Issues Related to Dose Units and Damage Correlation

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from nuclear reaction to point defects

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Some Definitions -1

I. particle fluence, (unit area)$^{-1}$

a) depends only on irradiation source term and can be quoted at a point or averaged over a surface or volume

b) often quoted as a free-field particle fluence but the actual fluence will be modified by particle absorption and scattering when a test object is in place – i.e. material perturbs local flux

II. absorbed dose

a) depends on:

1. particle fluence
2. particle type
3. particle energy spectrum
4. material

b) not dependent on:

1. exposure conditions such as T, mechanical loads
2. previous dose or dose rate

Some Definitions -2

III. damage correlation parameter

a. at a minimum depends on

  1) particle fluence / absorbed dose
  2) specific damage parameter being monitored: e.g. electrical resistivity, swelling, hardening

b) successful application will depend on:

  1) damage rate and previous damage
  2) exposure conditions such as T, mechanical loads
  3) dopants, alloy elements, and impurities in material
  4) previous damage, thermomechanical treatment
  5) correlated damage mechanisms such as transmutation production
    - notably helium and hydrogen
    - solid transmutation products can also be significant, e.g. silicon production in aluminum where $\varphi_{th}=2.5\text{x}10^{26}$ n/m^2 (~6 months in HFIR) converts 1% of Al to Si

Illustrate difference between dose and exposure parameter: Norwegian and Australian models in Hawaii

What is dpa?

- based on a measure of absorbed dose, specifically the energy per atom of kinetic energy absorbed by a material
- the NRT or modified Kinchin-Pease model provides a what of estimating the number of stable atomic displacements (Frenkel pair) produced by the excess kinetic energy:

$$\nu_{NRT}=0.8 \cdot T_d / (2 \cdot E_d)$$

- the NRT was developed to specifically enable the direct comparison of very different irradiation environments, e.g. reactor spectra with very different thermal-to-fast neutron flux ratios, and charged particle irradiation with neutron irradiation
- no one ever believed it predicted the “right” number of FP

Development of dpa as an improved damage correlation parameter

Table 1: definition of terms

term	definition	typical or recommended value
E_p	atomic recoil energy, PKA energy	---
T_d, $T_d(E_p)$	damage energy, amount of PKA energy dissipated in elastic collisions	calculate from LSS stopping powers
η (E_p)	number of displacements created by recoil with specified PKA energy	---
κ	correction factor to account for realistic (as opposed to hard sphere) atomic scattering	0.8
L^*	cascade multiplication threshold	$2E_d/\kappa$ or 100 eV in NRT model
E_d	atomic displacement threshold energy	40 eV (iron)
E_c	maximum energy below which a vacancy will capture an atom	40 eV (iron)
E_b	atomic binding energy to lattice site	0^*
* model dependent, $L=(E_d+E_c+E_b)/\kappa$, K-P and NRT use $E_d=E_c$ and $E_b=0$		

I. Kinchin and Pease model [1]

$$\eta(E_p) = \begin{cases} 0, 0 < E_p < E_d & \text{(1a)} \\ 1, E_d \le E_p < 2E_d & \text{(1b)} \\ \dfrac{E_p}{2E_d}, E_p \ge 2E_d & \text{(1c)} \end{cases}$$

$$\frac{E_c}{2E_d}, E_p \ge E_c$$

Assumed sharp displacement threshold, only electronic stopping above a cutoff value, hard sphere collision cross section, no lattice effects

II. original NRT (modified Kinchin-Pease) [2]

$$\eta(E_p) = \begin{cases} 0, 0 < T_d < E_d & \text{(2a)} \\ 1, E_d \le T_d < \dfrac{2E_d}{\kappa} \quad \text{or} \quad 1, E_d \le T_d < L & \text{(2b)} \\ \dfrac{\kappa T_d}{2E_d}, T_d \ge \dfrac{2E_d}{\kappa} \quad \text{or} \quad \dfrac{\kappa}{L}, T_d \ge L & \text{(2c)} \end{cases}$$

Improved K-P model: binary collision models set $\kappa=0.8$ for more realistic scattering, damage energy calculated by theory from Lindhard, et al., NOTE:

Robinson and Oen [3,4] noted an inconsistency in the original NRT formulation that arises from using a damage energy calculated from a model that is independent of any consideration of a threshold in a threshold-based displacement model. They argue that $\eta(L)$ in Eqn. (2c) should equal 1. However, since Td(100)=86.63 eV and L=100, $\eta(L)<1$. This can be corrected by replacing L with Td(L) in Eqn. (2). This increases the number of displacements in Eqn. (2c) by the ratio of 100/86.63=1.15430.

References:

1. G.H. Kinchin and R.S. Pease, “The Displacement of Atoms in Solids by Radiation,” Reports on Progress in Physics 18 (1955) 1-51.
2. M.J. Norgett, M.T. Robinson, and I.M. Torrens, Nucl. Engr. and Des. 33 (1975) 50-54.
3. M.T. Robinson and O.S. Oen, J. Nucl. Mater. 110 (1982) 147-149.
4. M.T. Robinson, J. Nucl. Mater. 216 (1994) 1-28.

