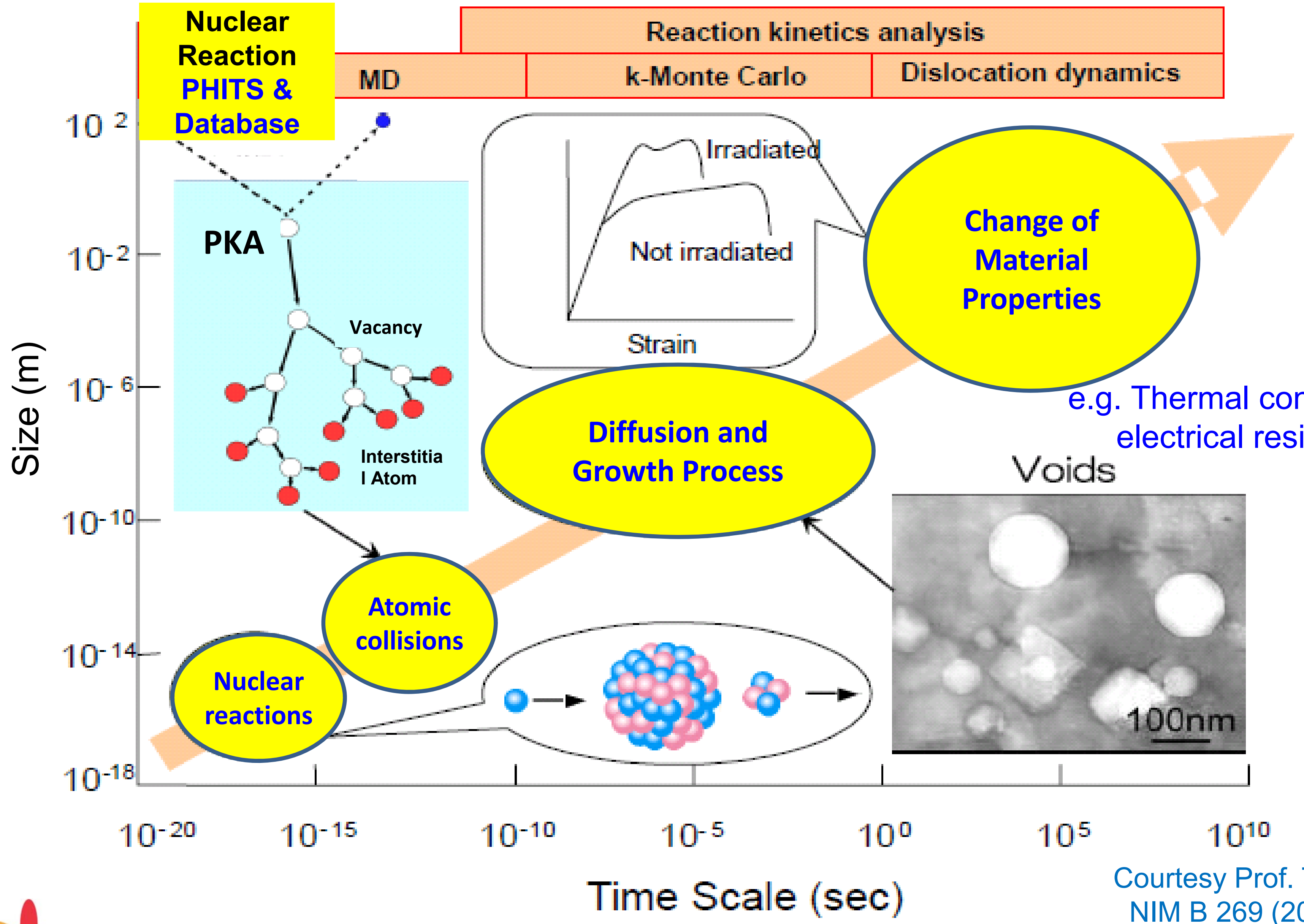
IAEA/TM on Primary Radiation Damage: from nuclear reaction to point defect
1-4 Oct. 2012, VIC, Room A2712, IAEA, Vienna, Austria

A Calculation Method of PKA, KERMA and DPA from Evaluated Nuclear Data with an Effective Single-particle Emission Approximation (ESPEA)
&
Introduction of Event Generator Mode in PHITS Code

Tokio FUKAHORI and Yosuke IWAMOTO
Japan Atomic Energy Agency
fukahori.tokio@jaea.go.jp

Microscopic Effects on Material



Nuclear Reaction
PHITS & Database

Reaction kinetics analysis

MD

k-Monte Carlo

Dislocation dynamics

Nuclear reactions

Atomic collisions

Diffusion and Growth Process

Change of Material Properties

e.g. Thermal conductivity, electrical resistivity

Courtesy Prof. T. Yoshiie,
NIM B 269 (2011) 1740.

Introduction

JENDL PKA/KERMA File (JENDL/PK)

- Purpose

  to supply fundamental data for the estimation of the radiation damage in solid materials

  to supply the PKA data to the FENDL-2 project as a trial task of ESPERANT, processing from the JENDL Fusion File below 20 MeV

- Incident Particle: neutron (< 50 MeV)

- Elements Included in the File: 29 elements, 78 isotopes

  H, Li, Be, B, C, N, O, Na, Mg, Al, Si, Cl, K, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Ge, Zr, Nb, Mo, W, Pb, Bi

ESPERANT Code

Processed from Neutron Data in the JENDL High Energy File up to 50 MeV by Using Effective Single-Particle Emission Approximation (ESPEA)

Introduction

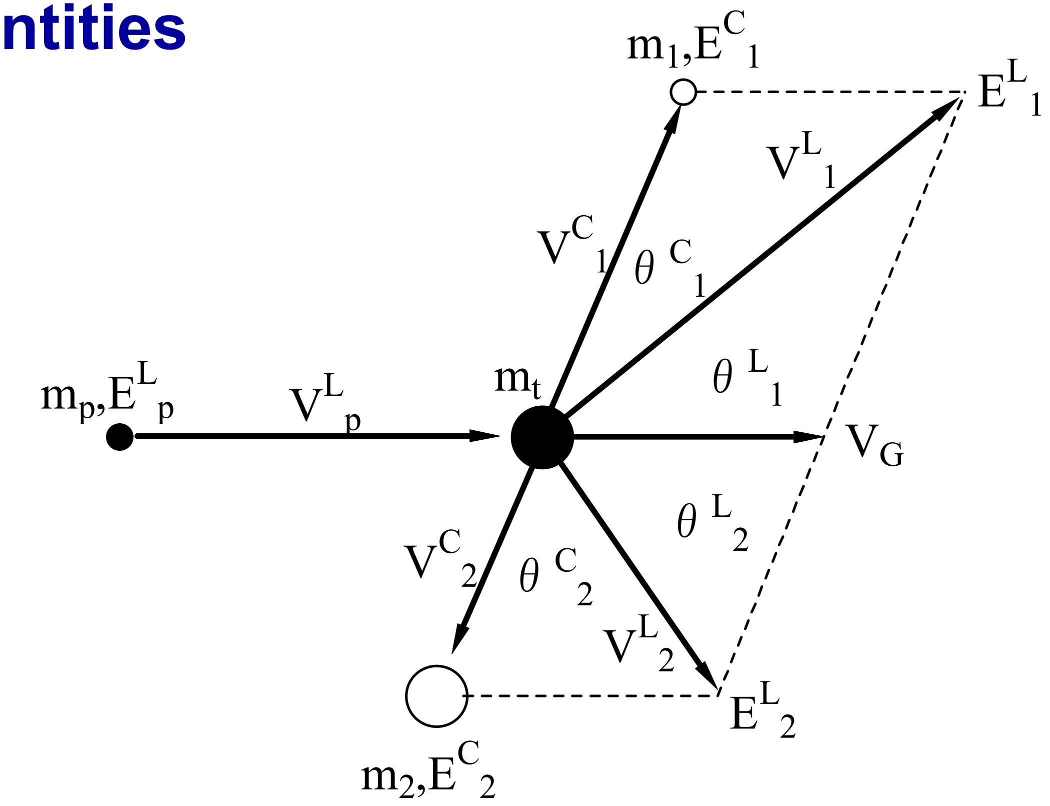
JENDL PKA/KERMA File (JENDL/PK)

Target Quantities and Proposal for MF Numbers

MF	Quantities (PKA File)	Quantities (KERMA File)
3	cross sections	KERMA factors
4	angular distributions for discrete levels	-
6	double-differential light particles and PKA cross sections	-
63	-	DPA cross sections
66	damage energy spectra	-

Introduction

Target Quantities



C, L : CMS and LAB

p, t, 1, 2 : incident particle, target nucleus, outgoing particle and residual nucleus

E, V, m, θ : energy, velocity, mass and emitted angle ($\mu = \cos\theta$)

$\boldsymbol{DDX_{1C}(E_{pL},E_{1C},\mu_{1C})}$: DDX of emitted particle in CMS (given)

$\boldsymbol{DDX_{2C}(E_{pL},E_{2C},\mu_{2C})}$: PKA spectrum in CMS

Introduction

Target Quantities

PKA Spectrum for particle

$$DDX_2^C(E_p^L, E_2^C, \mu_2^C) = \frac{m_2}{m_1} DDX_1^C(E_p^L, E_1^C, \mu_1^C)$$

$$E_2^C = \frac{m_1}{m_2} E_1^C \qquad \mu_2^C = -\mu_1^C$$

PKA Spectrum for γ-ray

$$DDX_2^C(E_p^L, E_2^C, \mu_2^C) = \frac{m_2 c^2}{E_\gamma} DDX_\gamma(E_p^L, E_\gamma, \mu_\gamma)$$

$$E_2^C = \frac{E_\gamma^2}{2m_2 c^2} \qquad \mu_2^C = -\mu_\gamma$$

Introduction

Target Quantities

Damage Energy Spectra: σ_{D}

$$\sigma_D(E_p^L, E_2^L, \mu_2^L) = E_D(E_2^L) \cdot DDX_2^L(E_p^L, E_2^L, \mu_2^L)$$

E_{D} by Lindhard-Robinson in energy unit of eV

$$E_D(E_2^L) = \frac{E_2^L}{1 + k \cdot g(\varepsilon)}$$

$$k = 0.13372 \cdot Z^{2/3} / A^{1/2}$$

$$g(\varepsilon) = 3.48008\varepsilon^{1/6} + 0.40244\varepsilon^{3/4} + \varepsilon$$

$$\varepsilon = E_2^L \big/ 86.931 Z^{7/3}$$

DPA Cross Section: σ_{DPA}

$$\sigma_{DPA}(E_p^L) = \iint \nu(E_2^L)\sigma_D(E_p^L, E_2^L, \mu_2^L) dE_2^L d\mu_2^L$$

$$\nu(E_2^L) = \frac{\kappa}{2\varepsilon_d} E_D(E_2^L)$$

$$\kappa = 0.8$$

ε_{d}: threshold energy for displacement

KERMA Factor for x-Reaction: $KERMAx(E_{\mathrm{p}}^{\mathrm{L}})$

$$KERMA_x(E_p^L) = \iint (E_{1x}^L + E_{2x}^L) DDX_{2x}^L(E_p^L, E_{2x}^L, \mu_{2x}^L) dE_{2x}^L d\mu_{2x}^L$$

Effective Single-Particle Emission Approximation

Normalization Factor for ESPEA

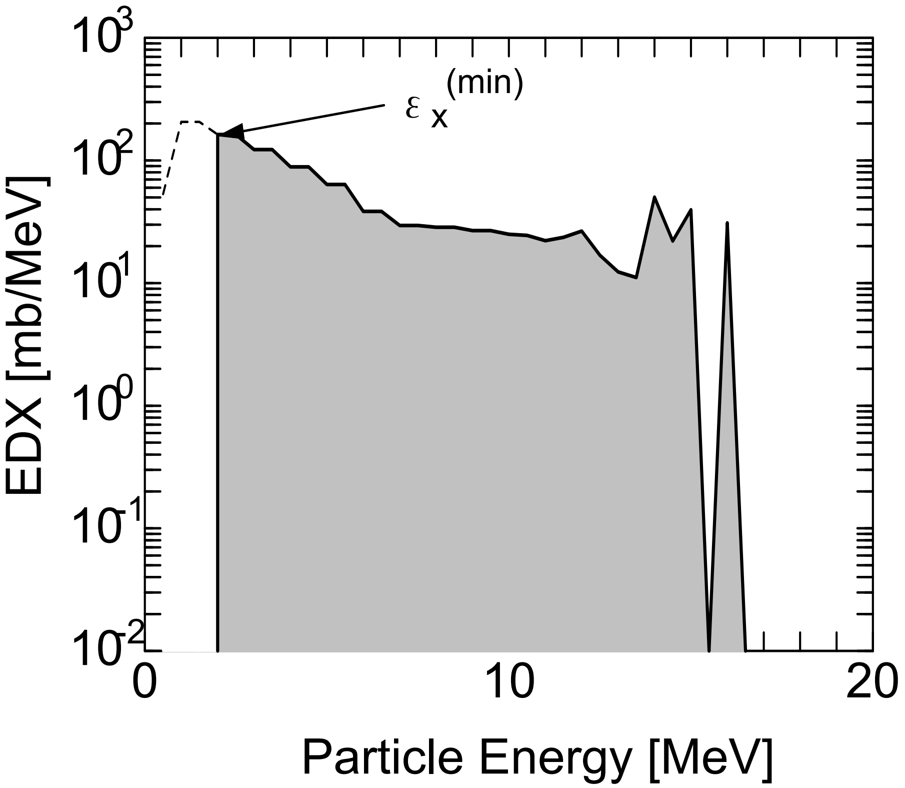
$$R = \frac{\sigma_R}{\sum_x \int_{\varepsilon_x^{(\min)}} d\varepsilon_x \int d\mu_x \sigma_x (E_p^L, \varepsilon_x, \mu_x)}$$

σ_R:	total reaction cross section
σ_x:	each particle emission channel
$\varepsilon_x^{(\min)}$:	lower limit of energy for spectrum considered.

$$\int_{\varepsilon_x^{(\min)}} \varepsilon_x f_x(\varepsilon_x) d\varepsilon_x = \left[\frac{m_t}{m_p + m_t} E_p^L + Q_x\right] \Big/ \left[1 + \left(\frac{m_{1x}}{m_{2x}}\right)^2\right]$$

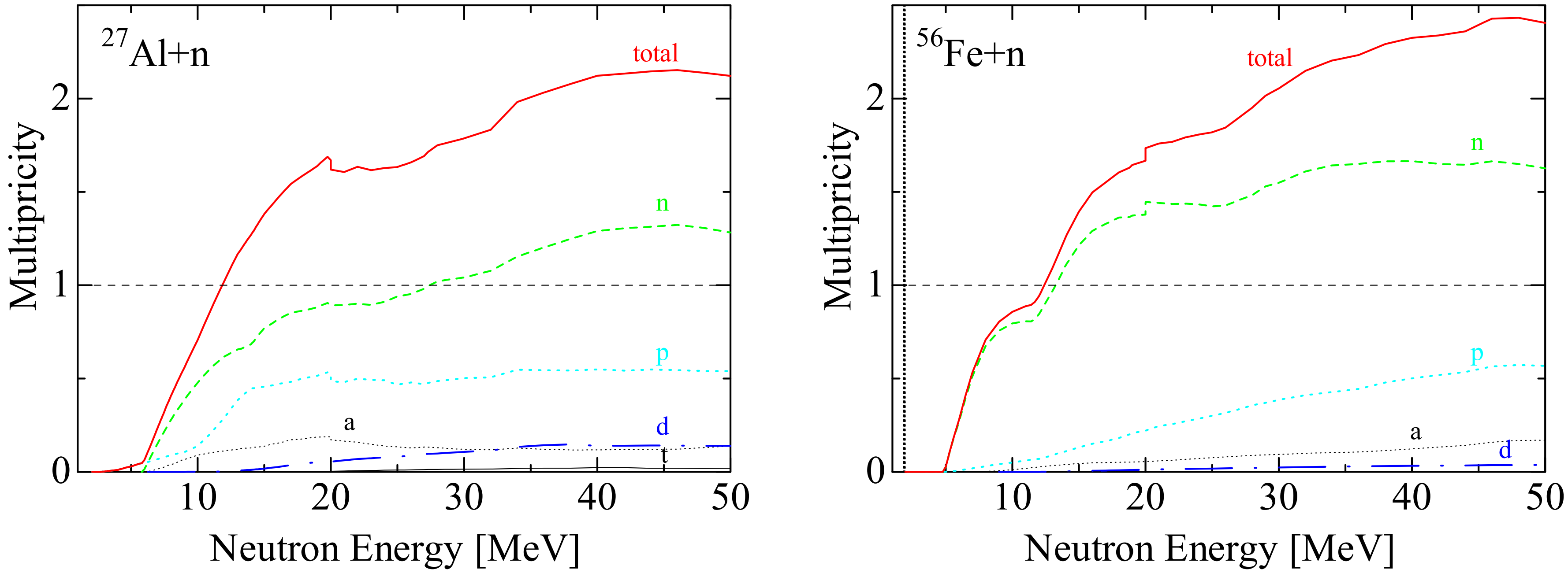
$$\int_0^\infty f_x(\varepsilon_x) d\varepsilon_x = 1$$

