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DPA calculation for proton and heavy ion incident reactions in wide-energy region using PHITS code

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- Introduction
- Implementation of DPA model in PHITS
- Comparison with other results
- Summary

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 :

DPA$=\phi\, t\, \sigma$

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

ϕt : the irradiation fluence.

ϕ: the product of the ion beam density

t : the bombardment time

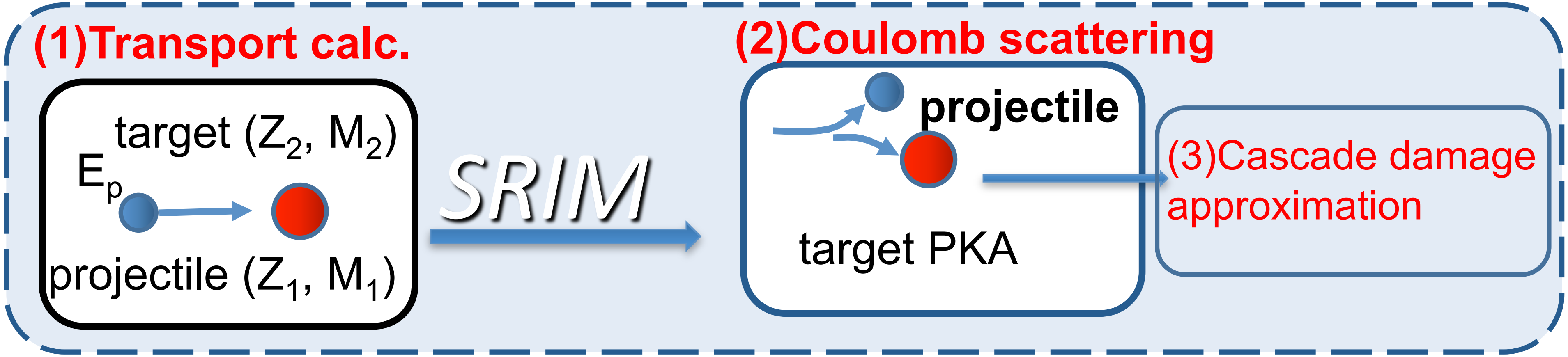
For example, 10 dpa means each atom in the material has been displaced from its site within the structural lattice of the material an average of 10 times.

DPA number is a useful measure in correlating results determined by different particles and fluxes in an irradiation environment.

Introduction ~radiation damage calculation ~

SRIM (Transport of Ions in Matter):

J.F. Ziegler, et al., The stopping and range of ions in matter (2008) see www.srim.org



- SRIM code has been developed in the low-energy region.
- As SRIM can not treat nuclear reaction,
damage calculation by PKA created by the secondary is not considered.

The DPA models in **the advanced Monte Carlo particle transport code systems** have been modified, respectively.

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

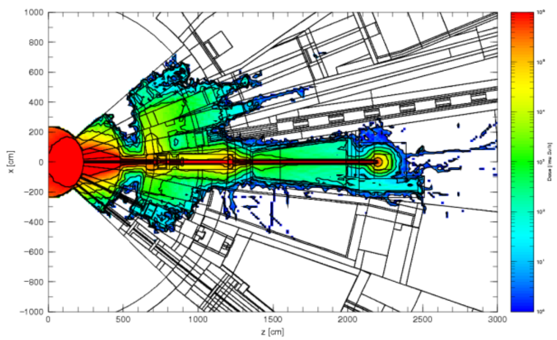
Transport and collision of all particles over wide energy range

in 3D phase space
with magnetic field & gravity

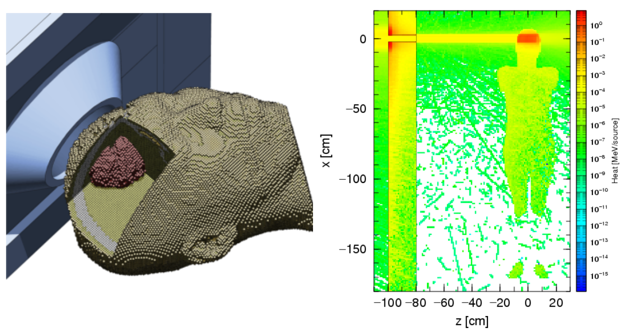
neutron, proton, meson, baryon
electron, photon, heavy ions

