MCNPX Calculation of DPA

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Radiation Damage

- 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

Radiation Damage

- 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

DPA Cross Section

- 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 did not predict actual number of Frenkel pairs, provided means of correlation for steels and other mid-atomic weight metals

DPA Cross Section

- 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

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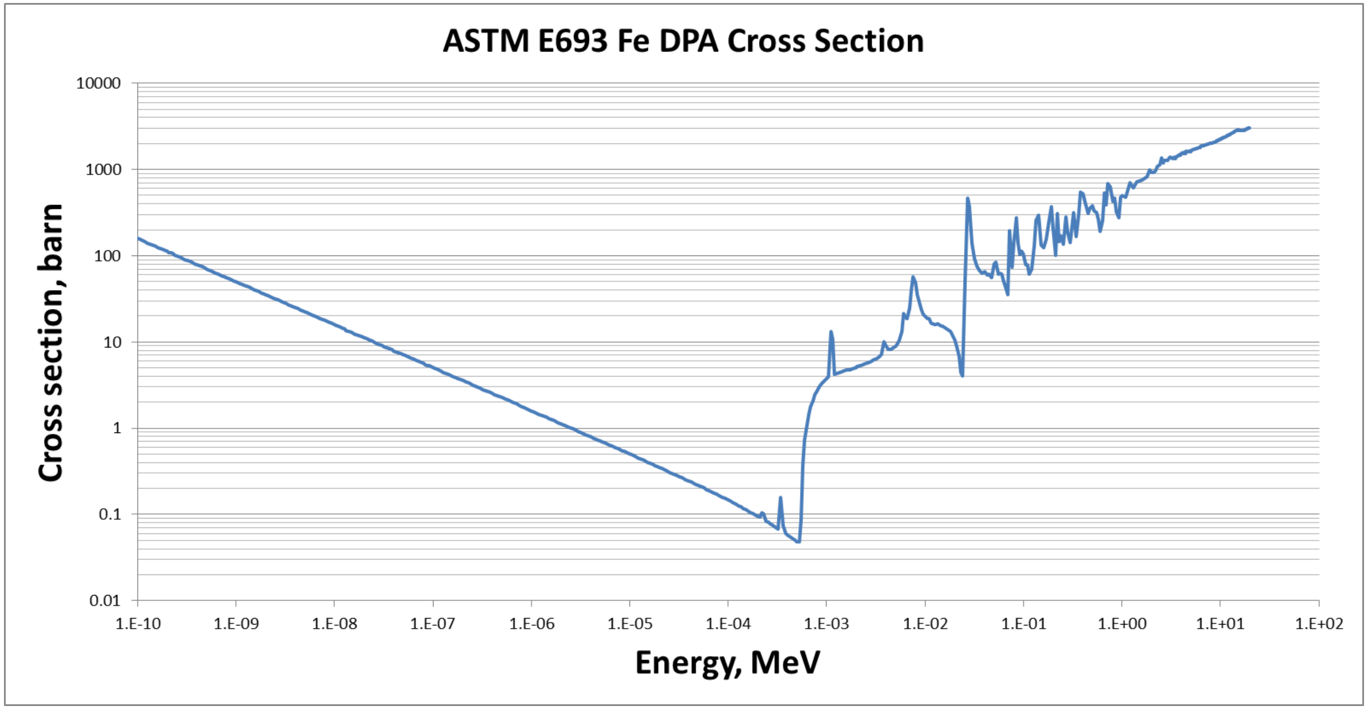
- ASTM E693 Standard Practice for Characterizing Neutron Exposures in Iron and Low Alloy Steels in Terms of Displacements Per Atom
- Energy dependent neutron dpa cross section that is multiplied with neutron energy spectrum to calculate dpa



ASTM E521 Neutron Radiation Damage by Charged Particle Irradiation

- 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

$$\begin{array}{ll} N_d = 0 & T < T_d \\ N_d = 1 & T_d \leq T < 2T_d/\beta \\ N_d = \beta T_{dam}/2T_d & T \geq 2T_d/\beta \end{array}$$