Q_x:	Q-value of reaction ***x***
f_x:	normalized ***DDX***1C of reaction ***x***



Effective Single-Particle Emission Approximation

Particle Multiplicity



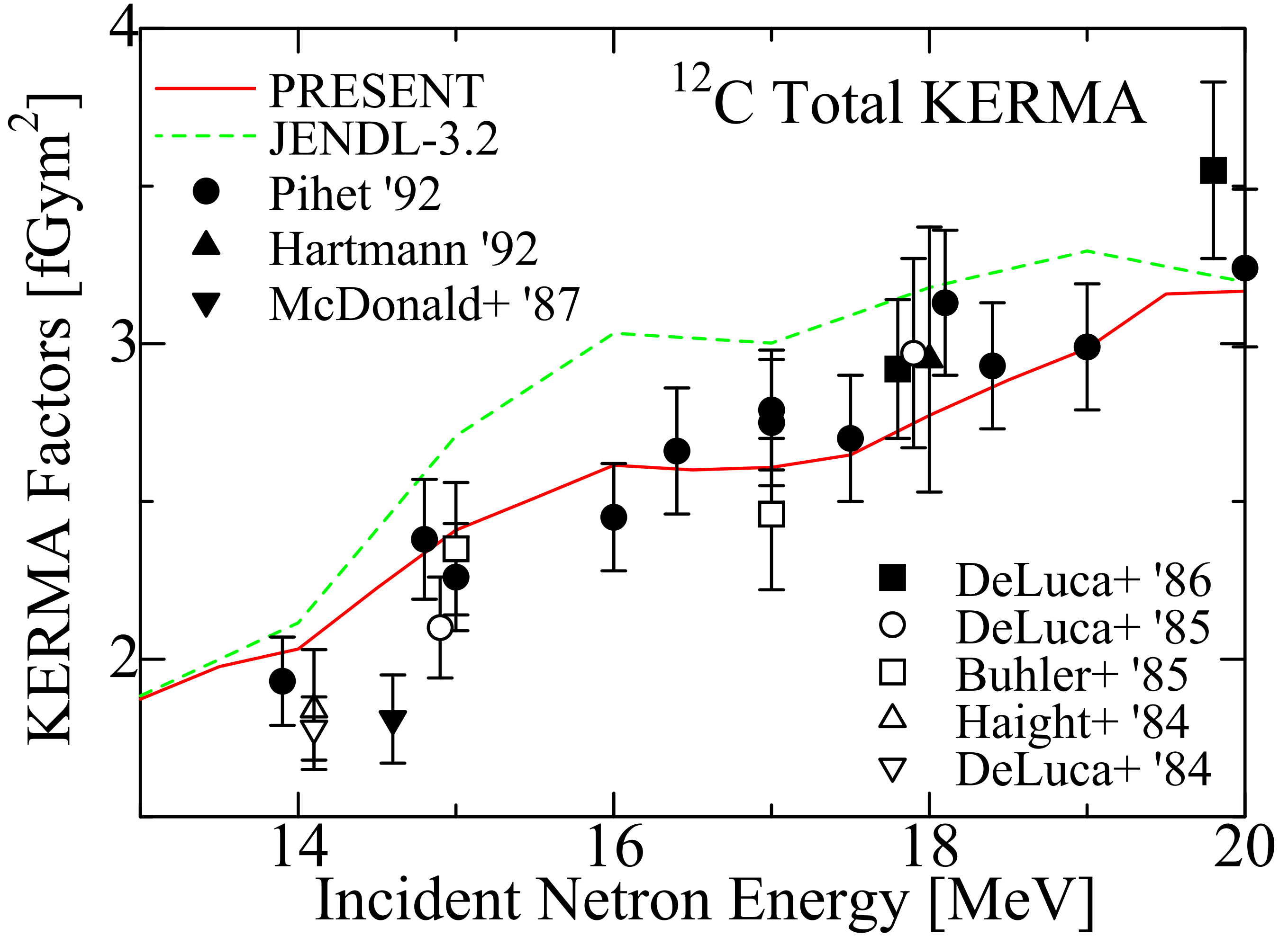
JENDL PKA/KERMA File (JENDL/PK)

Compilation of threshold energy for displacement: ε_d

Atomic Number	Symbol	ε_d [eV]	Atomic Number	Symbol	ε_d [eV]
4	Be	31	27	Co	40
6	C	31	28	Ni	40
12	Mg	25	29	Cu	40
13	Al	27	40	Zr	40
14	Si	25	41	Nb	40
20	Ca	40	42	Mo	60
22	Ti	40	47	Ag	60
23	V	40	74	W	90
24	Cr	40	79	Au	30
25	Mn	40	82	Pb	25
26	Fe	40		others	25

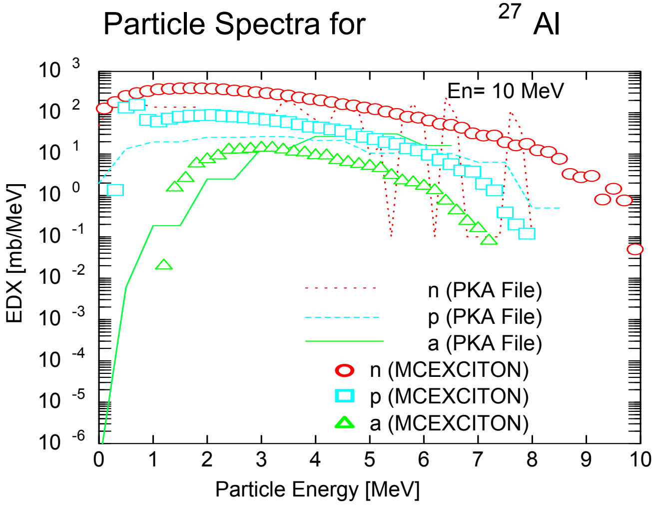
JENDL PKA/KERMA File (JENDL/PK)

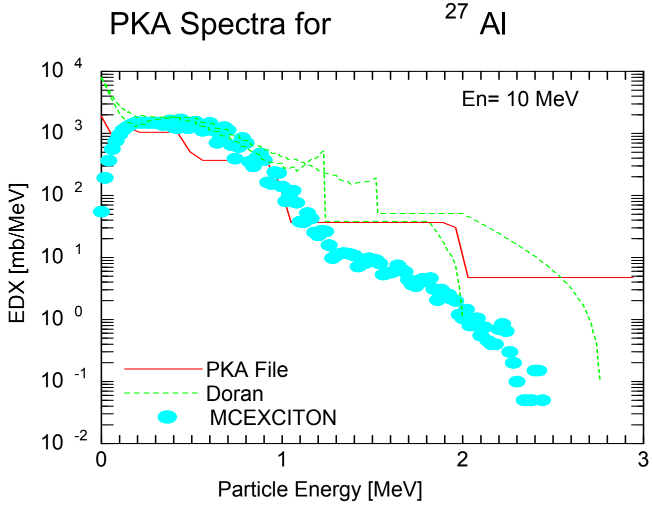
KERMA Factor of ^{12}C

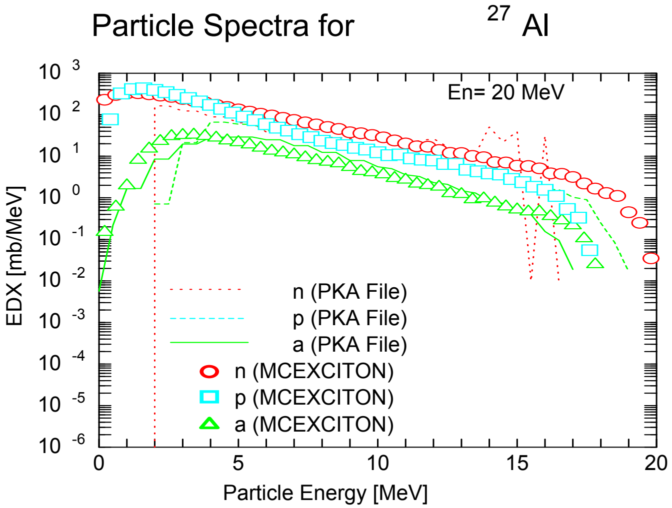


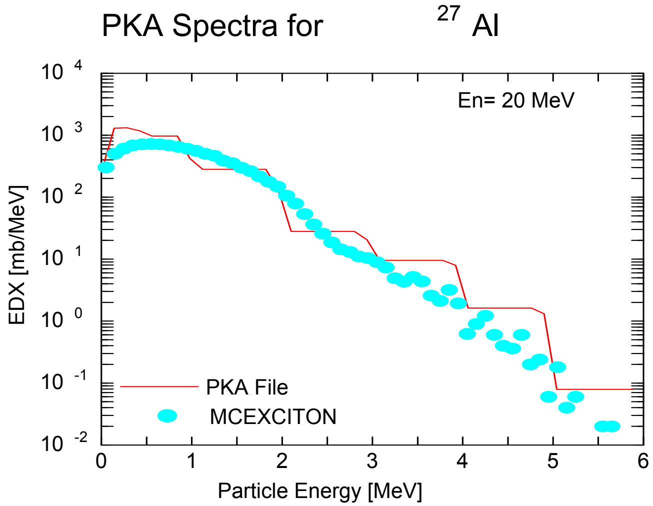
JENDL PKA/KERMA File (JENDL/PK)

Particle and PKA Spectra of ^{27}Al at 10 and 20 MeV


Particle Spectra for ^{27}Al

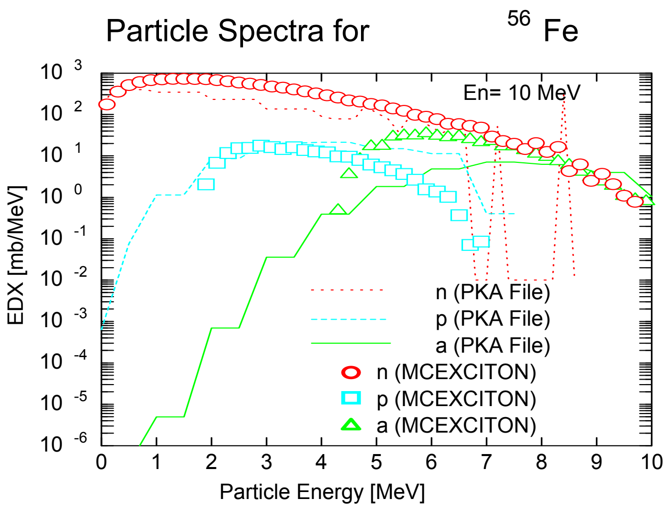

PKA Spectra for ^{27}Al

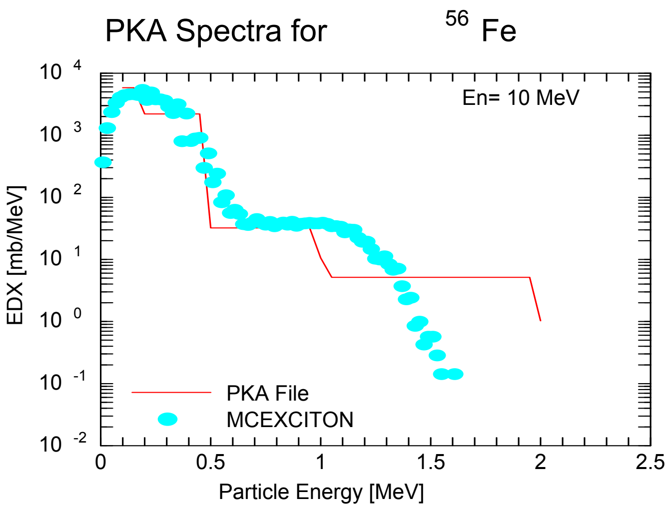

Particle Spectra for ^{27}Al

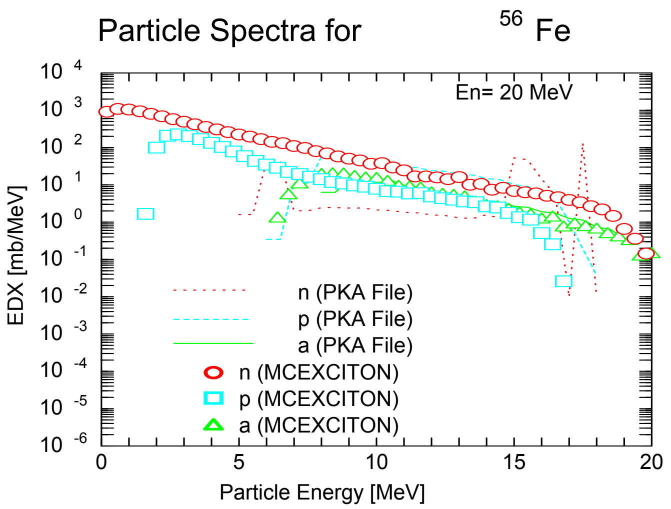

PKA Spectra for ^{27}Al

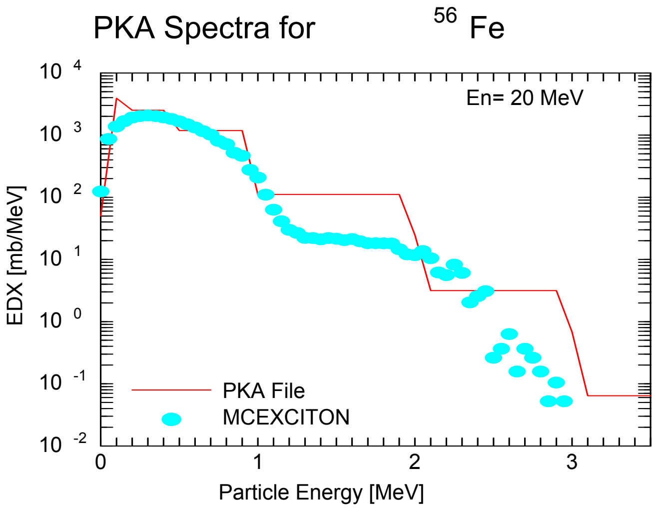
JENDL PKA/KERMA File (JENDL/PK)

