MCNPX Calculation of DPA

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Radiation damage can change the mechanical properties of materials and is important for high-power beams on targets, collimators, windows, and beam dumps.

Change in properties can affect lifetimes: ductility, tensile strength, embrittlement, cracks, swelling, elongation irradiation creep, phase transformation, segregation of alloys, thermal conductivity, electrical resistivity, thermal expansion.

Displacements per atom (DPA) is used to quantify radiation damage (number of times an atom is displaced during the irradiation period).

DPA cannot be measured since only a small fraction of the displaced atoms lead to permanent lattice defects.
Radiation Damage

- Lots of data for reactor neutrons <20 MeV
- Not much data for high energy charged particles
- Difficult to transfer physical property changes from reactor neutrons to particle beams
- Complex effects of particle irradiation on material properties
  - Temperature healing
  - Production of impurities
  - Grain size
  - Rate of irradiation (dpa/s)
  - Energy of particle irradiation
  - Limited particle irradiation depth compared to bulk neutron irradiation

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Radiation damage in materials results from nuclear collisions and reactions which produce energetic recoil atoms of the host material or reaction products.

These recoiling atoms generate electronic excitations in host material that displace additional host atoms – this is displacement damage.

In metals this is the only process that leads to permanent damage.

Displacements per atom is routinely used to characterize irradiations.

Only initial displacements of atoms from lattice sites are calculated.

Many displaced atoms recombine with holes in the lattice, especially at elevated temperatures.

Measure of total damage energy deposited in a material, and changes in physical and mechanical properties are fundamentally related to the available energy.
Displacement cross section is used to characterize and compare radiation damage from neutrons and charged particles in crystalline materials.

In 1975 Norget, Torrens and Robinson proposed the NRT-dpa standard. Number of displacements = $0.8T_d/2E_d$

- $0.8$ factor was determined from binary collision models to account for realistic scattering.
- $E_d$ is the minimum energy required to create a stable Frankel pair.

NRT DPA has been widely used and has proven useful for correlating radiation damage phenomena:

- Comparing thermal and fast spectrum neutron irradiations.
- Comparing charged particle with neutron irradiation.
- While not predicting the actual number of Frenkel pairs, provided means of correlation for steels and other mid-atomic weight metals.
NRT-dpa has limitations
- Some material property changes are sensitive to results of nuclear collisions
- Others are more sensitive to ionization effects
- Limited to metals, not applicable to compound materials (treated by mathematical weighting of separate elements)
- Does not account for recombination of atoms during cascade evolution
- Cannot be directly measured or validated
- Has no uncertainties/covariances

NRT DPA methodology incorporated into
- ASTM E693 Standard Practice for Characterizing Neutron Exposures in Iron and Low Alloy Steels in Terms of Displacements Per Atom (DPA)
- ASTM E521 Standard Practice for Neutron Radiation Damage Simulation by Charged Particle Irradiation
ASTM E693 DPA for Neutron Exposures in Iron and Low Alloy Steels

- ASTM E693 Standard Practice for Characterizing Neutron Exposures in Iron and Low Alloy Steels in Terms of Displacements Per Atom
- Energy dependent neutron dpa cross section that is multiplied with neutron energy spectrum to calculate dpa
ASTM E521 Standard Practice for Neutron Radiation Damage Simulation by Charged Particle Irradiation

Calculation of damage energy per atom per unit fluence for neutrons, light ions, heavy ions, and electrons

All possible reactions that transfer energy to an atom of the medium to displace it must be considered

Damage energy is converted to DPA using NRT model

\[
N_d = \begin{cases} 
0 & \text{if } T < T_d \\
1 & \text{if } T_d \leq T < 2T_d/\beta \\
\beta T_{\text{dam}}/2T_d & \text{if } T \geq 2T_d/\beta
\end{cases}
\]

\[\beta = 0.8, \quad T_d = 40 \text{ eV}\]
Monte Carlo particle transport code merging MCNP (<20 MeV for neutrons) and LAHET tracking high energy particles

