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
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:

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

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

\( \phi t \): the irradiation fluence. \( \phi \): 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.

- **(1) Transport calc.**
  - projectile \((Z_1, M_1)\)
  - target \((Z_2, M_2)\)

- **(2) Coulomb scattering**
  - projectile
  - target PKA

- **(3) Cascade damage approximation**

- 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~

(1) Transport calc.

\[
E_p \rightarrow \text{projectile (Z}_1, M_1) \rightarrow \text{target (Z}_2, M_2) \rightarrow \text{secondary particle (Z'}_1, M'_1) \rightarrow E'_p
\]

(3) Cascade damage approximation

- No Coulomb scattering in old PHITS.
- Result calculated by old PHITS are smaller than SRIM one.

130 MeV/u \(^{76}\text{Ge}\) into W
Number of source: \(9.45 \times 10^{16}\)
Displacement energy = 90 eV

No Coulomb scattering in old PHITS.

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

<table>
<thead>
<tr>
<th>Incident particle type</th>
<th>Incident energy range</th>
<th>target</th>
</tr>
</thead>
<tbody>
<tr>
<td>proton, $^{3}$He, $^{48}$Ca</td>
<td>1 MeV/u ~ 1 GeV/u</td>
<td>Cu, W</td>
</tr>
</tbody>
</table>
Implementation of DPA model in PHITS

~Overview of DPA model~

(1) Transport calc.

SRIM

(2) Coulomb scattering

NEW PHITS

(3) Cascade damage approximation

old PHITS

E_p

projectile (Z_1, M_1)

target (Z_2, M_2)

(2) Coulomb scattering

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

(3) Cascade damage approximation

target PKA
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.
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 $f(t^{1/2})$.

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

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

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

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

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

- **Transferred energy from projectile and secondary to target atom**
  $$T = T_{\text{max}} \times \frac{t}{\varepsilon_p^2}$$

$\varepsilon \Rightarrow$ large
$\theta \Rightarrow$ large
$b \Rightarrow$ small (impact parameter)
(3) Cascade damage approximation

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

Number of defects predicted by NRT


**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.

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

\[ k_{\text{cascade}} = 0.1337 \frac{1}{Z_{\text{target}}^6} (Z_{\text{target}}/A_{\text{target}})^{1/2} \]
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.
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.
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.
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 severe underestimation where projectile energy is high enough to create nuclear reactions.
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”.

For $^{48}$Ca and $^{238}$U, the contribution of PKA’s created by the secondary is small.

For proton and $^3$He beams, contribution of Coulomb scattering by PKA created by the secondary particles increases with energies.

Displacement cross section of heavy ion is much higher than that of light ion.
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 severe 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

\[ \nu(T_i) = \eta \cdot N_{NRT}, \]

\( \eta \): the defect production efficiency

copper\(^8\): \( \eta = 0.7066 T_{\text{dam}}^{-0.437} + 2.28 \times 10^{-3} T_{\text{dam}} \),

tungsten\(^8\): \( \eta = 1.0184 T_{\text{dam}}^{-0.657} + 5.06 \times 10^{-3} T_{\text{dam}} \),

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


- Cross-section is just at the \textit{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.

Useful to estimate DPA easily for proton machine.
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 \( f\left(t^{1/2}\right) \).

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

- **Dimensionless collision parameter** \( t \)
- **Dimensionless energy** \( \varepsilon \)
- **Maximum transferred energy** \( T_{\text{max}} \)
- **Transferred energy from projectile and secondary to target atom** \( T = \frac{T_{\text{max}}}{\varepsilon_p^2} \times t \)

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

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

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

\[ \varepsilon = E_p a_{TF} M_2 / Z_1 Z_2 e^2 (M_1 + M_2) \]

\[ T_{\text{max}} = \frac{4 M_1 M_2}{(M_1 + M_2)^2} E_p \]
**Introduction**

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

Institution: JAEA, RIST and KEK

\[
\text{PHITS} = \text{Monte Carlo particle transport} + \text{JAM} + \text{JQMD}
\]

<table>
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<tr>
<th><strong>Transport</strong></th>
<th>Neutron, Photon, Electron Transport by Nuclear Data</th>
</tr>
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<tbody>
<tr>
<td><strong>JAM</strong></td>
<td>Hadron-Nucleus Collisions up to 200 GeV</td>
</tr>
<tr>
<td><strong>JQMD</strong></td>
<td>Nucleus-Nucleus Collisions by Molecular Dynamics</td>
</tr>
</tbody>
</table>

**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/](http://phits.jaea.go.jp/)