Overview of ‘classical’ or ‘standardized’ DPA calculation stemming from the reactor world.

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Purpose

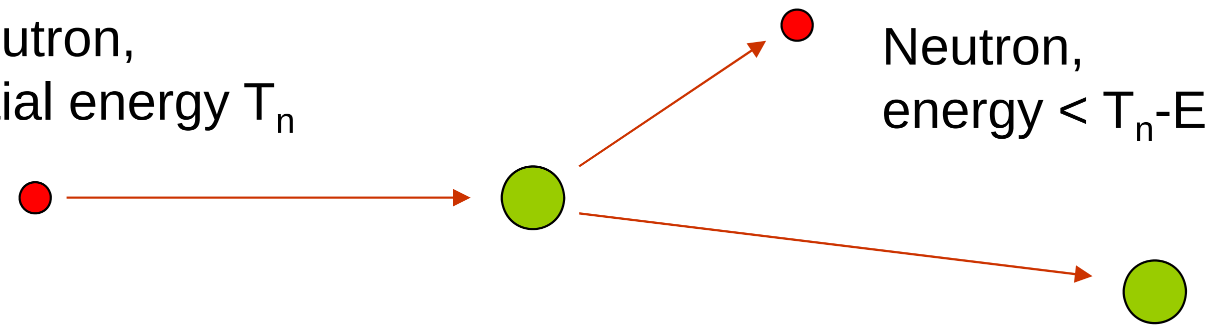
- Overview of ‘classical’ or ‘standardized’ DPA calculation stemming from the reactor world.
  - Current Status
  - Details of accepted Methodology
  - Known Limitations
- Limited discussion of implications (to RaDIATE) of limitations

Introduction

- The key steps in evaluating the damage dose for a material exposed to a flux of neutrons are

    1. Determination of the neutron energy spectrum.
    2. Determination of the total fluence of neutrons passing through the material.
    3. Evaluation of the **Primary Knock-On Atom (PKA)** energy spectrum
    4. **Evaluation of the number of atomic displacements produced in the material.**