up to 100 GeV/n

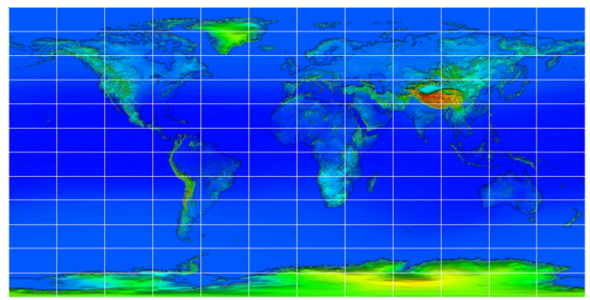
Application Fields



Accelerator Design



Radiation Therapy

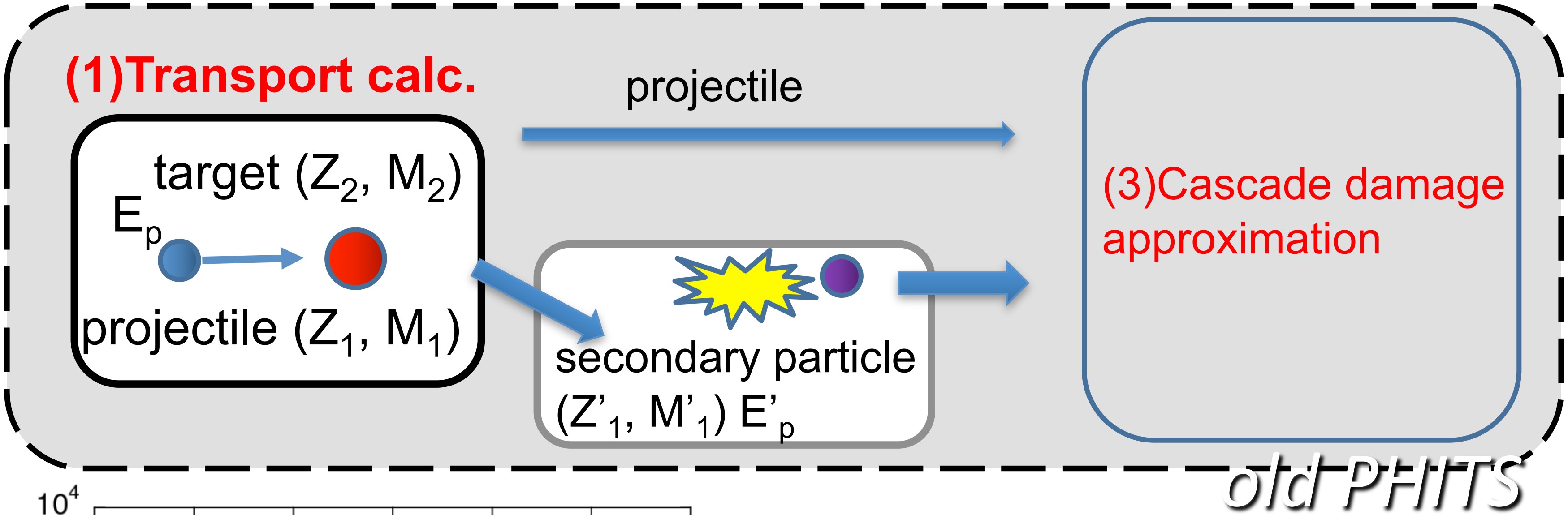


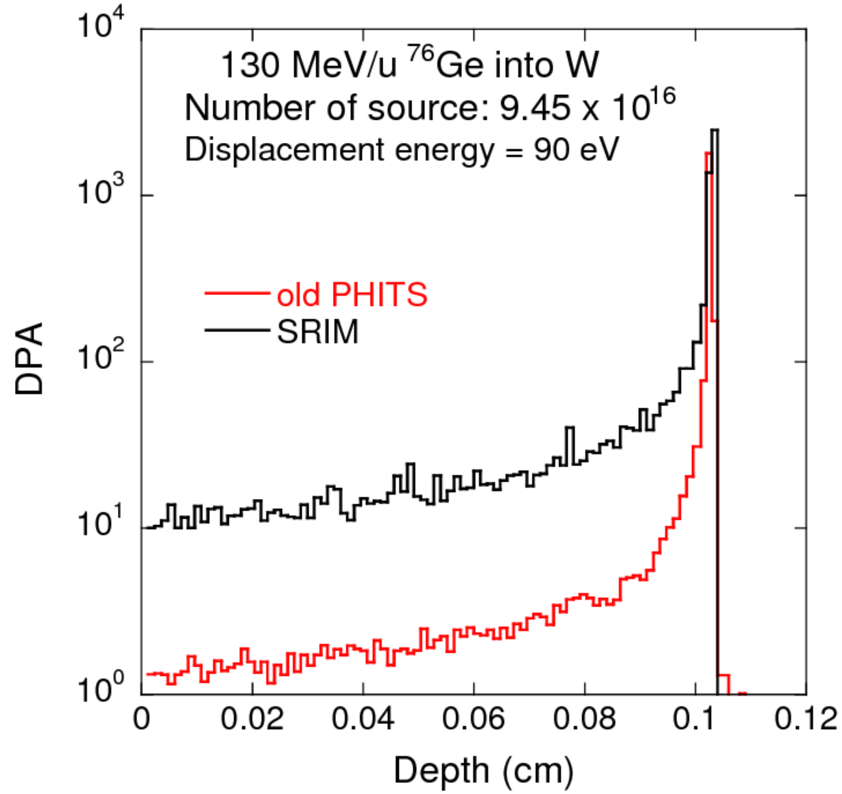
Space Application

http://phits.jaea.go.jp

available from NEA databank

Introduction
~DPA model in old PHITS~





- No Coulomb scattering in old PHITS.

- Result calculated by old PHITS are smaller than SRIM one.

Introduction

Purpose

➢Implementation of DPA model in PHITS code including Coulomb scattering and nuclear reaction model.

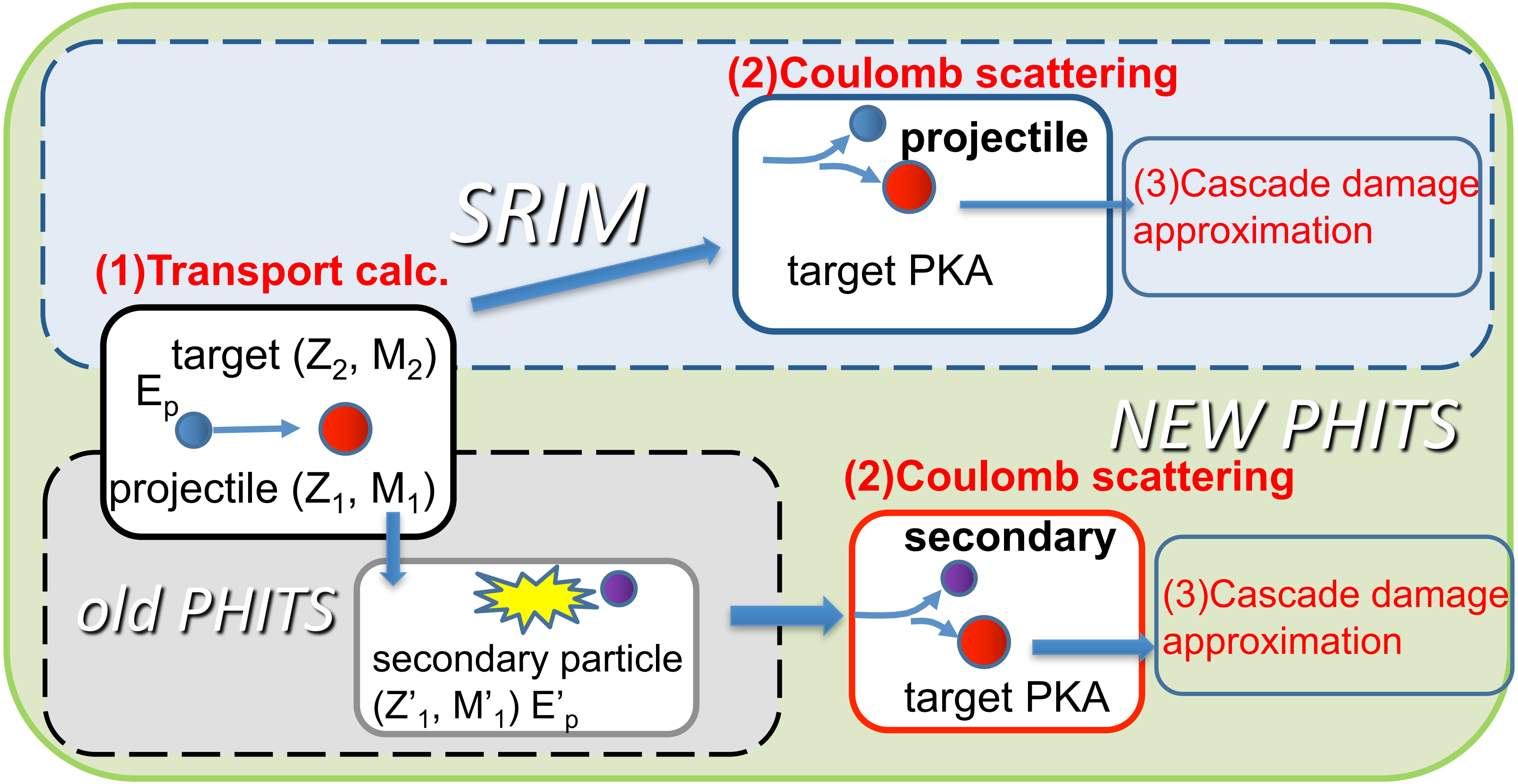
➢Comparison PHITS results with SRIM results and a few data.

✓Calculation condition

1. 130 MeV/u ^{76}Ge into W
2.