$\beta = 0.8,\ T_d = 40$ eV

MCNPX

- 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

MCNPX

- 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

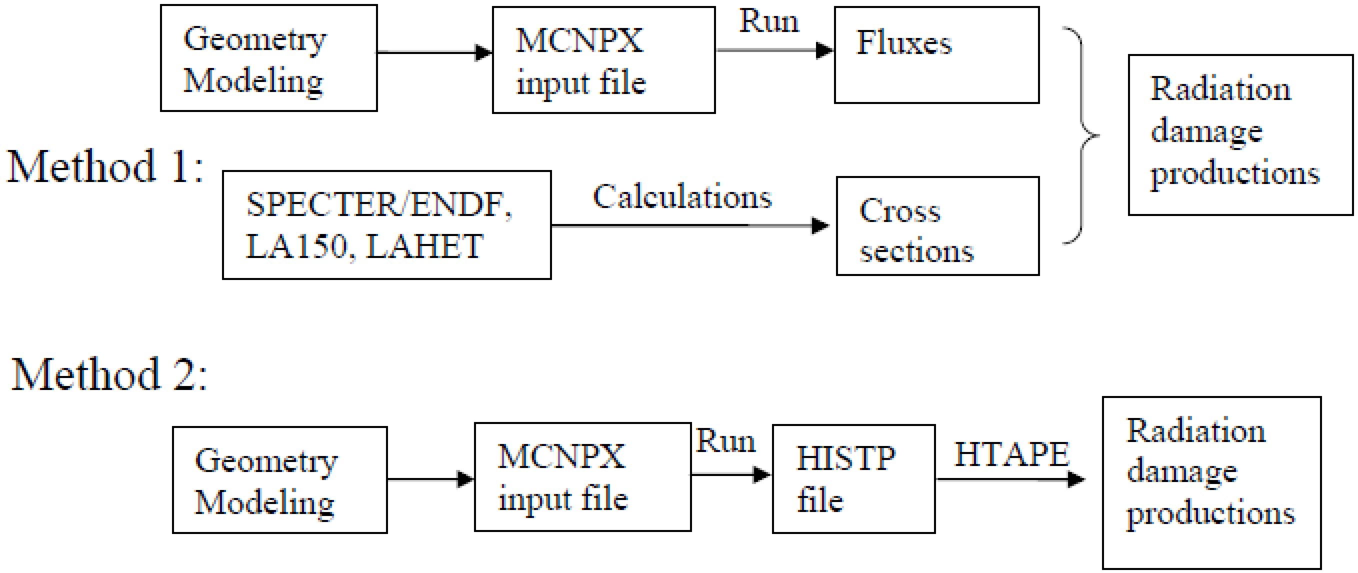
- Advantages
  - Explicit modeling of complicated geometries
  - Can select physics treatment from available options
  - Monte Carlo tracking of particle interactions
  - Extensive cross section library for low energy reactions <20 MeV
  - Physics treatment for when cross sections are not available
  - 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

MCNPX

- 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

MCNPX Calculation of DPA

- 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 < 20MeV
    - 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

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

Radiation Damage

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$$DPA = \int \sigma_{disp}(E) \frac{d\emptyset(E)}{dE} dE$$

$\emptyset(E)$: fluence (particles/cm^2)
$\sigma_{disp}\ (E)$: displacement cross section (barns)