Particle and PKA Spectra of ^{56}Fe at 10 and 20 MeV

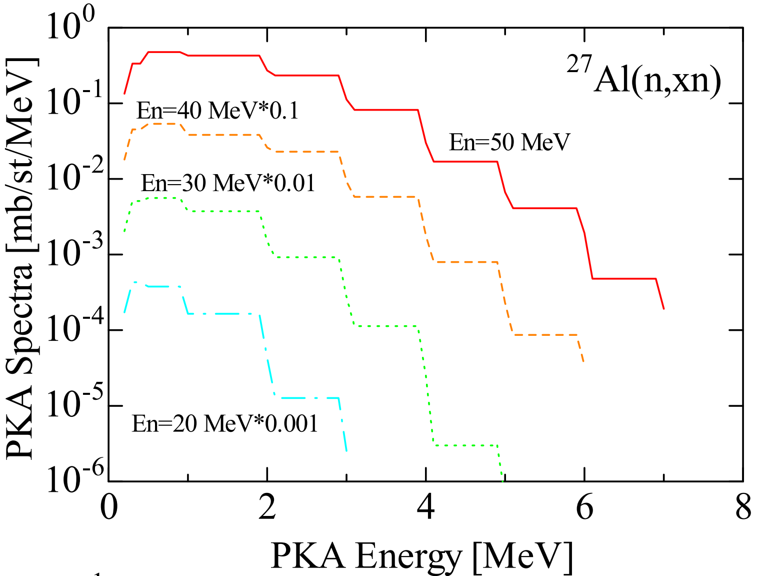


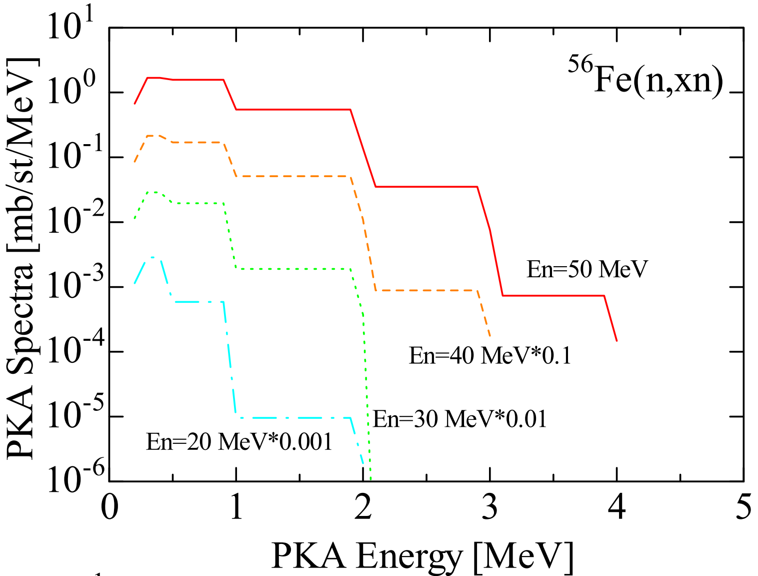


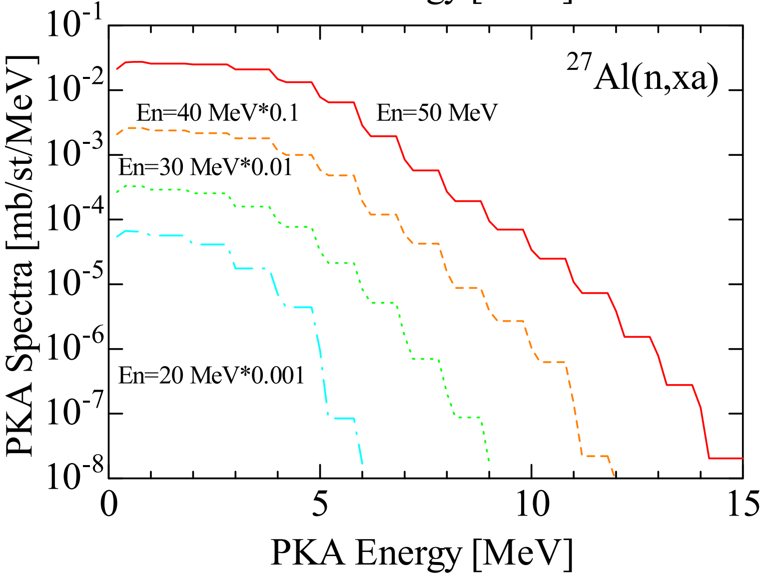


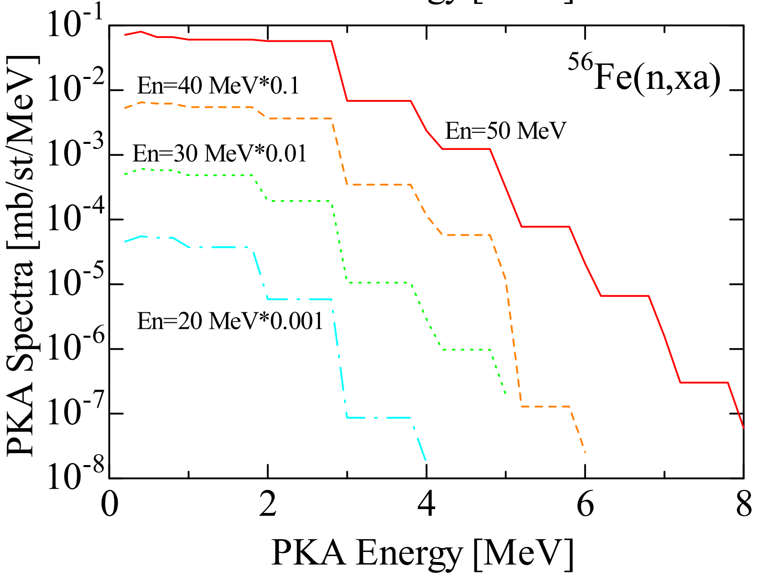


PKA Spectra of ^{27}Al and ^{56}Fe at Other Incident Energies



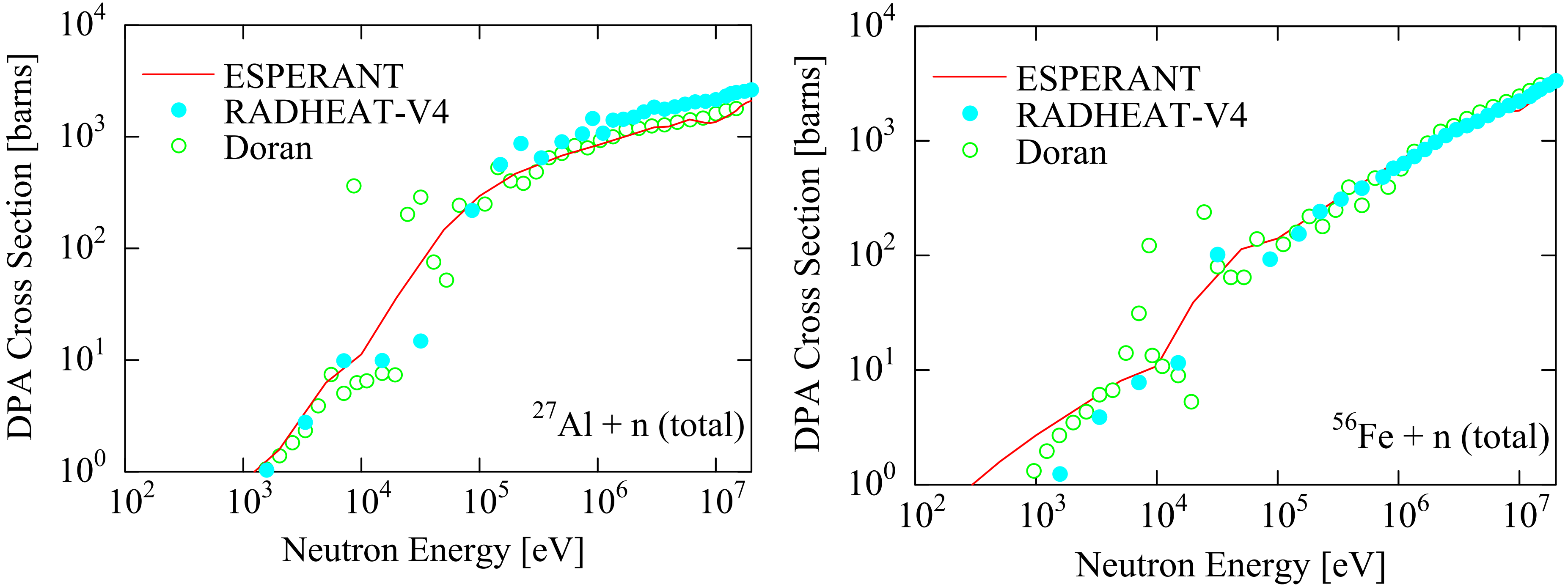






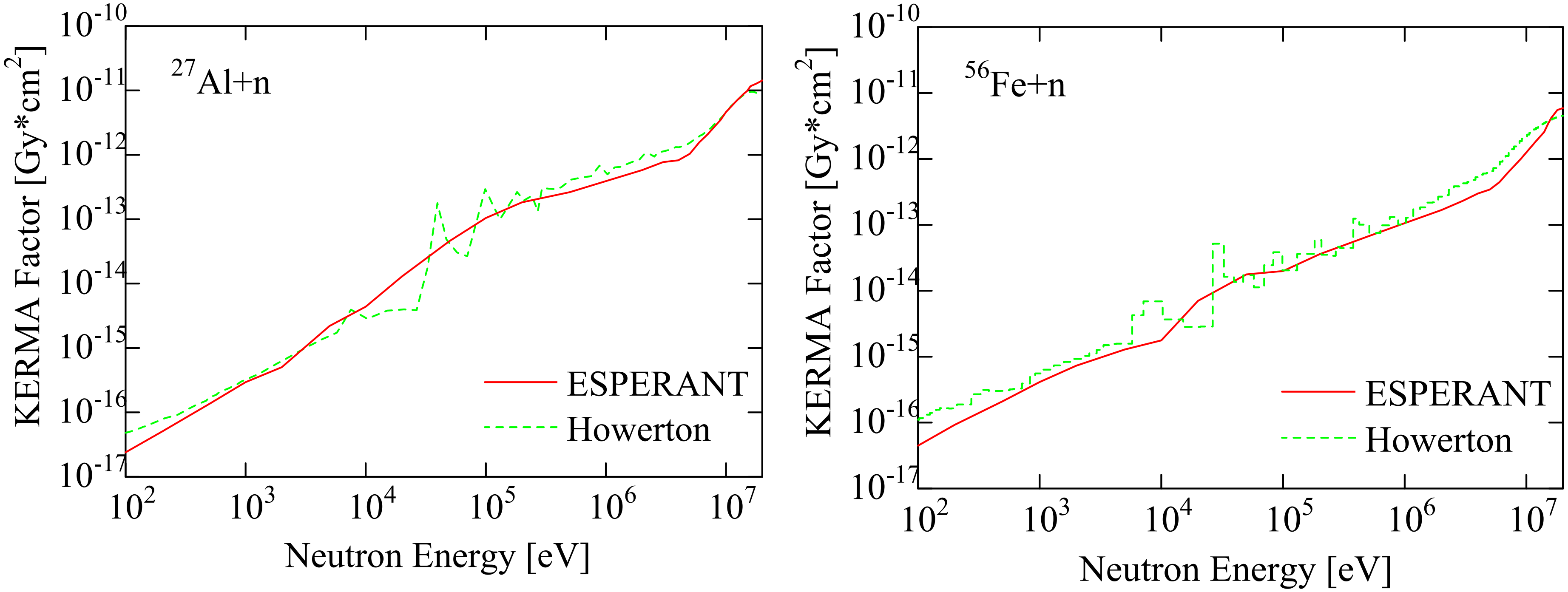
JENDL PKA/KERMA File (JENDL/PK)

DPA Cross Sections of ^{27}Al and ^{56}Fe



JENDL PKA/KERMA File (JENDL/PK)

KERMA Factors of ^{27}Al and ^{56}Fe



Displacement Damage Calculation in PHITS

Nuclear Reaction Model

Simulate many body phenomena by generating an event in the calculation

- Any observables
- Coincident data, pulse height…
- Energy is conserved in an "Event"

Event Generator

Nuclear Data Library

Solve the Boltzmann Equation using the test particle method for one-body phase space distribution

- Only one-body observables
- No correlated quantities
- Energy is conserved in average

Not Event Generator

We sometimes would like to know beyond one-body observables…

- Pulse-height distribution of detector irradiated by low-energy neutrons
- Dose equivalent based on Q(L) relationship (Siebert and Schuhmacher 1995)
- Deposition energy distribution in semi-conductor devices

Y. Iwamoto et al., *Nucl. Instr. and Meth. B* 274, 57-64 (2012).

Event Generator Mode in PHITS

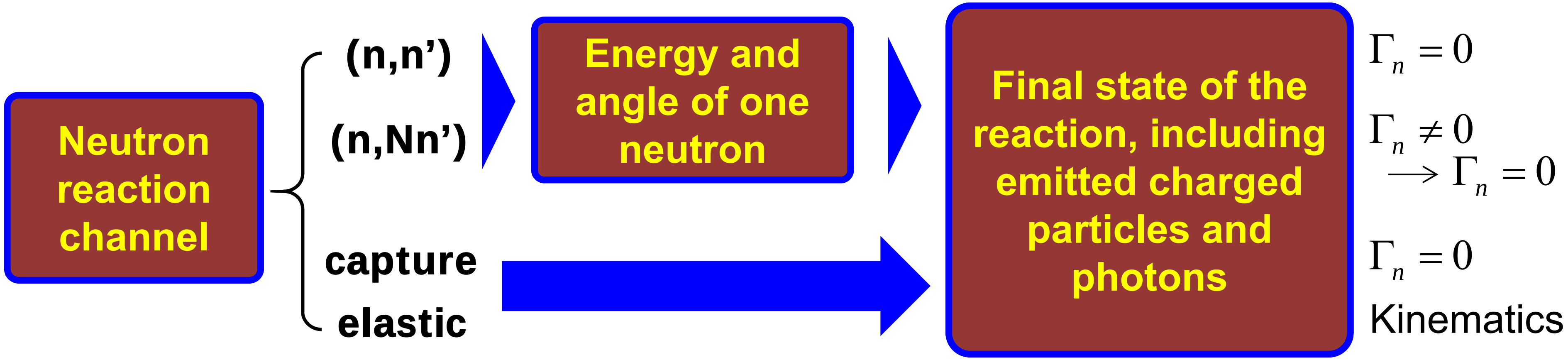
Nuclear Data Library

- Channel cross section
- Inclusive DDX of neutron

\+

Special Evaporation Model

- Binary decay of recoiled nucleus
- Neutron decay width Γ_n is adjusted



Neutron reaction channel

(n,n')

(n,Nn')

capture

elastic

Energy and angle of one neutron

Final state of the reaction, including emitted charged particles and photons

$\Gamma_n = 0$

$\Gamma_n \neq 0$

$\longrightarrow \Gamma_n = 0$

$\Gamma_n = 0$

Kinematics

Using this mode, we can determine …

- all ejectiles (neutrons, charged particles, recoil nucleus and photons) with keeping energy and momentum conservation
- deposit energy without using local approximation (Kerma factor)

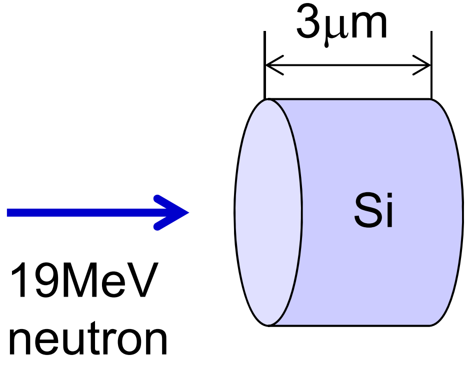
Y. Iwamoto, et al., Proc. of ND2007.

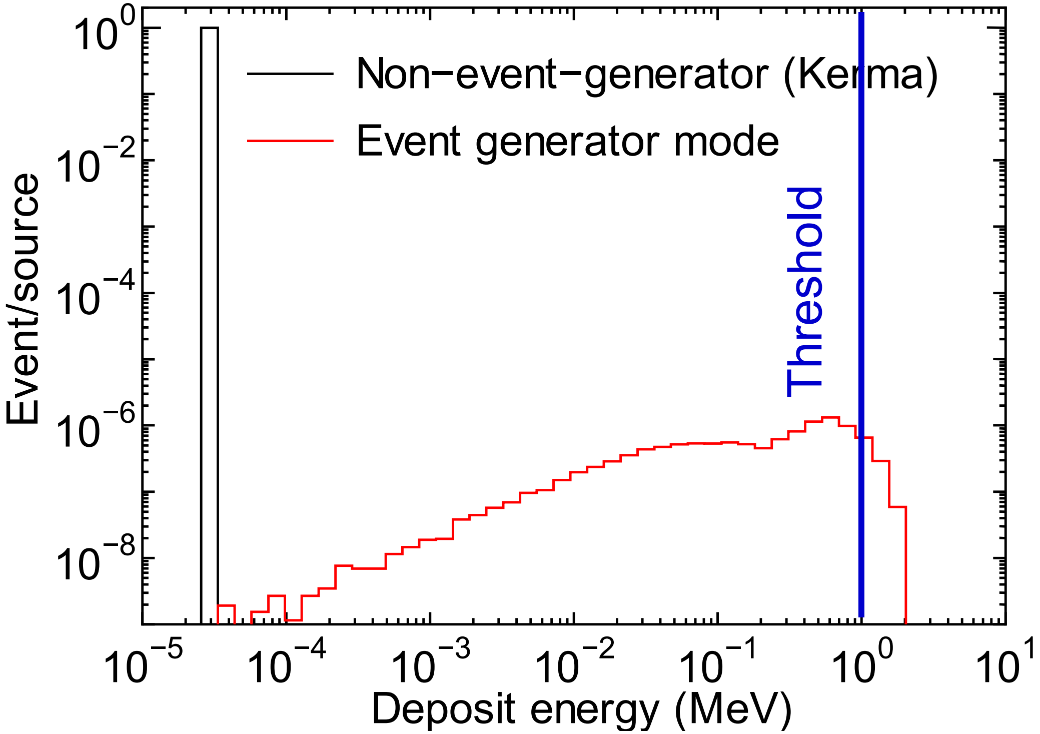
Example of Event Generator Mode

Single Event Upset (SEU) of Semi-conductor Devices

- SEU occurs when deposition energy exceeds a certain threshold
- SEU probability = 0 from non-event generator simulation
- SEU probability = 10^{-6}/source from event generator simulation

→ Critical mistake!





Deposition energy distribution in 3μm Si

DPA Calculated in PHITS

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

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

ϕ : irradiation fluence (particles/cm^2)

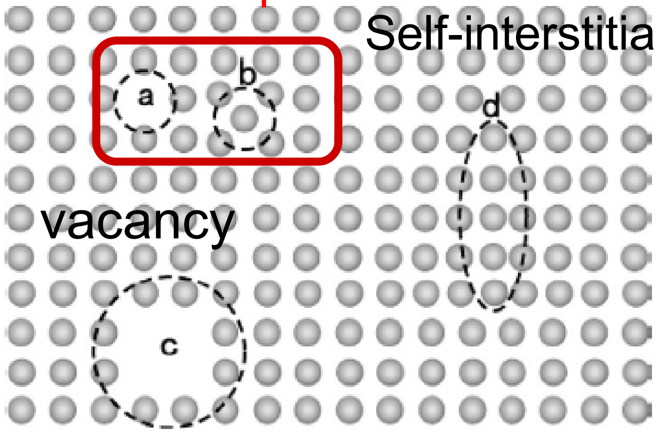
$$\mathbf{DPA}=\int \sigma_{disp}(E)\phi(E)dE$$

Related to the number of Frenkel pairs N_F:

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

N_i : number of particles

Frenkel pair



Note: liquid is not damaged.

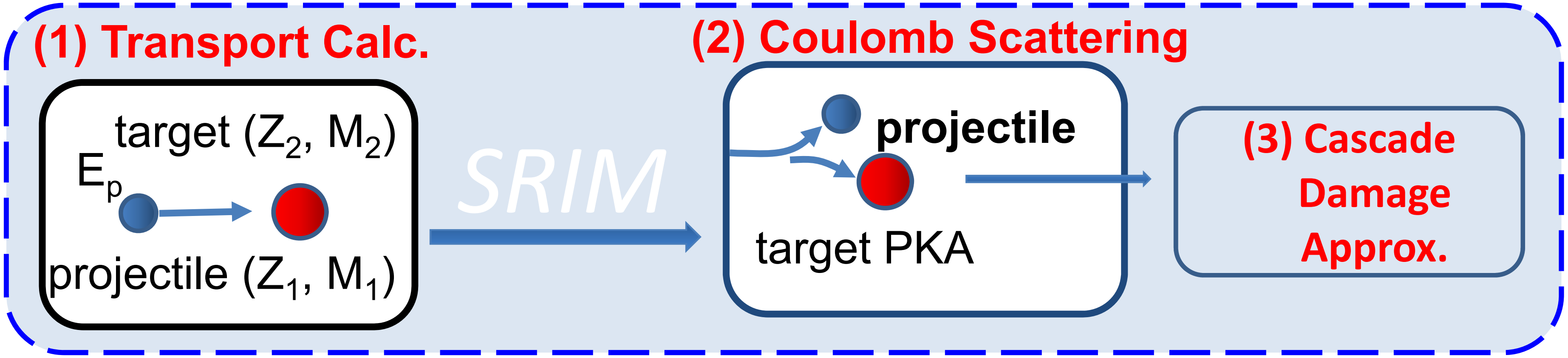
DPA is used to compare radiation damage by different radiation sources.

Not much is known for high energy protons, neutrons, and heavy-ions

Radiation Damage Calculation in PHITS

SRIM (Transport of Ions in Matter): Major code for radiation damage calc.

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



✓transport charged particles.

