

DPA Calculational Methodologies Used in Fission and Fusion Reactor Materials Applications

David Wootan - david.wootan@pnnl.gov, 1-509-372-6865

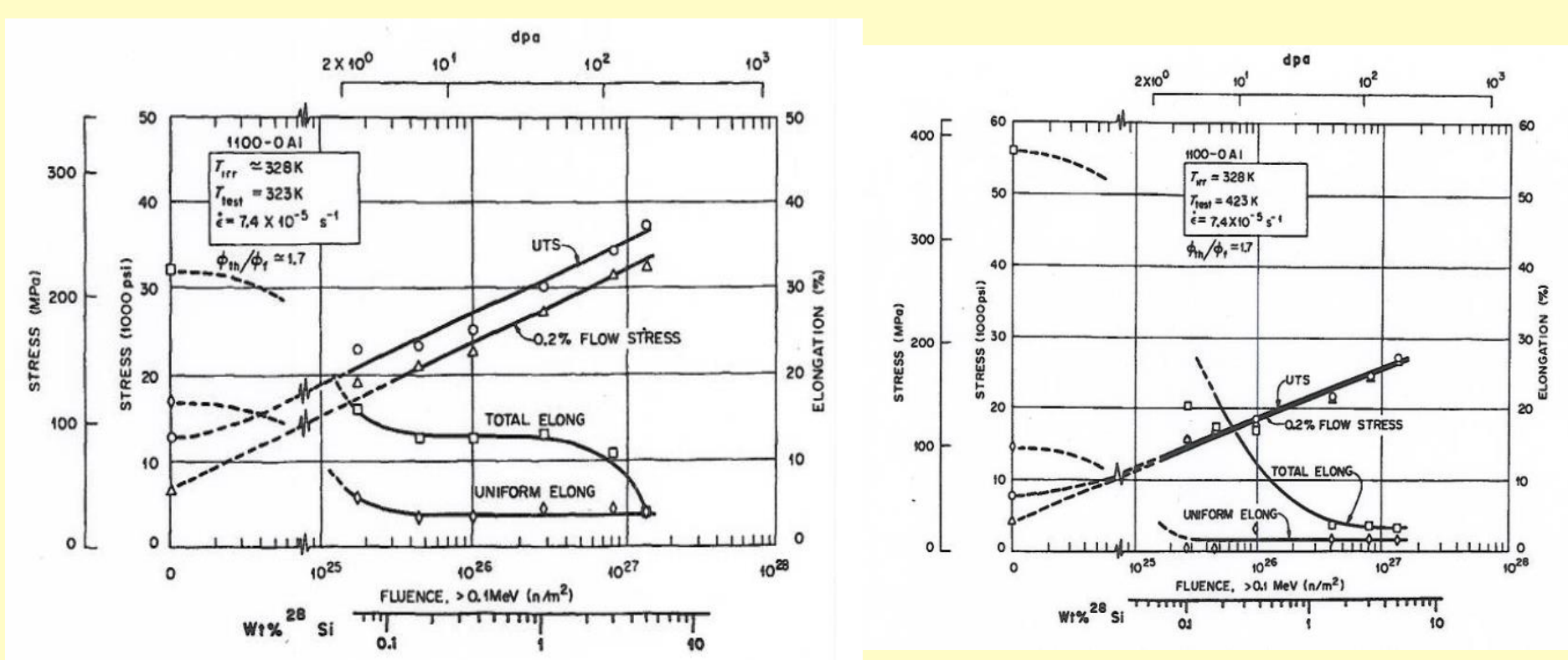


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Radiation Damage and DPA

- Displacements per atom (DPA) is used to quantify radiation damage (number of times an atom is displaced during the irradiation period). 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 main process that leads to permanent damage, but generated He and H also contribute to radiation damage.
- DPA cannot be measured since only a small fraction of the displaced atoms lead to permanent lattice defects and the concentration of permanent defects is a function of irradiation conditions (especially temperature). Only the initial displacements of atoms from lattice sites are calculated. Many displaced atoms recombine with holes in the lattice, especially at elevated temperatures.
- Radiation damage can change the mechanical properties of materials and is important for high-power beams on targets, collimators, windows, and beam dumps. Examples of properties that can affect lifetimes include ductility, tensile strength, embrittlement, cracks, swelling, elongation irradiation creep, phase transformation, segregation of alloys, thermal conductivity, electrical resistivity, thermal expansion.
- Much more damage data is available for reactor neutrons <20 MeV than for high energy charged particles.
- It is difficult to extrapolate physical property changes from reactor neutrons to charged particles because of the complex effects of particle irradiation on material properties, such as temperature healing, production of impurities from nuclear reactions and ion implantation, grain size, rate of irradiation (DPA/s), energy of particle irradiation, limited particle irradiation depth compared to bulk neutron irradiation.
- For reactor irradiations, correlations of change in material properties with accumulated neutron DPA also depend on temperature, as shown in these figures.