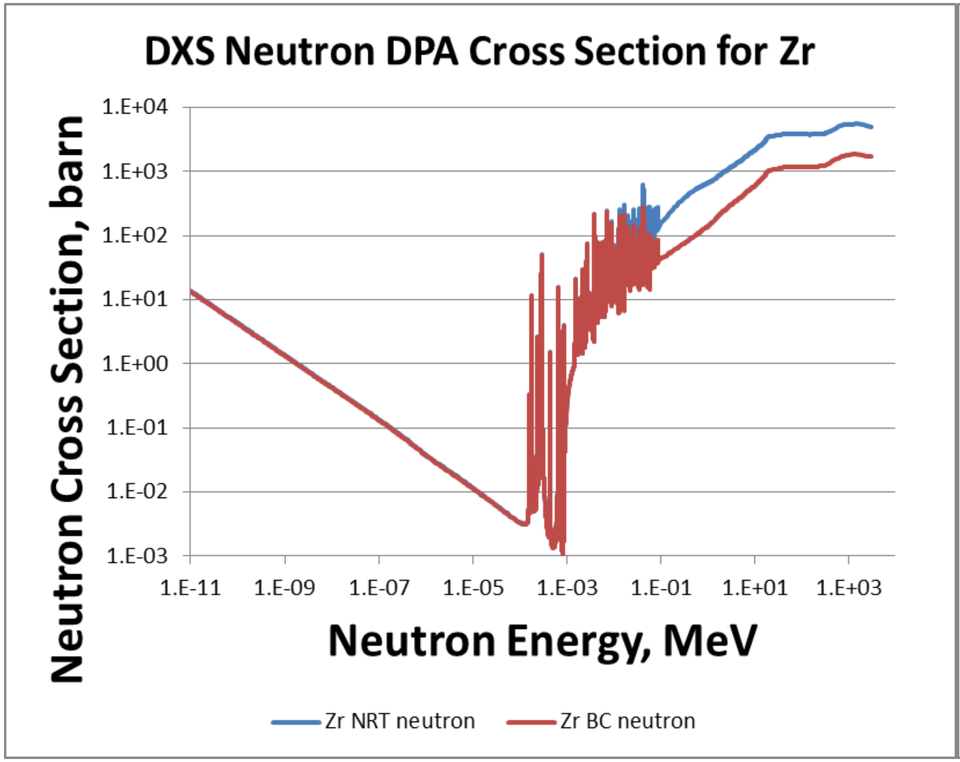
- DPA is calculated by folding displacement cross section with particle spectrum
  - Energy dependent particle spectrum (neutron, proton) calculated with transport model (MCNPX)
  - Neutron spectrum folded with neutron dpa cross section,
  - Proton spectrum folded with proton dpa cross section
  - Main difference between proton and neutron displacement cross section is Coulomb interaction of charged particle at low energies

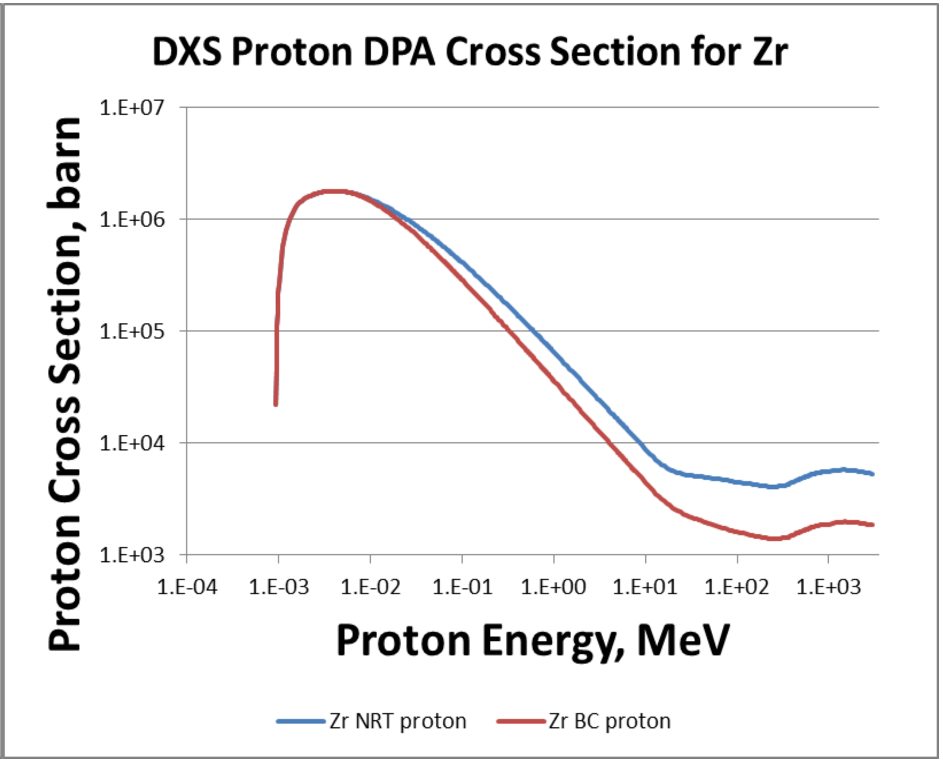
DPA Cross Section

- 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,

DPA Cross Section

- IAEA Nuclear Data Section database DXS includes both NRT and MD-BCA DPA cross sections
- MD-BCA DPA are substantially lower than NRT





DPA Cross Section

- 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,3He), (n,4He), (n,γ), β-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.)