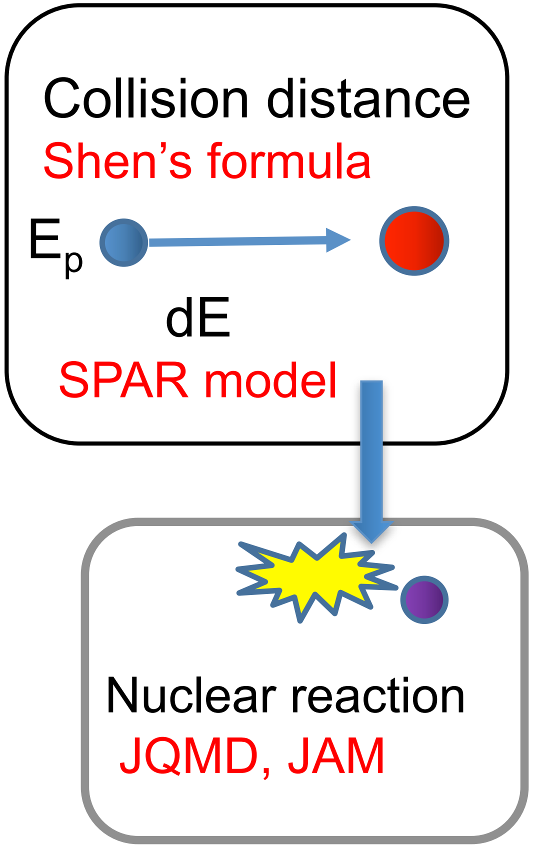
Incident particle type	Incident energy range	target
proton, ^{3}He , ^{48}Ca	1 MeV/u ~ 1 GeV/u	Cu, W

Implementation of DPA model in PHITS
~Overview of DPA model~



(1)Transport calculation

H. Iwase, K. Niita, T. Nakamura, J. Nucl. Sci. and Technol. 39 (2002) 1142-1151.



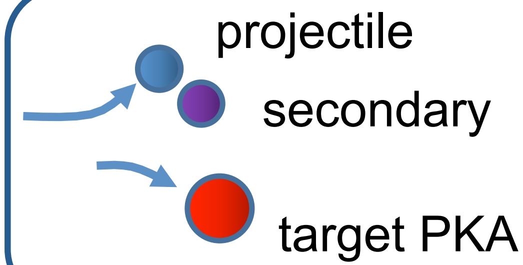
- Collision distance is calculated using the total reaction cross section produced by Shen’s formula.

- **SPAR calculates**
  Stopping power and ranges
  using different procedure for each of three (β,z) region.

- **Nuclear reaction** produces secondary particles using physics models JQMD or JAM.

(2) Coulomb scattering

M. Nastasi et. al., "Ion-Solid Interaction: Fundamentals and Applications (Cambridge Solid State Science Series)



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

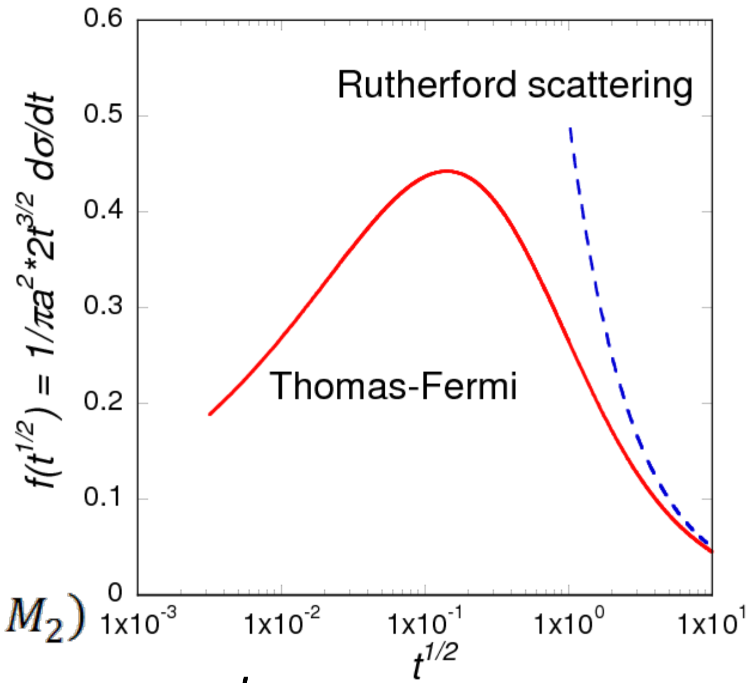
T: transferred energy, (Z_2, M_2)

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*

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

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

- Transferred energy from projectile and secondary to target atom

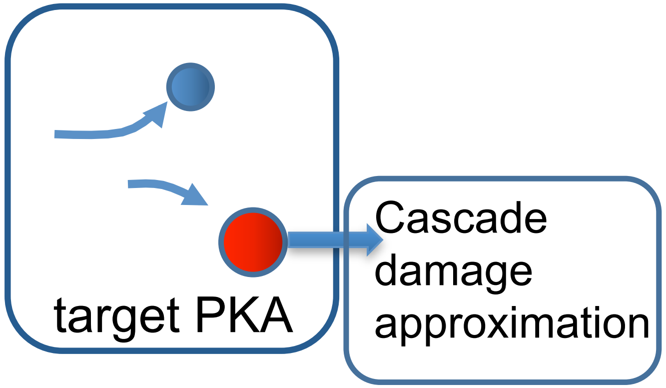
$$T = T_{\max} \times \frac{t}{\varepsilon_p^2}$$

ε ⇒ *large*

θ ⇒ *large*

b ⇒ *small (impact parameter)*

(3) Cascade damage approximation



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 predicted 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*

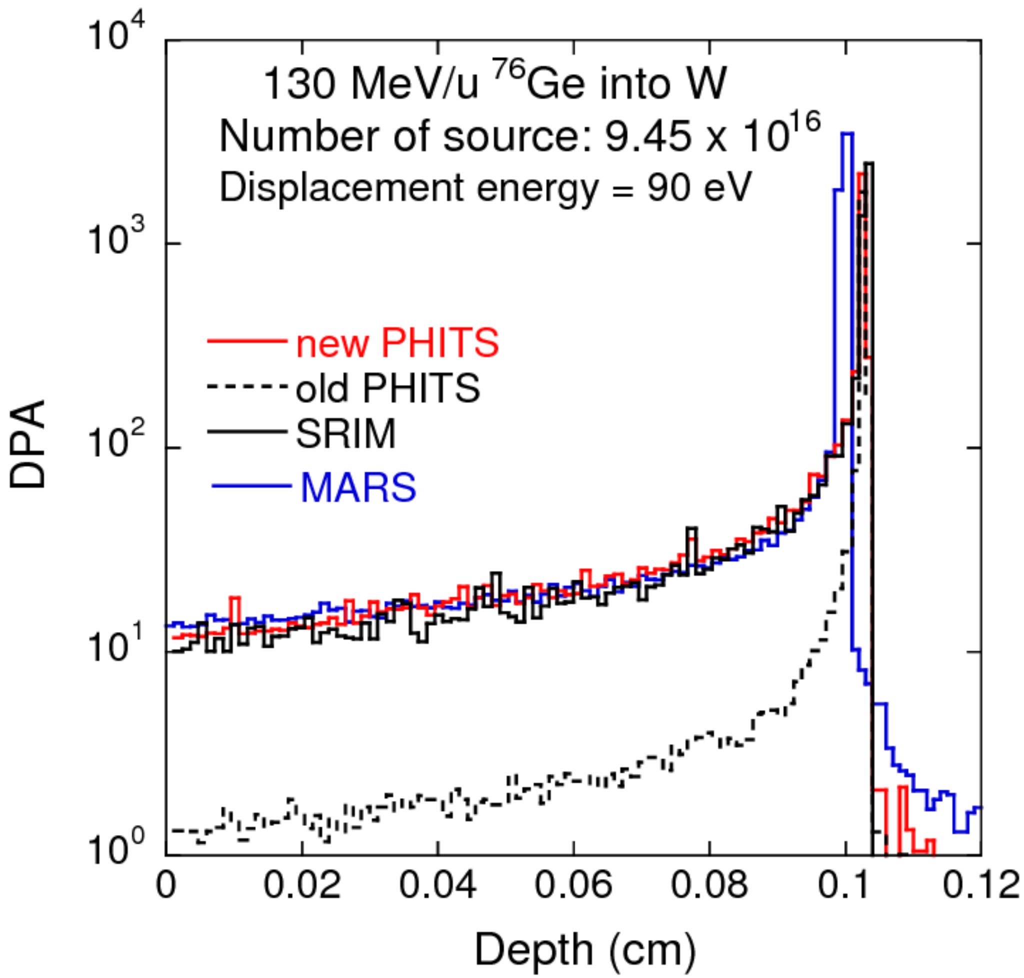
T_d: the value of the threshold displacement energy. 30 eV for Cu and 90 eV for W