Introduction: PKA

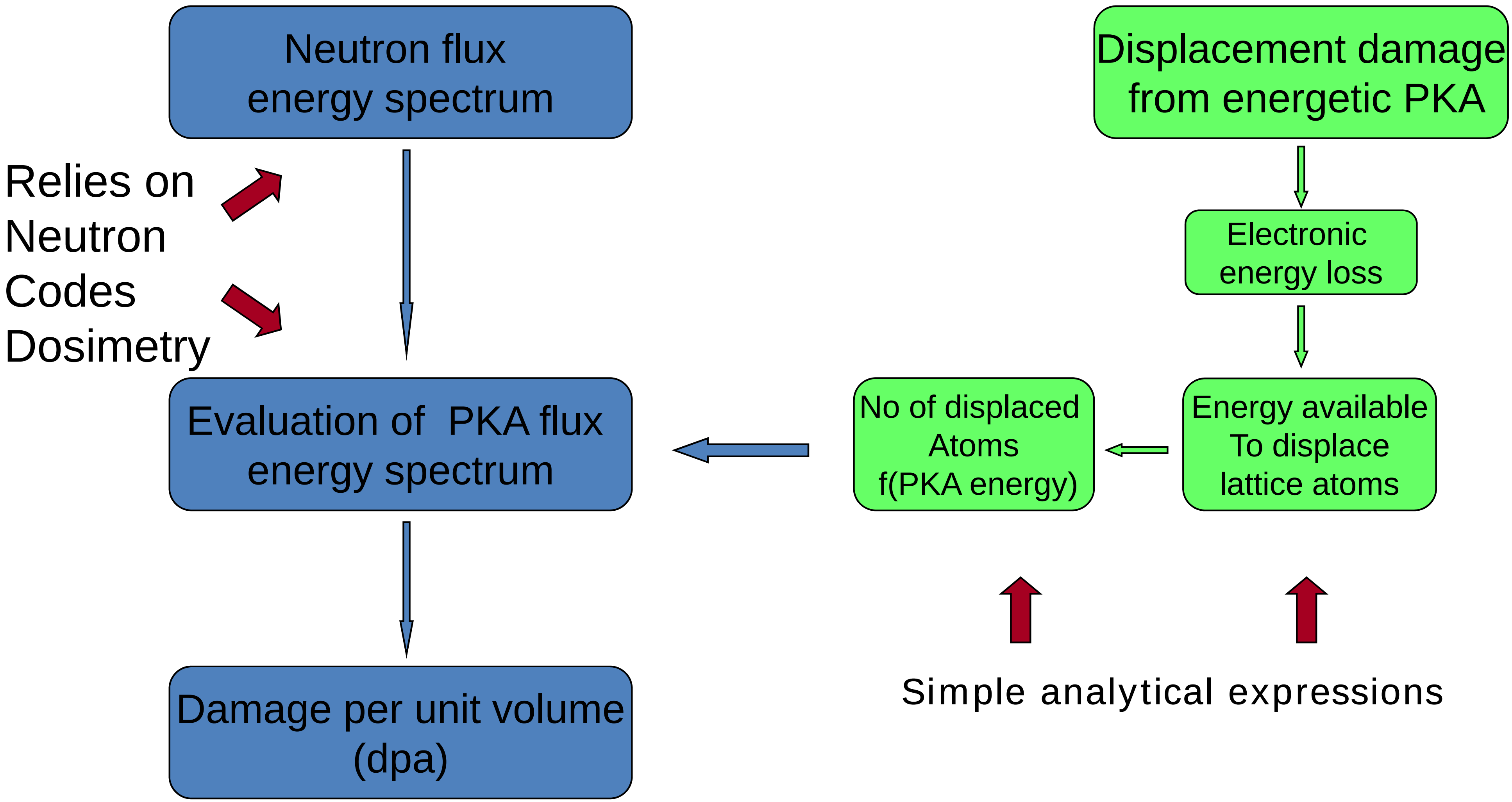


- Typical PKA energies
  - Thermal neutrons
    - Average PKA Fe 400eV
  - Fast neutrons >.1MeV
    - Fe PKAs few eV to 10s of keV
- ~40eV required (E_d) to create a stable displaced atom and vacancy in Fe (damage)

Well above E_d,

- PKA has sufficient kinetic energy itself to displace other lattice atoms from their sites.

Introduction: Current Methodology



Current Methodology

Introduction IV

- Evaluation of the number of atomic displacements produced in the material by the energetic neutrons.
  - Evaluation of the energy and fluxes of energetic primary knock-on atoms (PKA) set up in the lattice by the (fast) neutrons.