✓no treatment of nuclear reaction and nuclear elastic scattering
no production of PKAs created by the secondary particles

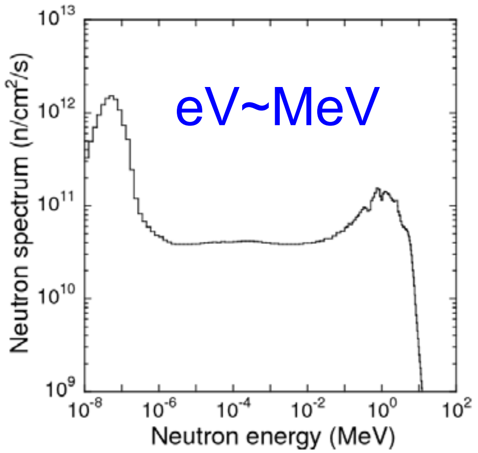
to extend to high-energy region and to incident neutrons

The DPA models in the advanced Monte Carlo particle transport codes have been developed. Development of DPA model including Coulomb scattering and a nuclear reaction model.(**e.g. PHITS, MARS, FLUKA, MCNP**)

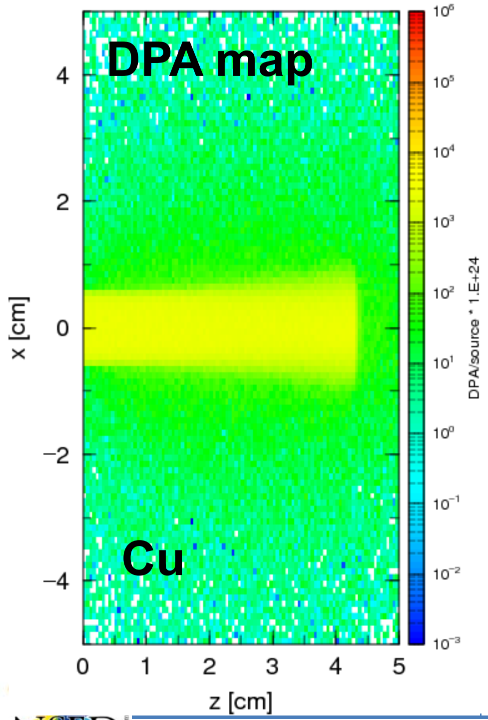
Effects of Nucl. Reaction and Elastic Scattering

Calculation Condition

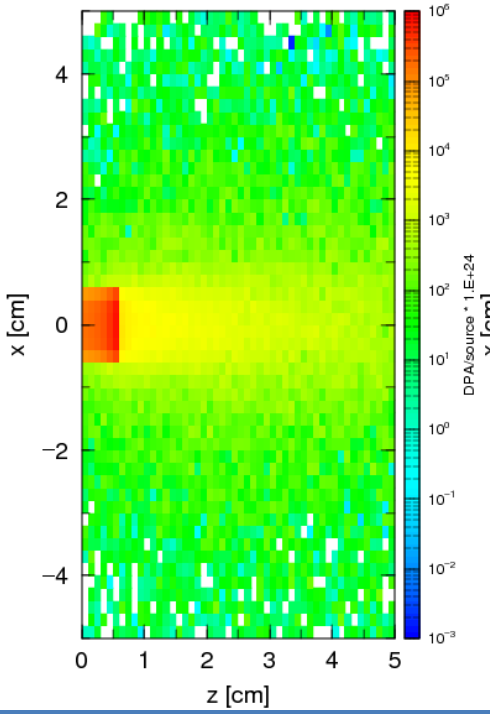
- ✓Beam size: 1cm^2
- ✓Target: 5 cm radius x depth Cu
- ✓Displacement energy: 30 eV



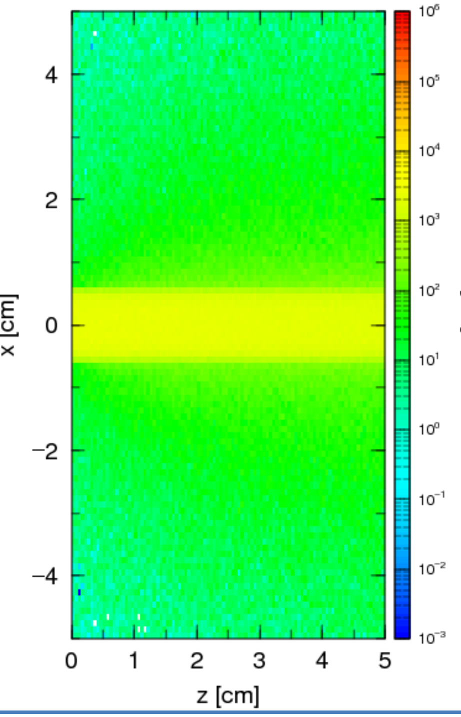
(1)200 MeV proton



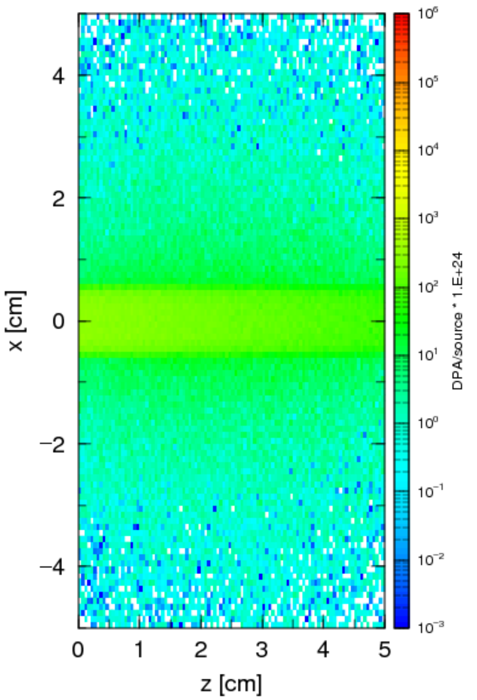
(2)200 MeV/u ^{48}Ca



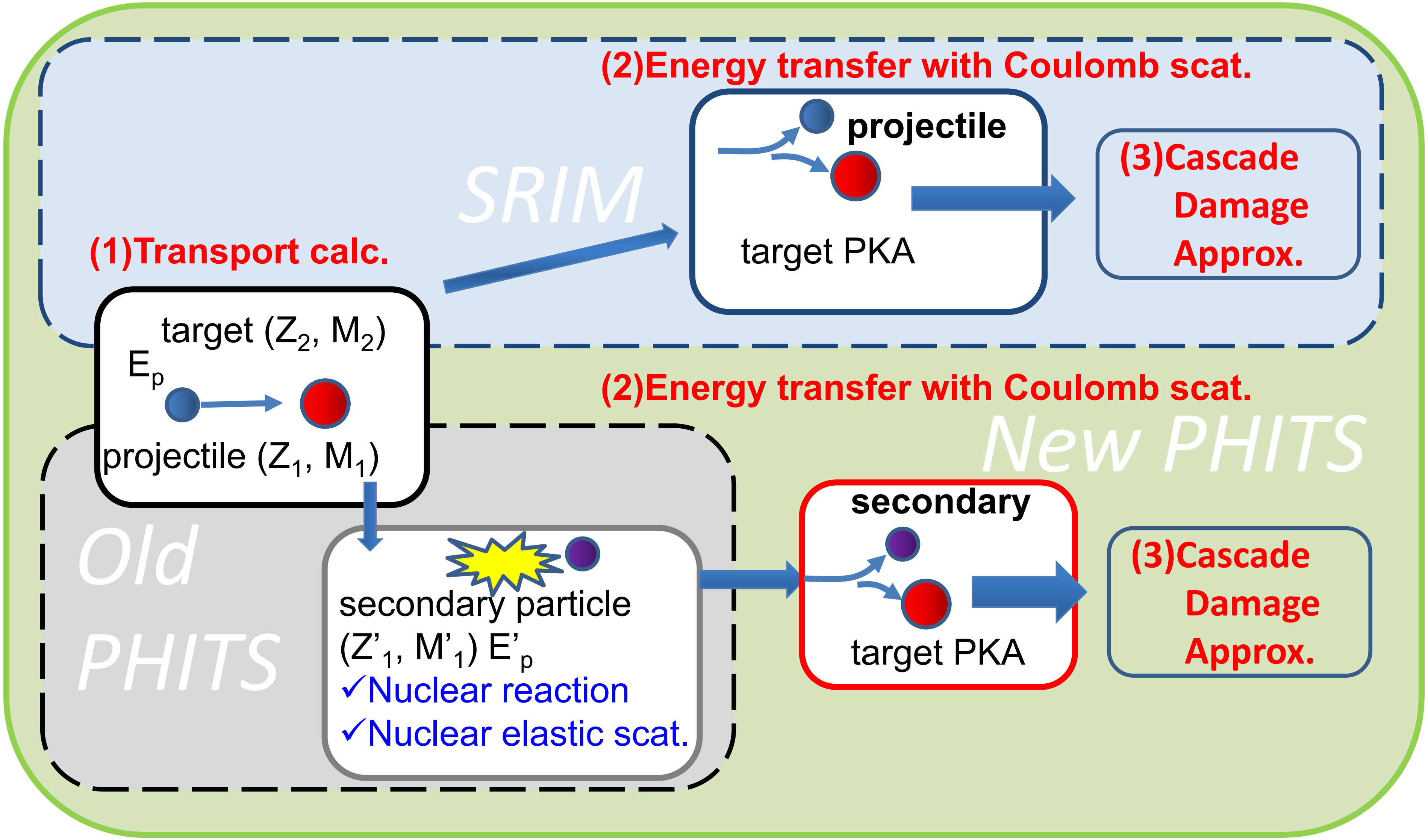
(3)200 MeV neutron



(4)Reactor Neutron



Implementation of DPA model in PHITS



SRIM

(1)Transport calc.

target (Z_2, M_2)

E_p

projectile (Z_1, M_1)

(2)Energy transfer with Coulomb scat.

projectile

target PKA

(3)Cascade Damage Approx.

Old PHITS

secondary particle (Z'_1, M'_1) E'_p

✓Nuclear reaction

✓Nuclear elastic scat.

New PHITS

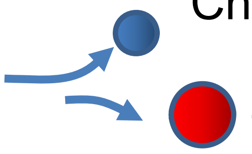
(2)Energy transfer with Coulomb scat.

secondary

target PKA

(3)Cascade Damage Approx.

(2) Energy transfer with Coulomb scattering in PHITS



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

leads to the deflection of the particles

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

Coulomb scat. cross section: one parameter

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

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

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

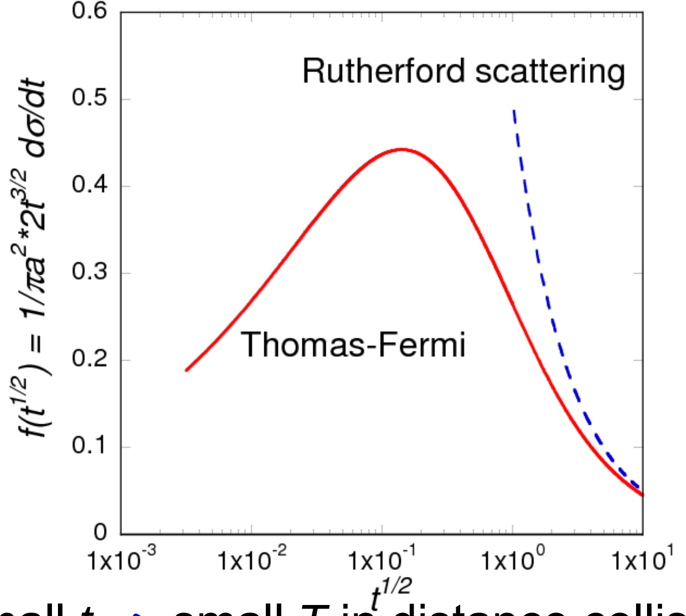
ε :dimensionless energy

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

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

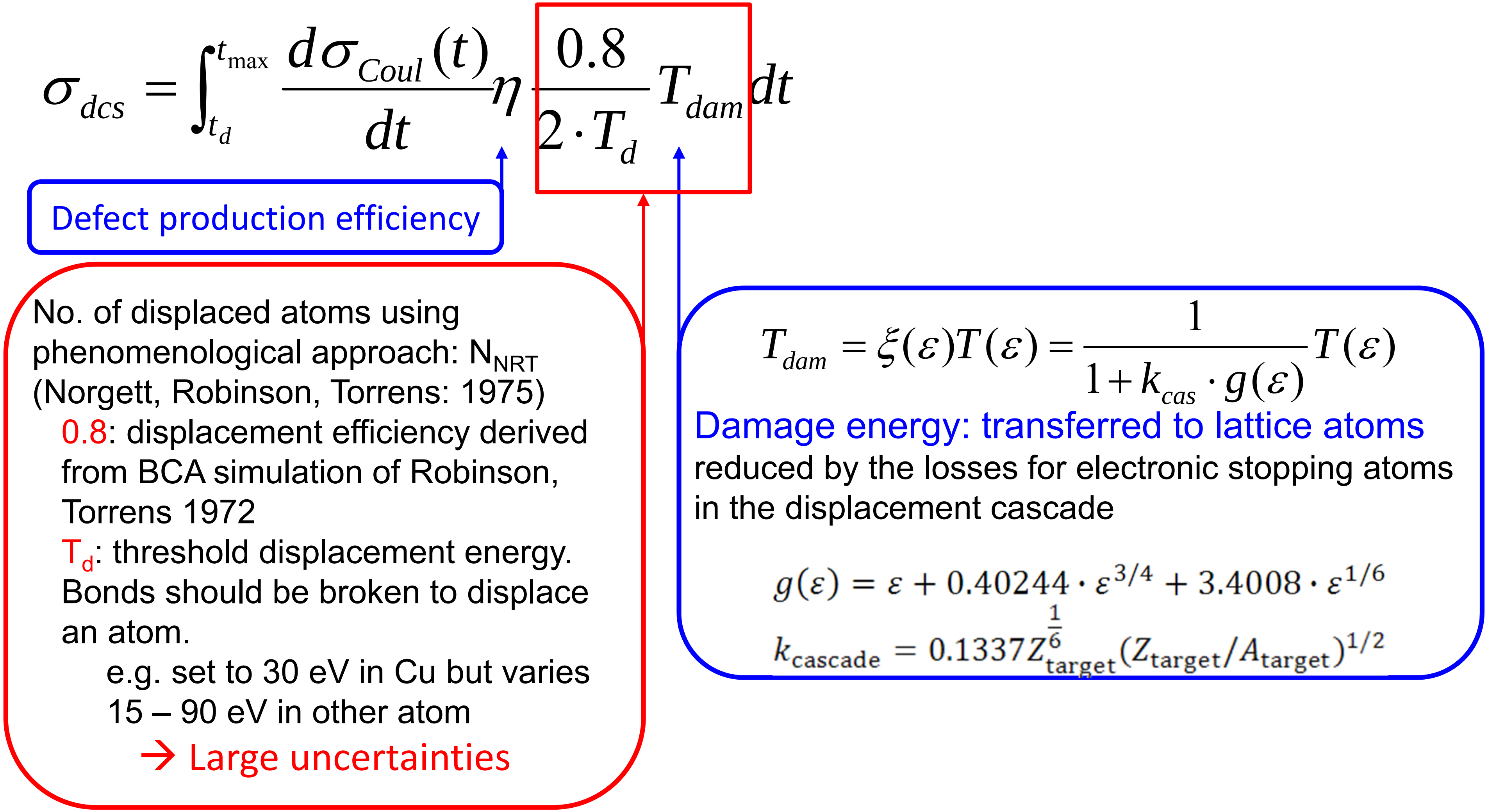


Small *t* → small *T* in distance collisions

Large *t* → large *T* in close collisions

(3) Cascade Damage Approximation in PHITS

Displacement Cross Section (dcs)



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

Defect production efficiency

No. of displaced atoms using phenomenological approach: N_{NRT} (Norgett, Robinson, Torrens: 1975)

0.8: displacement efficiency derived from BCA simulation of Robinson, Torrens 1972

T_d: threshold displacement energy. Bonds should be broken to displace an atom.

e.g. set to 30 eV in Cu but varies 15 – 90 eV in other atom

→ Large uncertainties

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

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

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

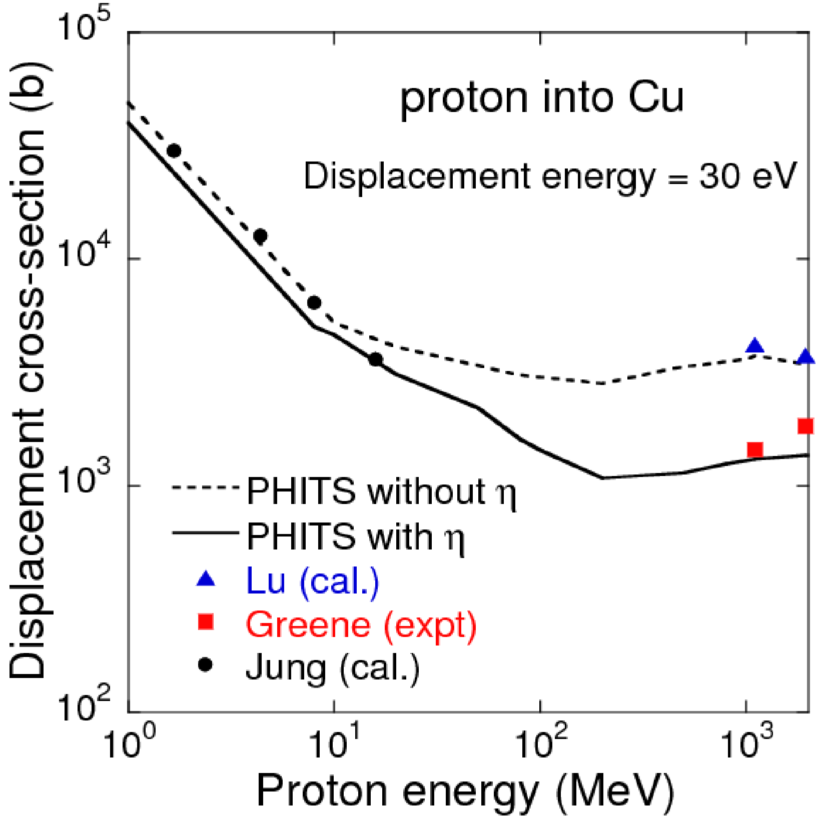
$$k_{cascade} = 0.1337 Z_{target}^{\frac{1}{6}}(Z_{target}/A_{target})^{1/2}$$

Efficiency of Defect Production in PHITS

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

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

N_D: number of stable displacements at the end of collision cascade ⬅ MD and BCA
N_{NRT}: number of defects calculated by NRT model



Displacement cross section with η reproduces the experimental data in the high-energy region.

