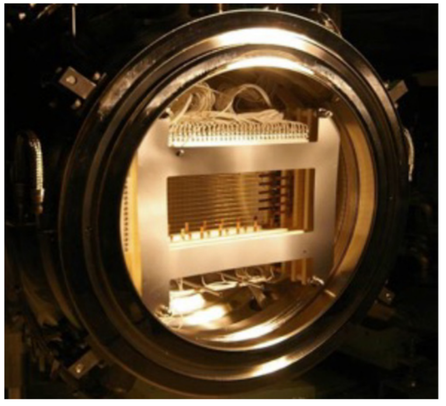
Radiation damage calculation in PHITS and benchmarking experiment for cryogenic-sample high-energy proton irradiation

Y. Iwamoto, H. Matsuda, S. Meigo, D. Satoh, JAEA
T. Nakamoto, M. Yoshida, KEK
Y. Ishi, Y. Kuriyama, T. Uesugi, , H. Yashima T. Yoshiie,
KURNS, Kyoto University
T. Shima, RCNP, Osaka University
R. M. Ronningen, FRIB, Michigan State University
K. Niita, RIST

Contents

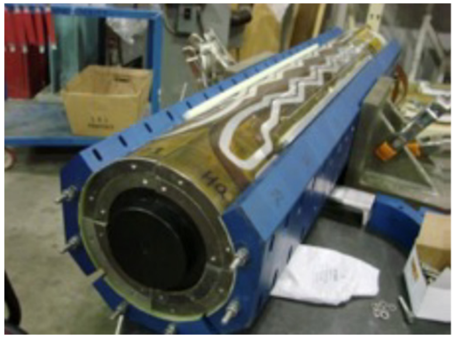
Introduction

Prediction of usable lifetime of materials under high-energy (E>100 MeV) particle irradiation is essential for the accelerator design.

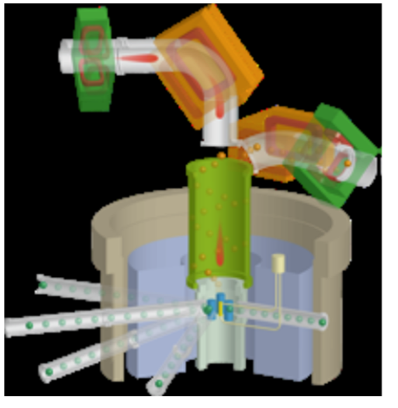


Beam windows in J-PARC MLF (Al alloy)

Beam window in neutrino facility (Ti alloy)



CERN LHC superconducting magnet (Nb alloy)



2nd target in J-PARC MLF (W)

Displacement per atom (DPA) value is used as a damage-based exposure unit.

Microscopic effects on material

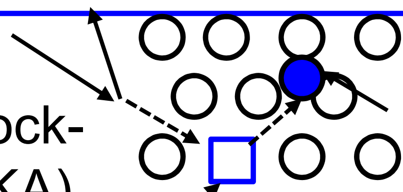
DPA: average number of displaced atoms per atom of a material

DPA = $\sigma_d \phi$

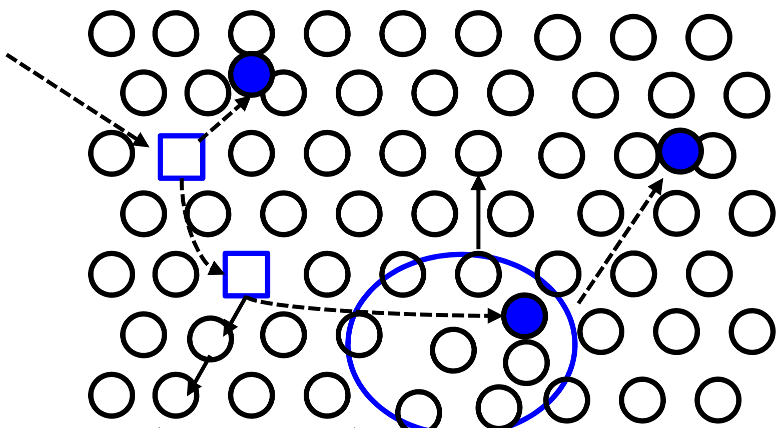
$\boldsymbol{\sigma_d}$: **displacement cross-section (m^2)**

ϕ: irradiation fluence (particles/m^2)

i.e. 1 dpa mean each atom has been displaced from its lattice site an average of 1 times.



Frenkel-pairs causes cascade damage.



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

Cascade damage deals with primary damage state only,

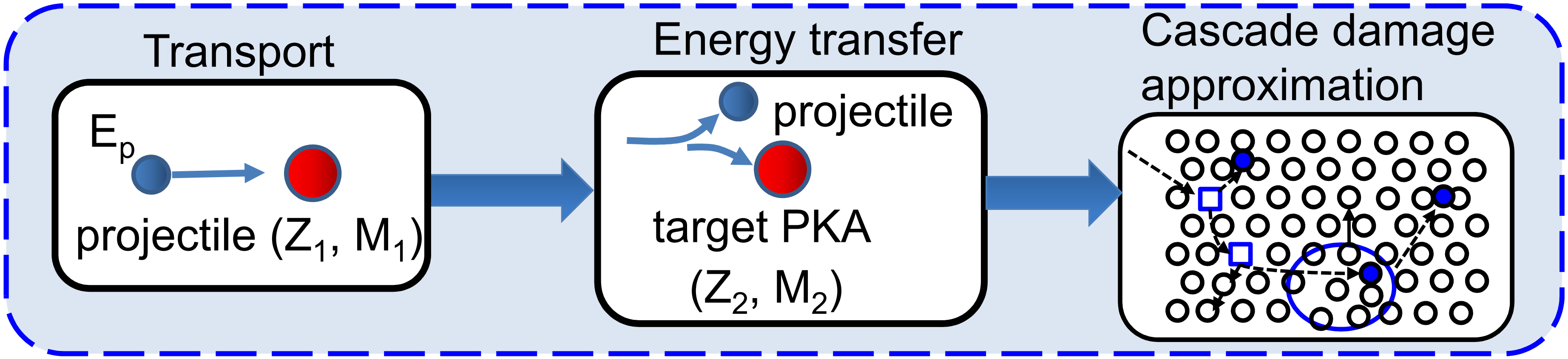
i.e. damage produced during first few ps. Long-range thermally activated defect motion is excluded.

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



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, MARS, FLUKA, MCNP

Contents

Overview of PHITS

Particle and Heavy Ion Transport code System

Development

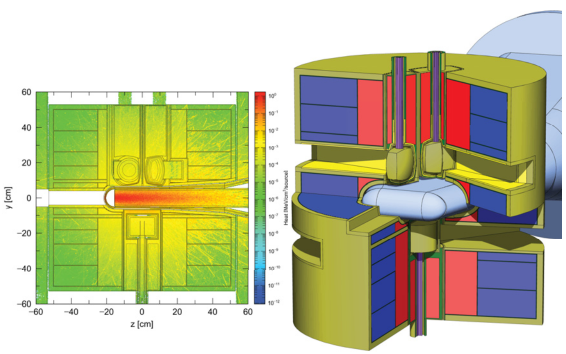
JAEA (Japan), RIST (Japan), KEK (Japan), Technische Universitat Wien(Austria)
RIKEN (Japan), CEA (France), Kyushu Univ. (Japan)