  - Evaluation of the displacements from a given energy PKA

- Frequently the number of displacements produced in a given irradiation is evaluated per unit volume and quoted as the average displacements per atom.
  - Hence the unit dpa.
    - Thermal Reactor Pressure Vessel 15mdpa
    - Core internal in LWR 1-10 dpa
    - Fast Reactor cladding ~ 100 dpa.

Dpa: Current status - Usage

- Importance of the level of damage or dpa is that frequently it can become a ‘measure’ of the change in bulk properties in-service.

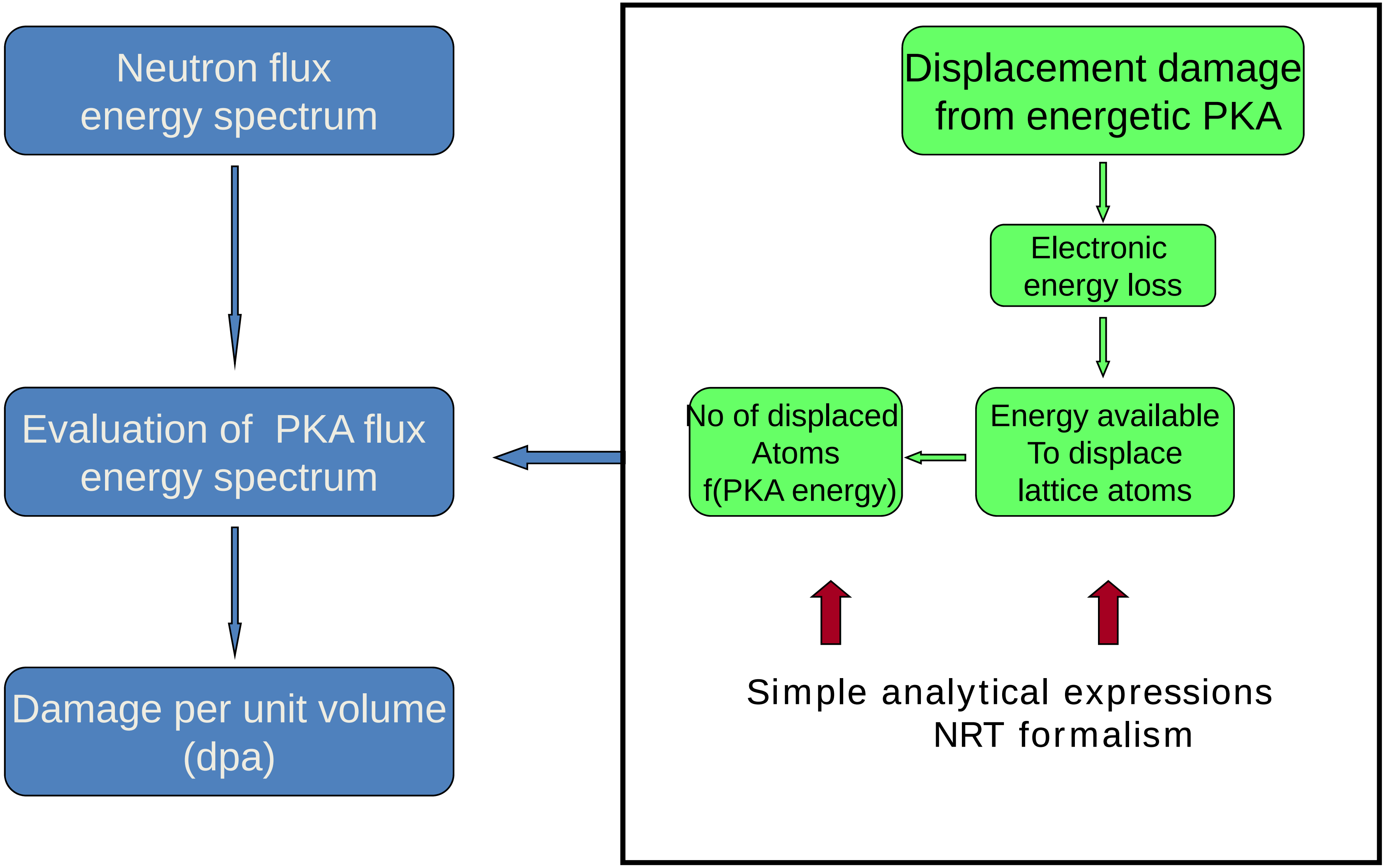
- Frequently, interested in either
  - Using data on property change from a simulation to predict behaviour of component in-service reactor.
  - Comparing response in different irradiations