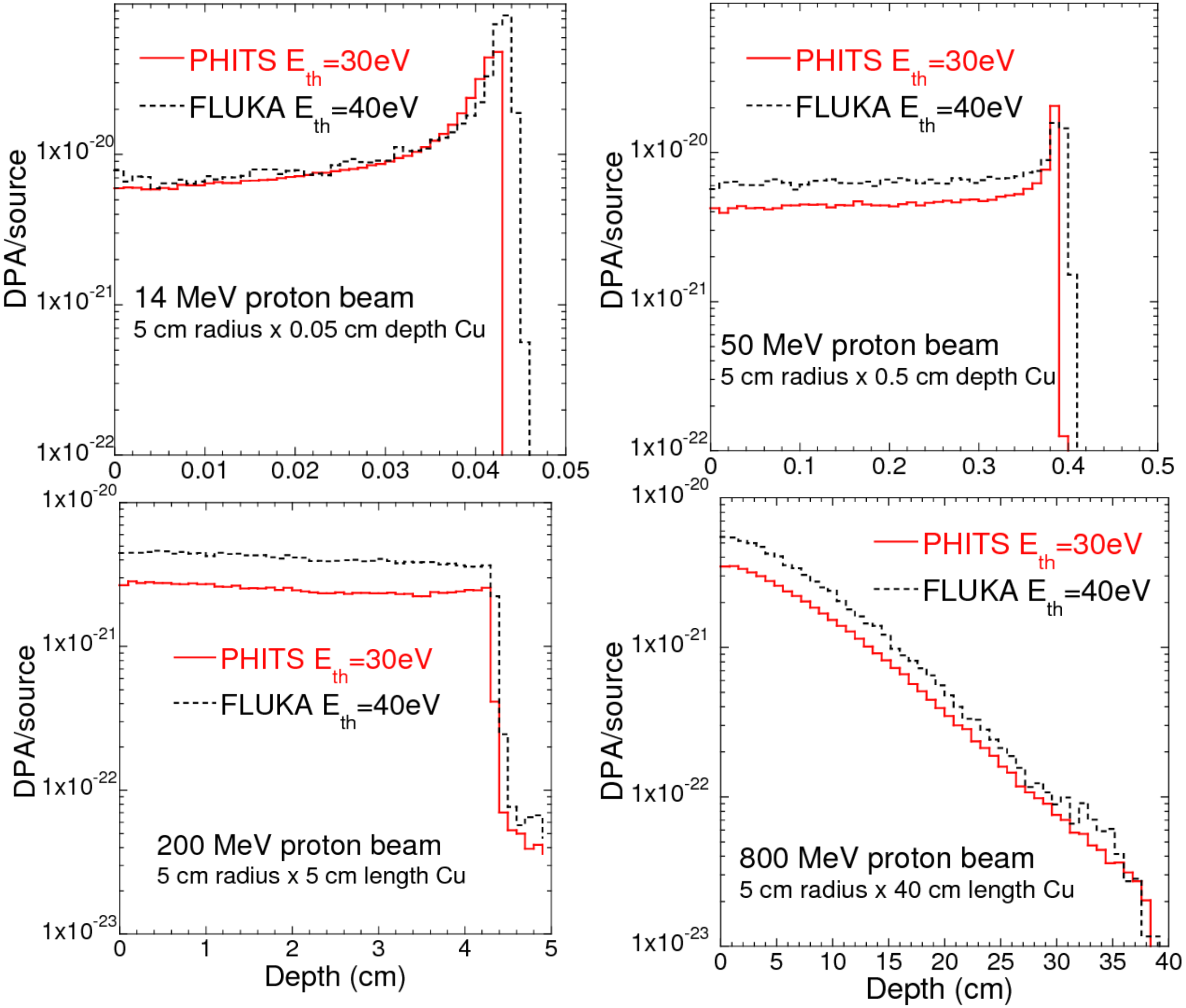
Comparison with Other Codes

A) Proton into Cu

well-developed hadronic cascades.

✓Nuclear reactions occur before the stopping range is reached.

DPA by PKA's directly created by the secondary are increased with energy.



DPA Estimations using PHITS

$$DPA_{total} = \int \sigma_{proj}(E_{proj})\phi_{proj}(E_{proj})dE_{proj} + \sum_{i} \int \sigma_{i}(E_{i})\phi_{i}(E_{i})dE_{i}$$

$DPA_{projectile}$

$\sigma_{proj}(E)$: dcs of proj. (cm^2)

$\phi_{proj}(E)$: fluence of proj. in a region (particles/cm^2)

Remarks: 0 for neutron

$DPA_{secondary}$

i: type of sequential particles

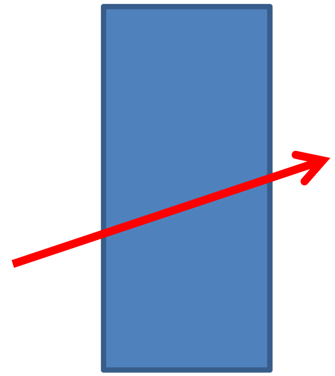
$\sigma_{i}(E)$: dcs of secondary (cm^2)

$\phi_{i}(E)$: fluence of secondary in a region (particles/cm^2)

needs scattering and reaction models

PHITS calculates dcs and fluence of all charged particles event by event.

PHITS Simulation



Average energy E_{ave} of a charged particle in a region

↓ (E_{ave}, M_1, Z_1)

Displacement Cross Section: σ

e1 e2

Range(e1) Range(e2)

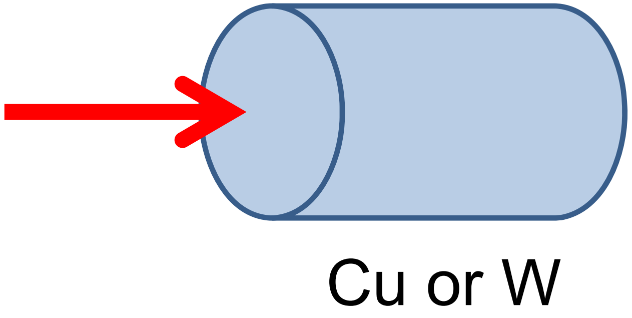
delt=Range(e1)-Range(e2)

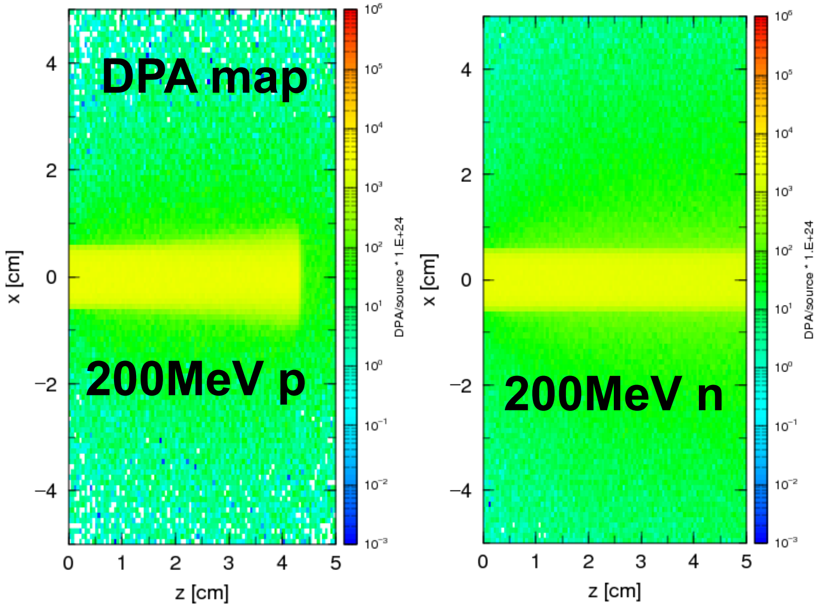
$$DPA = \frac{\sum(\sigma \times delt \times dens)}{\sum dens \times Volume}$$

Comparison with Other Codes

Calculation Condition

Beam area: 1cm^2
Target: 5 cm radius x depth Cu



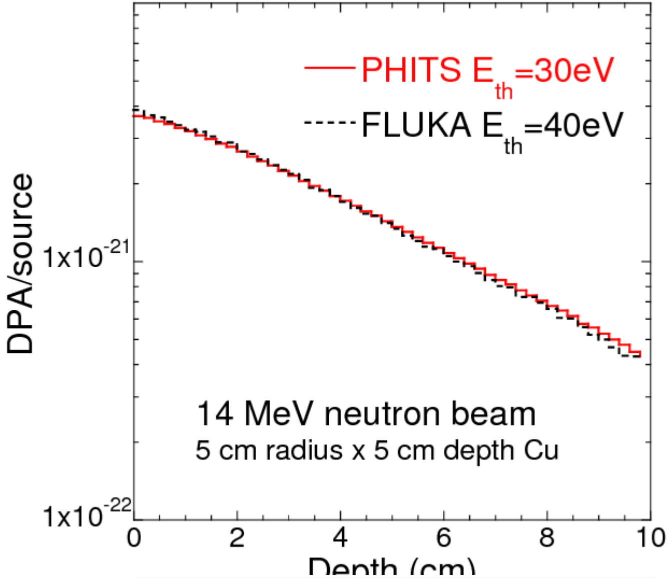


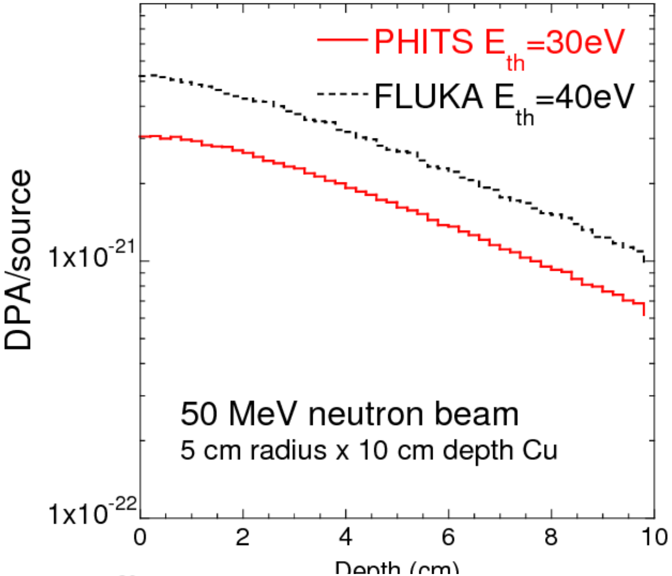
Codes: PHITS(Bertini/GEM), FLUKA(Peanut/ABLA), MARS

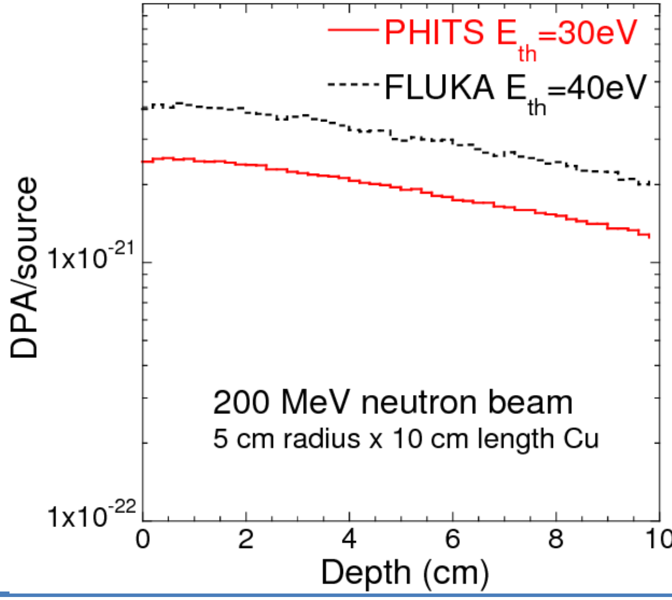
case	Incident particle	Energy(MeV/nucleon)	target	code
A)	proton	14, 50, 200, 800	Cu	PHITS,FLUKA
B)	neutron	14, 50, 200, 800	Cu	PHITS,FLUKA
C)	^{76}Ge	130	W	PHITS,FLUKA, MARS

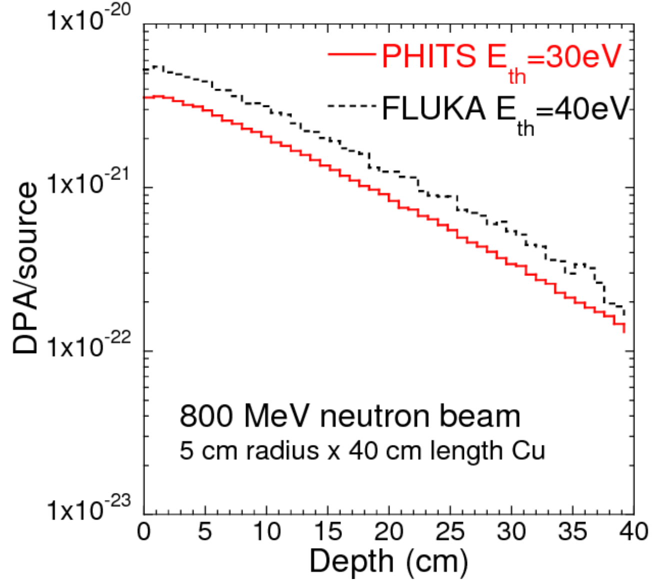
Comparison with Other Codes

B) Neutron into Cu







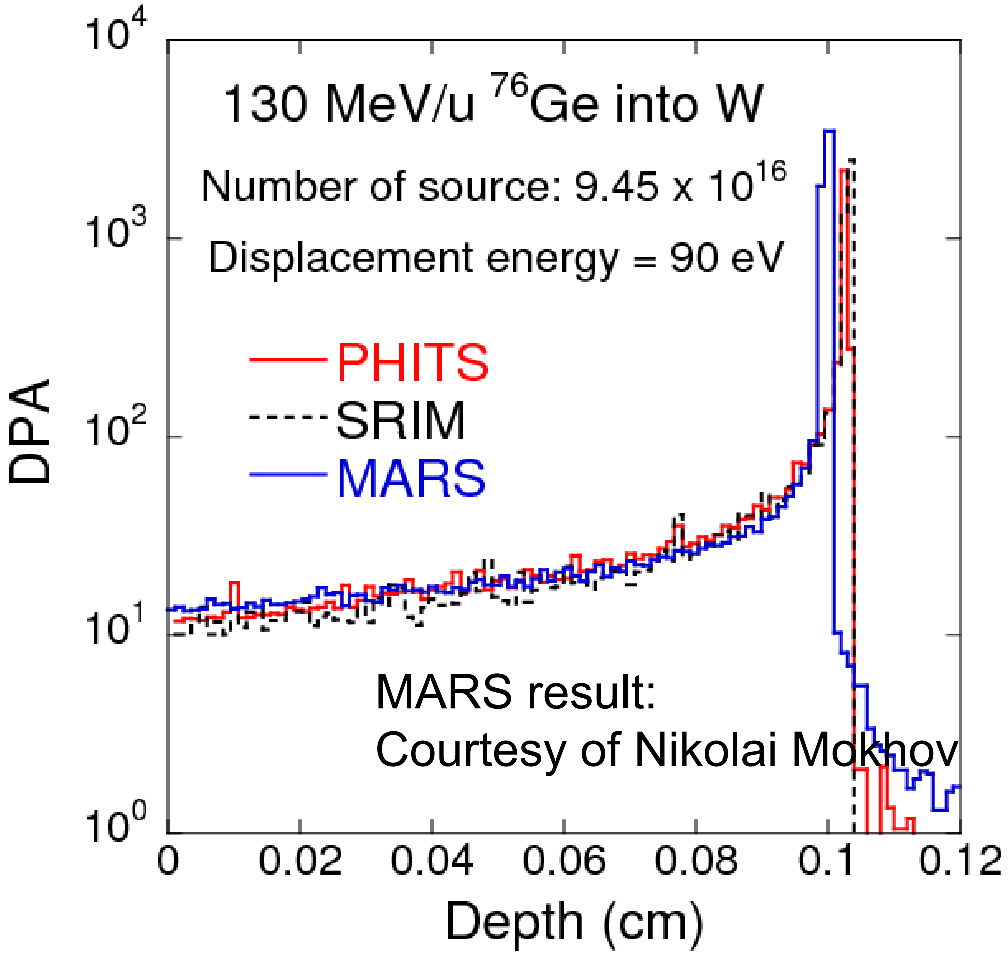


✓ Secondary created by nuclear elastic scattering and reaction contributes DPA values.

✓ PHITS results give good agreement with FLUKA ones with in a factor of 1.7.

Comparison with Other Codes

C) Heavy Ion into W

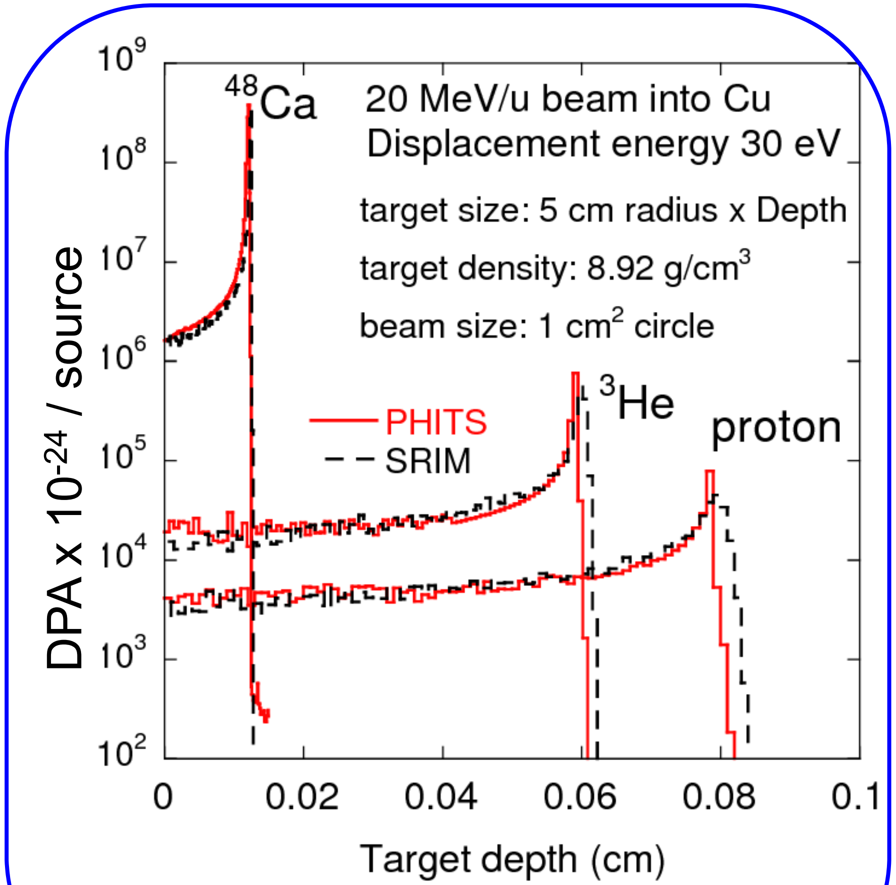


✓Coulomb scattering cross section of ^{76}Ge is much higher than that of light ion.

