# Development of displacement damage model in PHITS and comparison with other codes in a high-energy region

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## Abstract

*The PHITS code (Monte Carlo Particle and Heavy Ion Transport code System) was further developed to include the displacement damage model. The screened Coulomb scattering and the nuclear reaction model was used to evaluate the energy of the target PKA (Primary Knock on Atom) created by the projectile and the secondary particles. These latter include all particles created from the sequential nuclear reactions. It was found that the PKA created by the secondary particles is more dominant than a target PKA created by the projectile in DPA (Displacement per Atom) calculations for proton and neutron induced reactions at energies above 20 MeV. Recently, radiation damage models in other codes such as FLUKA, MARS and MCNP have also been developed. As there is little experimental data in this high-energy region, an intercomparison among Monte Carlo codes such as FLUKA, MARS and MCNP used in the radiation damage calculation is one way to improve models or have a consistent approach. As an example, for the reactions between 130 MeV/u $^{76}$Ge ions and tungsten, it was found that DPA values calculated with the PHITS are in good agreement with those of SRIM, which is one of the major codes used to estimate radiation damage in the low-energy region and MARS. For the neutron and proton beams in the energy range from 10 MeV to 1 GeV, the PHITS results agree with those of FLUKA within a factor of two. Further intercomparison among the codes such as MARS, FLUKA, MCNP and PHITS should be carried out, as well as measurements of displacement damage cross-sections.*

## Introduction

As the power of proton and heavy-ion accelerators increases, the prediction of the structural damage to materials under irradiation is essential. Radiation damage of materials is usually measured as a function of the average number of displaced atoms per all atoms in a material, DPA. For example, ten dpa means each atom in the material has been displaced from its lattice site of the material an average of ten times. DPA serves as a quantitative measure of damage: DPA=$\phi t \sigma_{damage}$; $\sigma_{damage}$ is the displacement cross-section; and $\phi t$ is the irradiation fluence, i.e. the product of the ion beam flux and the bombardment time. The level of the radiation damage in DPA units is used, for example, to estimate radiation damage of those materials experiencing significant irradiation by primary and "secondary particles" which include all particles created from the sequential nuclear reactions at high-energy, high-intensity facilities such as the Facility for Rare Isotope Beams (FRIB) [1], J-PARC facility [2], European Spallation Source (ESS) [3], and others. The DPA value is a useful measure in correlating results determined by different particles and fluxes in an irradiation environment. However, it is difficult to measure the DPA value in high-energy reactions and the relationships between DPA and material property are at present unclear.

SRIM [4] is one of the major codes used to estimate radiation damage in the low-energy region. SRIM treats the transport of projectile with its Coulomb scattering and makes an approximation of cascade damage. As SRIM does not treat nuclear reactions, the calculated damage is that produced by the primary knock-on atom, PKA, because damage created by the "secondary particles" produced in nuclear reactions is not considered. On the other hand, the nuclear reaction models in the advanced Monte Carlo particle transport code systems such as PHITS [5], MARS15 [6], FLUKA [7] and MCNP [8] have been developed for the calculation of radiation shielding and protection. These codes treat nuclear reactions and create the "secondary particles". Recently, these codes were enhanced with the capability of making realistic predictions of radiation induced damage to materials for the high-energy heavy ion region.

In this paper, we describe the radiation damage model which includes Coulomb scattering and the nuclear reaction in the improved PHITS and compare the improved PHITS results with the prediction of the FLUKA, MARS15 and SRIM. The details (incident particle, energy, target, and Monte Carlo code) of the different calculations are given in Table 1.

