Radiation damage calculation in PHITS

Y. Iwamoto\textsuperscript{1}, K. Niita\textsuperscript{2}, T. Sawai\textsuperscript{1}, R.M. Ronningen\textsuperscript{3}, T. Baumann\textsuperscript{3}

\textsuperscript{1} JAEA, \textsuperscript{2}RIST, \textsuperscript{3}MSU/NSCL
Introduction

Radiation damage model in PHITS

Radiation damage calculation
  • proton, heavy-ion, neutron incidences

Example of heat calculations

Summary
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:

\[ \text{DPA} = \phi \ t \ \sigma \]

\( \sigma \) : the Displacement cross-section.

\( \phi t \) : 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
Introduction

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Summary
Overview of radiation damage model in PHITS

(1) Transport
- projectile
- Secondary particle by nuclear reaction
- Recoil atom by nuclear elastic scattering

(2) Energy transfer to target recoil atom by Coulomb scattering
- Recoil atom by Coulomb

(3) Cascade damage approximation
- target atom
- Recoil atom
Radiation damage model in PHITS(1)

(1) Transport

(2) Energy transfer to target recoil atom with Coulomb scattering

(3) Cascade damage approximation

Models in PHITS

<table>
<thead>
<tr>
<th>Collision distance between particles</th>
<th>Total reaction cross section produced by systematic formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stopping power dE/dx and ranges</td>
<td>SPAR based on Bethe formula</td>
</tr>
<tr>
<td>Nuclear reaction</td>
<td>Intra-nuclear cascade model</td>
</tr>
<tr>
<td>E&gt;20MeV, all particles</td>
<td></td>
</tr>
<tr>
<td>E&lt;20MeV, low energy neutron</td>
<td>Nuclear data, event generator</td>
</tr>
</tbody>
</table>
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 $f(t^{1/2})$.

\[ d\sigma_{\text{scat.}} = \frac{\pi a_{TF}^2}{2} \frac{f\left(\frac{1}{t^{2}}\right)}{t^{3/2}} \, dt \]

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

Thomas-Fermi $\lambda=1.309$, $m=1/3$, $q=2/3$

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

- Dimensionless energy $\varepsilon = \frac{E_p a_{TF} M_2 / Z_1 Z_2 e^2 (M_1 + M_2)}{T_{\text{max}} \times \frac{t}{\varepsilon_p}}$

- Transferred energy from projectile and secondary to target atom
Radiation damage model in PHITS(3)

(1) Transport

(2) Energy transfer to target recoil atom with Coulomb scattering

(3) Cascade damage approximation

Damage energy

\[ \sigma_{\text{damage}} = \int_{t_d}^{t_{\text{max}}} \frac{d\sigma_{\text{scat.}}}{dt} \cdot \frac{0.8}{2 \cdot T_d} \frac{T}{1 + k_{\text{cascade}} \cdot g(\varepsilon)} dt \]

Number of defects developed by NRT


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
Introduction

Radiation damage model in PHITS

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Example of heat calculations

Summary
Comparison new PHITS with other code

MARS result:
Courtesy Nikolai Mokhov

MARS also folds with Coulomb scattering and nuclear reaction.

Agreement is very good except for old PHITS.

DPA=$\phi t \sigma_{\text{damage}}$
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 severe underestimation where projectile energy is high enough to create nuclear reactions.
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

- Neutron

- Secondary particle by nuclear reaction

- Recoil atom by nuclear elastic scattering

- Target atom

- Recoil atom by Coulomb
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.

14MeV neutrons

Al: 1mmx1mm x50mm

PHITS can calculate detail dpa distribution in a target.

SRIM code cannot calculate dpa for neutrons.

DPA value decrease with depth, exponentially.

Elastic scattering and capture are dominant.

PHITS fit

fit
Introduction

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Example of heat calculations

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

Proton beam at 12 GeV


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
- 

\( ^{48}\text{Ca} \) 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.

Neutron

Proton

Nuclei
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

<table>
<thead>
<tr>
<th>Setting</th>
<th>Target isotope</th>
<th>Bρ* [Tm]</th>
<th>Be target thickness [mm]</th>
<th>Average current [μA]</th>
<th>Heat load [W]</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>$^{31}$Ne</td>
<td>8.2</td>
<td>15</td>
<td>0.53</td>
<td>11.9</td>
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<tr>
<td>II</td>
<td>$^{32}$Ne</td>
<td>8.4</td>
<td>20</td>
<td>2.25</td>
<td>42.6</td>
</tr>
<tr>
<td>III†</td>
<td>$^{24}$O</td>
<td>8.1</td>
<td>15</td>
<td>3.5</td>
<td>32.7</td>
</tr>
<tr>
<td>IV†</td>
<td>$^{33}$Al</td>
<td>7.0</td>
<td>10</td>
<td>3.7</td>
<td>26.8</td>
</tr>
</tbody>
</table>

Heat load (PHITS) [W]

12.0
63.8
45.9
34.4

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