energy: 30 eV

(1)200 MeV proton into Cu

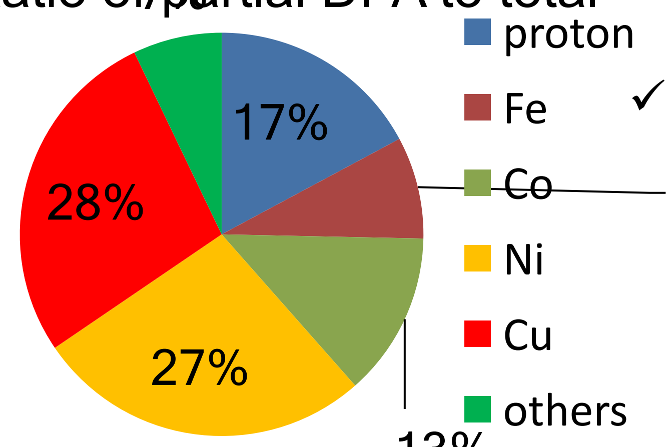
DPA distribution



Energy spectra in Cu



Ratio of partial DPA to total

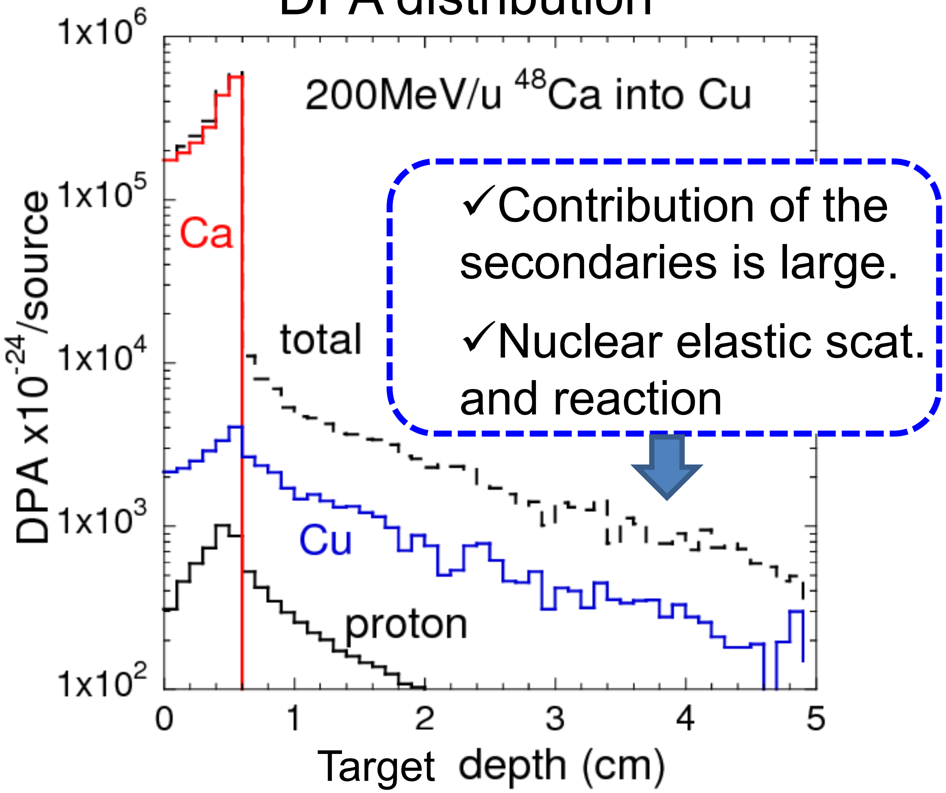


✓ Types of Particles around Cu increase due to nuclear reactions and these particles contribute to total DPA .