**Table 1: Calculations performed with Monte Carlo codes**

| Case | Incident particle | Energy (MeV/nucleon) | Target | Monte Carlo code |
|---|---|---|---|---|
| A | proton | 14,50,200,800 | $^{63}$Cu | PHITS, FLUKA |
| B | neutron | 14,50,200,800 | $^{63}$Cu | PHITS, FLUKA |
| C | $^{76}$Ge | 130 | $^{184}$W | PHITS, MARS15, SRIM |

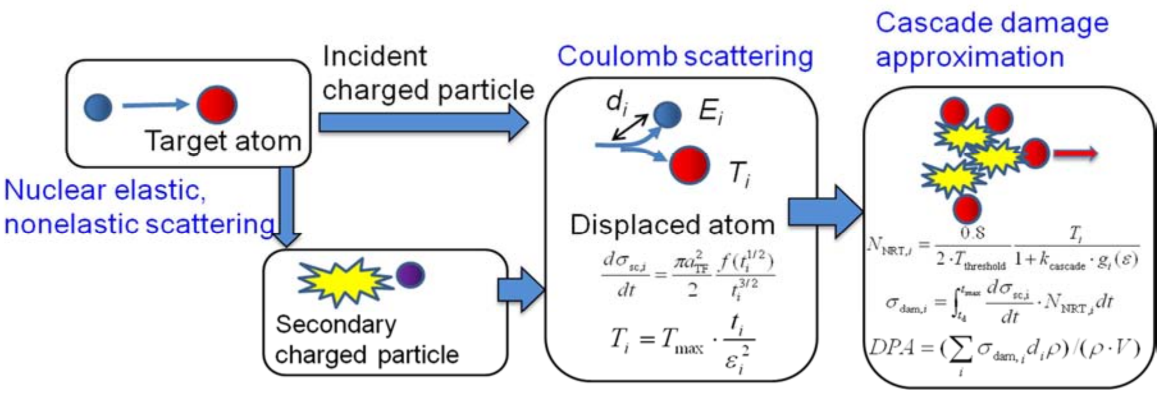
## DPA calculation in PHITS

### *Overview of DPA calculation in PHITS*

High-energy ions travelling through a target lose their energy in three ways; nuclear reaction, electron excitations and Coulomb scatterings. The lower the projectile energy is, the higher the energy transfer to the target atom via Coulomb scattering is. The target atom directly hit by the projectile has usually much lower energy than the projectile itself and, therefore, has a larger cross-section for Coulomb scattering with other target atoms. Thus, the primary knock-on atom (PKA) creates localised cascade damage where many target atoms are displaced from their original lattice site and the number of interstitials will be equal to the number of vacancies. These point defects and their clusters affect the macroscopic properties, such as hardness.

The conditions of various irradiations will be described by using the damage energy to characterise the displacement cascade. This is defined as the initial energy of target PKA, corrected for the energy lost to electronic excitations by all of the particles composing the cascade. There are mainly two processes to produce the target PKA for heavy-ions and proton incident reactions, as shown in Figure 1. One is the Coulomb scattering due to PKA's directly created by the projectile, and the other is that due to PKA's created by the secondary particles. In this work, the energy of the secondary charged particles is obtained by PHITS calculations using the nuclear reaction model of JQMD and Bertini for heavy-ion and proton, respectively, and the evaporation model of GEM [5]. Details of the model are presented in our previous paper [9].

**Figure 1: Overview of DPA calculations in PHITS**




### *Coulomb scattering with target atom*

To simplify differential cross-section calculations even further, J. Lindhard, V. Nielsen, and M. Scharff [10] introduced a universal one-parameter differential scattering cross-section equation in reduced notation:

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

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

where $t$ is a dimensionless collision parameter defined by:

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

$t \equiv \varepsilon^2 \frac{T}{T_{max}} = \varepsilon^2 \sin^2\left(\frac{\theta_c}{2}\right) t \equiv \varepsilon^2 \frac{T}{T_{max}} = \varepsilon^2 \sin^2\left(\frac{\theta_c}{2}\right)$where $T$ is the transferred energy to the target and $T_{max}$ is the maximum transferred energy as:

$$T_{max} = \frac{4M_1 M_2}{(M_1 + M_2)^2} E_p \qquad (3)$$

where $E_p$ is the energy of incident and secondary charged particle. $\varepsilon$ is the dimensionless energy as:

$$\varepsilon \equiv \frac{a_{TF}}{d_c} = \frac{a_{TF} E}{Z_1 Z_2 e^2} \qquad (4)$$

$\varepsilon \equiv \frac{a_{TF}}{d_c} = \frac{a_{TF}E}{Z_1 Z_2 e^2}$In the above expression, $d_c$ is the unscreened (i.e. Coulomb) collision diameter or distance of closest approach for a head-on collision (i.e. b=0), and $a_{TF}$ is the screening distance.