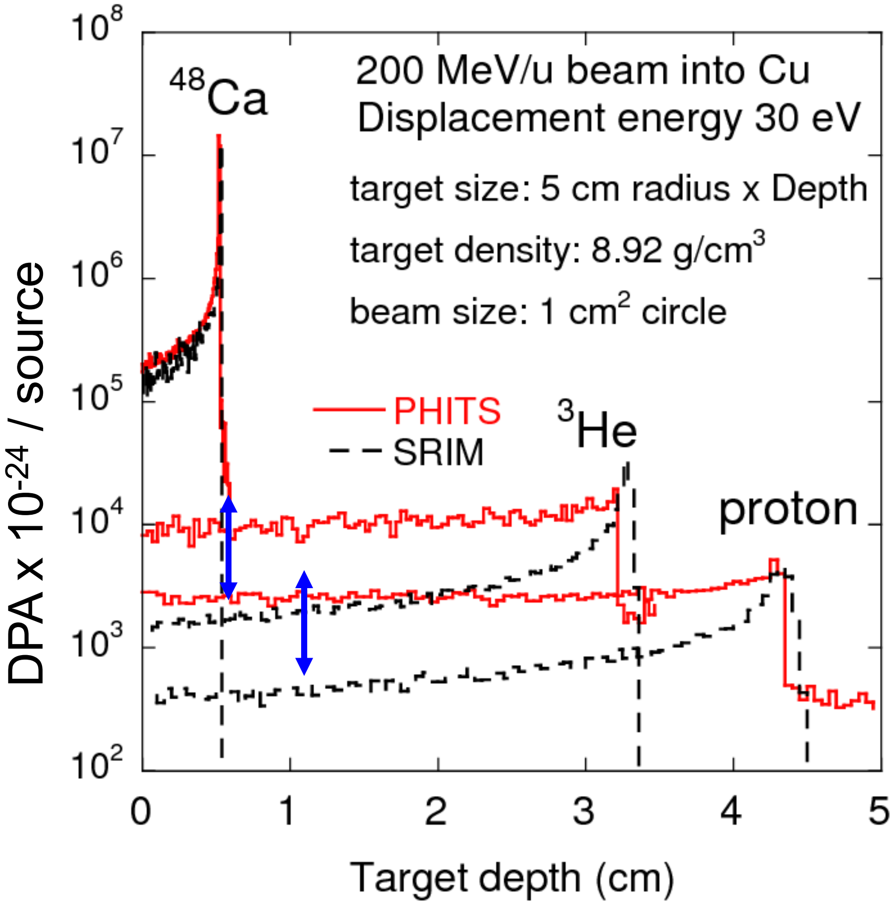
➡ Characteristic of developed hadronic cascades is not appeared.

✓Agreement is good.

Comparison of PHITS with SRIM



✓PHITS results are in good agreement with SRIM results.



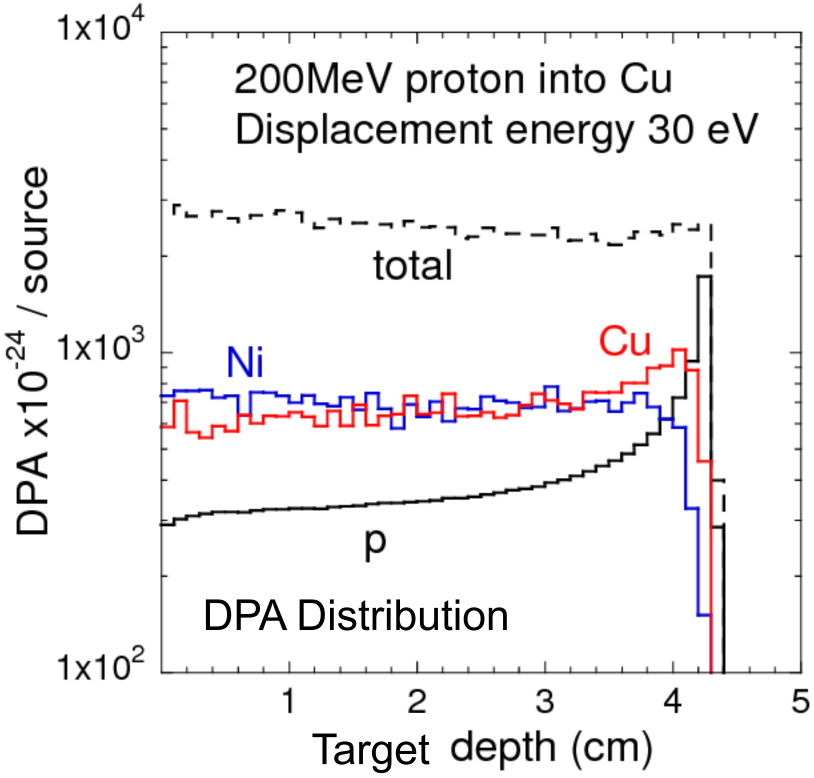
What are the differences between two results?

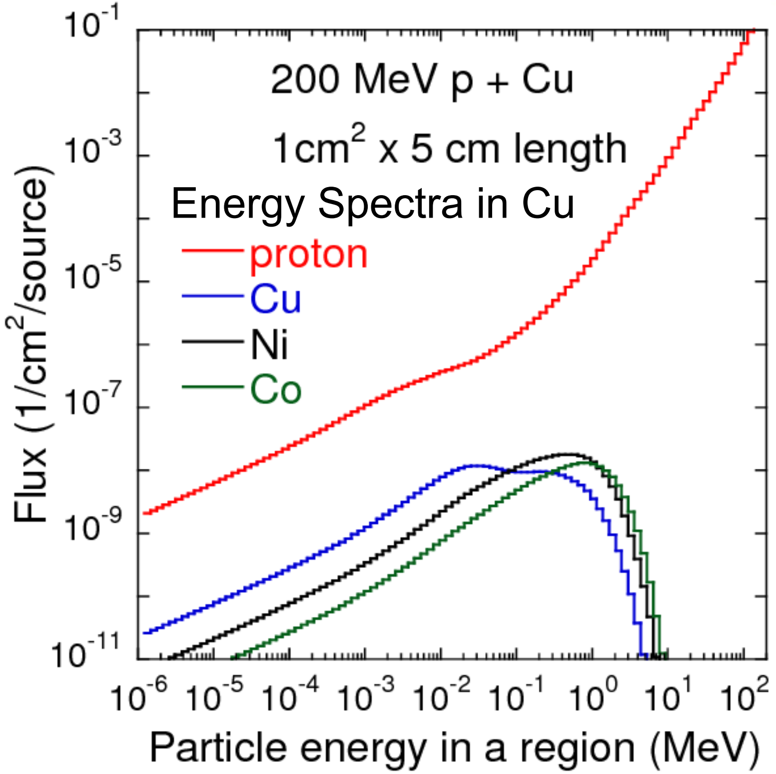
→ Secondary particles created from sequential nuclear reactions

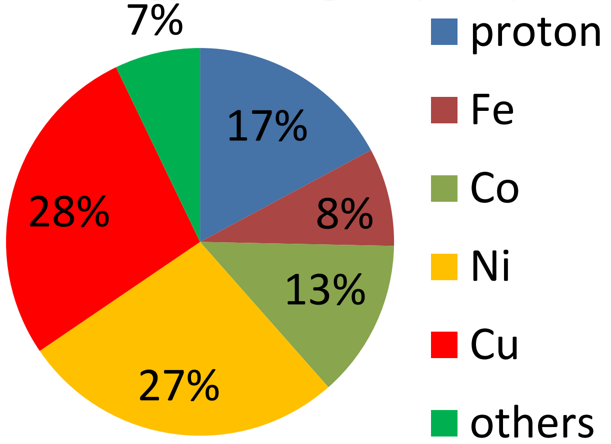
What particles contribute to the DPA value? → Next Slides

Comparison of PHITS with SRIM

C) Heavy Ion into W





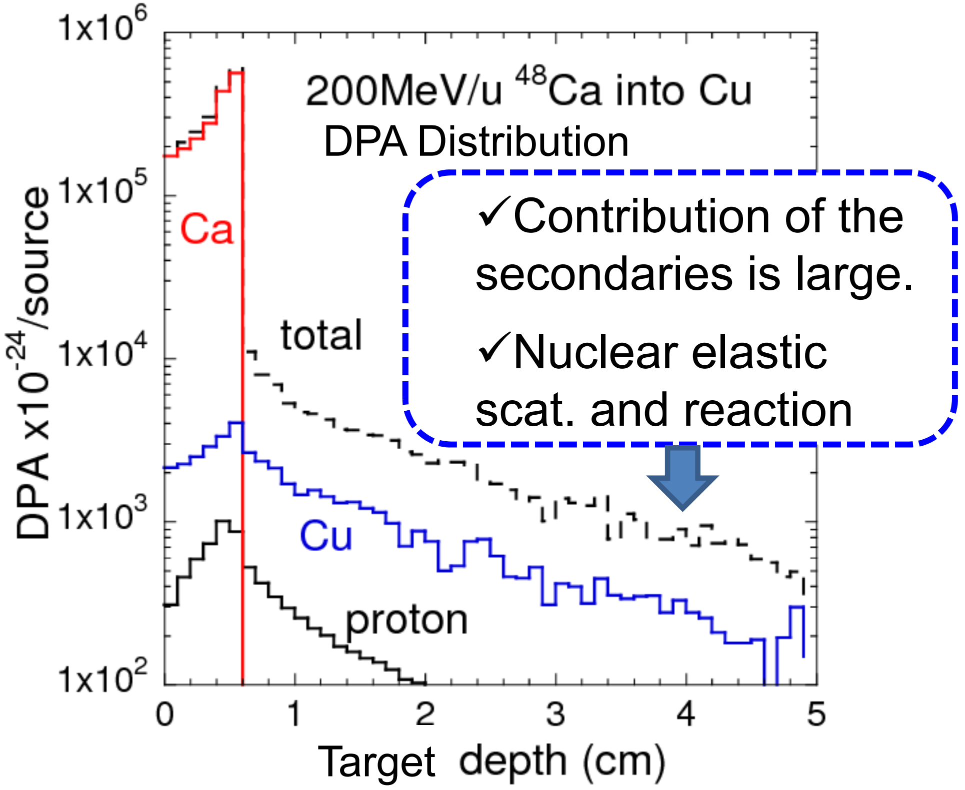


✓ Types of Particles around Cu increase due to nuclear reactions and these particles contribute to total DPA .

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

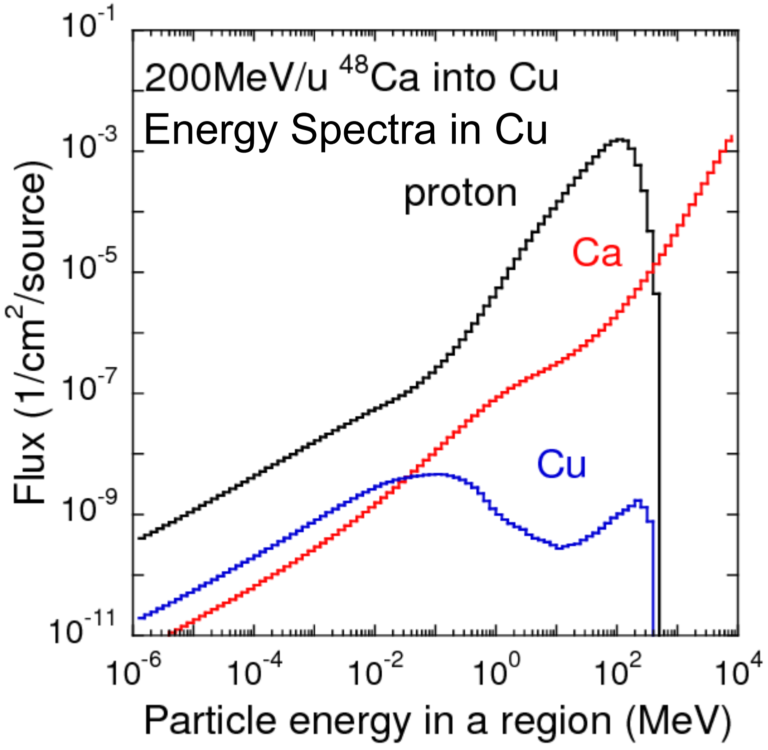
Comparison of PHITS with SRIM

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

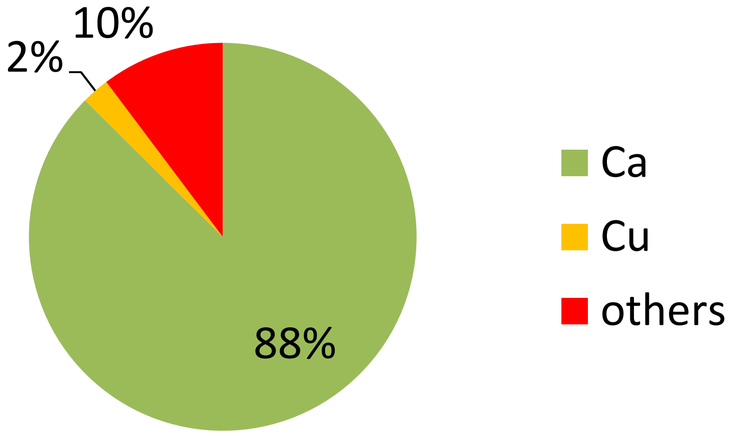


✓Contribution of the secondaries is large.

✓Nuclear elastic scat. and reaction

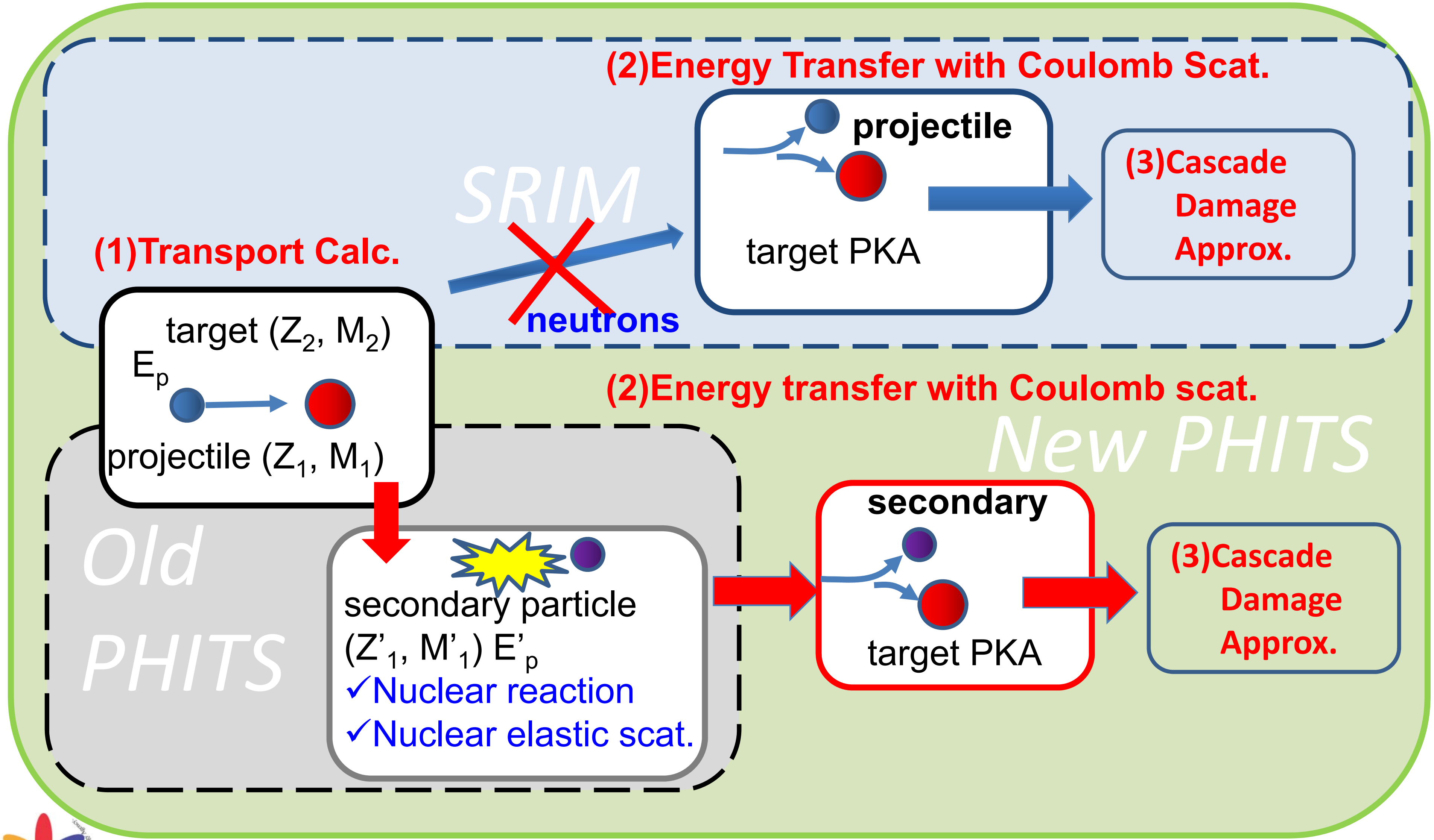


DPA produced by the primary beam is much larger than DPA produced by other contributors.