Capability

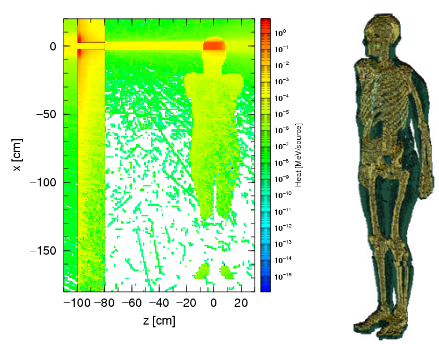
Transport and collision of various particles over wide energy range

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

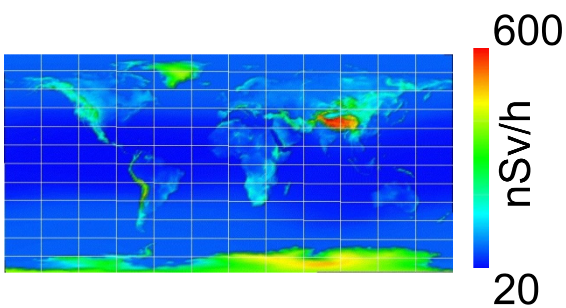
Application Fields



Accelerator Design



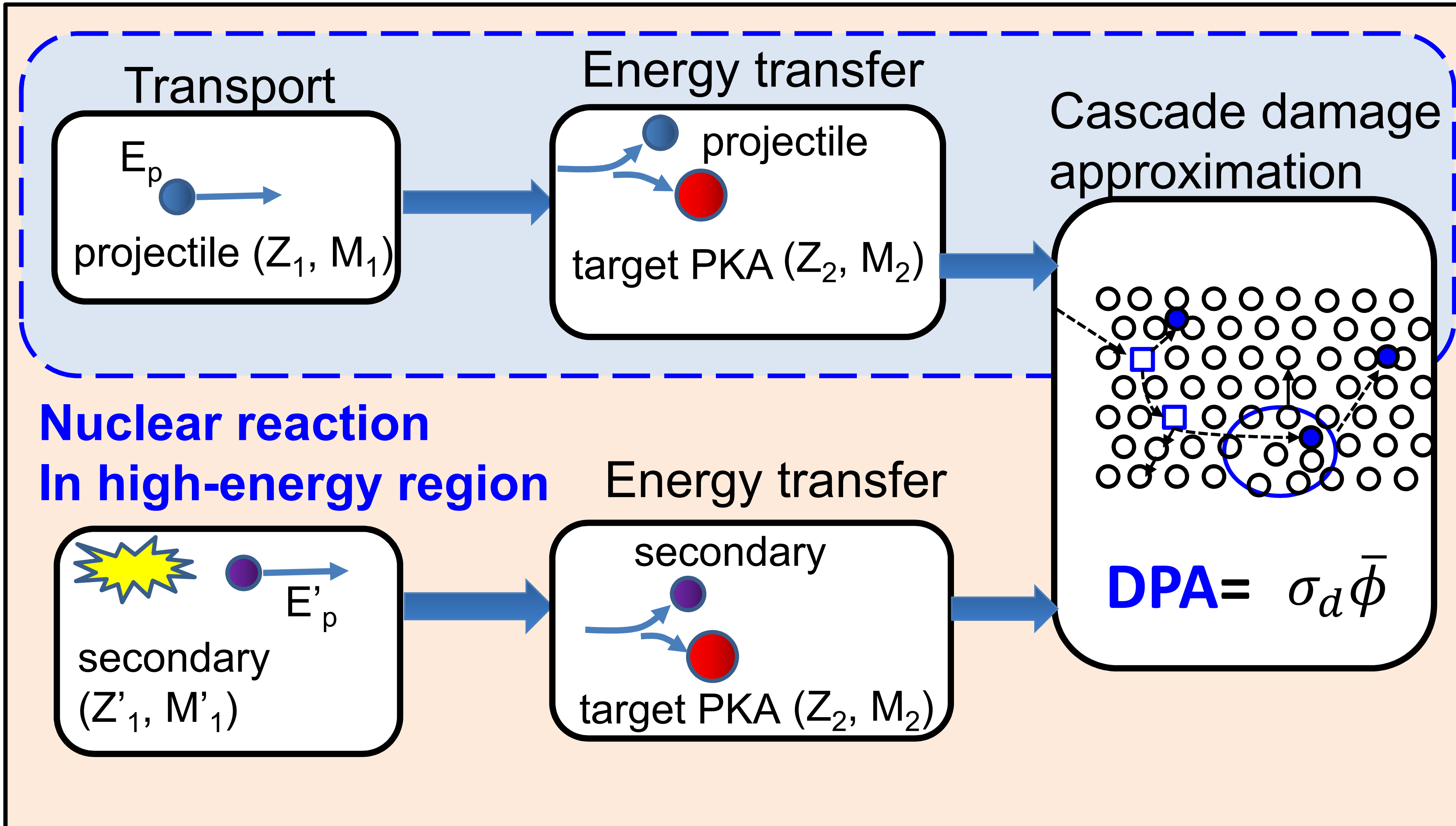
Radiation Therapy



Space Application

T. Sato et al., J. Nucl. Sci. Technol., 55 (2018) 684-695.

Radiation damage model in PHITS

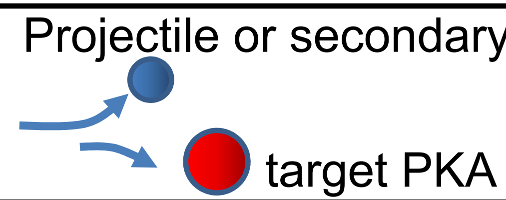


Y. Iwamoto et al., Nucl. Instr. Meth. B 274 (2012) 57-64.

Displacement cross-section with standard approximation

$$\sigma_{\mathrm{NRT}} = \int_{t_\mathrm{d}}^{t_\mathrm{max}} d\sigma_{\mathrm{sc}}/dt \cdot N_{\mathrm{NRT}} dt$$

$d\sigma_{\mathrm{sc}}/dt$: Coulomb scattering cross section using dimensionless collision parameter t



N_{NRT}: Number of displaced atoms using phenomenological approach
Norgett, Robinson and Torrens, Nuclear Engineering and Design, 33 (1975) 50-54.

The standard approach has been a simple equation for more than 40 years.

$$N_{\mathrm{NRT}} = (0.8 \cdot T_\mathrm{d})/(2 \cdot E_\mathrm{d})$$

T_d :damage energy available to generate atomic displacements by elastic collisions

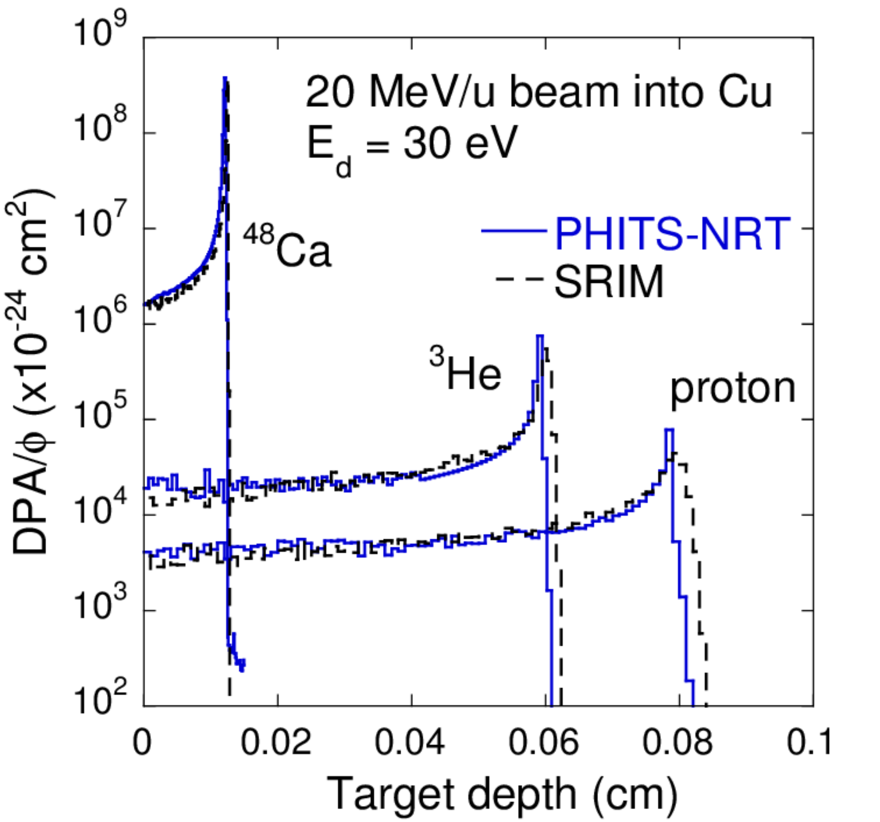
$$T_\mathrm{d} = T/(1 + k_{\mathrm{cascade}} \cdot g(\varepsilon))$$