Lindhard *et al*. considered $f\,(t^{1/2})$ to be a simple scaling function and the variable *t* to be a measure of the depth of penetration into the atom during a collision, with large values of *t* representing small distances of approach. $f\,(t^{1/2})$ can be generalised to provide a one parameter universal differential scattering cross-section equation for interatomic potential such as screened and unscreened Coulomb potentials. The general form is:

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

$$f(t^{1/2}) = \lambda t^{1/2-m}\left[1+(2\lambda t^{1-m})^q\right]^{-1/q} \quad (5)$$

where λ, m, and q are fitting variables, with λ=1.309, *m*=1/3 and *q*=2/3 for the Thomas-Fermi version [11] of $f(t^{1/2})$. The value of $t^{1/2}$ increases with an increase in a dimensionless energy $\varepsilon$, scattering angle in the CM system, and impact parameter. The Coulomb scattering cross-section in the energy region above the displacement threshold energy can be calculated from the following expression:

$$\sigma_{\mathrm{sc}} = \int_{t_{\mathrm{d}}}^{t_{\max}} \frac{d\sigma_{\mathrm{sc}}}{dt} \cdot dt \quad (6)$$

where $t_{max}$ in dimensionless is equal to $\varepsilon^2$ from equation (2) when $\theta=\pi$. $t_d$ is the displacement threshold energy in dimensionless given by equation (4). Displacement threshold energy $T_{threshold}$ is typically in the range between 20 and 90 eV for most metal.

***Displacement cross-sections***

To estimate the damage cross-sections the NRT formalism of Norgett, Robinson, and Torrens and Robinson [12] is employed as a standard to determine that fraction of the energy of the PKA of the target which will produce damage, e.g. further nuclear displacements. The displacement cross-sections, which indicate the scattering cross-section multiplied by the number of defects, can be evaluated from the following expression:

$\sigma_{\mathrm{damage}} = \int_{\mathrm{t_d}}^{\mathrm{t_{max}}} \mathrm{d}\sigma/\mathrm{dt} \times \nu\left(\mathrm{Z_{target}}, \mathrm{A_{target}}, \mathrm{T_{target}}\right)\mathrm{dt}\ \sigma_{\mathrm{damage}} = \int_{\mathrm{t_d}}^{\mathrm{t_{max}}} \mathrm{d}\sigma/\mathrm{dt} \times \nu\left(\mathrm{Z_{target}}, \mathrm{A_{target}}, \mathrm{T_{target}}\right)\mathrm{dt}$

$$\sigma_{\mathrm{damage}} = \int_{t_{\mathrm{d}}}^{t_{\max}} \frac{d\sigma_{\mathrm{sc}}}{dt} \cdot N_{\mathrm{NRT}}\, dt \quad (7)$$

where $N_{NRT}$ is the number of defects based on the Kinchin and Pease formula [13] modified by Norgett *et al*. and using the Lindhard slowing-down theory, in irradiated material calculated by:

$$N_{\mathrm{NRT}} = \frac{0.8 \cdot T_{\mathrm{damage}}}{2 \cdot T_{\mathrm{threshold}}} \quad (8)$$

The constant 0.8 in the formula is the displacement efficiency given independent of the PKA energy, the target material, or its temperature. The value is intended to compensate for forward scattering in the displacement cascade of the atoms of the lattice. $T_{damage}$ is the “damage energy” transferred to the lattice atoms reduced by the losses for electronic stopping in the atom displacement cascade and is given by Norgett, Robinson, and Torrens.

$$T_{\mathrm{damage}} = \frac{T}{1 + k_{\mathrm{cascade}} \cdot g(\varepsilon)} \qquad (9)$$

where $T$ is the transferred energy to target atom given by Equation (2) as:

$$T = T_{\max} \cdot \frac{t}{\varepsilon_{\mathrm{p}}^2} \qquad (10)$$

where $\varepsilon_{\mathrm{p}}$ is the dimensionless projectile energy given by Equation (4) and the projectile energy $E_{\mathrm{p}}$. The parameters $k_{\mathrm{cascade}}$, and $g(\varepsilon)$ are as follows:

$$k_{\mathrm{cascade}} = 0.1337 Z_{\mathrm{target}}^{1/6} (Z_{\mathrm{target}} / A_{\mathrm{target}})^{1/2} \qquad (11)$$

$$g(\varepsilon) = \varepsilon + 0.40244 \cdot \varepsilon^{3/4} + 3.4008 \cdot \varepsilon^{1/6} \qquad (12)$$