See ASTM E521 for additional details and table of recommended E_d values

See ASTM E693 for iron dpa cross section for neutron irradiation a standard dpa cross section for iron has been developed based on physical nuclear scattering cross sections and the assumptions from the NRT model about defect production, from ASTM E683

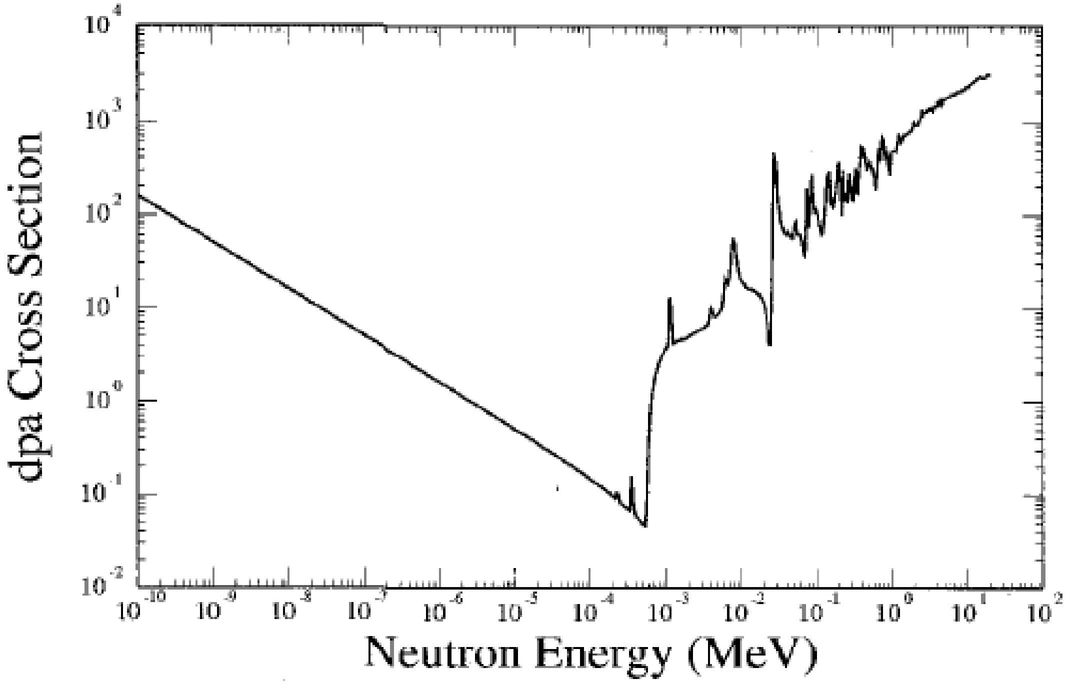
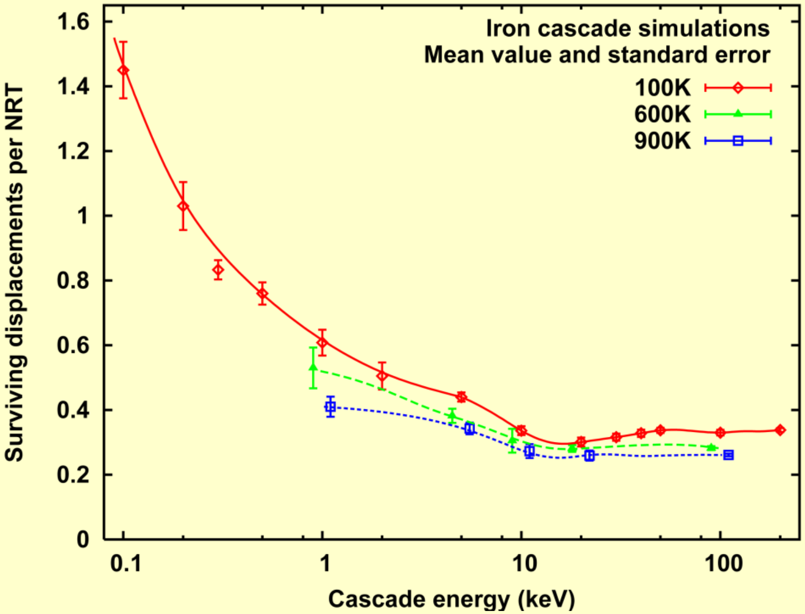