In 1975 Norget, Torrens and Robinson proposed the NRT-DPA standard.

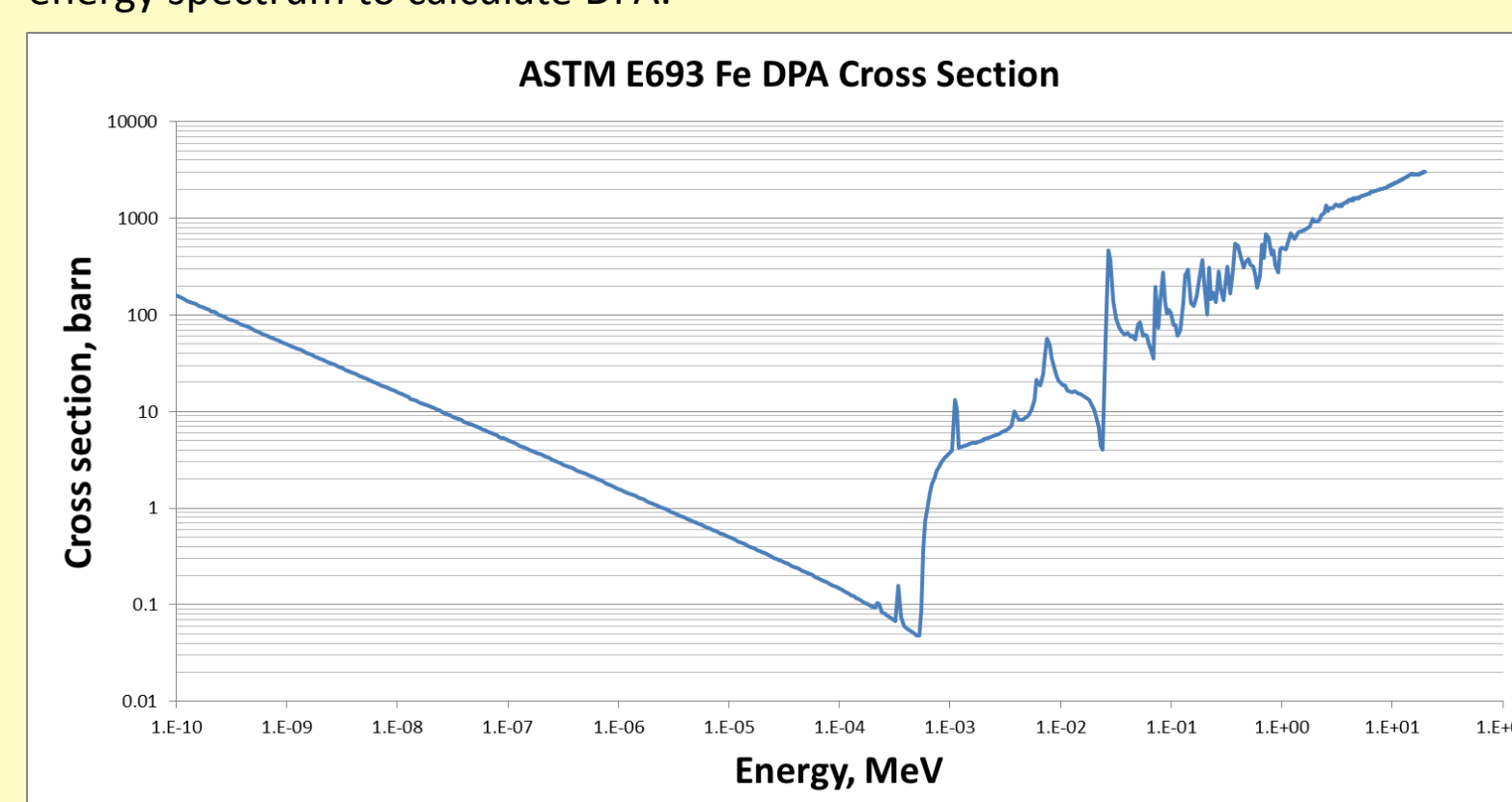
$$\text{number of displacements} = 0.8T_d/2E_d$$

The 0.8 factor was determined from binary collision models to account for realistic scattering, and 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 such as comparing thermal and fast spectrum neutron irradiations and comparing charged particle with neutron irradiation. While NRT DPA did not predict the actual number of Frenkel pairs, it provided a means of correlating radiation damage for steels and other mid-atomic weight metals. This methodology has been incorporated into ASTM E693 and ASTM E521 Standard Practices.