$\varepsilon$ is the dimensionless transferred energy given by Equations (4) and (10). Note that this calculation does not include the self-healing of lattice defects.

### *DPA values*

DPA value is calculated from the following expression:

$$DPA = (\sum_i \sigma_{\mathrm{damage},\ i} d_i \rho) / (\rho \cdot V) \qquad (13)$$

where $d_i$ is the travelling length of incident charged particles and secondary ones in the target calculated by using SPAR code [14]. $\rho$ and $V$ is the atomic density and volume of the target, respectively.

## DPA calculations using PHITS and other codes

Based on the above formalisms, we calculated DPA distributions in thick Cu and W for various beams listed in Table 1 and compared to calculated results using FLUKA, MARS15 and SRIM codes. Beam area was 1 cm$^2$ and target geometry was cylinder with 5 cm radius and each depth. All the calculated results were normalised by the number of incident particles.

### *Case A: Proton into Cu using PHITS and FLUKA*

Figure 2 shows calculated results for 14, 50, 200 and 800 MeV protons. Displacement threshold energy $T_{\mathrm{threshold}}$ was 30 eV in PHITS and 40 eV in FLUKA for Cu. For the proton beams in the energy range from 10 MeV to 1 GeV, the PHITS results agree with those of FLUKA within a factor of two. In higher energy, nuclear reactions occur before the stopping range is reached and DPA values produced by PKA directly created by the secondary are increased with energy. For 800 MeV, well-developed hadronic cascades are appeared.

### *Case B: Neutron into Cu using PHITS and FLUKA*

Figure 3 shows calculated results for 14, 50, 200 and 800 MeV neutrons. PHITS results also agree with those of FLUKA within a factor of two because the production of secondary particles in PHITS is almost the same as that in FLUKA. Note that neutron cannot create the radiation damage in the model. Secondary charged particles created by nuclear elastic and nonelastic scattering contribute to the damage calculation.

### *Case C: $^{76}$Ge into W using PHITS, MARS15 and SRIM*

Figure 4 shows calculated results by using PHITS, SRIM and MARS15. We selected "Quick Calculation of Damage" as the SRIM option for DPA calculations. The damage calculated with this option is from the statistical estimates based on the Kinchin-Pease formalism. SRIM treats only Coulomb scattering for the projectile and cannot produce "secondary particles" from nuclear reactions. MARS15 code is Monte Carlo transport code for an accurate description of radiation effects in numerous applications at high-power beam facilities. The improved PHITS results were close to SRIM and MARS15 results for DPA values produced by PKA directly created by the $^{76}$Ge projectiles. In the 130 MeV/u $^{76}$Ge and tungsten system, Coulomb scattering created by the $^{76}$Ge projectiles is more dominant than that created by the "secondary particles" produced by nuclear reactions.