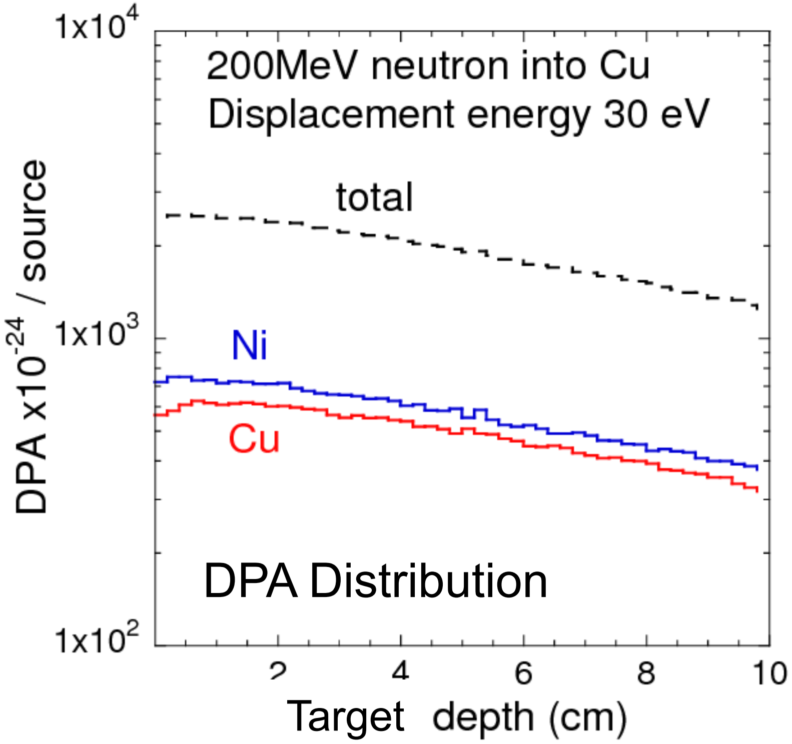
Comparison of PHITS with SRIM

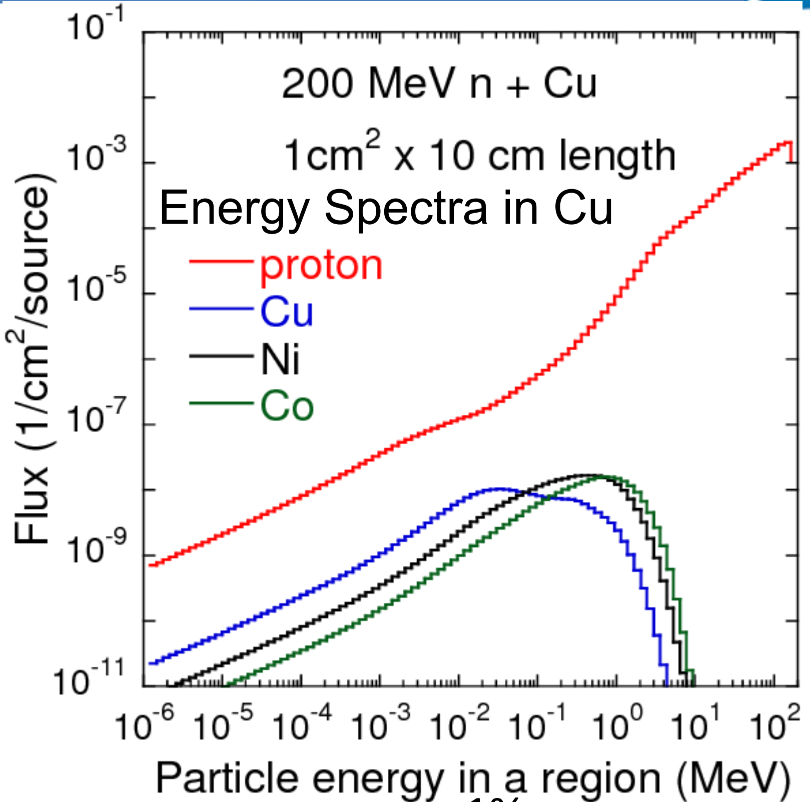
Concept of DPA Model for Neutrons



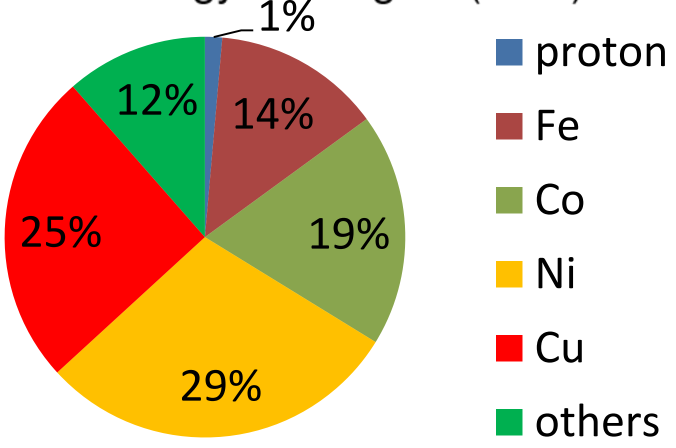
Comparison of PHITS with SRIM

(3)200 MeV Neutron into Cu



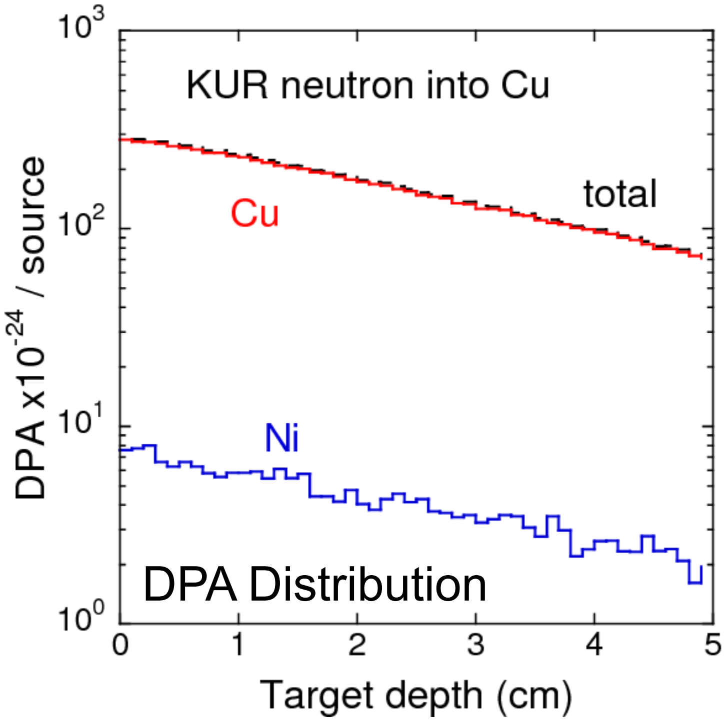


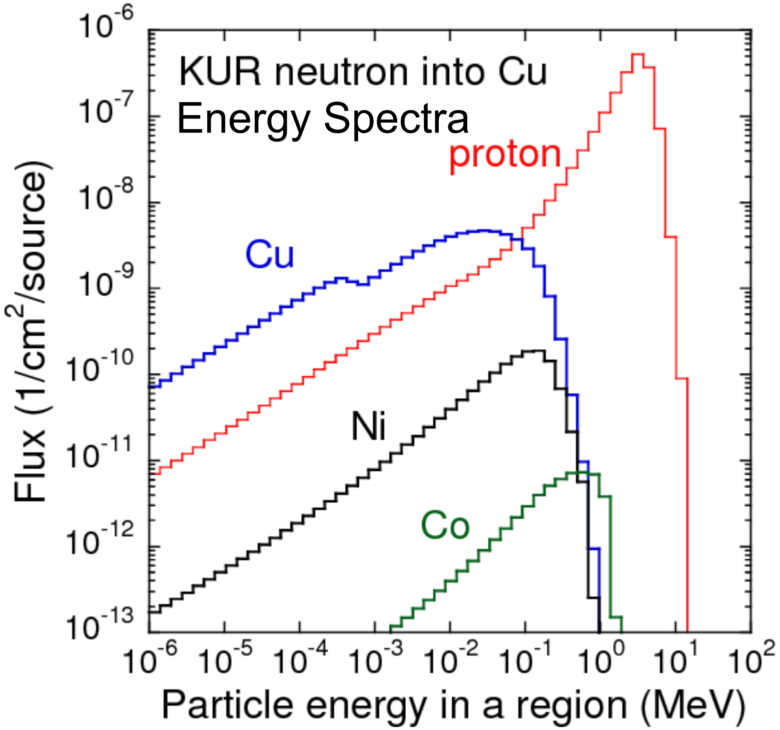
- ✓Contributions to total DPA by various particles around Cu increase due to nuclear reactions.
- ✓Secondary particle distributions for neutron are similar with that for protons.



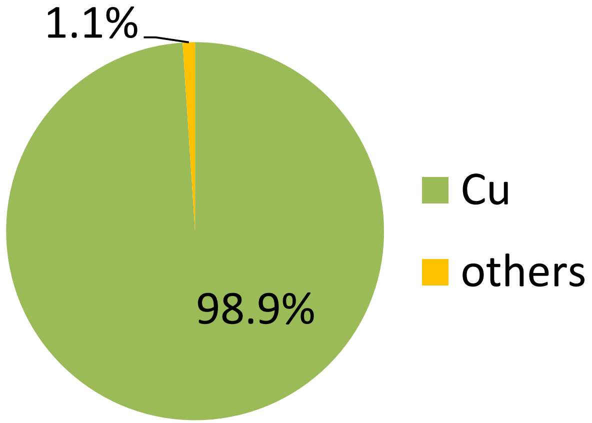
Comparison of PHITS with SRIM

(4)Reactor Neutron into Cu





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



Comparison of PHITS with SRIM

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/u ^{48}Ca	-	99.8	-	-	-	-	0.2
200MeV/u ^{48}Ca	-	88	-	-	-	2	10
Reactor neutron	-	-	-	-	-	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.

Summary

✓The displacement calculation method from evaluated nuclear data file has been developed by using effective single-particle emission approximation (ESPEA).

✓The ESPEA can be used effectively below about 50 MeV, because of since multiplicity of emitted particles.

✓The displacement calculation method in PHITS has been developed.

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

✓ For heavy-ion beams, DPA created by the primaries are dominant to total DPA due to the large Coulomb scattering cross sections.

✓PHITS results agreement with FLUKA ones within a factor of 1.7. In the high-energy region above 10 MeV/nucleon, comparisons among codes and measurements of displacement damage cross section are necessary.

PHITS

Particle and Heavy Ion Transport code System

K. Niita[1], N. Matsuda[2], S. Hashimoto[2], Y. Iwamoto[2],
H. Iwase[3], T. Sato[2], S. Noda[2], H. Nakashima[2],
T. Fukahori[2], S. Chiba[4,2], L. Sihver[5]

1. *Research Organization for Information Science and Technology, RIST, Japan*
2. *Japan Atomic Energy Agency, JAEA, Japan*
3. *High Energy Accelerator Research Organization, KEK, Japan*
4. *Tokyo Institute of Technology, TITech, Japan*
5. *Chalmers University of Technology, Sweden*

Last update 2012/6/1

What is PHITS?

Capability

Transport and collision of all particles over wide energy range

in 3D phase space
with magnetic field & gravity

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

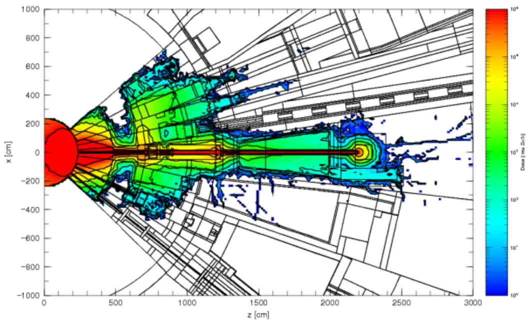
10^{-4} eV to 100 GeV/u

All-in-one-Package

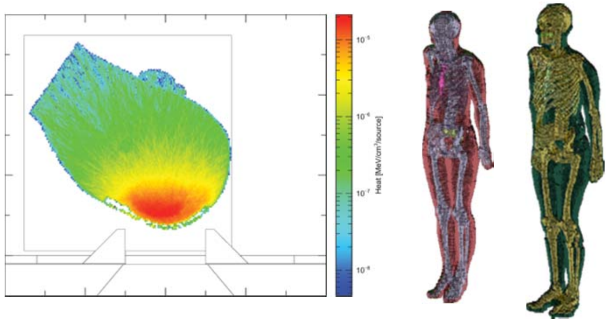
All contents of PHITS (source files, binary, data libraries, graphic utility etc.) are fully integrated in one package

OECD/NEA Databank, RSICC (USA, Canada etc.) and RIST (Japan)

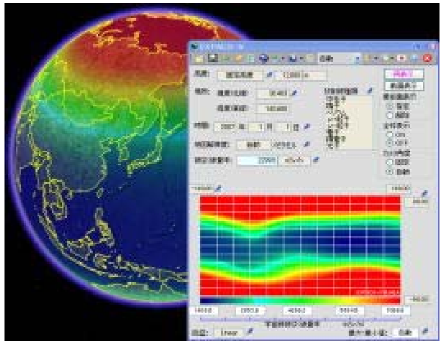
Applications



Accelerator Design

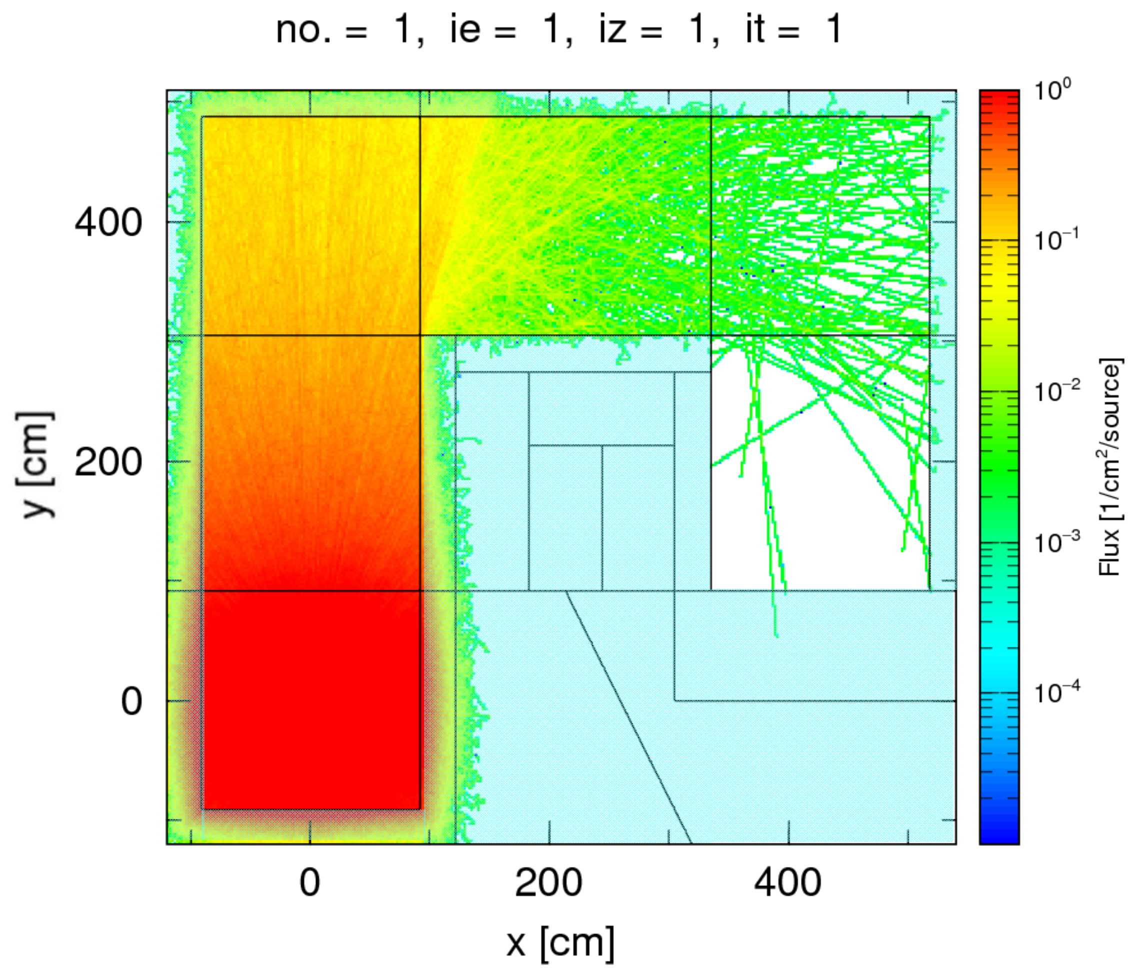


Radiation Therapy & Protection



Space & Geoscience

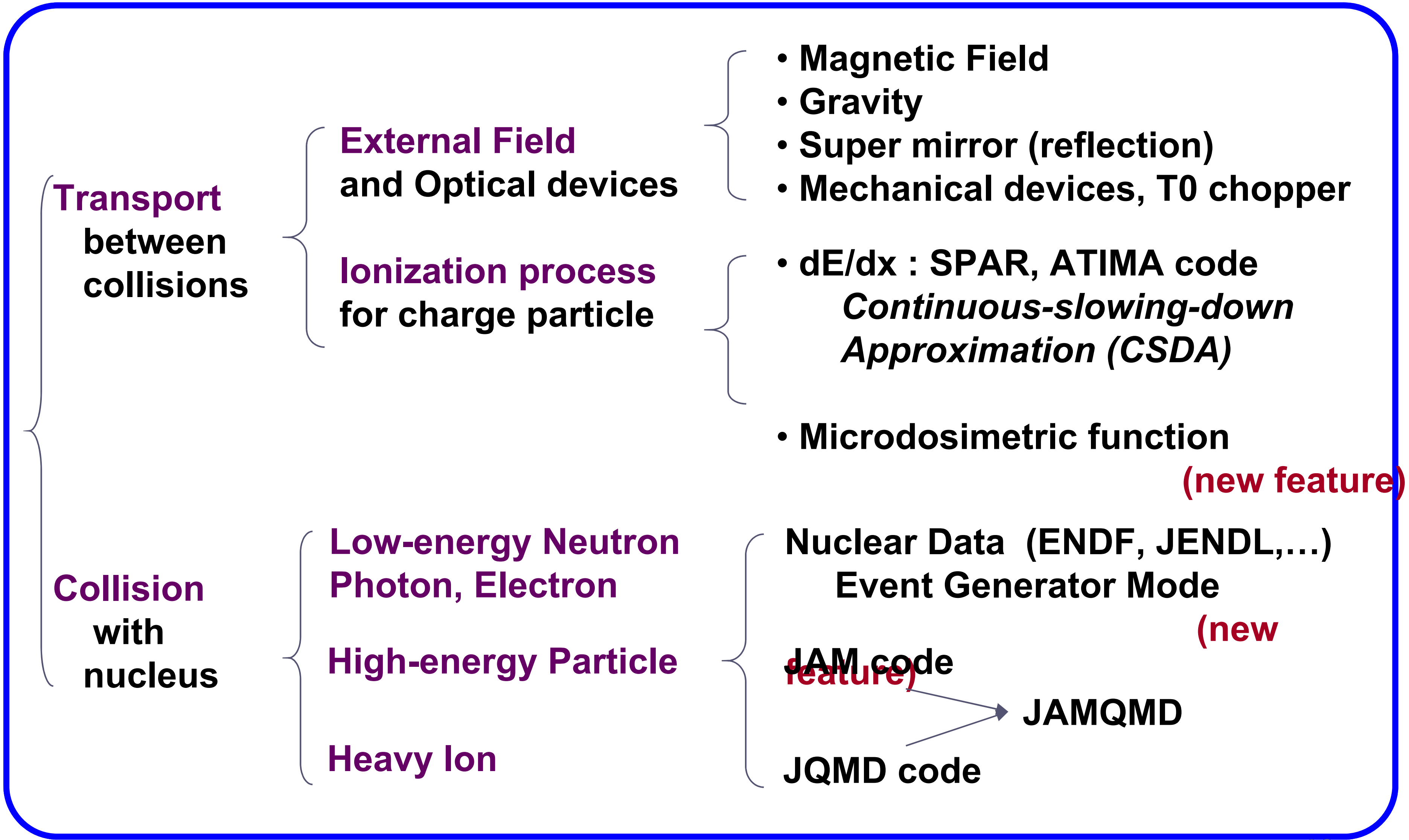
Example of PHITS Calculation



Motion of 100,000 photons produced from ^{137}Cs simulated by PHITS

Simulate the motion of each particle using the random walk method
→ Average behavior such as particle flux and mean deposition energy