NRT-DPA has limitations

- Some material property changes are sensitive to results of nuclear collisions while others are more sensitive to ionization effects.
- Limited to metals, but has been applied to compound materials like ceramics 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

ASTM E693 Standard Practice for Characterizing Neutron Exposures in Iron and Low Alloy Steels in Terms of Displacements Per Atom (DPA) specifies an energy dependent neutron DPA cross section that is multiplied with the neutron energy spectrum to calculate DPA.



ASTM E521 Standard Practice for Neutron Radiation Damage Simulation by Charged Particle Irradiation Specifies how to calculate 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 the NRT model:

$$N_d = 0 \quad T < T_d$$

$$N_d = 1 \quad T_d \leq T < 2T_d/\beta$$

$$N_d = \beta T_{dam}/2T_d \quad T \geq 2T_d/\beta$$

$$\beta = 0.8, T_d = 40 \text{ eV}$$

MCNPX and DPA Calculations

MCNPX is a Monte Carlo particle transport code merging MCNP (<20 MeV for neutrons) and LAHET for tracking high energy particles. It has been used as a simulation tool for accelerator and other physics work such as 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, and nuclear reactor analysis. MCNPX 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 for MCNPX includes cross sections up to 20 MeV for most isotopes and up to 150 MeV for the LA150 library cross sections. MCNPX includes intranuclear cascade/pre-equilibrium/evaporation models for neutral and charged particle reactions up to a few GeV. The physics models can be selected from:

- BERTINI/Dresner (default)
- ISABEL/ABLA
- INCL4/Dresner
- ISABEL/Dresner (default)
- CEM03
- INCL4/ABLA
- BERTINI/ABLA

A version of FLUKA or LAQGSM can be used in MCNPX to model higher energy interactions

Advantages

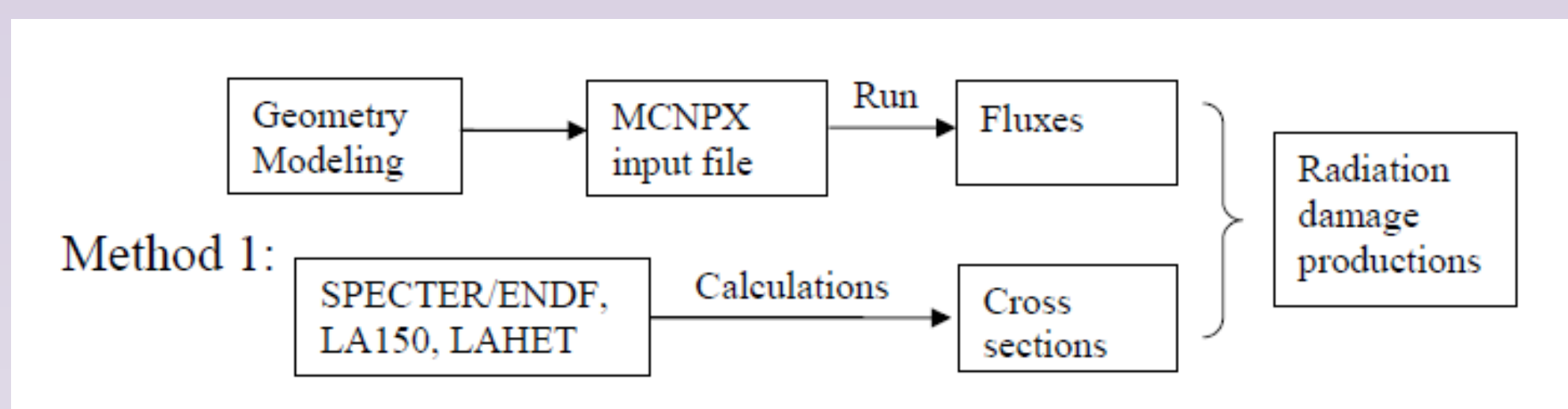
- Explicit modeling of complicated geometries
- Can select physics treatment from available options
- Monte Carlo tracking of particle interactions
- Extensive cross section library for low energy reactions <20 MeV
- Physics treatment for when cross sections are not available
- Calculates statistical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