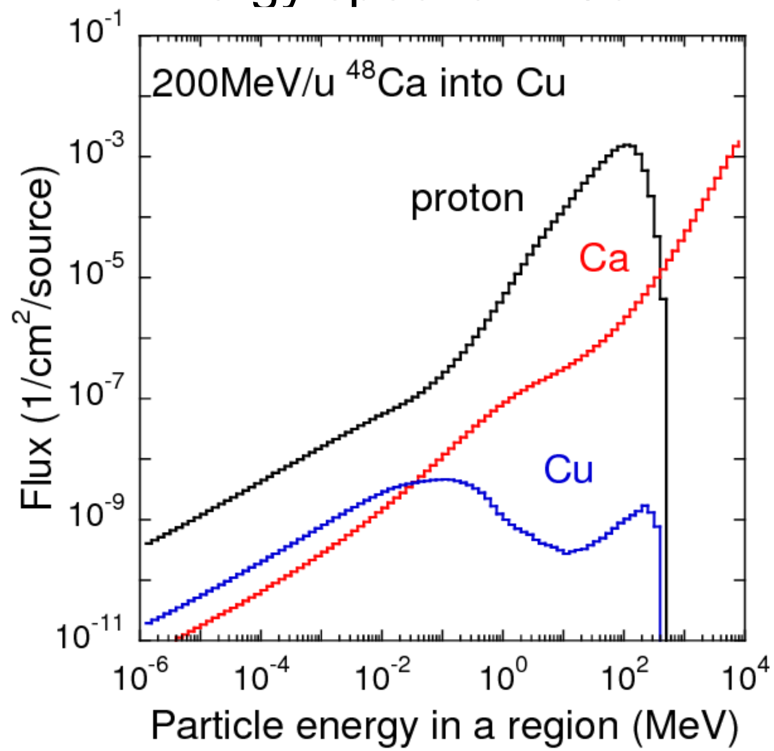
✓Proton DPA is smaller than for heavy-ions because Coulomb scattering cross section of proton is much smaller than that of heavy ions.