FIG. 1 ENDF/B-VI-based Iron Displacement Cross Section

see ASTM E683

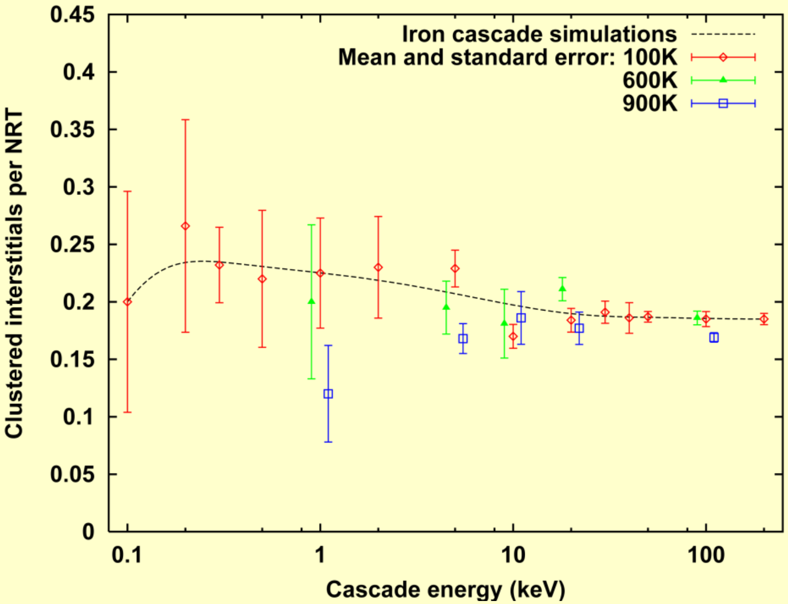
Compare MD results to NRT dpa

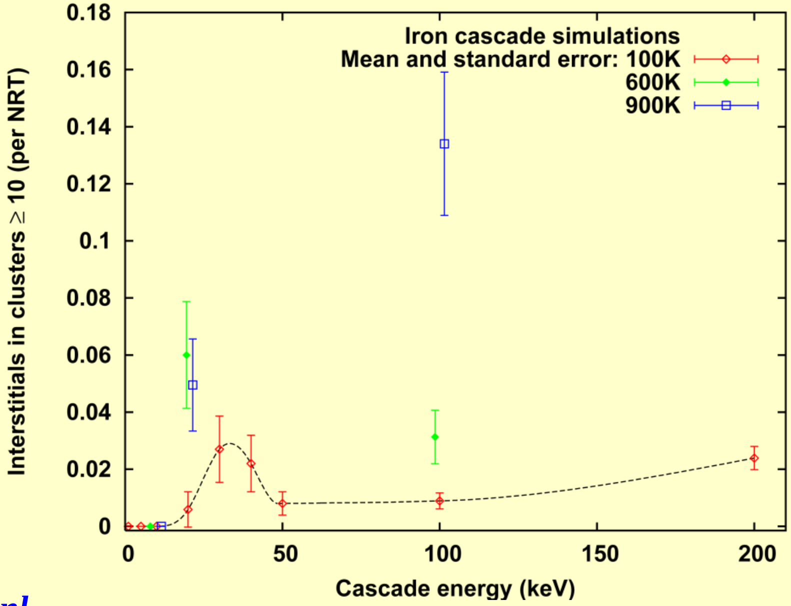


Finnis-Sinclair potential