MCNPX Method 1

Calculate Neutron and Proton Flux and fold with DPA cross section



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

Advantages

Straightforward, like other MCNP tallies, provides spatial distributions

Disadvantages

- Limited to energy range and materials in libraries
- Limited materials
- Average DPA for cell or material or spatial distributions

MCNPX cross sections can be based on traditional NRT or new methods such as Molecular Dynamics (MD), Binary Collision Approximation (BCA) or other simulations. MD-BCA DPA cross sections are substantially lower than NRT cross sections. Damage cross sections that can be used in MCNPX include:

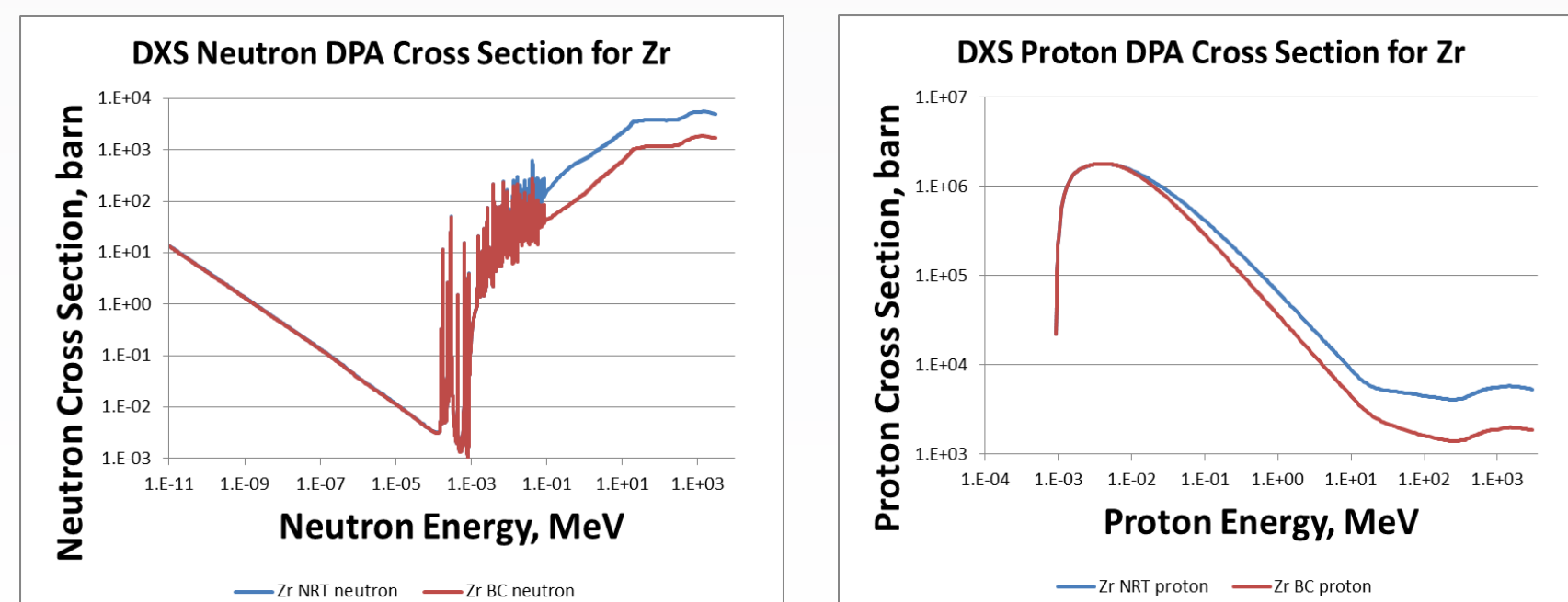
- ASTM E693 for neutrons up to 20 MeV in Fe, steel
- ENDF/B Evaluations for neutrons up to 20 MeV for most isotopes
- La150 neutron and proton cross sections up to 150 MeV for H, ³He, ⁴He, ⁶Li, ⁷Li, Be, ¹⁰B, ¹¹B, C, N, ¹⁶O, F, Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zr, Nb, Mo, ¹⁰⁷Ag, ¹⁰⁹Ag, Ta, ¹⁸²W, ¹⁸³W, ¹⁸⁴W, ¹⁸⁶W, Au, Pb
- Neutron dosimetry file IRDF-2002 contains neutron damage cross sections up to 20 MeV for Si, GaAs, Cr, Fe, Ni
- 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 for neutrons and protons < 3 GeV
 - ENDF/B-VII data processed with NJOY for neutrons < 20 MeV
 - Model physics for particle interactions > 20 MeV
- DPA cross section is the sum of proton or neutron elastic scattering and nonelastic interactions
- Gas (p,d,t,³He,⁴He) production in Cr, Fe, Ni, W for neutrons and protons < 3 GeV