T: PKA recoil energy

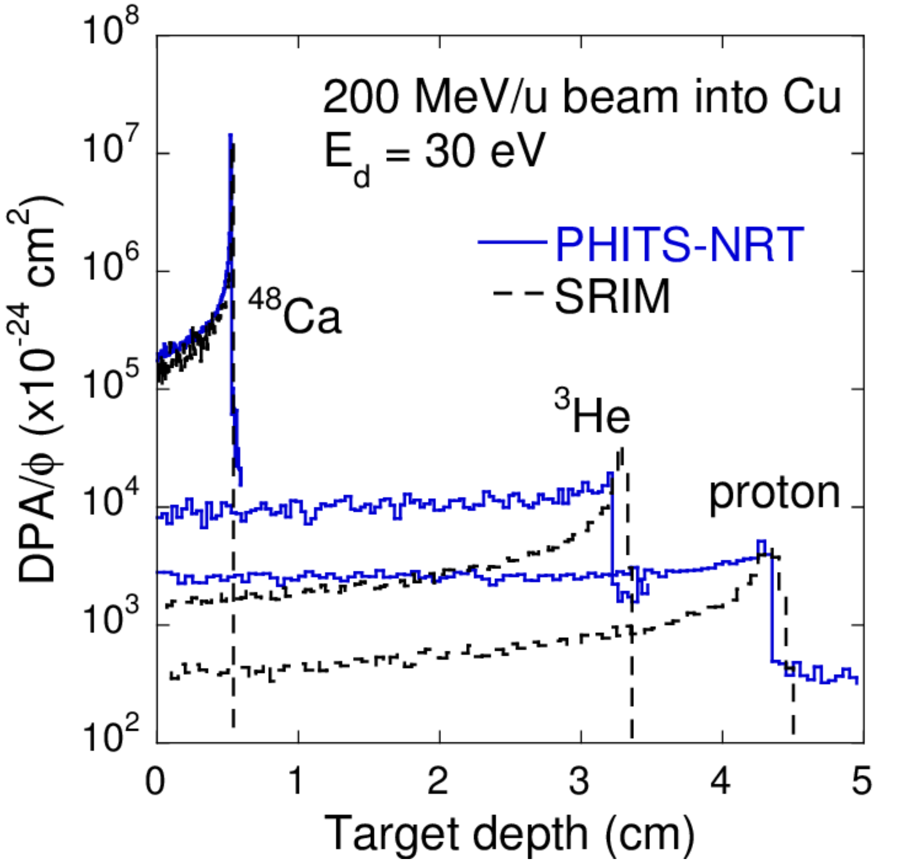
E_d: Displacement threshold energy. e.g. varies 15 – 90 eV for each atom.

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

Target depth dependence of DPA values in copper



Target depth distribution for 20 MeV/u proton, ^{3}He and ^{48}Ca



Target depth distribution for 200 MeV/u proton, ^{3}He and ^{48}Ca

Secondary particles produced by sequential nuclear reactions

Advanced Monte Carlo particle transport codes are essential for DPA calculations in high-energy region.

Displacement cross-section with new approximation

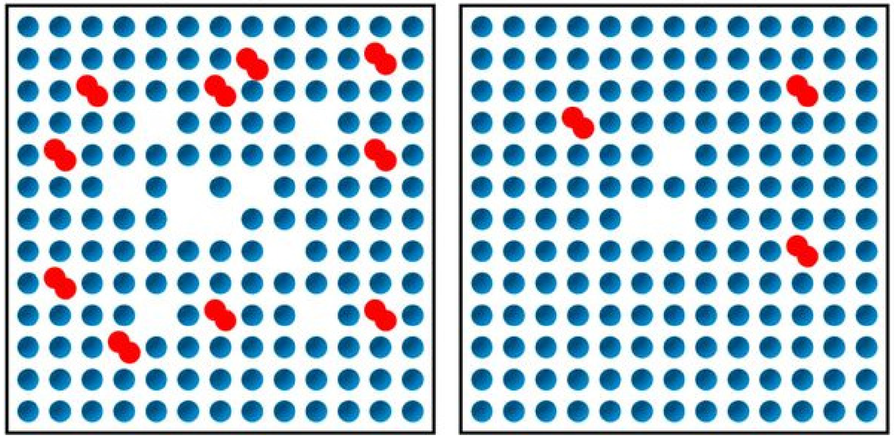


Figure 2 in the paper: K. Nordlund et al., Nature Communications 9 (2018) 1084.

Molecular Dynamic simulation study

athermal recombination between interstitial atom and vacancy

NRT-dpa damage model Actual damage production

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

addressed by new athermal recombination correction (arc-dpa) equation

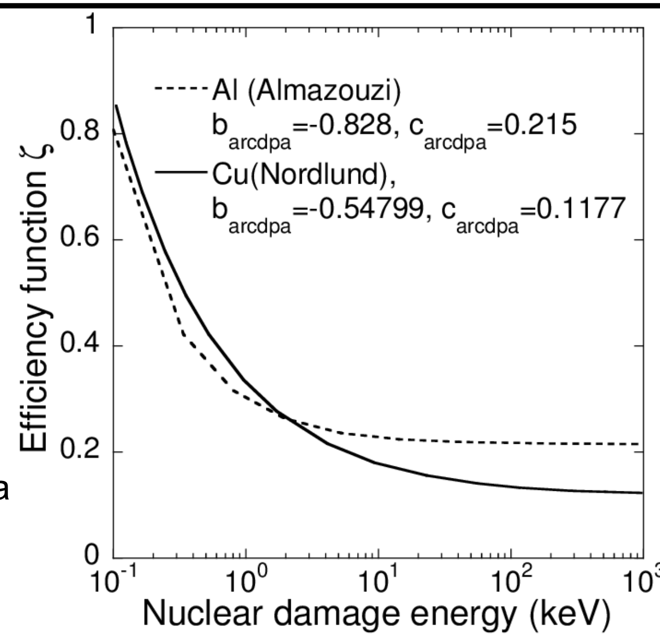
$$\sigma_{\mathrm{arc-dpa}} = \int_{t_\mathrm{d}}^{t_\mathrm{max}} d\sigma_{\mathrm{sc}}/dt \cdot N_{\mathrm{NRT}} \cdot \zeta dt$$

$$\zeta = \frac{1 - C_{\mathrm{arcdpa}}}{(2\,E_\mathrm{d}/0.8)^{b_{\mathrm{arcdpa}}}} T_\mathrm{d}^{b_{\mathrm{arcdpa}}} + C_{\mathrm{arcdpa}}$$