Physical Processes included in PHITS



Transport between collisions

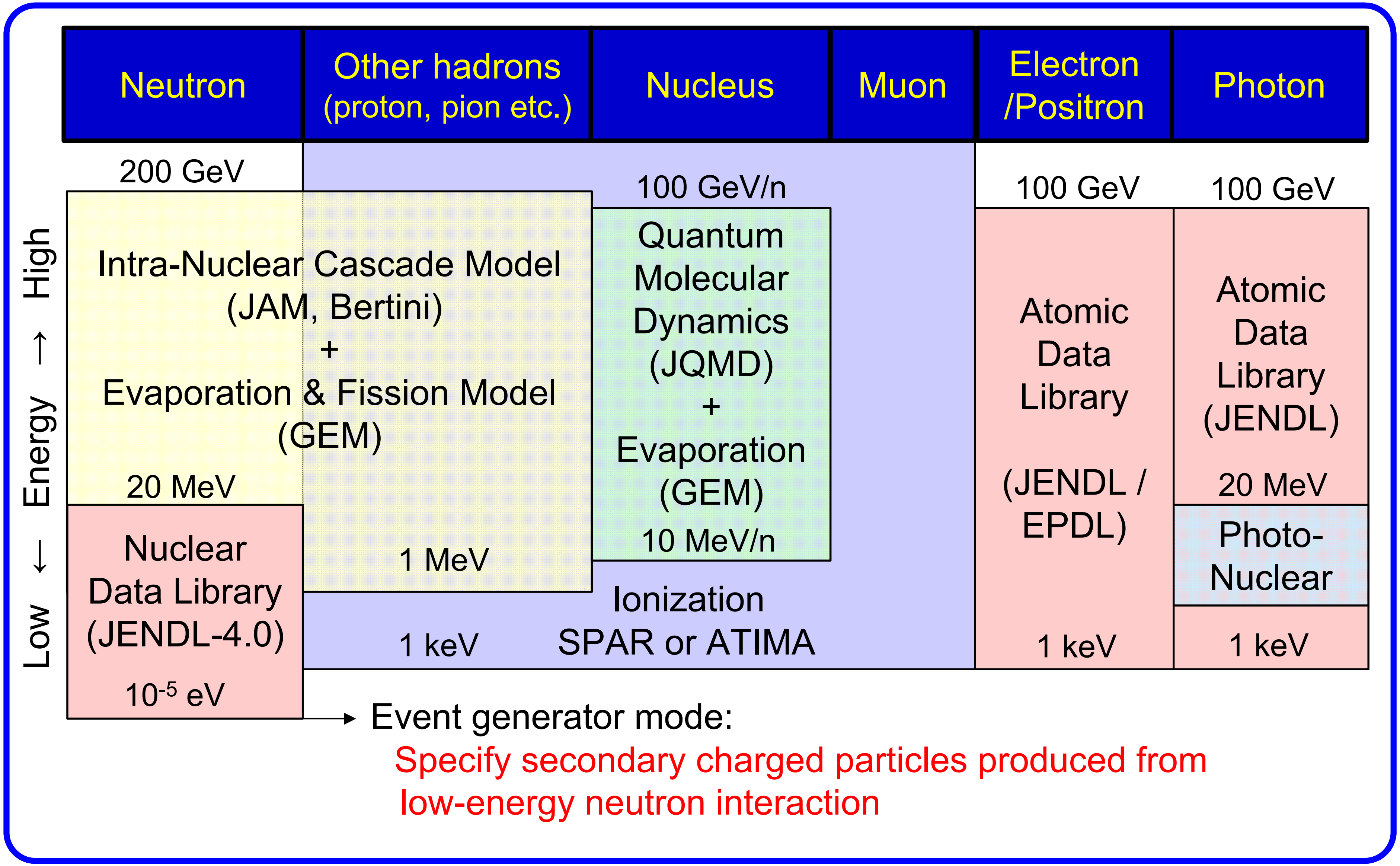
- **External Field** and Optical devices
  - Magnetic Field
  - Gravity
  - Super mirror (reflection)
  - Mechanical devices, T0 chopper
- **Ionization process** for charge particle
  - dE/dx : SPAR, ATIMA code
    Continuous-slowing-down Approximation (CSDA)
  - Microdosimetric function
    (new feature)

Collision with nucleus

- **Low-energy Neutron Photon, Electron**
  - Nuclear Data (ENDF, JENDL,…)
    Event Generator Mode
    (new feature)
- **High-energy Particle**
  - JAM code
- **Heavy Ion**
  - JQMD code

JAM code, JQMD code → JAMQMD

Map of Models used in PHITS



Neutron

Other hadrons (proton, pion etc.)

Nucleus

Muon

Electron /Positron

Photon

Low ← Energy → High

200 GeV

Intra-Nuclear Cascade Model (JAM, Bertini)
+
Evaporation & Fission Model (GEM)

20 MeV

1 MeV

Nuclear Data Library (JENDL-4.0)

10^{-5} eV

100 GeV/n

Quantum Molecular Dynamics (JQMD)
+
Evaporation (GEM)

10 MeV/n

Ionization
SPAR or ATIMA

1 keV

100 GeV

Atomic Data Library

(JENDL / EPDL)

1 keV

100 GeV

Atomic Data Library (JENDL)

20 MeV

Photo-Nuclear

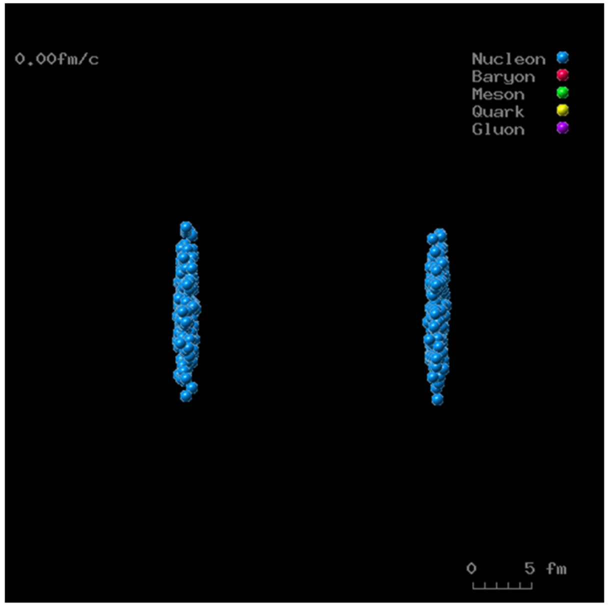
1 keV

Event generator mode:
Specify secondary charged particles produced from low-energy neutron interaction

Switching energies can be changed in input file of PHITS

JAM (Jet AA Microscopic Transport) Model

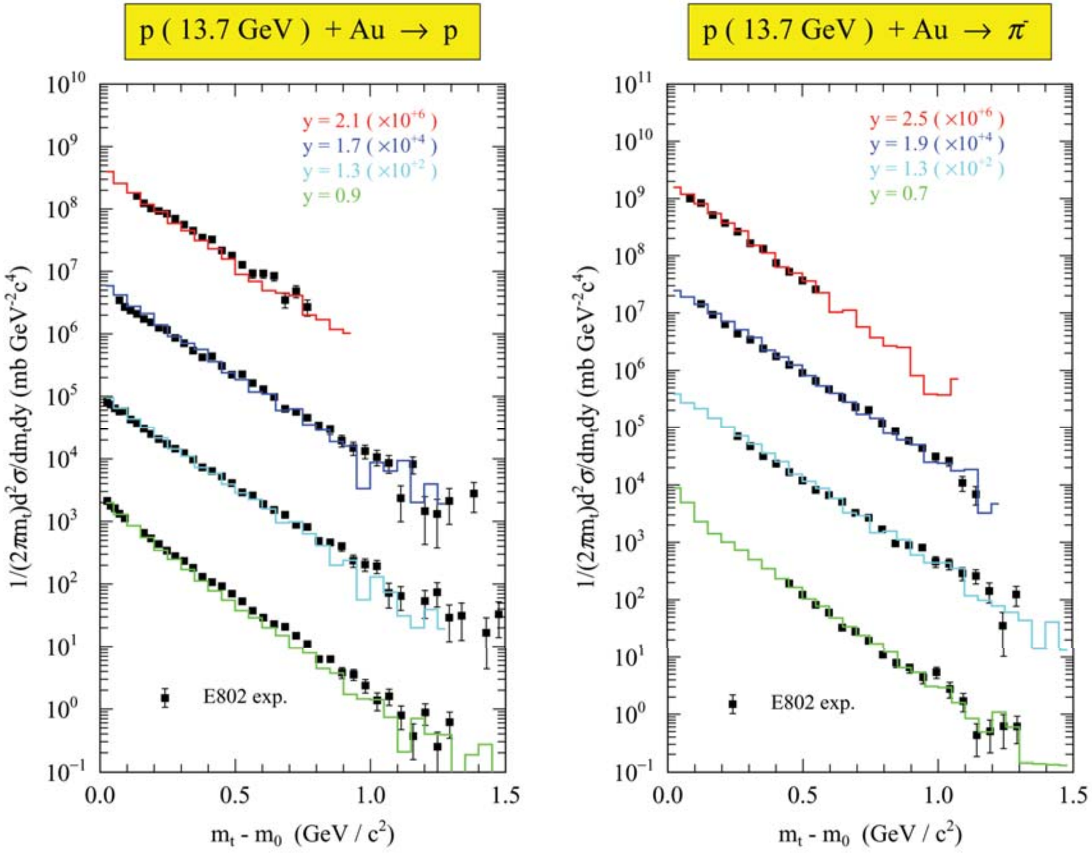
- ***JAM*** is a ***Hadronic Cascade Model***, which explicitly treats all established hadronic states including resonances with explicit spin and isospin as well as their anti-particles.
- We have parameterized all ***Hadron-Hadron Cross Sections***, based on ***Resonance Model*** and ***String Model*** by fitting the available experimental data.



Au+Au 200GeV/n in CM

119 kinds of Mesons

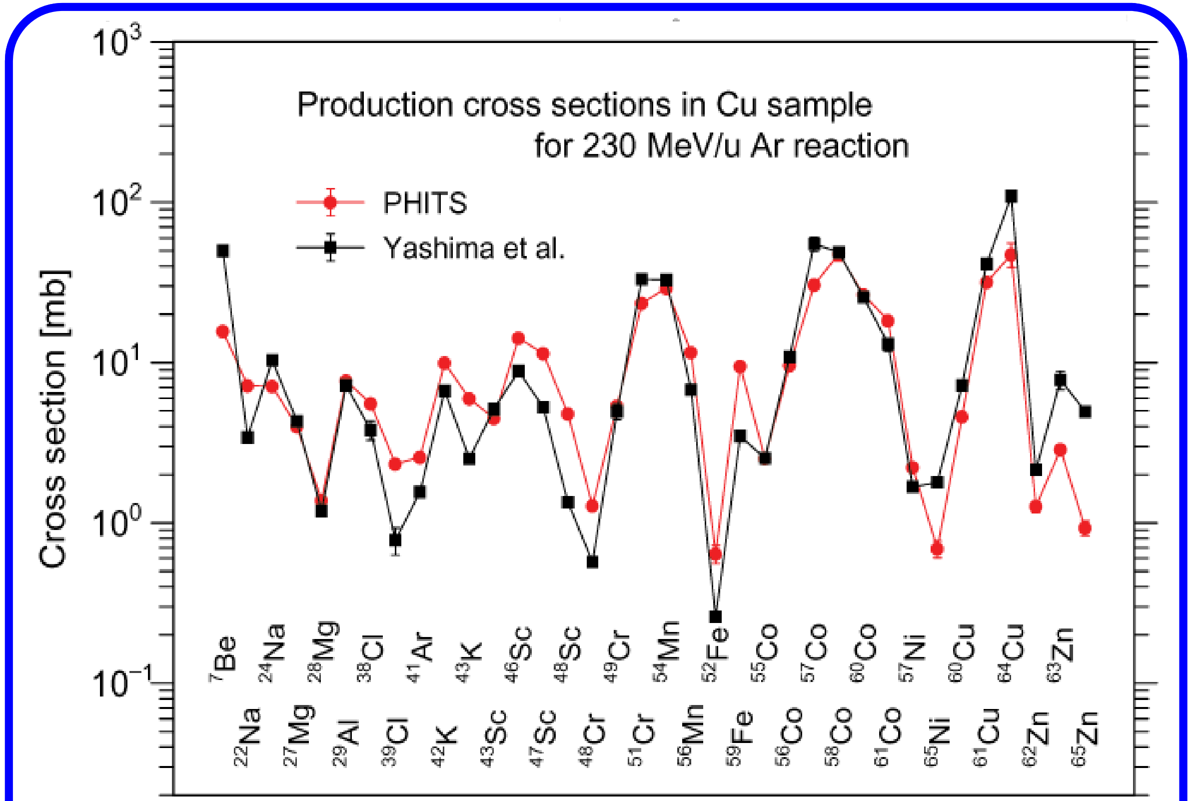
170 kinds of Baryons



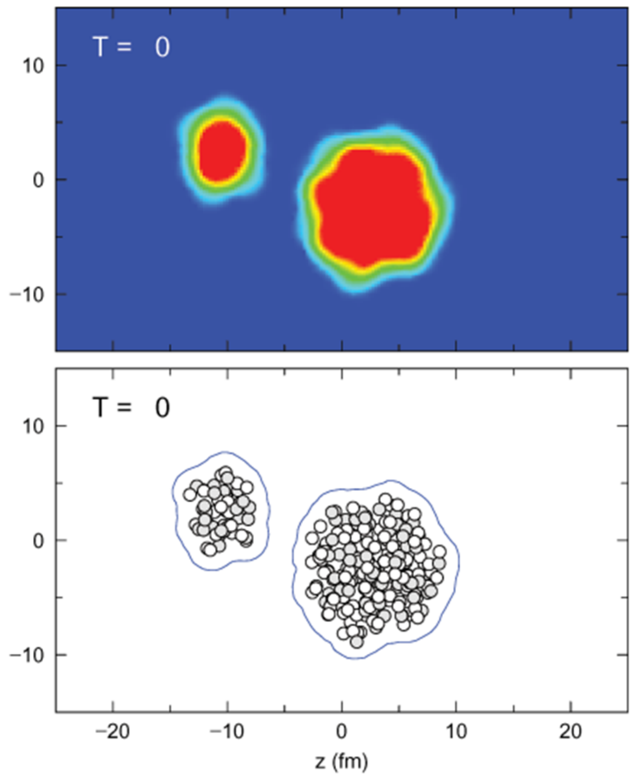
Y. Nara et al, Phys. Rev. C61 (2000) 024901

JQMD (JAERI Quantum Molecular Dynamics) Model

- ***JQMD*** can simulate the time evolution of nuclear reactions, considering the correlations between *every combination of nucleons* exist in the frame.
- Suit for simulating nucleus-nucleus interaction
- Time consumptive in comparison to cascade models



Production yields of residual nuclides



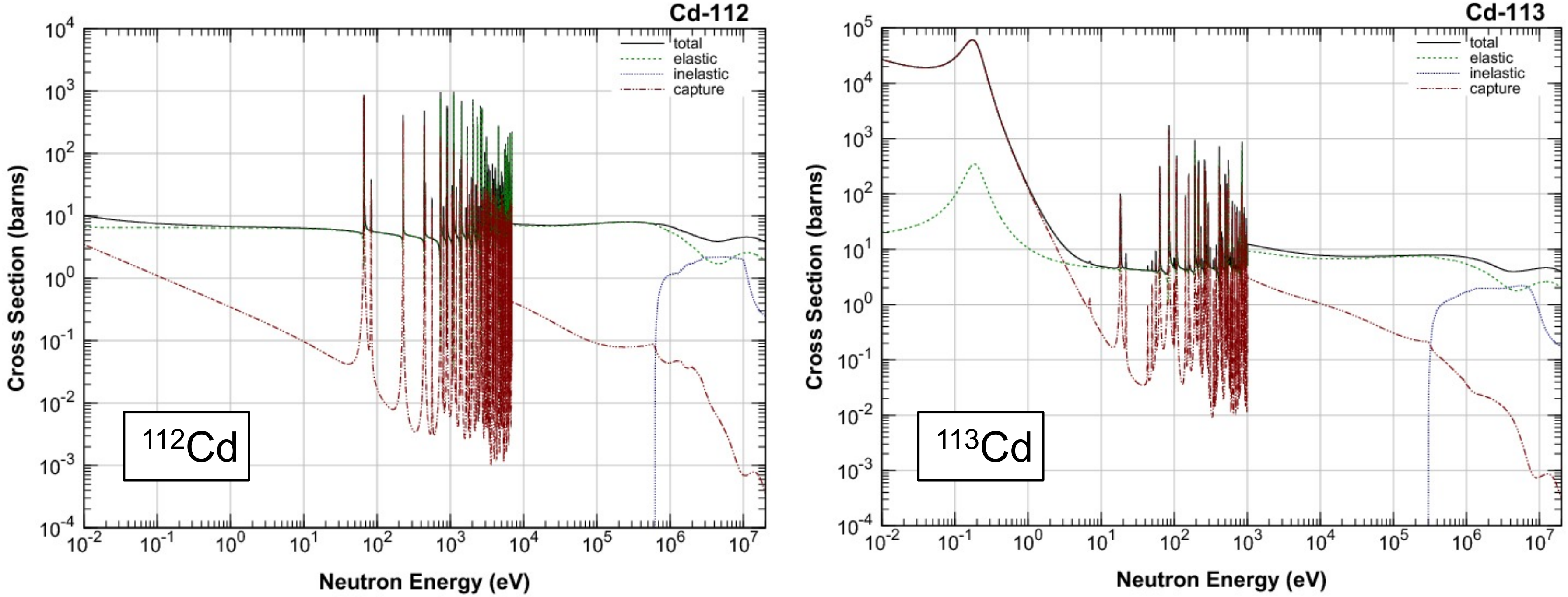
^{56}Fe 800 MeV/u on ^{208}Pb

K. Niita et al, Phys. Rev. C52 (1995) 2620

Nuclear Data Library

- ***Nuclear data libraries*** are necessary for simulating low-energy neutrons
- Cross sections of low-energy neutron significantly depend on shell structure

- PHITS Readable Format of nuclear data: ***ACE format*** (same as MCNP)
- Libraries: JENDL-4, ENDF etc. (for low-energy neutrons)
  LA150, JENDL-HE file (for high-energy neutrons and protons)



Neutron reaction cross sections of ^{112}Cd and ^{113}Cd taken from JENDL4.0