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

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

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

Comparison PHITS with SRIM and MARS

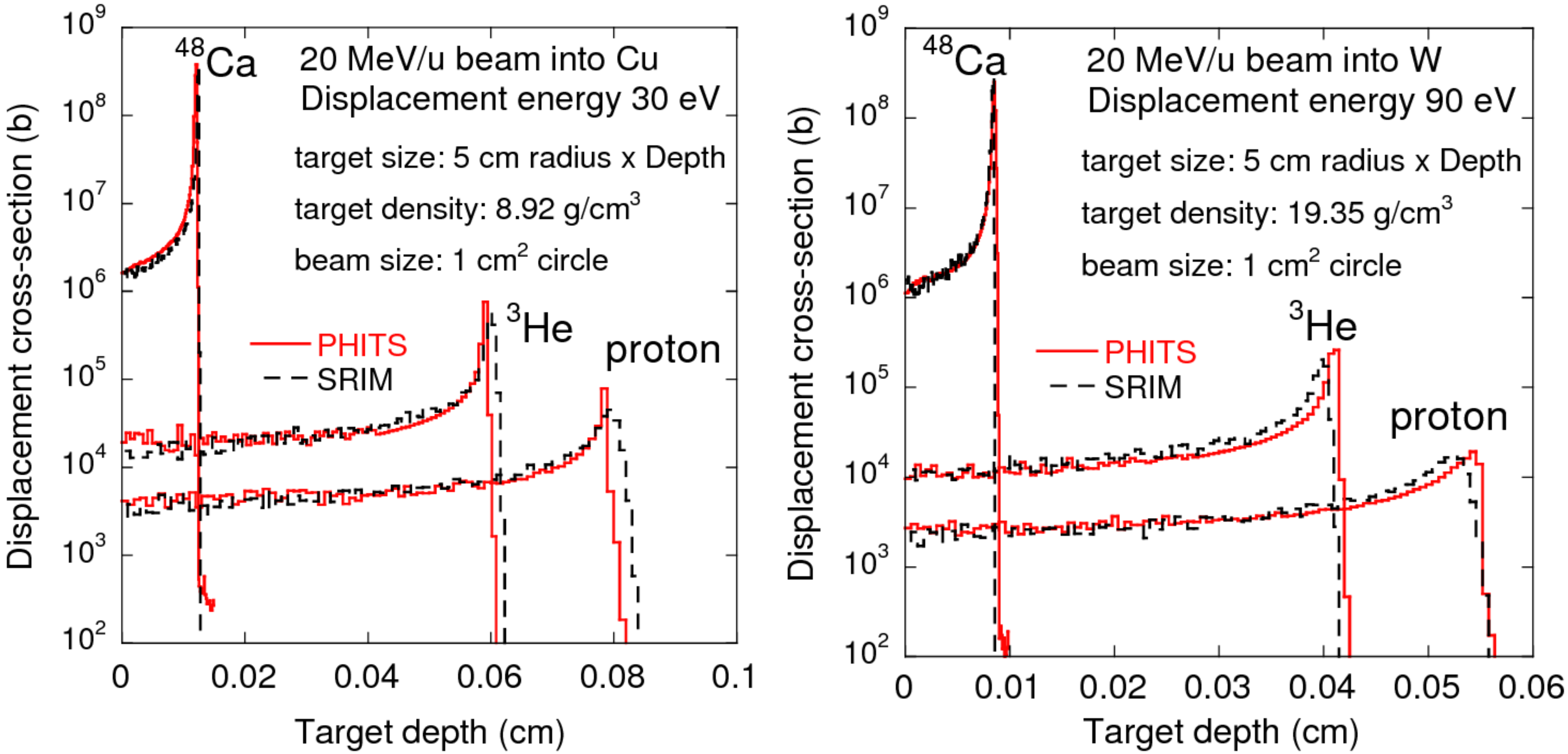


MARS result:
Courtesy Nikolai Mokhov

MARS also folds with Coulomb scattering and nuclear reaction.

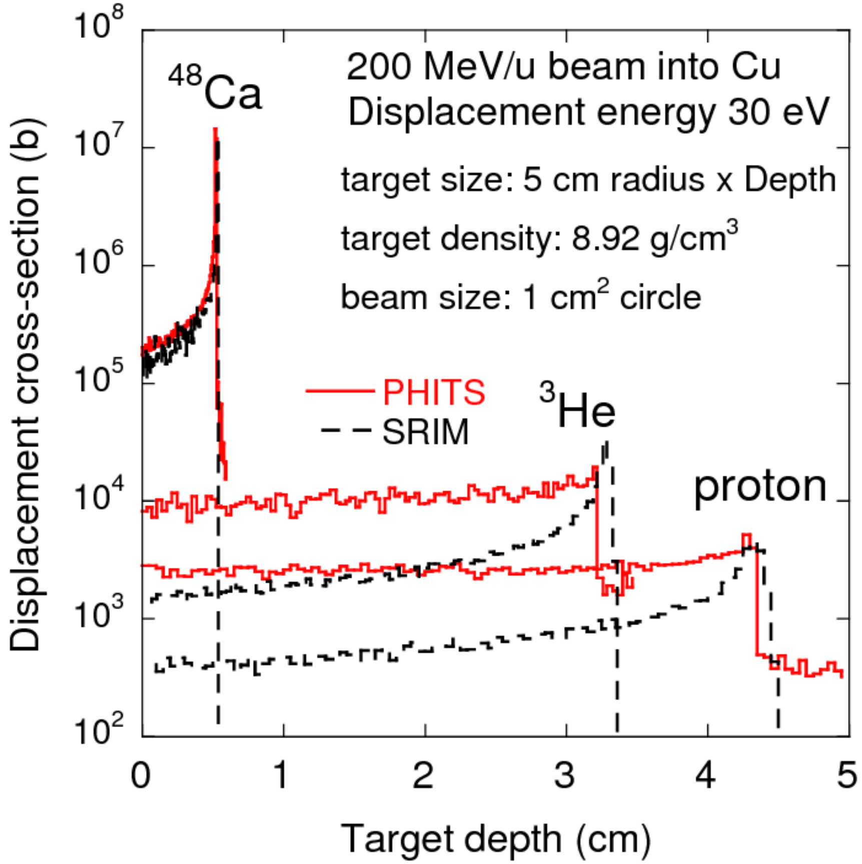
- Agreement is very good except for old PHITS.
- Coulomb scattering is important to calculate DPA.