- Dpa can be used as an exposure parameter or more usefully as a correlation parameter

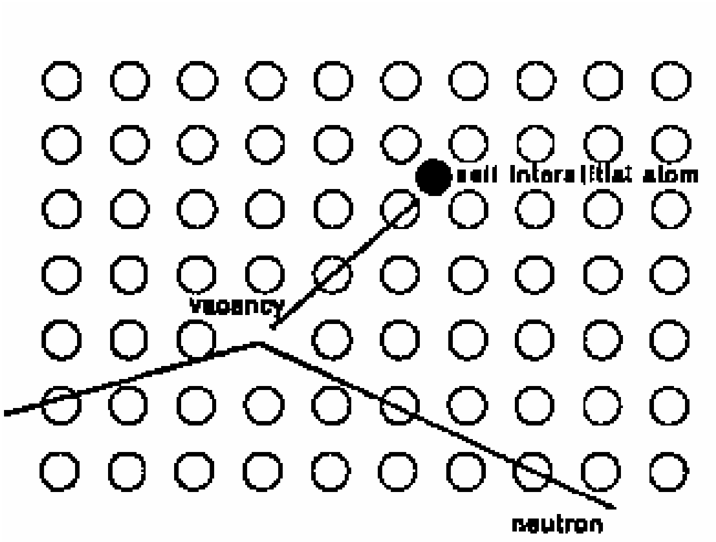
Dpa: Current status - Intl practice

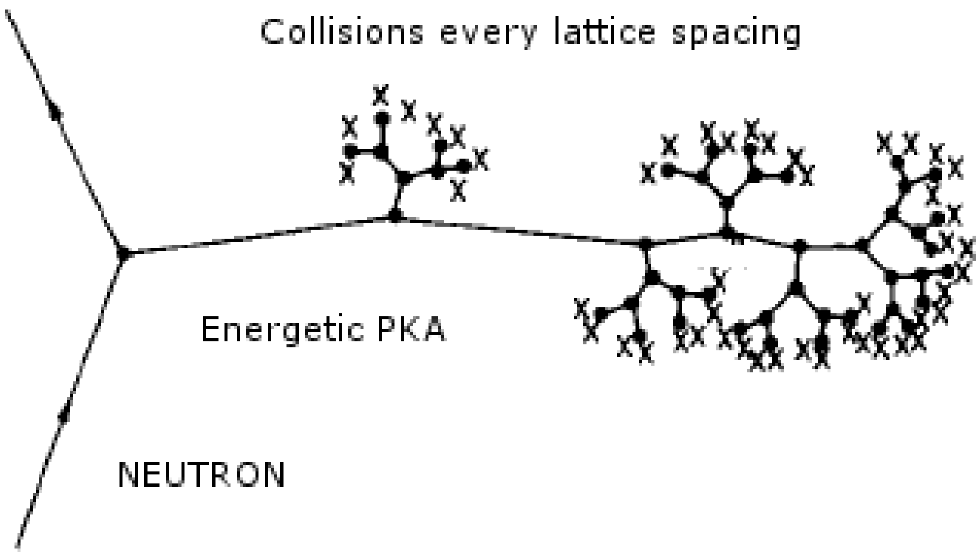
NATIONAL NUCLEAR LABORATORY

- Internationally accepted methodology for evaluating displacements from energetic PKA.
    - Methodology originally established in 1972.
    - Incorporated in ASTM Standard E693 75 (now ASTM E693-01 (2012))
        - Evaluates dpa from a flux of energetic neutrons
        - Standard has been re-approved since original formulation
- Dpa widely used in thermal, fast reactor and fusion material studies.
    - Use of dpa has been ‘accepted’ by Civil Nuclear Regulators
- **Understanding of the processes controlling damage production has developed since the 1970’s**
    - There are limitations in the current formulism
    - However, these limitations are judged not sufficiently severe to lead to revision of the ASTM Standard(s).
        - Note this is in the context of fast neutron irradiation