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

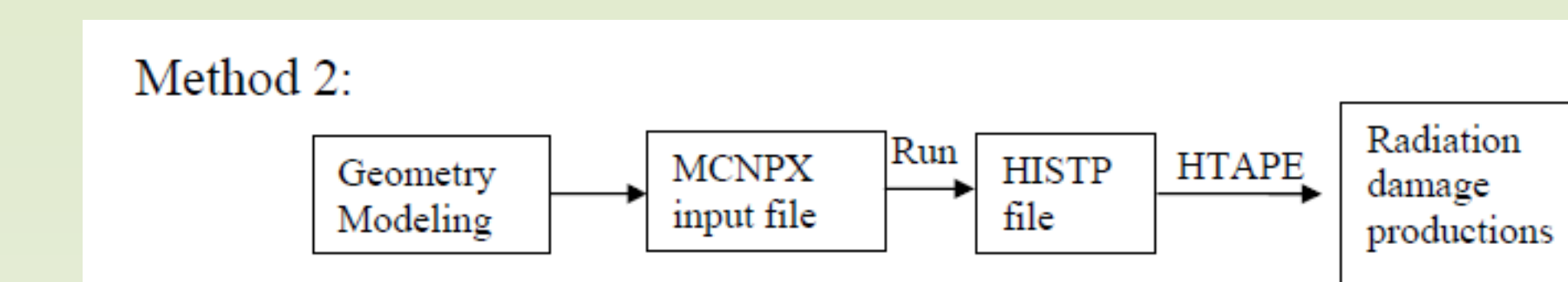
Proton DPA

- 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



MCNPX Method 2

Calculate DPA directly with MCNPX using HISTP/HTAPE



- Calculate neutron, proton transport at specific locations the same as method 1 but record histories on HISTP file. HISTP card included in input file produces history file of medium and high energy collision data.
- Read HISTP histories using HTAPE3X module of MCNPX and calculates damage energy spectrum, which is converted to DPA.

HTAPE3X INT=myinput OUTT=myoutput HISTP=file1

- IOP1=16 damage energy spectra
- Provides tables as function of input energy grid by cell or material and total
- Provides 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

Advantages

- Doesn't require separate DPA XS
- Includes most reaction mechanisms

Disadvantages

- Low energy neutron and proton collisions utilizing the tabulated MCNPX libraries are not included
- Only includes contributions from physics models
- Can underestimate damage if <20 MeV contributions are significant since interactions of neutrons < 20 MeV are not recorded in the HISTP file

Other Codes for Calculating DPA

SPECTER Code is Widely Used for Calculating Neutron Damage for Reactors

- Simplified neutron damage calculations compared to MCNPX
- Instead of calculating DPA in MCNPX, user inputs MCNPX calculated energy-dependent neutron spectrum to SPECTER, which 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,y), β -decay
- Limited to energy range from 10⁻¹⁰ to 20 MeV
- Limited to processed ENDF/B-V nuclear data

LR Greenwood and RK Smither, SPECTER: Neutron Damage Calculations for Materials Irradiations, ANL/FPP/7M-197 (1985)

SRIM Code is Widely Used for Calculating Damage for Ion Beams

- Stopping Range of Ions in Materials (SRIM) is a Monte Carlo simulation code for calculating ion deposition profiles in materials exposed to energetic beams of ions.
- Broadly applied because of relative power and ease of use
- Recommendations for computing DPA