Significant simulation tool for accelerator and other physics work: target design, isotope production, isotope destruction, accelerator driven energy systems proton and neutron therapy, imaging technology, shielding design, detection technology, neutrino experiment design, charged particle tracking in plasmas, single-event upsets in semiconductors, nuclear reactor analysis

Provides geometry-independent mesh tallies for visualization of flux, dose, energy deposition over continuous space volume without complicating particle transport through the geometry
Tabulated nuclear data
- < 20 MeV for most isotopes
- < 150 MeV for LA150 library cross sections: H, C, N, O, Al, Si, K, Ca, Cr, Fe, Ni, Cu, Nb, W, Hg, Pb, Bi

Intranuclear cascade/pre-equilibrium/evaporation model up to few GeV
- BERTINI/Dresner (default)
- ISABEL/Dresner (default)
- BERTINI/ABLA
- ISABEL/ABLA
- CEM03
- INCL4/Dresner
- INCL4/ABLA

Version of FLUKA or LAQGSM can be used in MCNPX for higher energy interactions
MCNPX

Advantages

- Explicit modeling of complicated geometries
- Can select physics treatment from available options
- Monte Carlo tracking of particle interactions
- Extensive cross section library for low energy reactions <20 MeV
- Physics treatment for when cross sections are not available
- Calculates statistical uncertainties
- Widely used for reactor analysis
- Same model can be used for shielding, activation studies
- Can calculate damage energy directly
- Mesh tally can provide spatial distributions independent of problem model
- Can add more XSs using NJOY
Disadvantages

- Calculations can take time to obtain adequate statistics on small regions.
- Damage energy calculations do not include tabular XS contributions.
- May need separate calculations of low energy (<20 MeV) and medium to high energy contributions.
Two methods for calculating DPA with model of specific geometry

- **Method 1** - Calculate flux and fold with DPA XS
- **Method 2** - Calculate DPA directly with MCNPX (HISTP/HTAPE)
MCNPX Calculation of DPA Method 1

- Calculation of neutron, proton spectrum at specific locations or for regular spatial mesh
- Fold neutron and proton DPA XS with neutron and proton flux spectrum
- Advantages
  - Straightforward, like other MCNP tallies, provides spatial distributions
- Disadvantages
  - Limited to energy range and materials in libraries
    - ENDF XS < 20 MeV
    - SPECTER limited to neutrons < 20 MeV
    - LA150 neutron and proton XS < 150 MeV
    - DXS DPA cross sections for neutrons, protons, H production, He production <3 GeV
  - Limited materials
  - Average DPA for cell or material or spatial distributions

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Calculating DPA with MCNPX with DPA Cross Section

► Neutron DPA
  ■ Tally neutron flux spectrum in MCNPX as function of energy
    ● F4 tally, Multiply by neutron dpa cross section for each material (spreadsheet)
    ● MESH tally type 1, neutron flux, response function is dpa cross section
      ◆ mfact keyword, mshmf3 energy dependent neutron dpa cross section

► Proton DPA
  ■ Tally proton flux spectrum in MCNPX as function of energy
    ● F4 tally, Multiply by proton dpa cross section for each material (spreadsheet)
    ● MESH tally type 1, proton flux, response function is dpa cross section
      ◆ mfact keyword, mshmf3 energy dependent proton dpa cross section
\[
DPA = \int \sigma_{\text{disp}}(E) \frac{d\phi(E)}{dE} dE
\]

\[\phi(E): \text{fluence (particles/cm}^2)\]
\[\sigma_{\text{disp}}(E): \text{displacement cross section (barns)}\]

- DPA is calculated by folding displacement cross section with particle spectrum
  - Energy dependent particle spectrum (neutron, proton) calculated with transport model (MCNPX)
  - Neutron spectrum folded with neutron dpa cross section,
  - Proton spectrum folded with proton dpa cross section
  - Main difference between proton and neutron displacement cross section is Coulomb interaction of charged particle at low energies
Cross sections can be based on traditional NRT or new methods such as Molecular Dynamics (MD), Binary Collision Approximation (BCA) or other simulations.