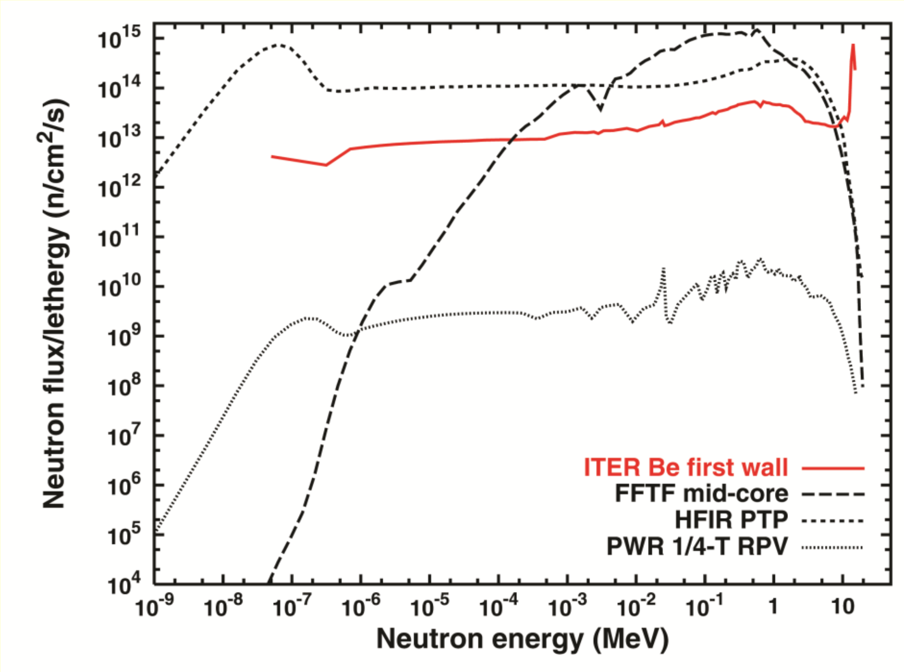
Note: temperature dependence

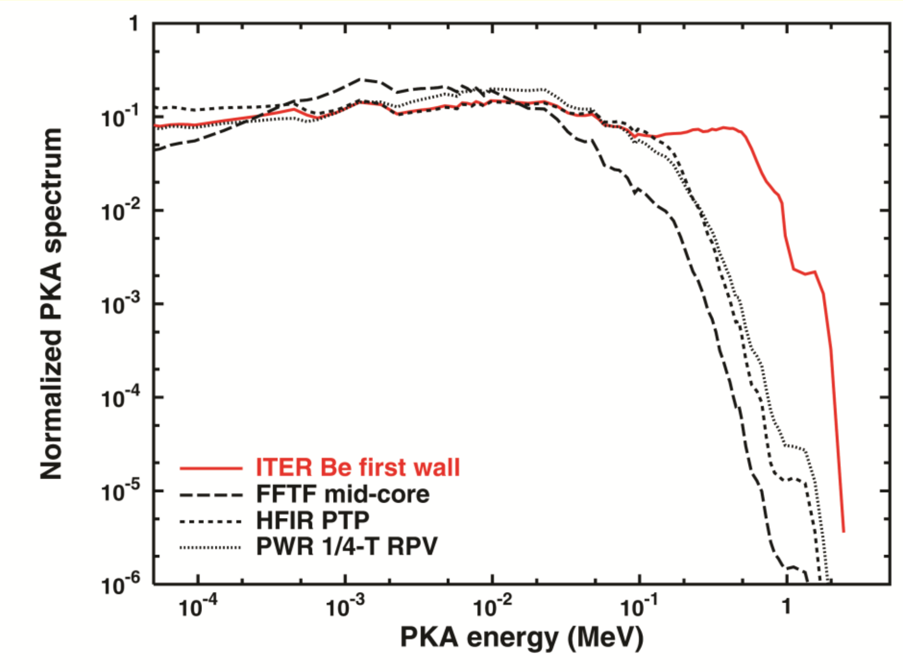
see Stoller





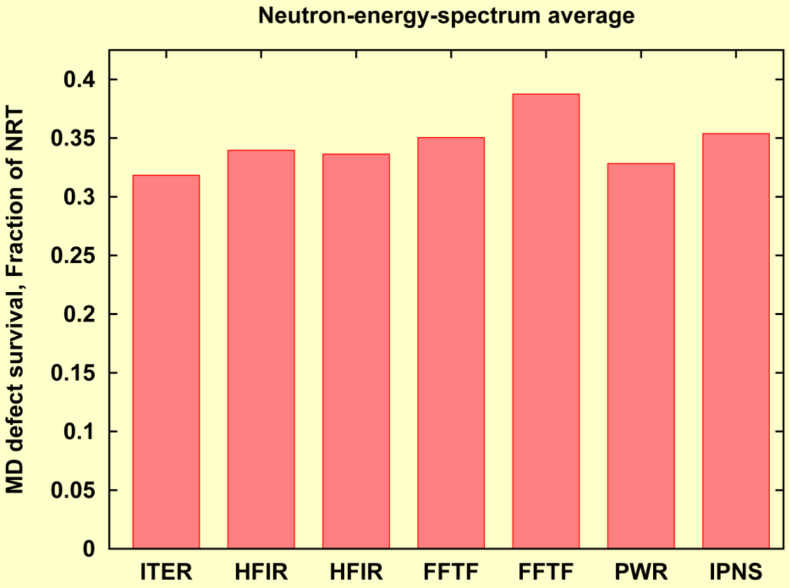
Typical neutron and iron pka energy spectra