(2)200 MeV/nucleon ^{48}Ca into Cu

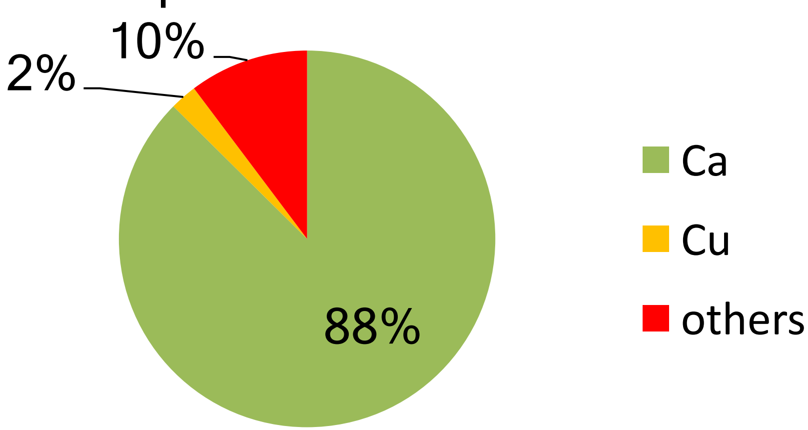
DPA distribution



Energy spectra in Cu



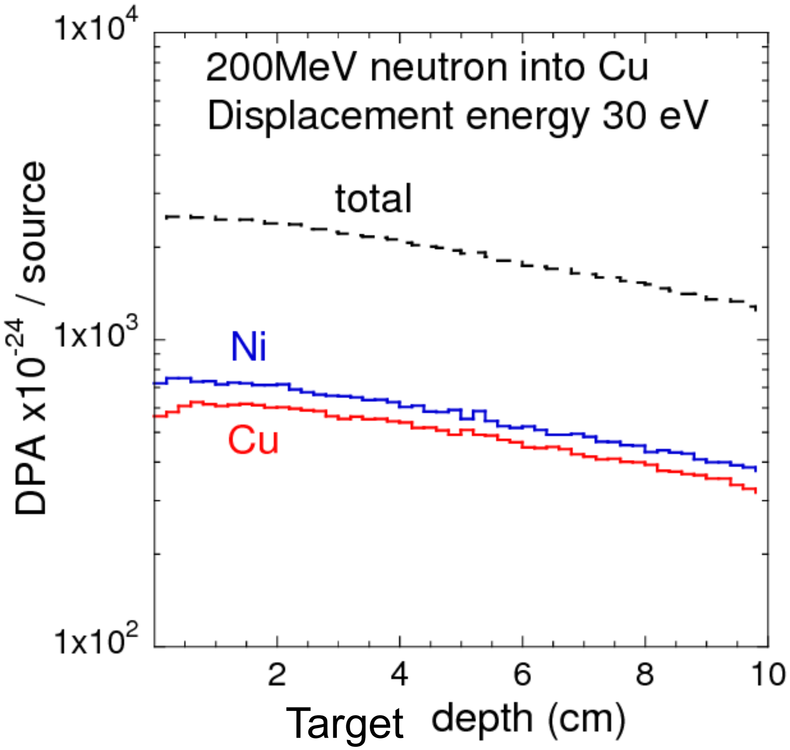
Ratio of partial DPA to total



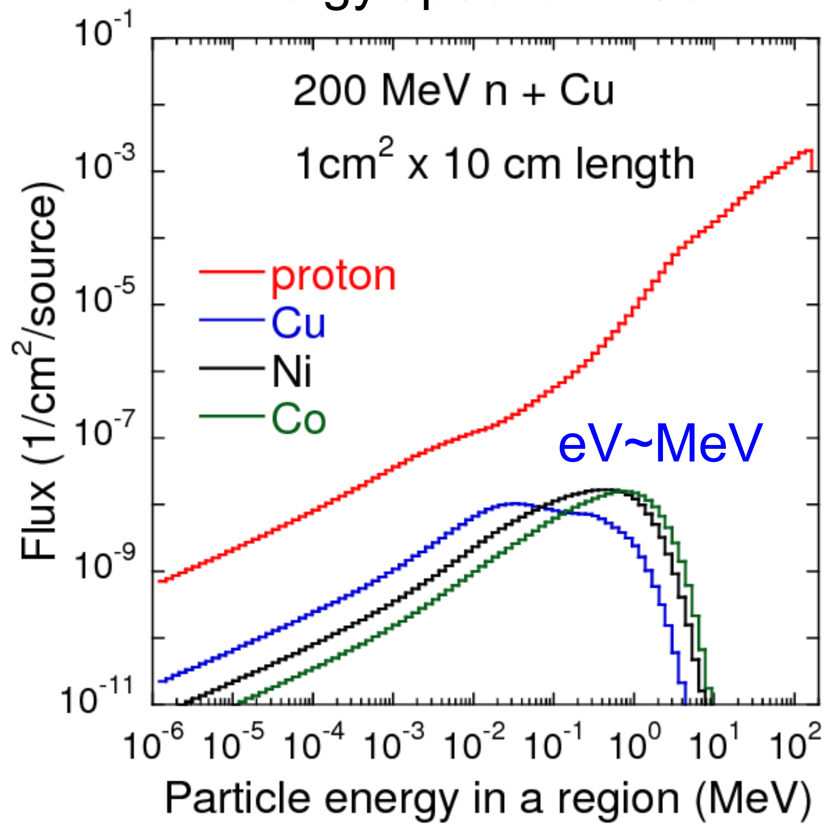
DPA produced by the primary beam is much larger than DPA produced by other contributors.

(3)200 MeV neutron into Cu

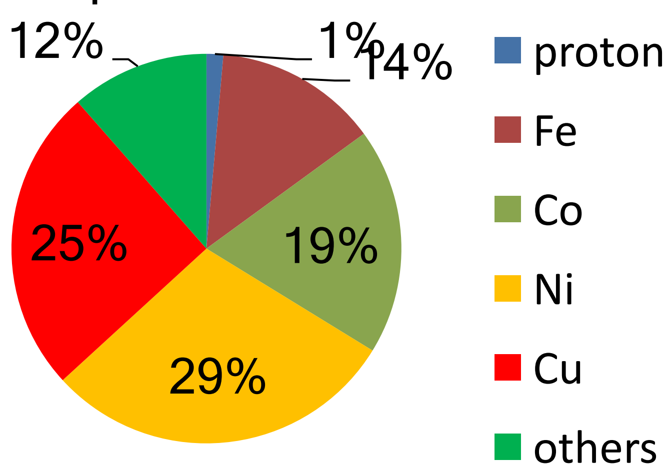
DPA distribution



Energy spectra in Cu



Ratio of partial DPA to total

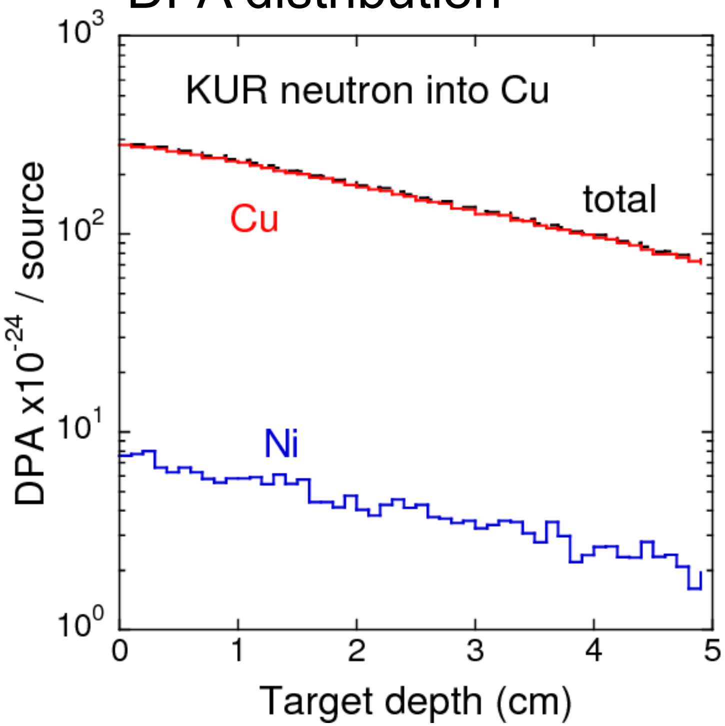


✓Contributions to total DPA by various particles around Cu increase due to nuclear reactions.