based on tabulated parameters: b_{arcdpa}, and c_{arcdpa}

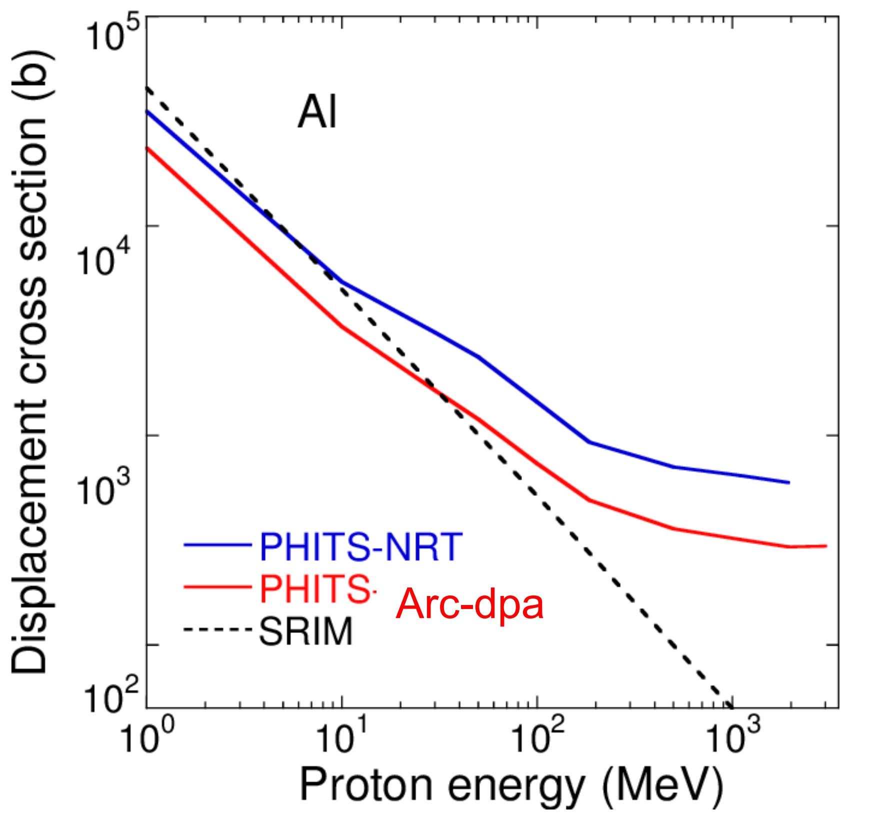
for Fe, Cu, Ni, Pd, Pt, W (Nordlund)
Al (Almazouzi)

➡ Implement into PHITS code

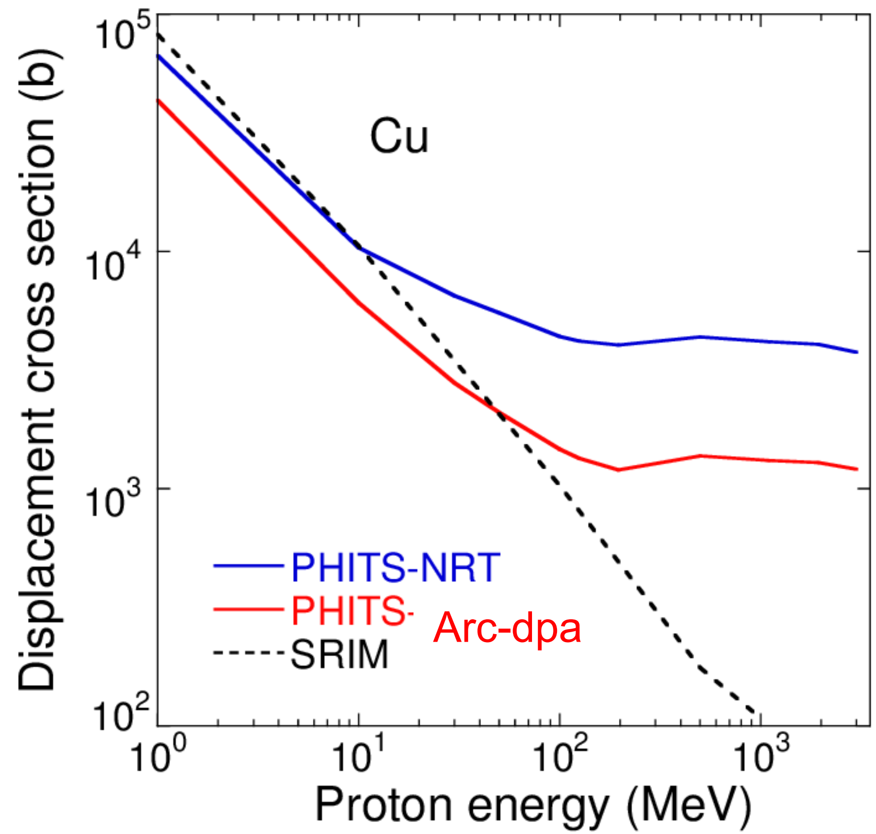


Efficiency function

Calculated displacement cross sections



Displacement cross section for p + Al



Displacement cross section for p + Cu

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

To Validate calculated results, experimental data is needed.

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

Contents

Irradiation on metal at cryogenic temperature

Recombination of Frenkel pairs by thermal motion is well suppressed.

Damage rate

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

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

$\overline{\Phi}$: Average Beam fluence($1/m^2$)

ρ_{FP}: Frenkel-pair resistivity (Ωm)

Resistivity increase is the sum of resistivity per Frenkel pair

BNL data (1.1, 1.9 GeV): Cryostat assembly for sample irradiation consisted of complicated system to deliver a flow of liquid cryogen.

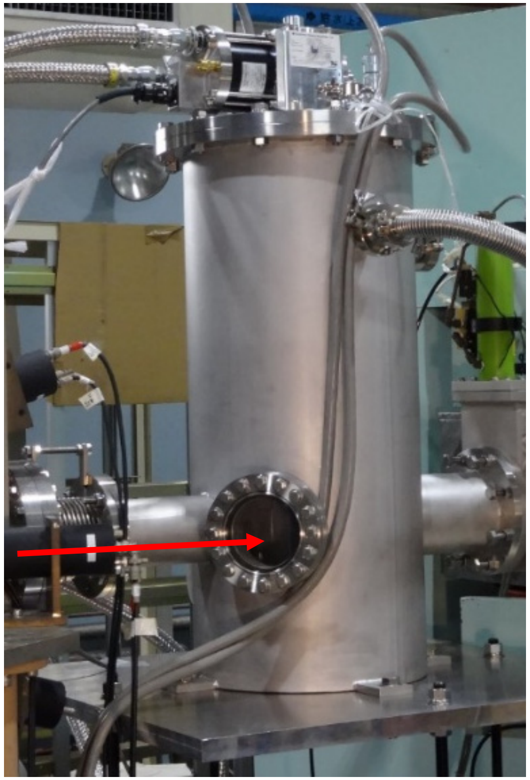
Hard to measure systematic data at other facilities with same device.