MD results: averaged over neutron (pka) energy spectrum

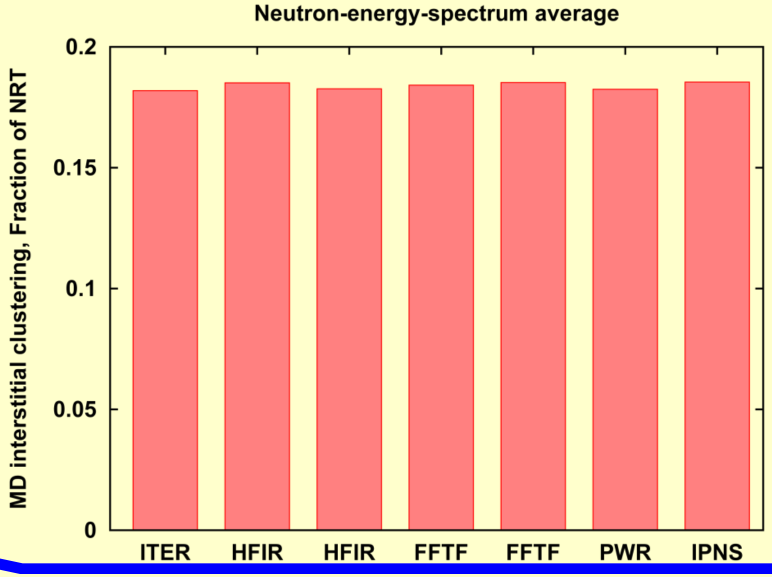
T=100K
Finnis-Sinclair potential

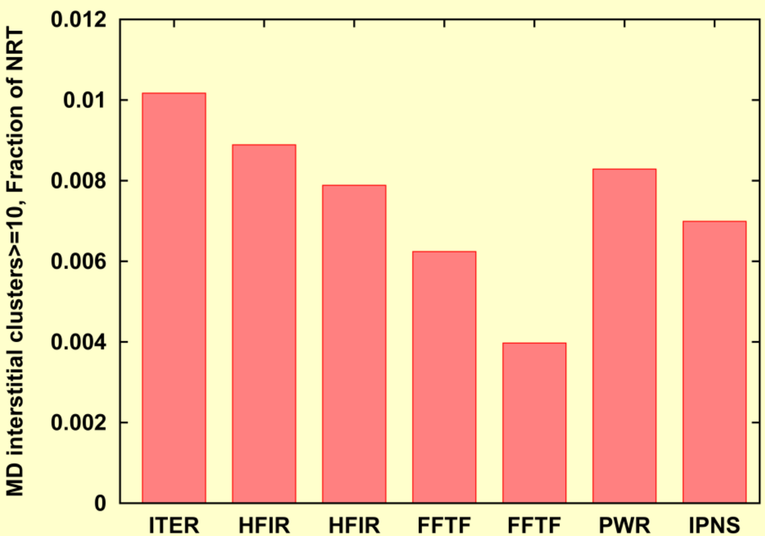


Absorbed energy

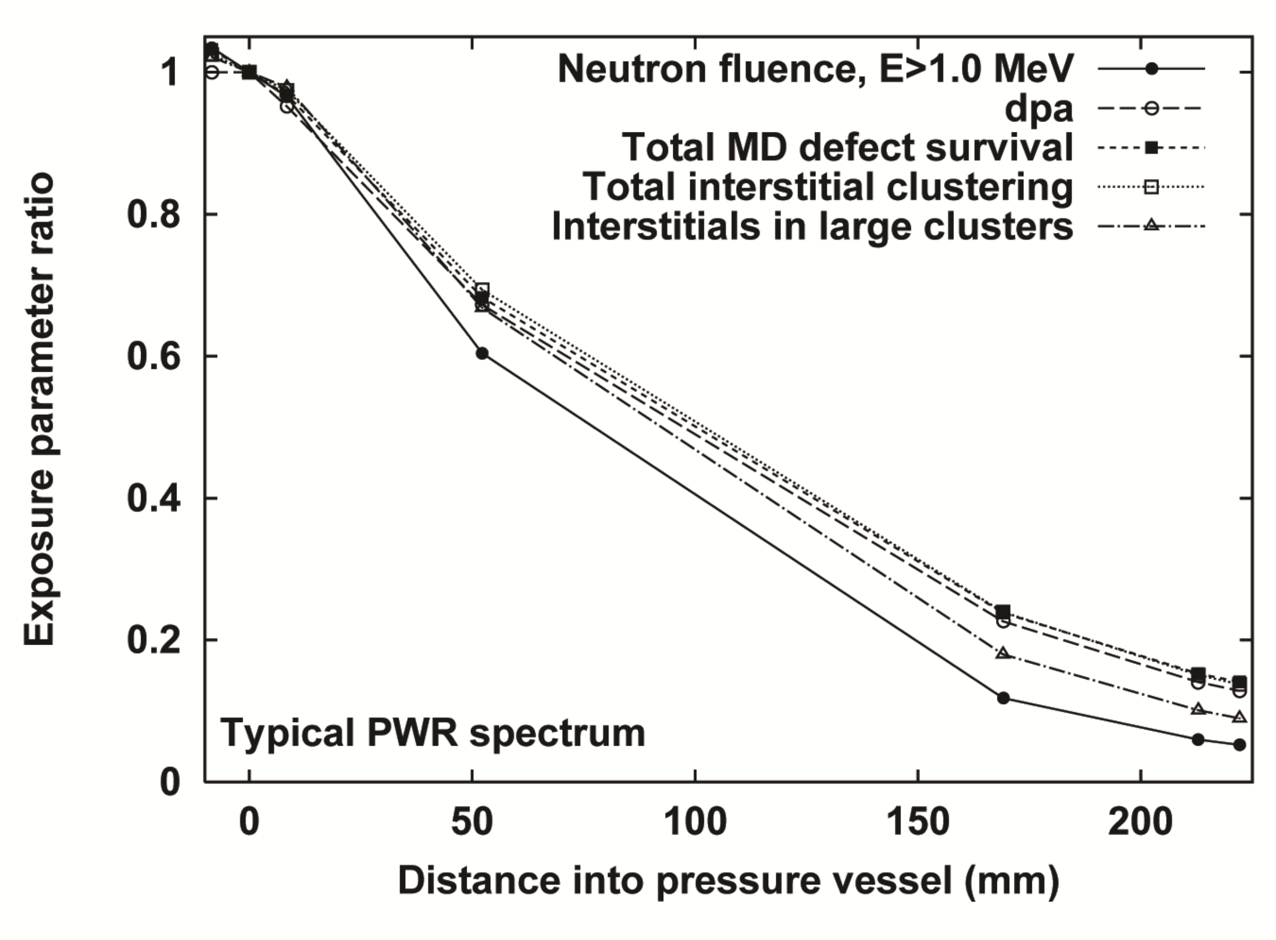
Significance to damage correlation?