Neutron flux energy spectrum
Evaluation of PKA flux energy spectrum
Damage per unit volume (dpa)
Displacement damage from energetic PKA
Electronic energy loss
Energy available To displace lattice atoms
No of displaced Atoms f(PKA energy)
Simple analytical expressions
NRT formalism

DPA: Point Defect production





- ~ 40eV required to create a stable Frenkel pair
- Collision or displacement cascade

Dpa: What is it

The number of surviving vacancies and interstitials N_D (so-called 'damage' dpa) that the events produce depends on PKA energy.

For very low recoil energies E this number is given by

$$N_D = 1 \qquad E_d < E_{dam} < 2E_d \qquad (1)$$

and for higher energies

$$N_D = k_d E_{dam} / 2E_d \qquad E_{dam} > 2E_d \qquad (2)$$

E_{dam} is expressed in keV and is the total energy available for displacing atoms, excluding energy losses due to electronic excitation

E_d is the displacement energy and is ~40eV for iron.

The quantity k_d is the damage efficiency for which a constant value of 0.8 was derived by Norgett, Robinson and Torrens (NRT) by means of a simple binary collision model. It was also assumed to be independent of target and temperature for all materials.

Dpa: What is it

- **Norgett et al. recommended the following method of evaluating E_{dam}:**

$$E_{dam} = E / (1 + Kg(\varepsilon))$$

$$\text{where } g(\varepsilon) = 3.4008\varepsilon^{1/6} + 0.40244\varepsilon^{3/4} + \varepsilon$$

$$K = 0.1337 Z_1^{1/6} (Z_1 / A_1)^{1/2}$$

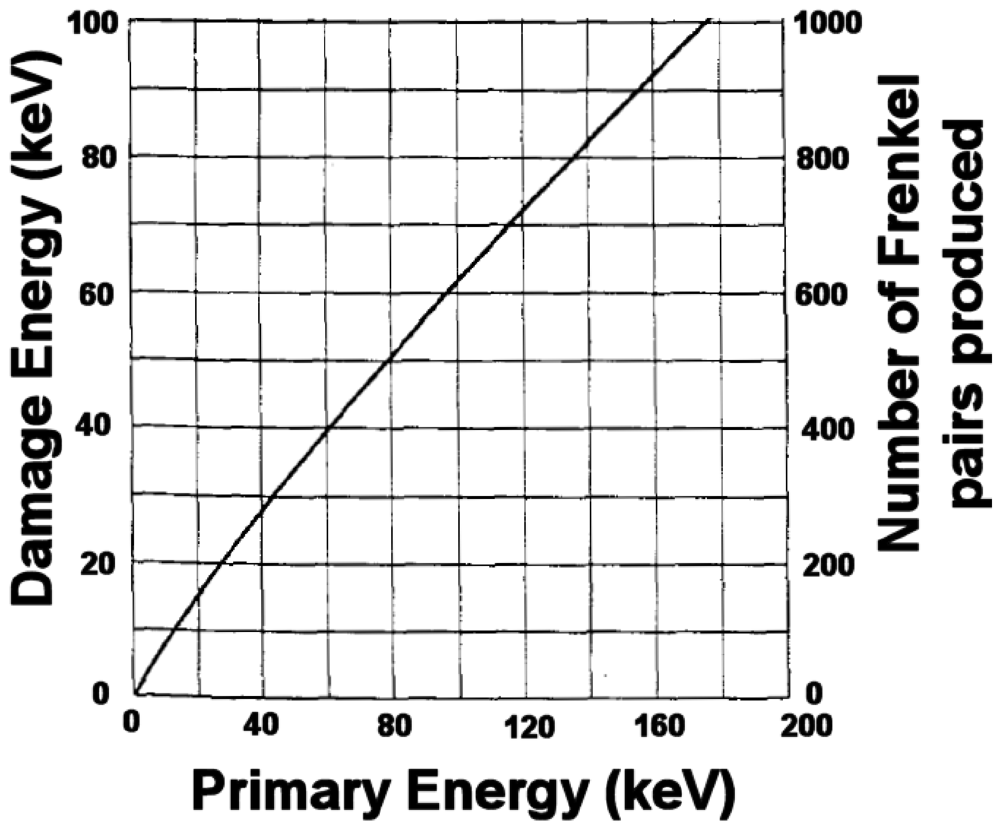
$$\varepsilon = a A_2 E / (2 Z_1 Z_2 e^2 (A_1 + A_2))$$

$$a = 0.8853 a_o / ((Z_1^{2/3} + Z_2^{2/3})^{1/2})$$

A_1 and Z_1 are the atomic mass and number of the moving particle and A_2 and Z_2 are the atomic mass and the number of the of the lattice atoms; a_o is the Bohr radius; and *e* is the electronic charge.