**Figure 2: Calculated results for 14, 50, 200 and 800 MeV protons into a thick Cu target using PHITS and FLUKA**

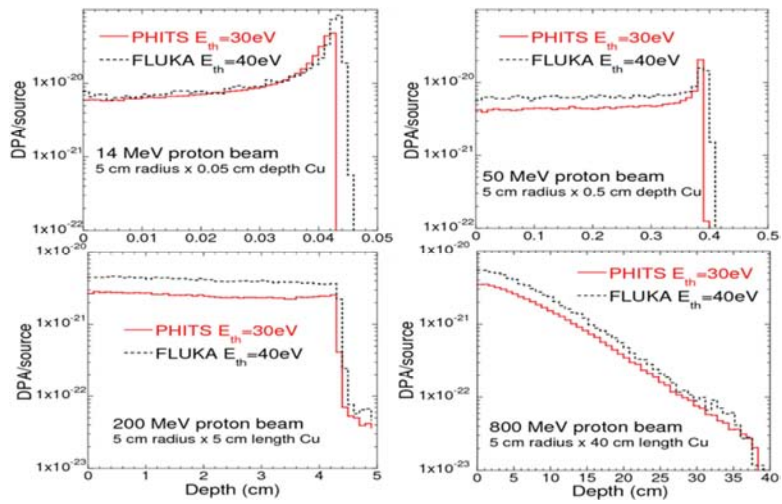



**Figure 3: Calculated results for 14, 50, 200 and 800 MeV neutrons into a thick Cu target using PHITS and FLUKA**

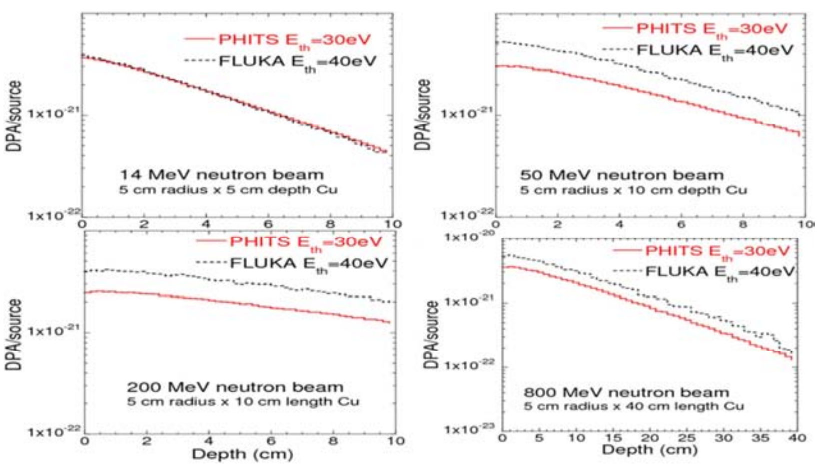
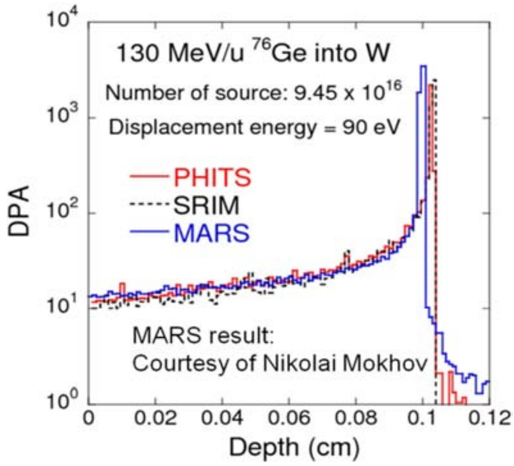


**Figure 4: Calculated results for 130 MeV/u $^{76}$Ge into W target using PHITS, SRIM and MARS15**




## Summary

The PHITS code was further developed to include the displacement damage model. The screened Coulomb scattering and the nuclear reaction model were used to evaluate the energy of the target PKA created by the projectile and the secondary particles. These latter include all particles created from the sequential nuclear reactions. It was found that the PKA created by the secondary particles is more dominant than a target PKA created by the projectile in DPA calculations for proton and neutron induced reactions at energies above 20 MeV. Recently, radiation damage models in other codes such as FLUKA, MARS, and MCNP have also been developed. As there are few experimental data in this high-energy region, an intercomparison among Monte Carlo codes such as FLUKA, MARS, and MCNP used in the radiation damage calculation is one way to improve models or have a consistent approach. As an example, for the reactions between 130 MeV/u $^{76}$Ge ions and tungsten, it was found that DPA values calculated with the PHITS are in good agreement with those of SRIM and MARS. For the neutron and proton beams in the energy range from 10 MeV to 1 GeV, the PHITS results agree with those of FLUKA within a factor of two. Further intercomparison among the codes such as MARS, FLUKA, MCNP and PHITS should be carried out, as well as measurements of displacement damage cross-sections. In the future, there is a need to consider new DPA values that go beyond the standard proposed by Norget, Robinson and Torrens (NRT) in 1975.

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