see Stoller and Greenwood





Variation in possible exposure parameters: RPV pressure vessel thru-thickness



Stoller and Greenwood, ASTM STP 1405, 2001

Damage function analysis or cross sections

- damage function analysis slightly predated the NRT dpa
- objective was to provide effective cross sections to permit comparisons of different irradiation environments
- developed in a similar way to how other cross sections are developed
  - try to determine which part of neutron energy spectrum was responsible for the specific radiation effect of interest, such as hardening or embrittlement
  - multiple irradiations in different environments
  - unfolding schemes to obtain the cross section

(see references on next slide)

A few damage function references

- REFERENCE: Serpan, C.Z., Jr., "Damage-Function Analysis of Neutron-Induced Embrittlement in A302-B Steel at 550 F (288 C)," Effects of Radiation on Substructure and Mechanical Properties of Metals and Alloys, ASTM STP 529, American Society for Testing and Materials, 1973, pp. 92-106 .
- REFERENCE: Yoshikawa, H. H. "Materials Performance Prediction from Irradiation Test Data," Effects of Radiation on Substructure and Mechanical Properties of Metals and Alloys. ASTM STP 529, American Society for Testing and Materials, 1973, pp. 337-348.
- REFERENCE: Simons, R. L., "Neutron Energy Dependent Damage Functions for Tensile Properties of 20 Percent Cold-Worked Type 316 Stainless Steel," Irradiation Effects on the Microstructure and Properties of Metals, ASTM STP 611, American Society for Testing and Materials, 1976, pp. 181-192.
- REFERENCE: Gold, R., Lippincott, E. P., McElroy, W. N., and Simons, R. L., "Radiation Damage Function Analysis," Effects of Radiation on Structural Materials. ASTM STP 683, J. A. Sprague and D. Kramer, Eds., American Society for Testing and Materials, 1979, pp. 380-401.

Complexity of general form of damage function (Gold, *et al.* reference)

Postulate 2

$$P(\tau, T, F, \alpha_i) = \int_t \int_E G_P(T, t, E, f, \alpha_i)\Phi(E, t)\,dE\,dt$$

- P is property being measured as a function of time, τ, temperature, T, neutron fluence, F, and metallurgical (such as composition) variables, α_i
- G is damage function, analogous to cross section
- $\Phi(E,t)$ is neutron flux