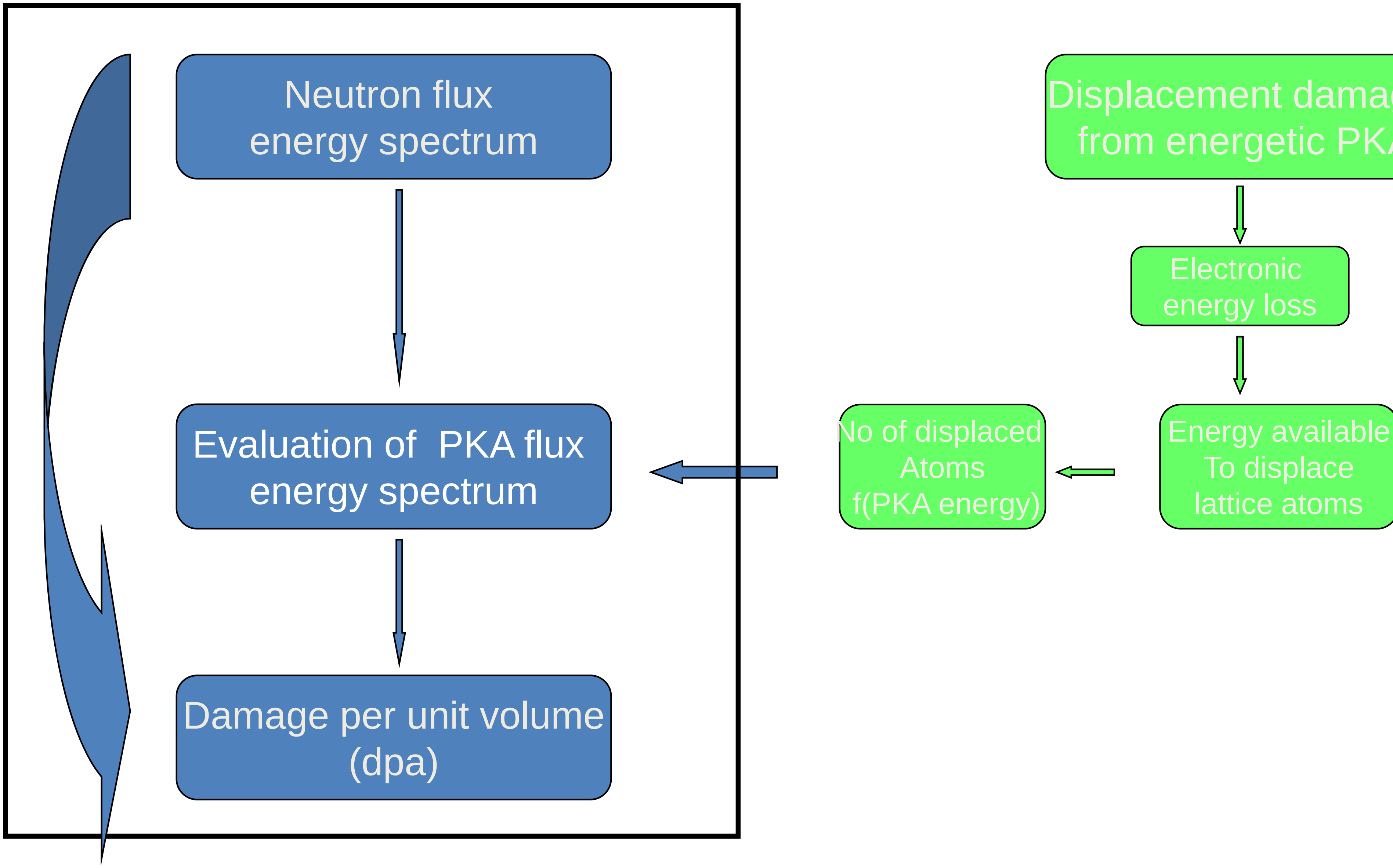
- **State of the art in early 1970s**

Dpa: What is it



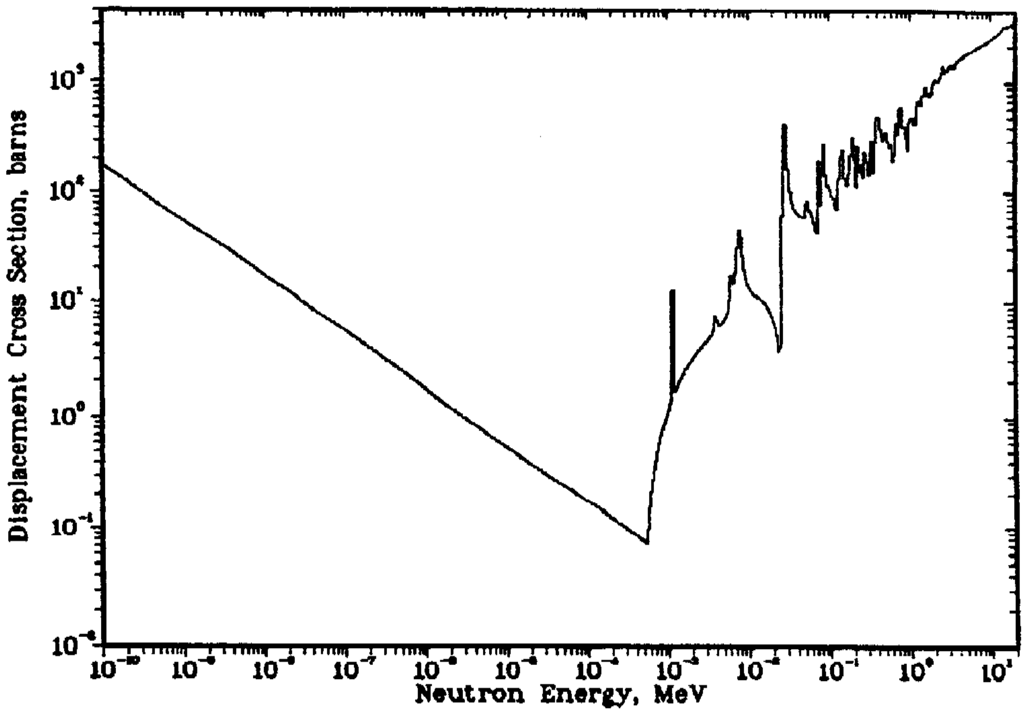
M.J. Norgett, M.T. Robinson and I.M. Torrens, "A Method of Calculating the Number of Atom Displacements in Irradiated Metals", AERE Report TP/494; CEA Report No. 4389; ORNL Solid State Division Report No. 72-70: 1972.
M. J. Norgett, M. T. Robinson, and I. M. Torrens, A proposed method of calculating displacement dose rates, Nucl. Engr. and Design 33, 50 (1975)