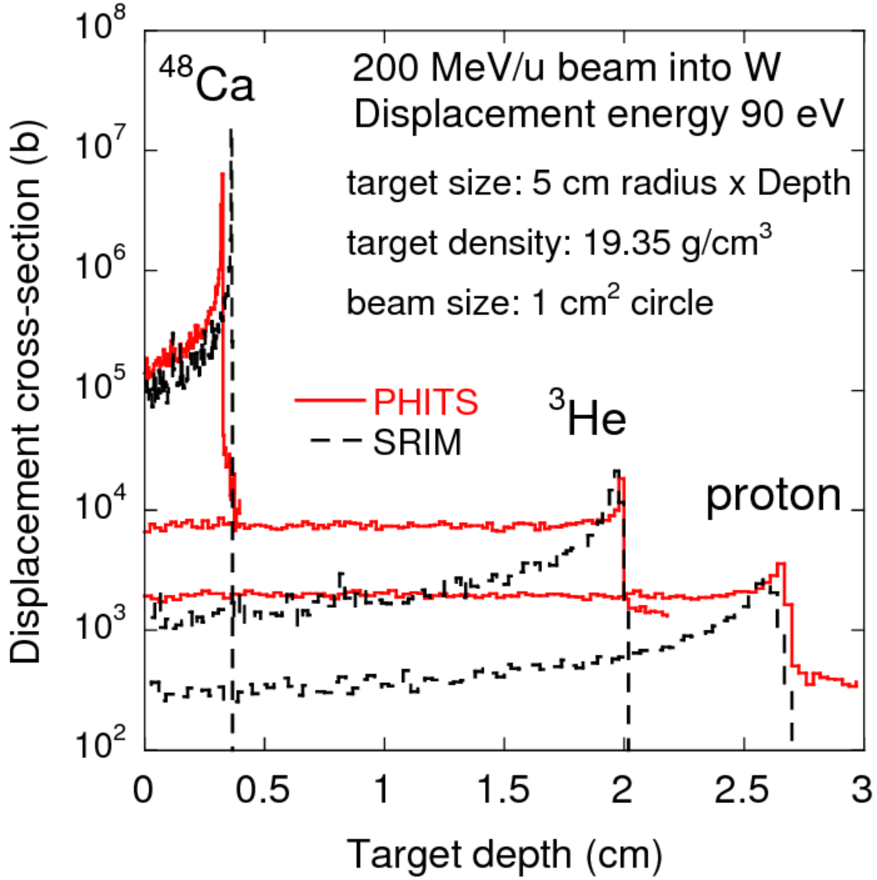
Comparison : 20 MeV/u beam



- At 20 MeV/u, the beam range in materials is less than the mean free path for nuclear reactions.
- PHITS results gives good agreements with SRIM ones.