Representative Damage Functions RPV embrittlement

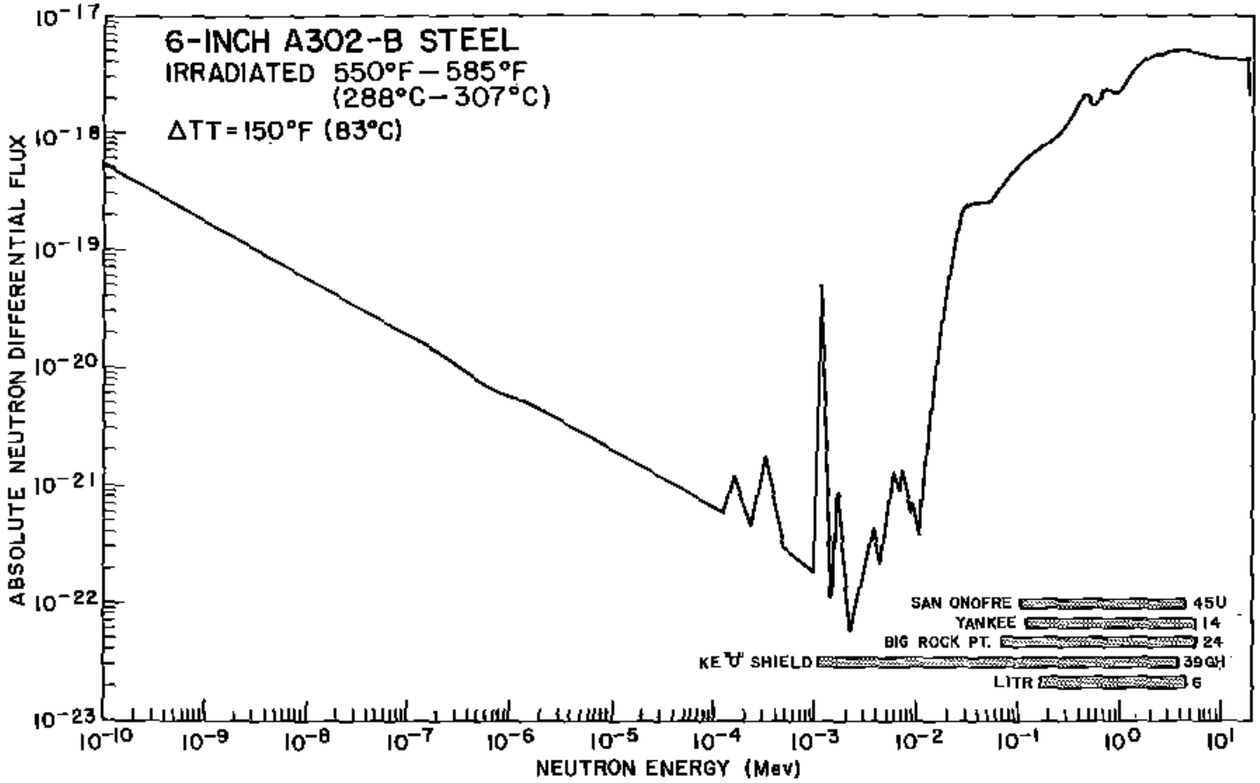


FIG. 2—*Absolute damage function for irradiation of A302-B steel at 550 to 585 F (288 to 307 C). Bars in the corner show the energy range of neutrons responsible for 90 percent of the nominal 150 F (83 C) transition temperature increase.*

Serpan reference – note how similar it is to dpa cross section

Representative Damage Functions 316SS total elongation

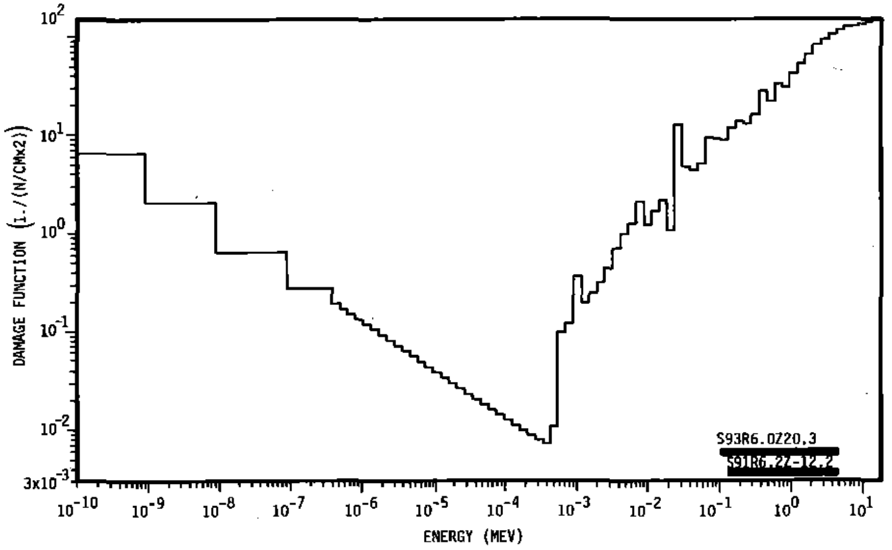


FIG. 3—*Damage function for 2 percent TE in 20 percent cold-worked Type 316 stainless steel irradiated at 593°C (1100°F) (using HEDL data only).*

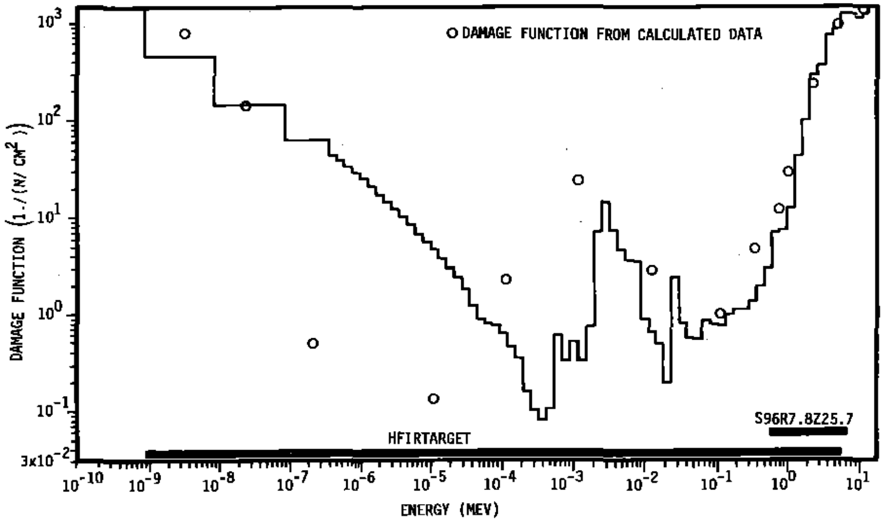


FIG. 4—*Damage function for 2 percent TE in 20 percent cold-worked Type 316 stainless steel irradiated at 593°C (1100°F) (using ORNL data only).*