ASTM Standard E693



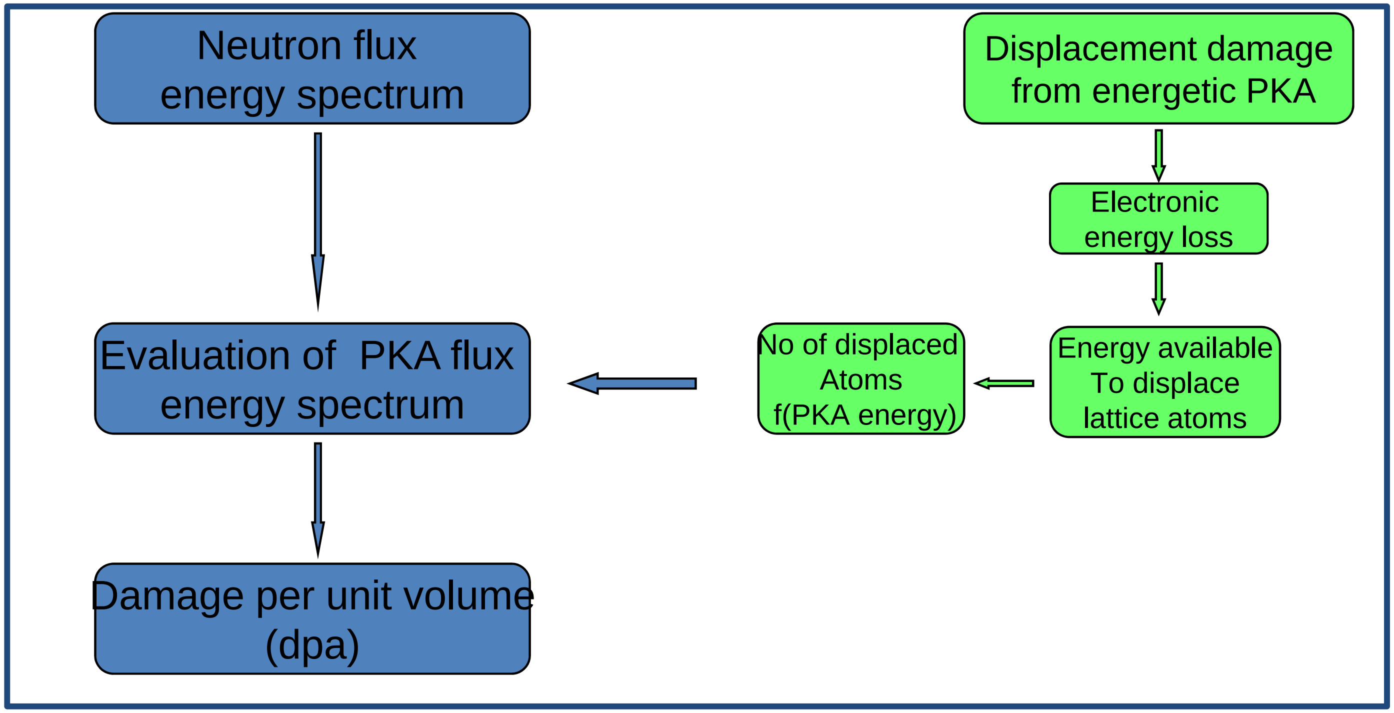
ASTM E693 Standard: Methodology

- Uses SAND II group structure for neutron energies and ENDFB IV neutron cross-sections
- Evaluates dpa cross-sections for each neutron energy group using the cross-sections above and the NRT formulism.



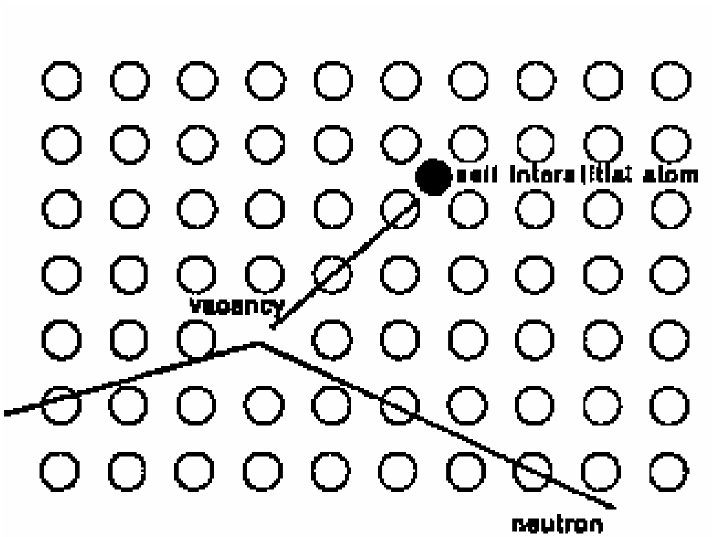
- Allows for a neutron energy cut-off of 10keV (i.e. no thermals)
- Dpa cross-sections specific to Fe but standard states methodology applies to all elements

Limitations in dpa methodology

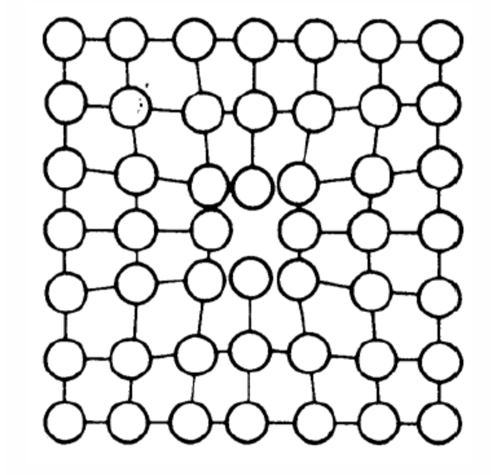


- Displacement damage production
  - Electronic loss (SRIM)
  - **No of displaced atoms from high energy PKA**

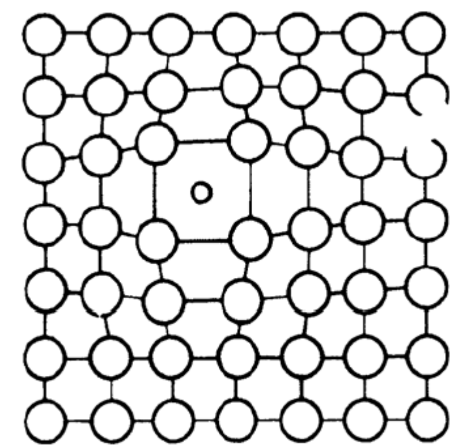
Point Defect pairs (Frenkel pair)