Comparison : 200 MeV/u beam

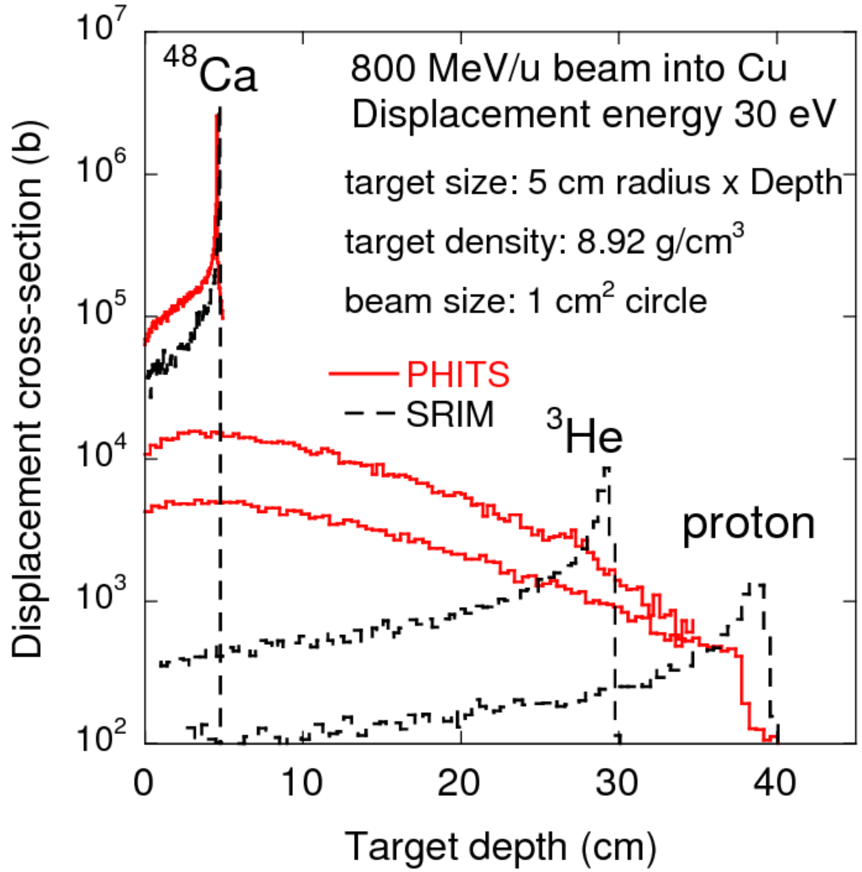


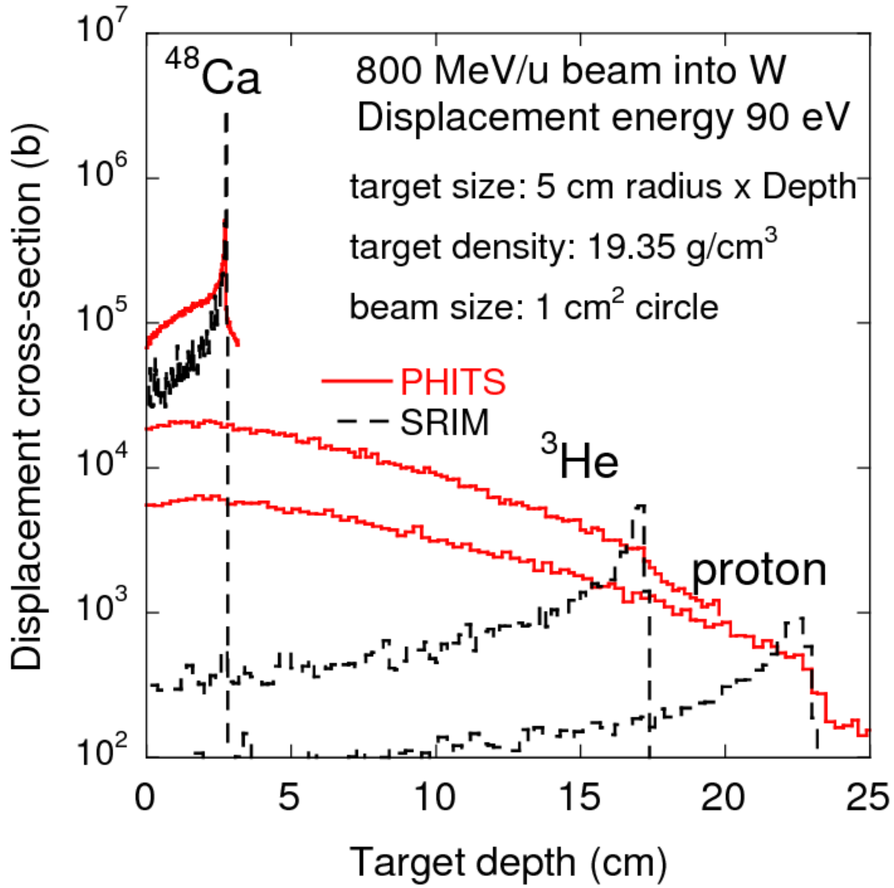


- PHITS results are larger than SRIM ones in tail part.

- Damage cross sections by PKA's directly created by the secondary are increased for proton and ^{3}He incidences.

Comparison : 800 MeV/u beam

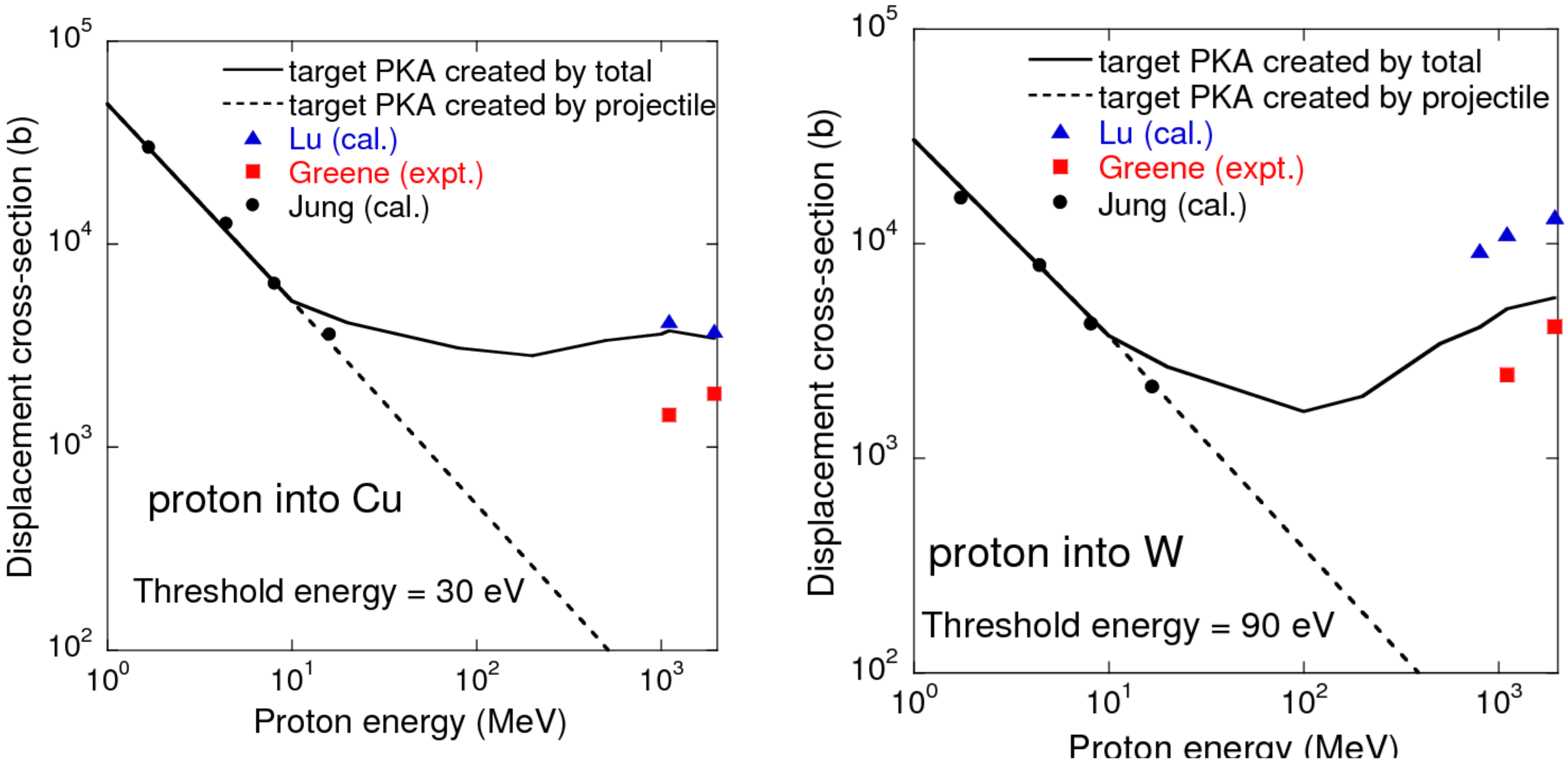




- At 800 MeV/u nuclear reactions occur before the stopping range is reached, and the curves show the characteristics of well-developed hadronic cascades.

- Damage calculation only by PKA's directly created by the projectile, such as SRIM, may lead to sever underestimation where projectile energy is high enough to create nuclear reactions.

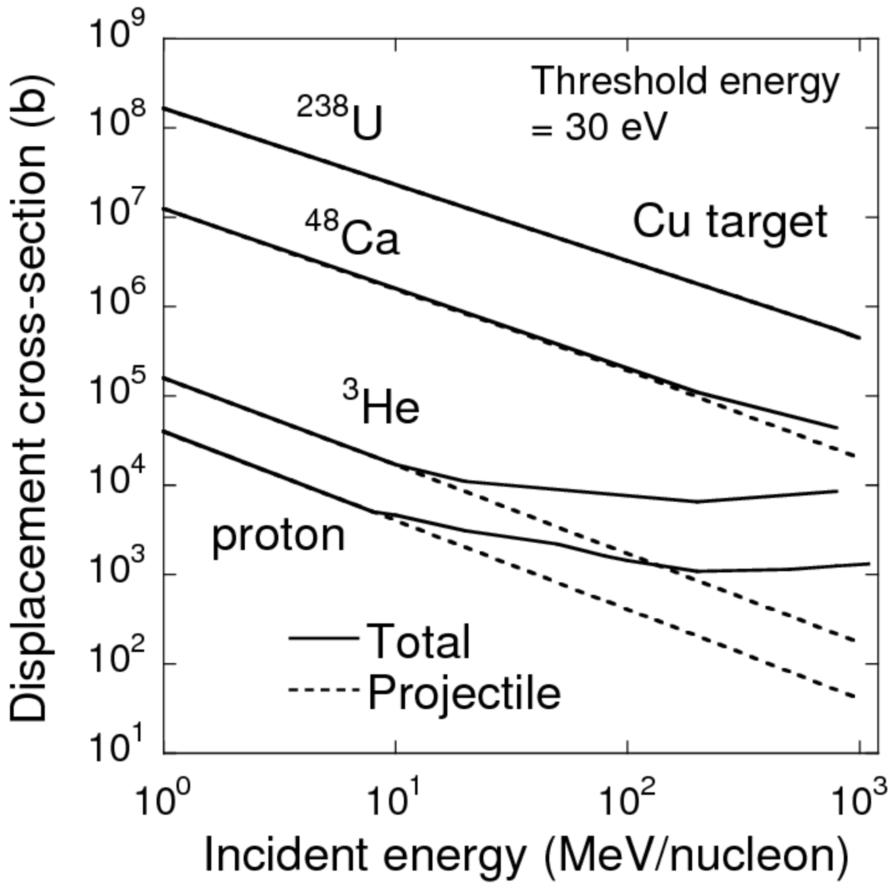
Comparison PHITS with other data for proton at surface