Development of liquid cryogen-free cooling system
Measurements of displacement cross sections of Al and Cu

Measurements of displacement cross section in Japan

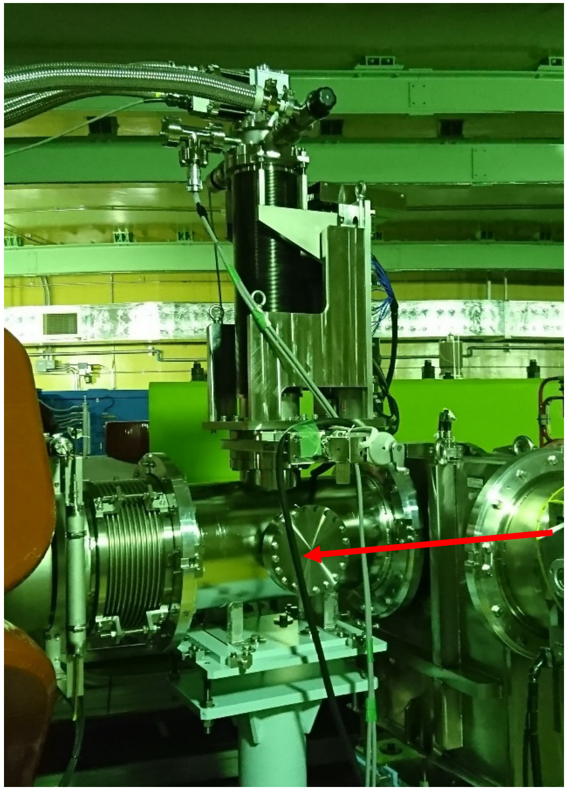
125 MeV proton+Cu
FFAG facility, Kyoto Univ.

Y. Iwamoto et al., J. Nucl. Mater., 458, (2015) 369-375.



200 MeV proton+Cu, Al
RCNP, Osaka Univ.

Y. Iwamoto et al., J. Nucl. Mater., 508, (2018) 195-202.

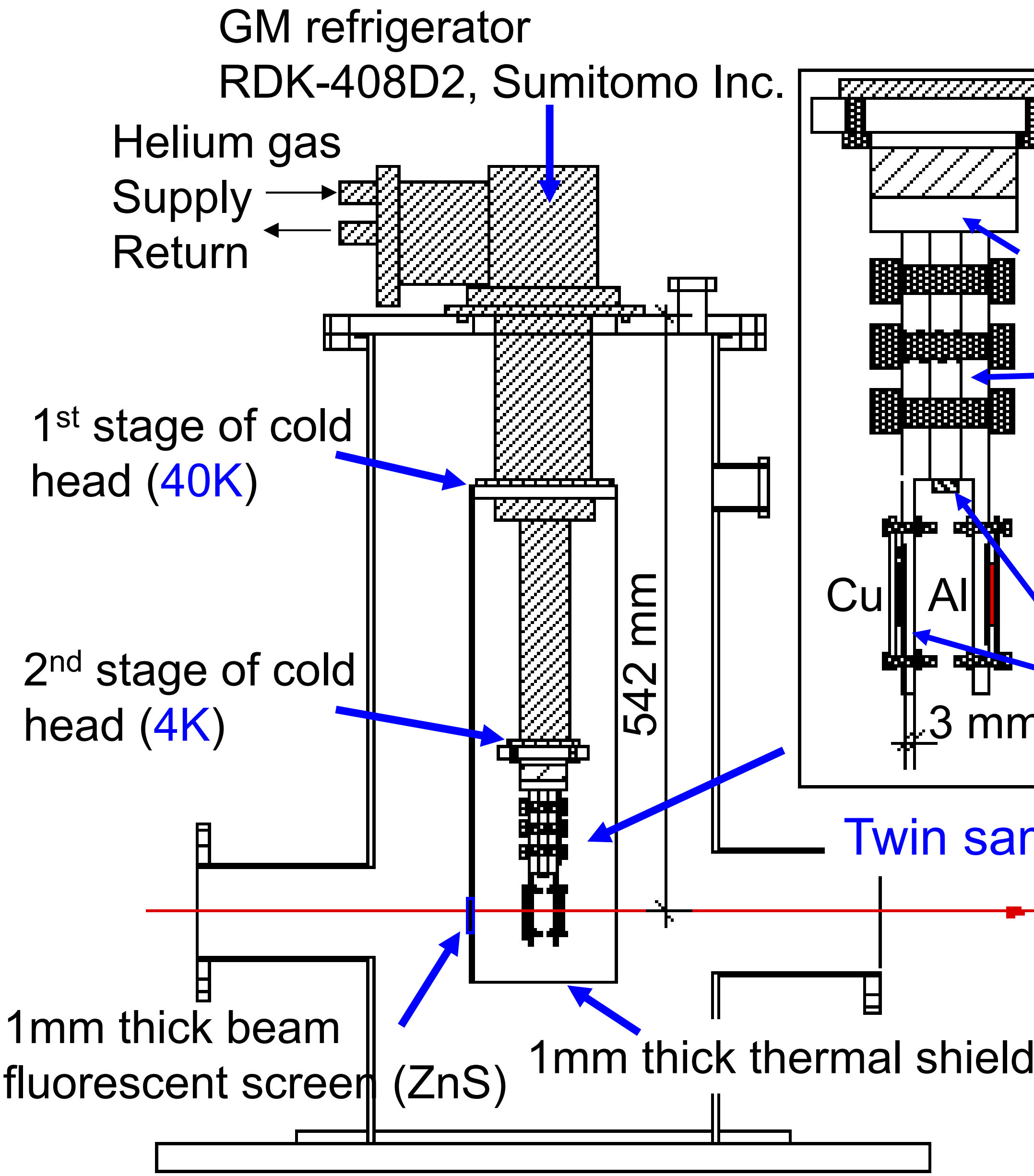


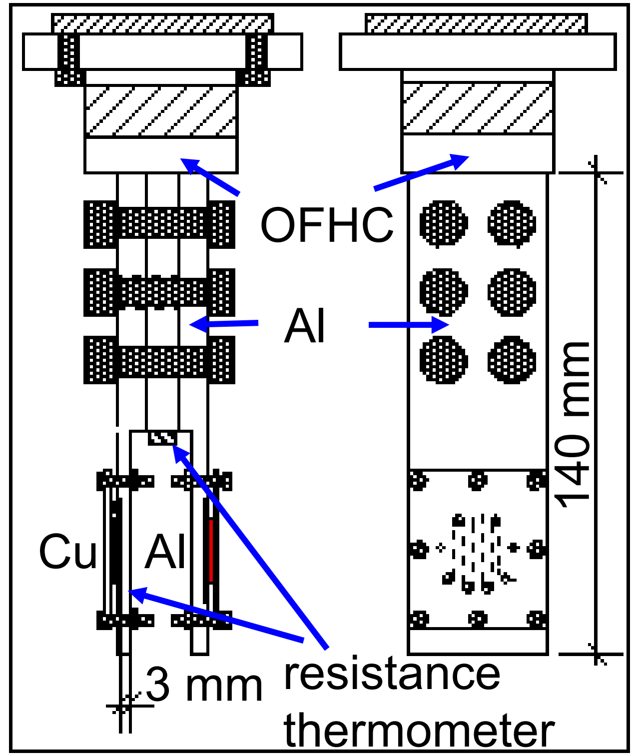
3 GeV proton+Cu
J-PARC

S. Meigo et al., presented at IPAC’18, 2018, MOPML045

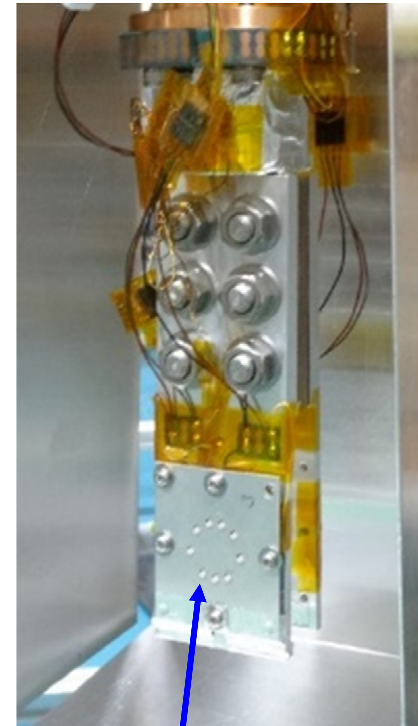
S. Meigo et al., presented at HB2018, 2018, TUP1WE03