Simons reference

Representative Damage Functions total elongation

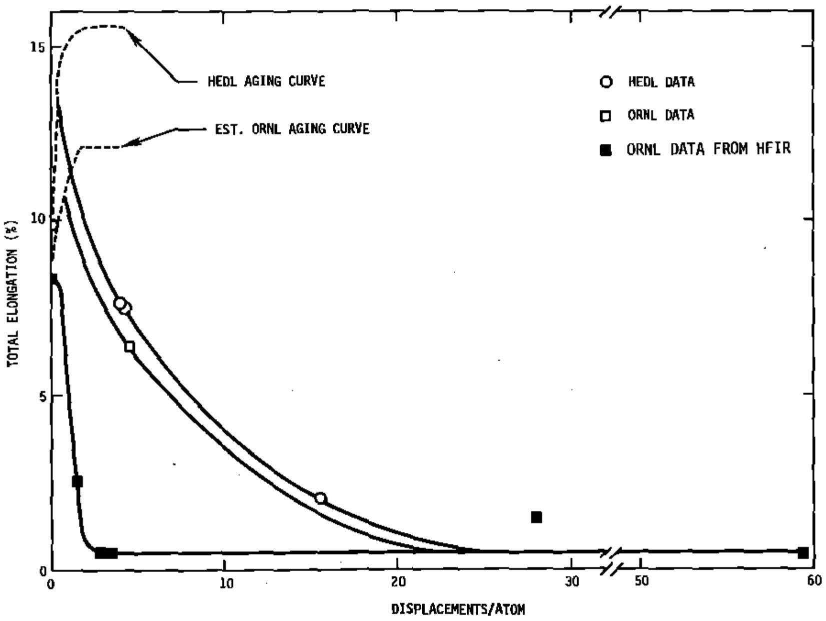


FIG. 2—*Total elongation of 20 percent cold-worked Type 316 stainless steel irradiated at 593°C (1100°F) versus displacements per atom.*

Compare HFIR and EBR-II data

1 – vs dpa

2 – vs (dpa*He/atom)$^{0.5}$

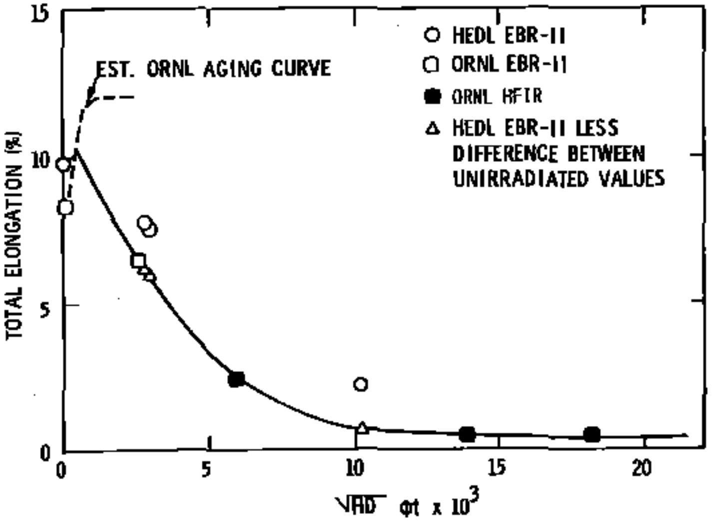


FIG. 5—*Total elongation in 20 percent cold-worked Type 316 stainless steel irradiated at 593°C (1100°F) versus square root of product of displacements and helium concentration.*

Simons reference

Summary/Comments

- each radiation-induced effect depends sensitively on a range of irradiation and material parameters
- this works against development of a universal exposure parameter
- MD simulations have advanced understanding of many details of displacement production, their results are not “right” either but are within 20 to 40% of the NRT displacements
  - generally consistent with cryogenic measurements of displaced atoms using resistivity change per FP

- Damage accumulation
  - primary damage provides source term only
    - commonly used, e.g. $G_{FP}=\eta G_{NRT}(1-f_{cl})$
  - microstructural evolution requires models such as:
    - mean field reaction rate theory
    - various Monte Carlo methods
    - models integrated with coarser length scale models
- the expectations of a replacement for the NRT dpa need to be carefully thought out – see slides (2) and (3)
  - a measure of dose? should not be function of T, dose rate, ...
  - a damage correlation parameter? many “new-dpa” required, all functions of many parameters
  - who is the customer and for what purpose? ... scientists? ... nuclear industry?