IAEA Nuclear Data Section database DXS in ENDF/B format includes both NRT and MD-BCA dpa cross sections as well as gas production cross sections:

- Al, Ti, V, Cr, Fe, Ni, Cu, Zr neutron, proton < 3 GeV
- ENDF/B-VII data processed with NJOY for neutrons <20 MeV
- Model physics for >20 MeV
- Dpa cross section is sum of proton or neutron elastic scattering and nonelastic interactions
- Gas (p,d,t,He3,He4) production in Cr, Fe, Ni, W neutron, proton < 3 GeV,
IAEA Nuclear Data Section database DXS includes both NRT and MD-BCA DPA cross sections

MD-BCA DPA are substantially lower than NRT

![DXS Neutron DPA Cross Section for Zr](image1)

![DXS Proton DPA Cross Section for Zr](image2)
Neutron damage cross sections

- ASTM E693 for E<20 MeV in Fe, steel
- ENDF/B Evaluations for E<20 MeV
- La150 cross section library includes:
  - H 3He 4He 6Li 7Li Be 10B 11B C N 16O F Na Mg Al Si P S Cl K Ca Ti V Cr
  - Mn Fe Co Ni Cu Zr Nb Mo 107Ag 109Ag Ta 182W 183W 184W 186W Au Pb

- Neutron dosimetry file IRDF-2002 also contains neutron damage cross sections <20 MeV that can be used by MCNP
  - Si  GaAs ASTM E722 electronic, Cr, Fe, Ni,
SPECTER Code for Calculating Neutron Damage

- Simplified neutron damage calculations
- User inputs calculated energy-dependent neutron spectrum
- SPECTER calculates spectral-averaged displacements, recoil spectra, gas production, and total damage energy for 41 isotopes at the same time
- Limited to neutron reactions
- Includes elastic scattering, multiple \((n,xn)\) reactions, \((n,d)\), \((n,t)\), \((n,3\text{He})\), \((n,4\text{He})\), \((n,\gamma)\), \(\beta\)-decay
- Limited to energy range from \(10^{-10}\) to 20 MeV
- Limited to ENDF/B-V nuclear data
MCNPX Calculation of DPA Method 2

- Calculate neutron, proton transport at specific locations the same as method 1 but record histories on HTAPE file
- HTAPE3X included with MCNPX (from LAHET) reads HTAPE histories and calculates damage energy spectrum, which is converted to DPA

Advantages
- Doesn’t require separate DPA XS
- Includes most reaction mechanisms

Disadvantages
- Only includes contributions from physics models
- Tabulated XS contributions are not included
- Can underestimate damage if <20 MeV contributions are significant
- Interactions of neutrons < 20 MeV are not recorded in HISTP file
MCNPX DPA Calculation Method 2

- HISTP card included in input file produces history file of medium and high energy collision data
  - Low energy neutron and proton collisions utilizing the MCNPX libraries are not included

- HTAPE3X INT=my_input OUTT=my_output HISTP=file1
  - IOPT=16 damage energy spectra
  - Provides tables as function of input energy grid by cell or material and total
    - total recoil, elastic recoil, total damage, elastic damage
  - Provides mean values of recoiling fragments and damage energy per history and mean energy per recoil
  - IOTP = -16 multiplies damage energy spectra by flux
Validating Methods

- Limited measurements to compare
- Since DPA cannot be measured, not sure what to compare to
- Large database of reactor neutron correlations of physical property changes to calculated DPA based on NRT
- Most of these cannot be recalculated with new more fundamental methods (neutron spectrum not available, not enough detail to model in new calculation, etc.)