Irradiation chamber and target assembly





Twin sample assembly

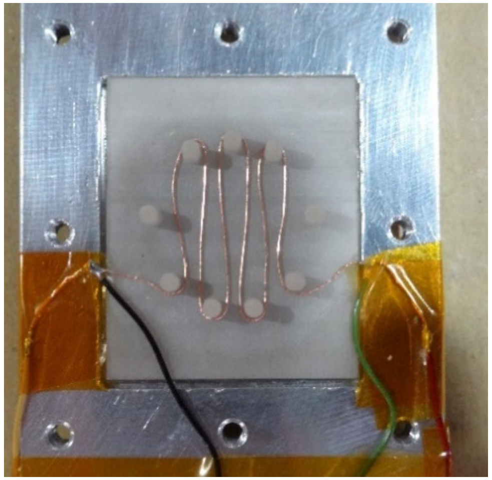


Samples at **3 K**

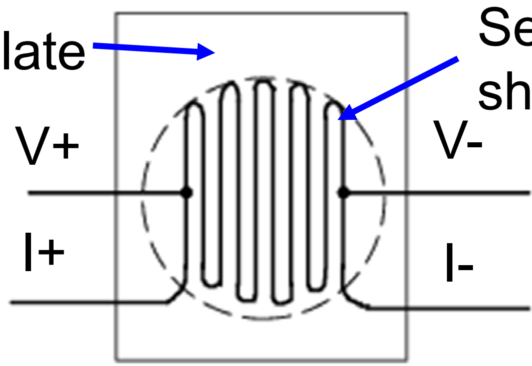
Measure the changes in electrical resistivity of two samples under 200 MeV proton irradiation

Schematic of the cryogenic irradiation chamber

Sample and electrical resistance measurement



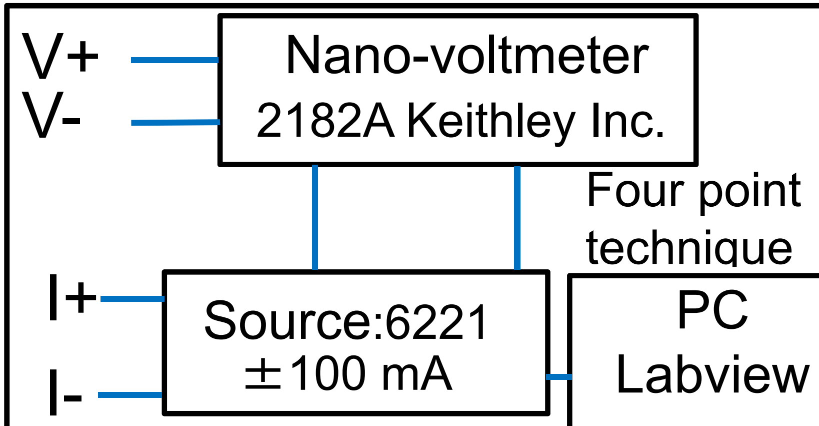
Material	Aluminum	Copper
Diameter (mm)	0.25	0.25
Length (mm)	123	134
Purity (%)	99.99	99.999
Electrical resistivity at room temperature(Ω m)	2.19×10^{-8}	1.47×10^{-8}
Electrical resistivity at 3 K(Ω m)	4.43×10^{-11}	2.02×10^{-11}



Cross section of wire

Electrical resistivity $\rho(\Omega m) = \frac{S(m^2)}{L(m)} * R(\Omega)$

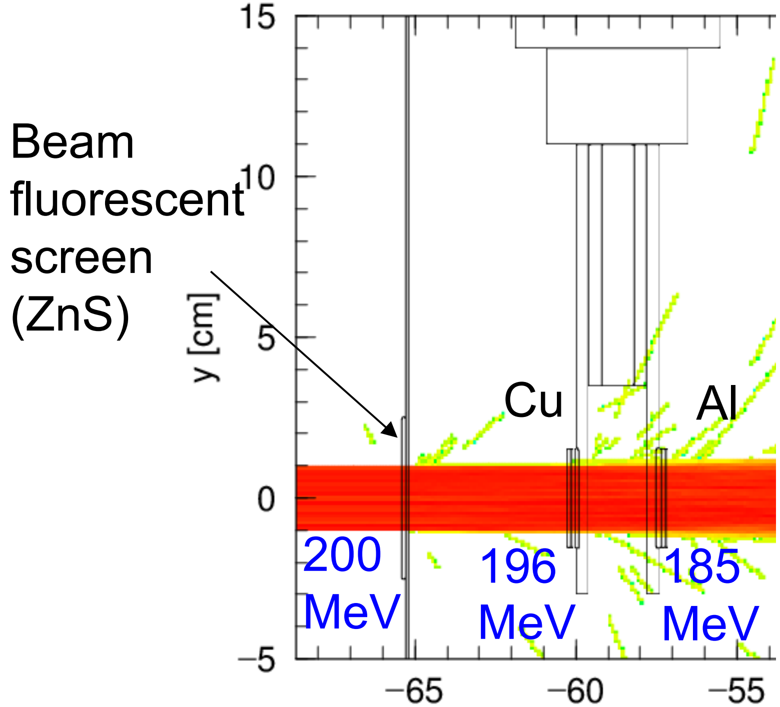
Length Resistance



Cancel effects of thermal electromotive force

Precision ±0.001μΩ @ 3 K

Beam profile



PHITS simulation

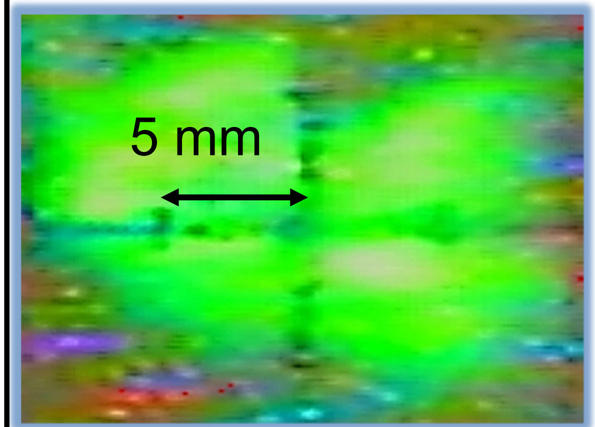


Image on screen

Adjusted beam area to cover sample with controlling magnetic field of magnets

Captured the beam shape on screen by portable camera.