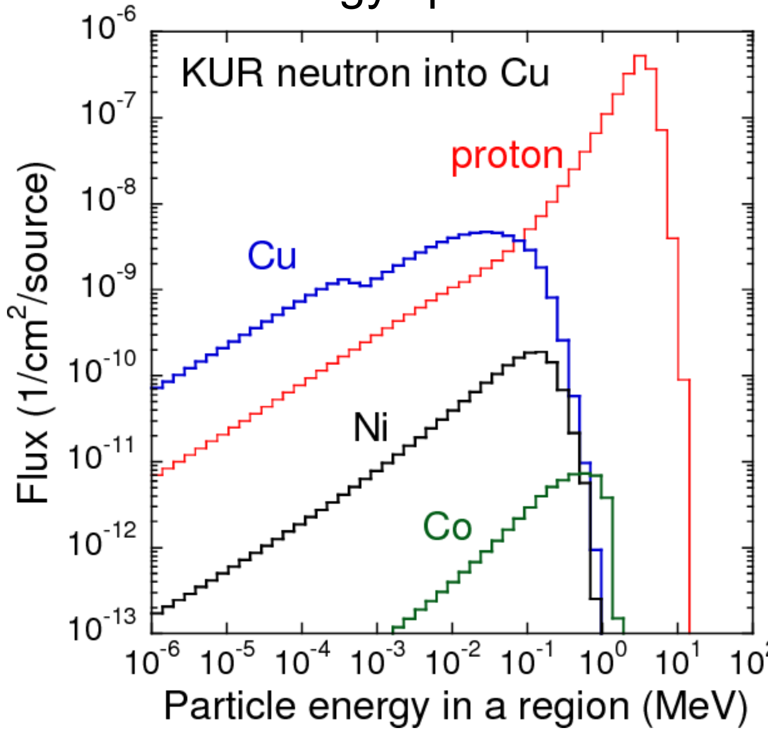
✓Secondary particle distributions for neutron are similar with that for protons.

(4)Reactor neutron into Cu

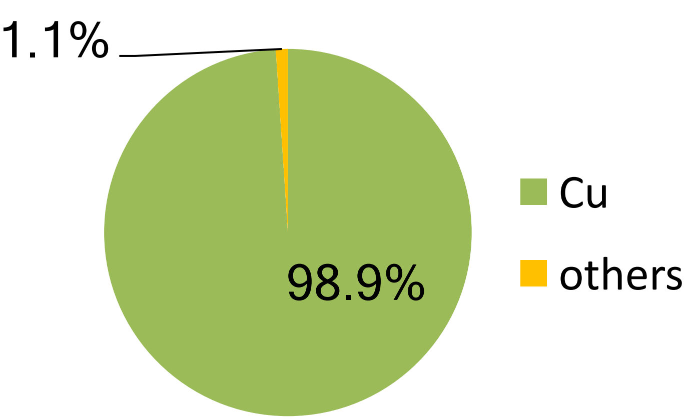
DPA distribution



Energy spectra



Ratio of partial DPA to total



For the low-energy neutron incidence, the target atom is scattered by incident neutron elastic scattering and it contributes to the DPA value

Summary of effect of nuclear reactions

5 cm radius and depth Cu target

	ratio of partial DPA to total (%)						
	proton	^{48}Ca	Fe	Co	Ni	Cu	others
14 MeV proton	89	-	-	-	2	6	3
200 MeV proton	17	-	8	13	27	28	7
14MeV/nucleon ^{48}Ca	-	99.8	-	-	-	-	0.2
200MeV/nucleon ^{48}Ca	-	88	-	-	-	2	10
Reactor neutron in Kyoto U.	-	-	-	-	-	99	1
14 MeV neutron	-	-	-	1	31	68	-
200 MeV neutron	1	-	14	19	29	25	12

Proton: DPA value created by projectile decreased with energy.
DPA created by secondary (Cu, Ni) increase with energy.

Neutrons: reactor: n-Cu elastic scattering produce Cu and contribute to DPA.
Secondary particles produced by nuclear reactions increase with neutron energy.