- For the cross sections below 20 MeV, the slope of -1 is seen for Coulomb scattering.
- At the energy region above 20 MeV, contribution of Coulomb scattering for the secondary particles increases with energies.
- At high energy region, discrepancy between data may be due to "the defect production efficiency".

A. Yu. Konobeyev, C.H.M. Broeders, U. Fischer, Proceedings of AccApp '07, 241 - 248.

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



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

Summary

- The DPA model in PHITS has been extended to include all contributions from not only nuclear reaction but also Coulomb scattering.

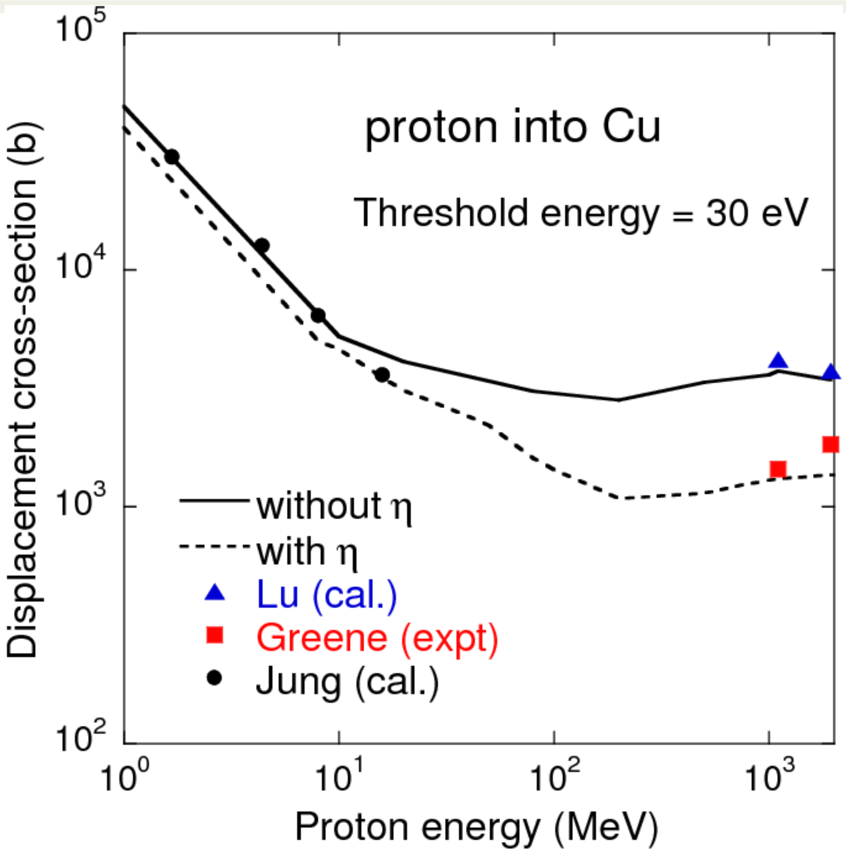
- PHITS results give good agreements with SRIM and MARS for 130 MeV/u ^{76}Ge into W.

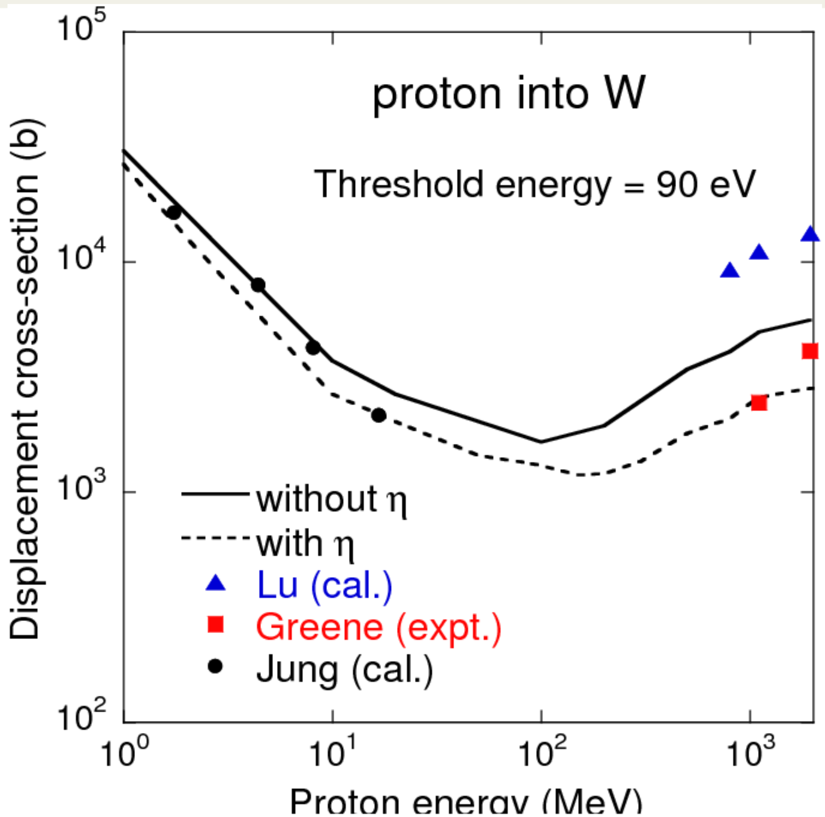
- Damage calculation only by PKA's directly created by the projectile, such as SRIM, lead to sever underestimation where projectile energy is high enough to create nuclear reactions.

- PHITS can make heavy-ion damage database not only at surface but also peak and averaged DPA in a cell.