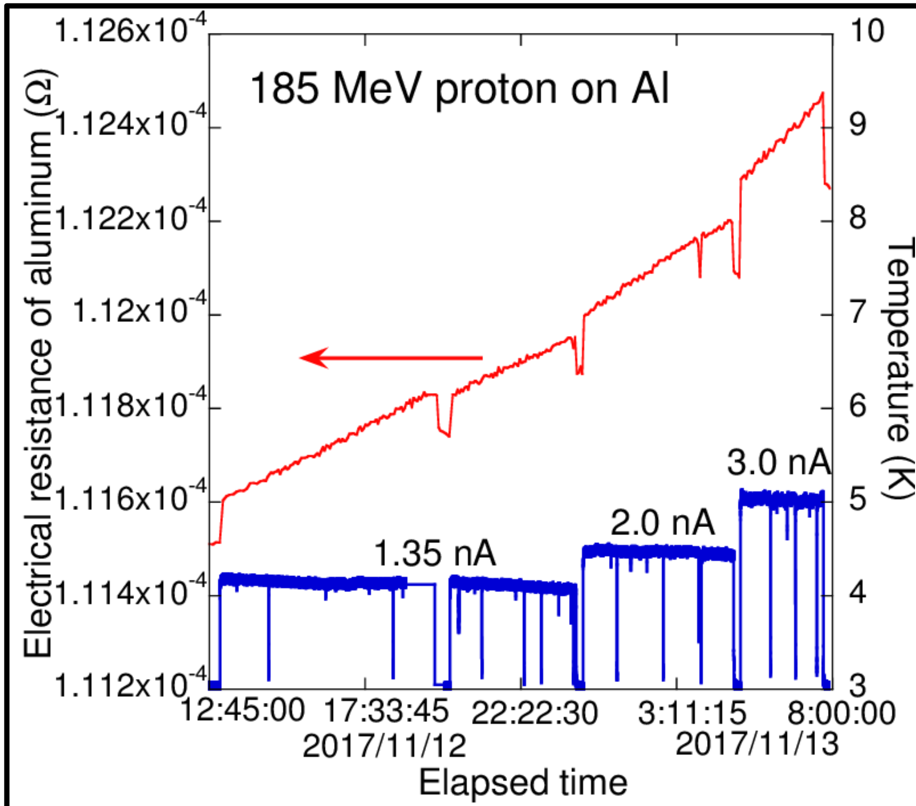
Estimation of uncertainty of displacement cross section due to beam profile (FWHM = 9.5 ± 2.5 mm) using PHITS

$$\boldsymbol{\sigma_d = \frac{DPA}{\bar{\Phi}}}$$

~4 %

➡ In future, beam profile monitor will be used at RCNP.

Electrical resistivity changes of wires during irradiation



- ✓ 5 K during 3 nA beam irradiation
- ✓ Total increase in resistance at 3 K: 0.76 μΩ for Al, 2.34 μΩ for Cu
- ✓ Total fluence: 3.89×10^{18} proton/m^2

Damage rate

$$D(\Omega \mathrm{m}^3) = \frac{\Delta\rho(\Omega \mathrm{m})}{\bar{\Phi}(1/\mathrm{m}^2)}$$

Electrical resistivity

Average beam fluence

Experimental damage rate

Beam		fusion neutron	125 MeV proton	200 MeV proton	1.94 GeV proton	3 GeV proton
		RTNS-II	KURRI-FFAG	RCNP	BNL	J-PARC
Damage rate (10^{-31} Ω m^3/particle)	Al	4.18	-	**1.31**	-	-
	Cu	2.48	**3.41**	**3.60**	3.66	**2.35**

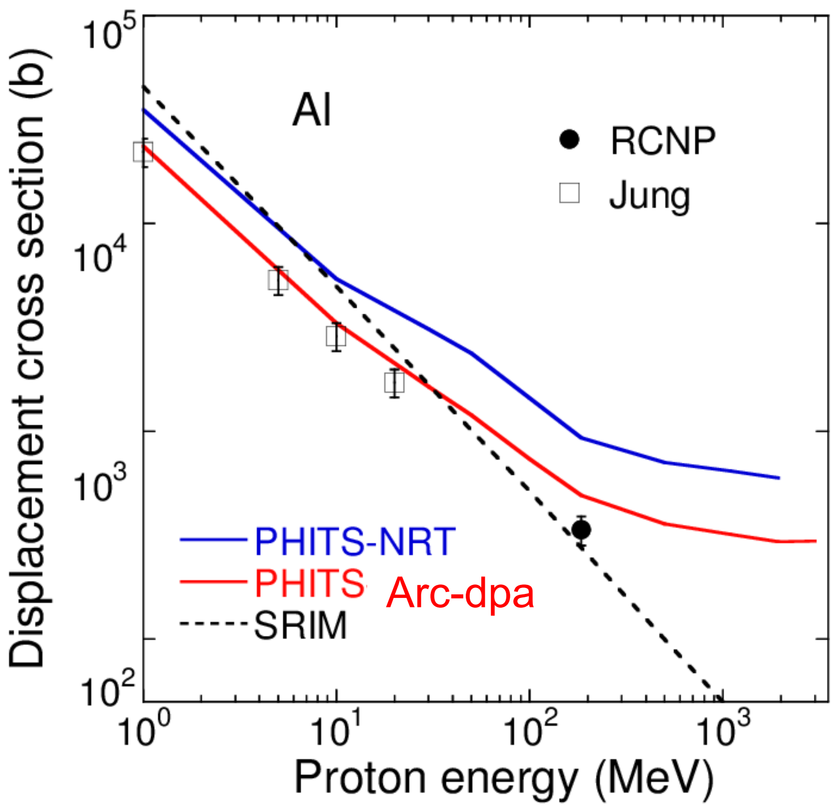
Comparison of experimental displacement cross sections with PHITS results

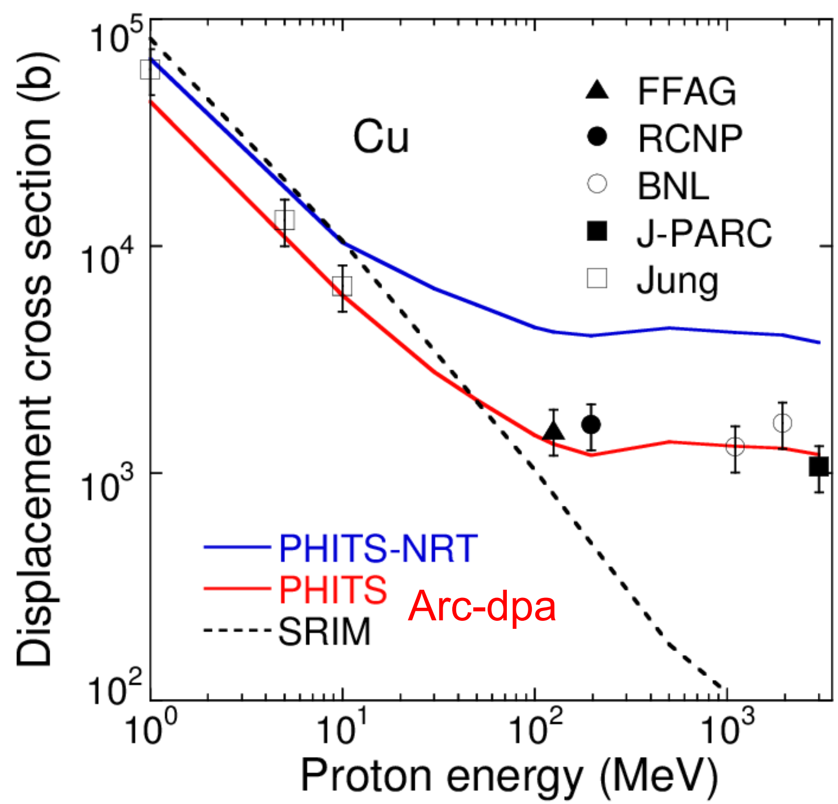
$$\sigma_{\mathrm{exp}}(\mathrm{m}^2) = \frac{1}{\rho_{\mathrm{FP}}(\Omega\mathrm{m})} D(\Omega\mathrm{m}^3)$$

➡ Damage rate (D)

➡ Change in resistivity per Frenkel-pair density (ρ_{FP})

Al:3.9±0.6 μΩm 15 % uncertainty Phys. Rev. B 8 (1973) 2604-2621.	Cu:2.2±0.5 μΩm 23 % uncertainty J. Nucl. Mater. 69&70 (1978) 644-649.