- Run SRIM using the "Quick" Kinchin and Pease option
- Choose the displacement threshold energy from ASTM E521
- Set the lattice binding energy to zero
- Compute the damage energy by

$$T_{dam} = E_i^p + E_T^p$$

- Use T_{dam} to calculate displacements by

$$\sqrt{N_{NRT}} = 0.8T_{dam}E_{PKA}/2E_d$$

Where

$$E_i^p = \text{beam energy lost to phonons}$$

$$E_T^p = \text{target atom energy lost to phonons}$$

$$E_d = \text{displacement threshold energy}$$

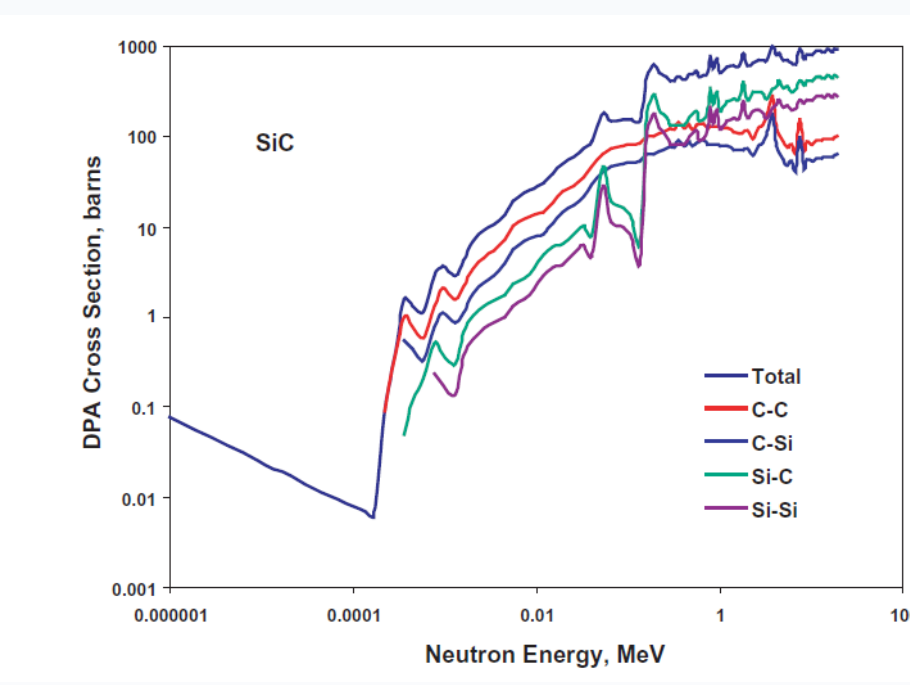
RE Stoller, et al., On the use of SRIM for computing radiation damage exposure, Nuclear Instruments and Methods in Physics Research B 310 (2013) 75-80

PNNL has Characterized Radiation Damage to Support a Variety of Fission and Fusion Applications

- Reactor structural materials testing and development in US and foreign fast reactors: FFTF (~40 DPA/yr), EBR-II (~25 DPA/yr), BOR-60, JOYO
- Reactor materials testing for thermal reactors: HFIR (~10 DPA/yr), HFBR, ATR (~15 DPA/yr), TRIGA, CANDU, BWR (~3 DPA/yr)
- Reactor pressure vessel surveillance of commercial LWRs
- Irradiation of materials in spallation neutron fields in proton accelerators: LANSCE
- Fusion materials irradiation testing: FFTF, EBR-II, HFIR
- Important transmutation effects, H and He gas production

Example: Displacement Damage in Silicon Carbide in Various Reactors

- Revised physical model for DPA for multi-component ceramic materials compared to metals
- Molecular dynamics simulations determined threshold energies
- Stopping powers from SRIM
- Damage functions integrated over PKA damage energy spectrum using SPECOMP code to generate total DPA cross section as function of neutron energy
- DPA cross section folded with neutron flux spectrum provides DPA rate



Total DPA cross sections in barns for SiC

Reactor	Position	DPA cross section, barns		DPA/efpy	
		Fe	SiC	Fe	SiC
BWR	Midplane	303	265	2.8	2.4
PWR	Midplane	311	262	3.7	3.1
HFIR	C5	300	263	12	11
ATR	Midplane	302	260	14	12
EBR-2	Midplane	390	423	25	27
HFIR	PTP midplane	191	158	33	28
FFTF	MOTA midplane	267	324	43	53

HL Heinrich, LR Greenwood, WJ Weber, RE Williford, Displacement damage in silicon carbide irradiated in fission reactors, Journal of Nuclear Materials 327 (2004) 175-181