Back-up slides

Contribution of defect production efficiency





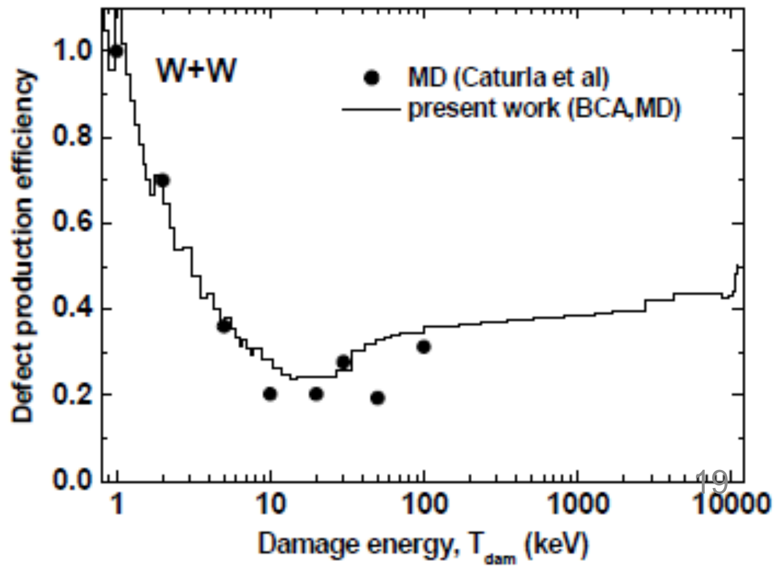
$\nu(T_i) = \eta \cdot N_{NRT}$, η: the defect production efficiency

copper[8]:

$$\eta = 0.7066\,T_{dam}^{-0.437} + 2.28\times10^{-3}\,T_{dam},$$

tungsten[8]:

$$\eta = 1.0184\,T_{dam}^{-0.667} + 5.06\times10^{-3}\,T_{dam},$$

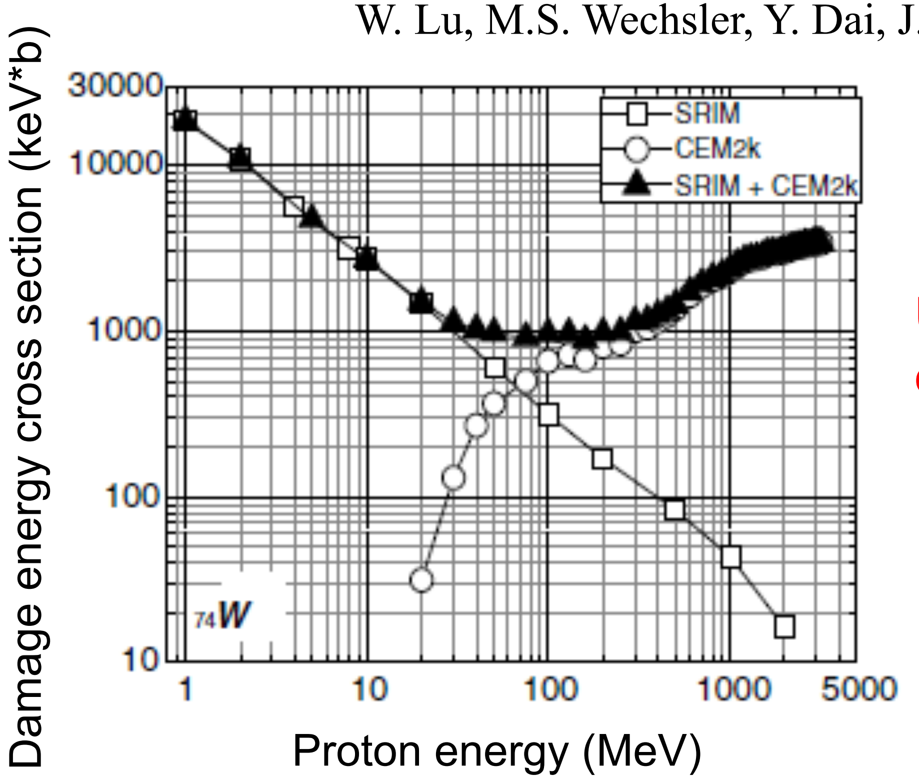


A. Yu. Konobeyev, et al., Proceedings of AccApp '07, 241 - 248.

Introduction ~similar work~

Displacement cross-sections were obtained for iron, copper and tungsten irradiated with protons at energies up to a few GeV using TRIM and nuclear reaction model.

W. Lu, M.S. Wechsler, Y. Dai, J. Nucl. Mater.356 (2006) 280-286.



Useful to estimate DPA easily for proton machine.

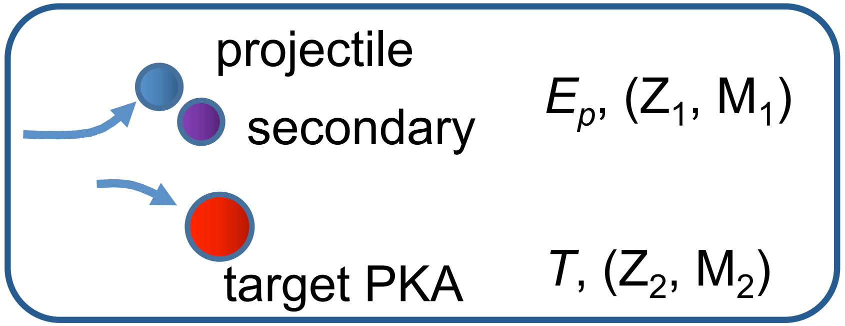
- Cross-section is just at the surface of material.
- No consideration for the DPA distribution in thick target.
- No consideration for heavy-ion incidence.

⇓

- Coulomb scattering and nuclear reaction should be folded for thick target calculation.

(2) Coulomb scattering

M. Nastasi et. al., "Ion-Solid Interaction: Fundamentals and Applications (Cambridge Solid State Science Series)



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

Thomas-Fermi λ=1.309, m=1/3, q=2/3

- Dimensionless collision parameter t $\quad t \equiv \varepsilon^2 \frac{T}{T_{max}} = \varepsilon^2 \sin^2\left(\frac{\theta_c}{2}\right)$
- dimensionless energy ε $\quad \epsilon = E_p a_{TF} M_2 / Z_1 Z_2 e^2 (M_1 + M_2)$
- Maximum transferred energy T_{max} $\quad T_{max} = \frac{4 M_1 M_2}{(M_1 + M_2)^2} E_p$
- Transferred energy from projectile and secondary to target atom $\quad T = \frac{T_{max}}{\varepsilon_p^2} \times t$

Introduction
~Overview of PHITS (Particle and Heavy Ion Transport code System)~

Institution: JAEA, RIST and KEK

PHITS = Monte Carlo particle transport + JAM + JQMD

Transport	Neutron, Photon, Electron Transport by Nuclear Data
JAM	Hadron-Nucleus Collisions up to 200 GeV
JQMD	Nucleus-Nucleus Collisions by Molecular Dynamics

Transport Particle and Energy

Proton	0 ~ 200 GeV
Neutron	10^{-5} eV ~ 200 GeV
Meson	0 ~ 200 GeV
Barion	0 ~ 200 GeV
Nucleus	0 ~ 100 GeV/u
Photon	1 keV ~ 1 GeV
Electron	1 keV ~ 1 GeV

External Field: Magnetic Field

Language and Parallelism

- FORTRAN 77
- MPI

Tally, Mesh and Graphic

- Tally: Track, Cross, Heat, Time, DPA, Product, LET
- Mesh: cell, r-z, xyz
- Graphic: ANGEL (PS generator)

K. Niita et al., JAEA-Data/Code 2010-022 (2010), see http://phits.jaea.go.jp/