Results calculated by standard model (NRT) overestimates the data by a factor of ~3.
New model(arc-dpa) gives good agreements with the data well.
The arc-dpa will be a basis for formulating more reliable.

Contents

Recovery of defects through annealing after beam irradiation

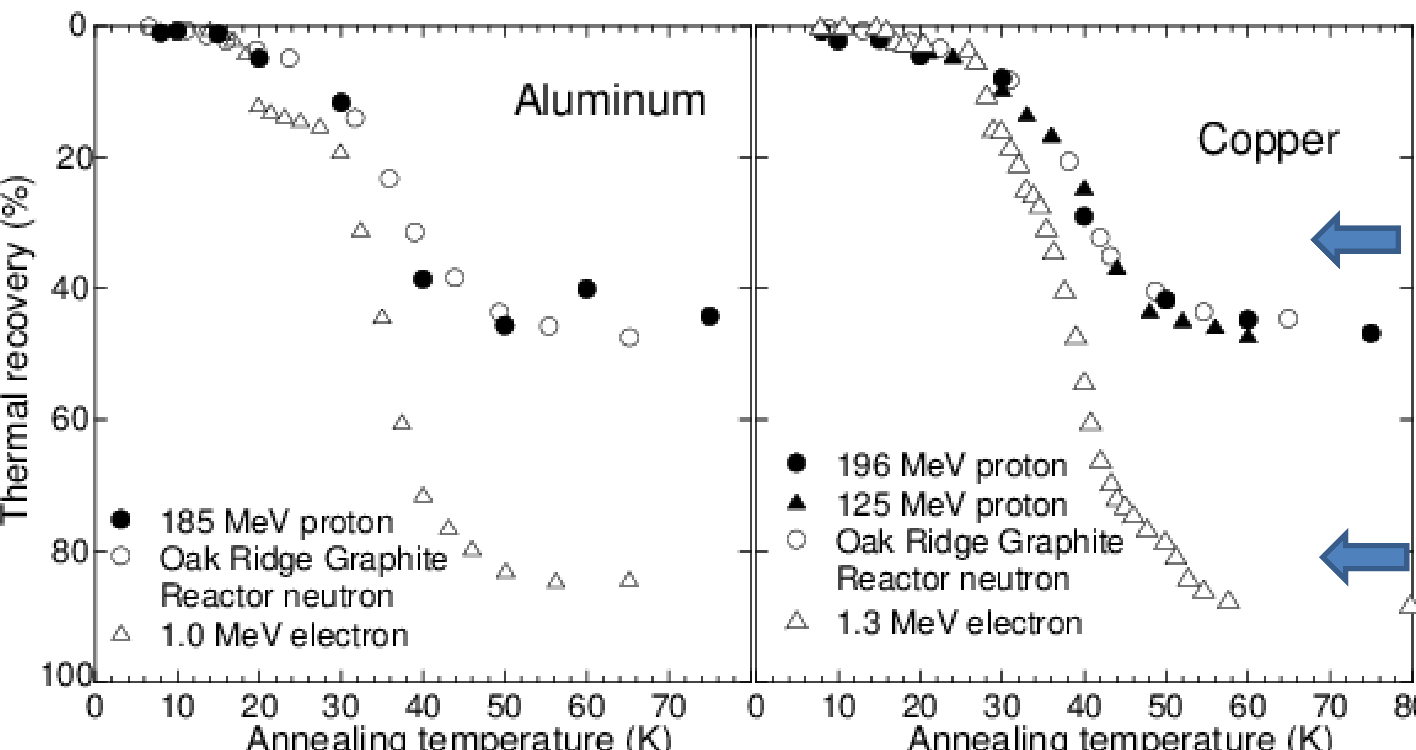
Annealing effects were observed up to certain temperatures by isochronal schedule.

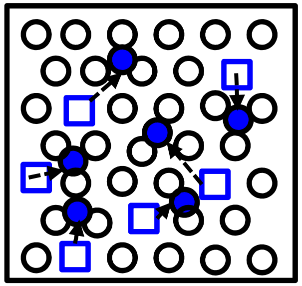
(1) Warming the sample to the annealing temperature using an electric heater.
(2) Holding sample temperature constant for about 10 min.
(3) Cooling the sample to 3 K.
(4) Measuring electrical resistivity of the sample at 3 K.

$$\text{Thermal recovery} = 1 - \frac{\Delta\rho}{\Delta\rho_0}(\%)$$

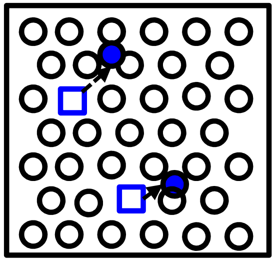
$\Delta\rho$ ← remaining radiation-induced resistivity increase

$\Delta\rho_0$ ← initial radiation-induced resistivity increase





Frenkel-pair density: Large (proton, neutron)



Frenkel-pair density: Small (electron)

Contents

1. Introduction

2. Radiation damage model in PHITS

3. Benchmarking experiments of displacement cross section

4. Recovery of defects through annealing after beam irradiation

5. Conclusion

Conclusion

The radiation damage model in PHITS has been developed.

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

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

We have developed cryogenic irradiation system and measured displacement cross sections of Al and Cu for 125, 200 MeV and 3 GeV proton irradiation.

The arc-dpa(new) reproduces the experimental data well for Cu and Al.

The arc-dpa will be used for efficient predictions of the usable lifetime.

Future plan

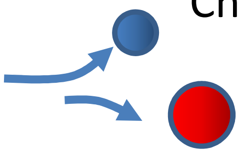
Continue to measure the data for various metals.
pure metal (Al, Fe, Ti, Nb, W), alloy

Arc-dpa parameters for various metals will be implemented in PHITS, when these parameters are opened.

This work is supported by JSPS KAKENHI Grant Number JP16H04638.

(2)Energy transfer with Coulomb scattering in PHITS

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



Charged particle

target PKA

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

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

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

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

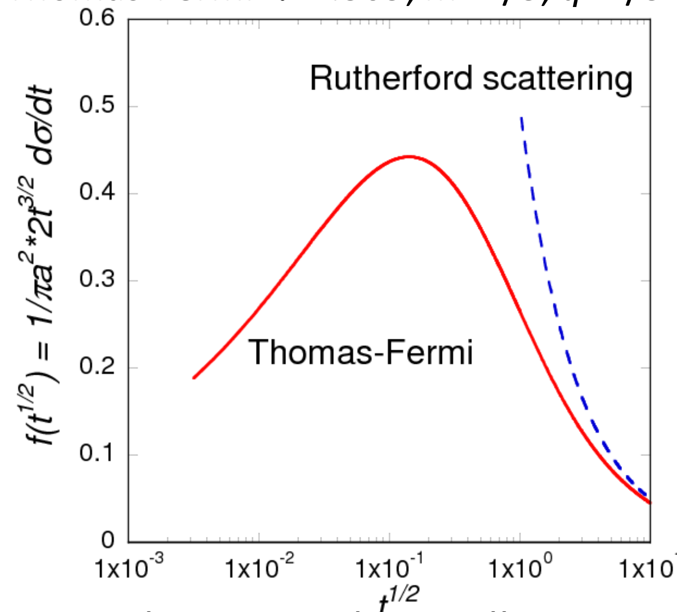
$\mathcal{E}$:dimensionless energy

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

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