Vacancy

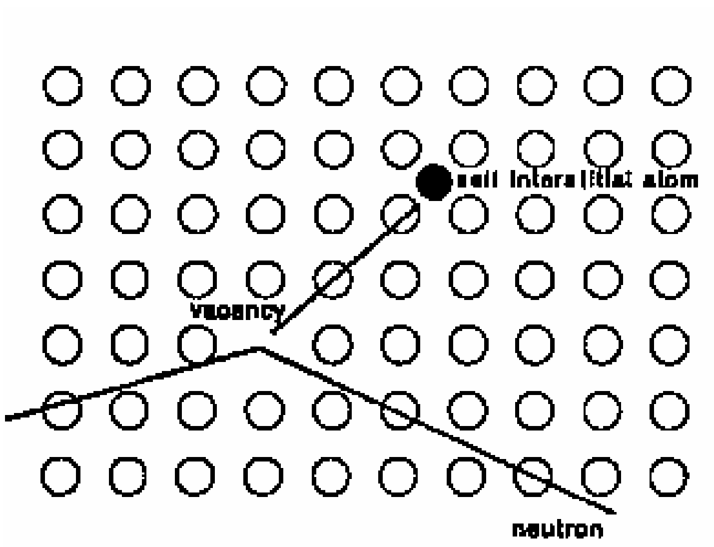


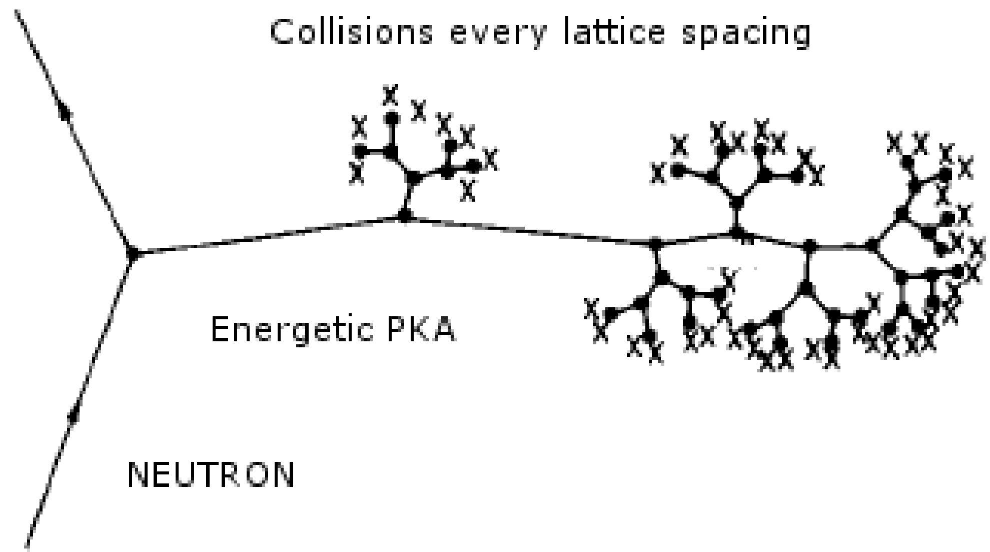
Interstitial



- ~ 40eV required to create a stable Frenkel pair
- At temperatures of interest both I’s and V’s are mobile

DPA: Point Defect production





- ~ 40eV required to create a stable Frenkel pair

http://www.liv.ac.uk/~afcalder/dispcasc.html

- Collision or displacement cascade
  - keV deposited in a small region
  - Sufficient energy to locally “melt” volume 10’s nm across
  - Complex event

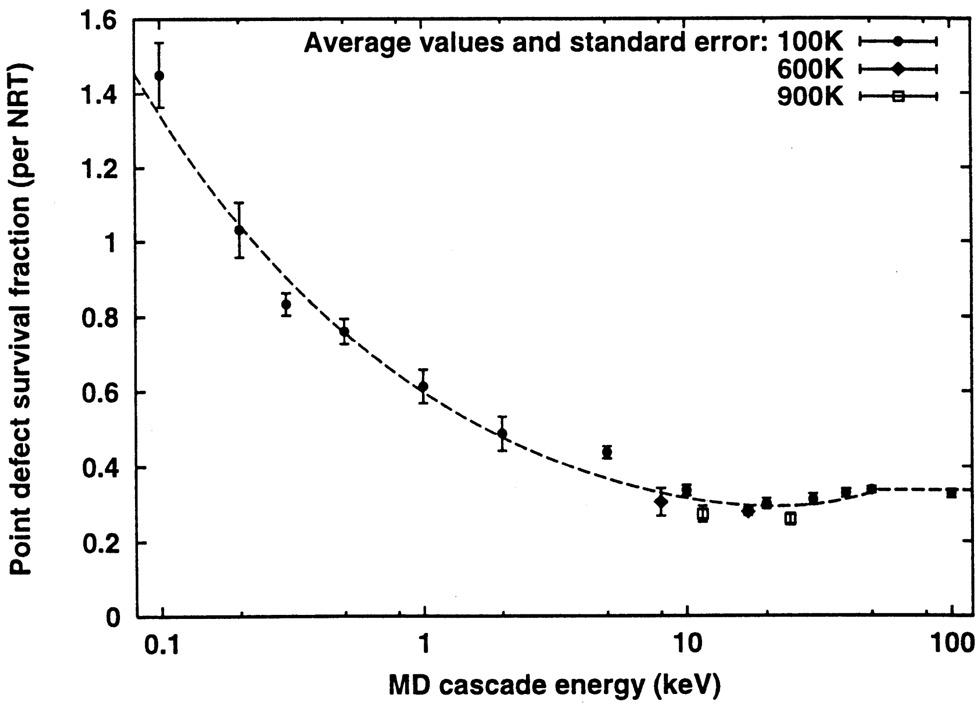
Treatment of Damage Production

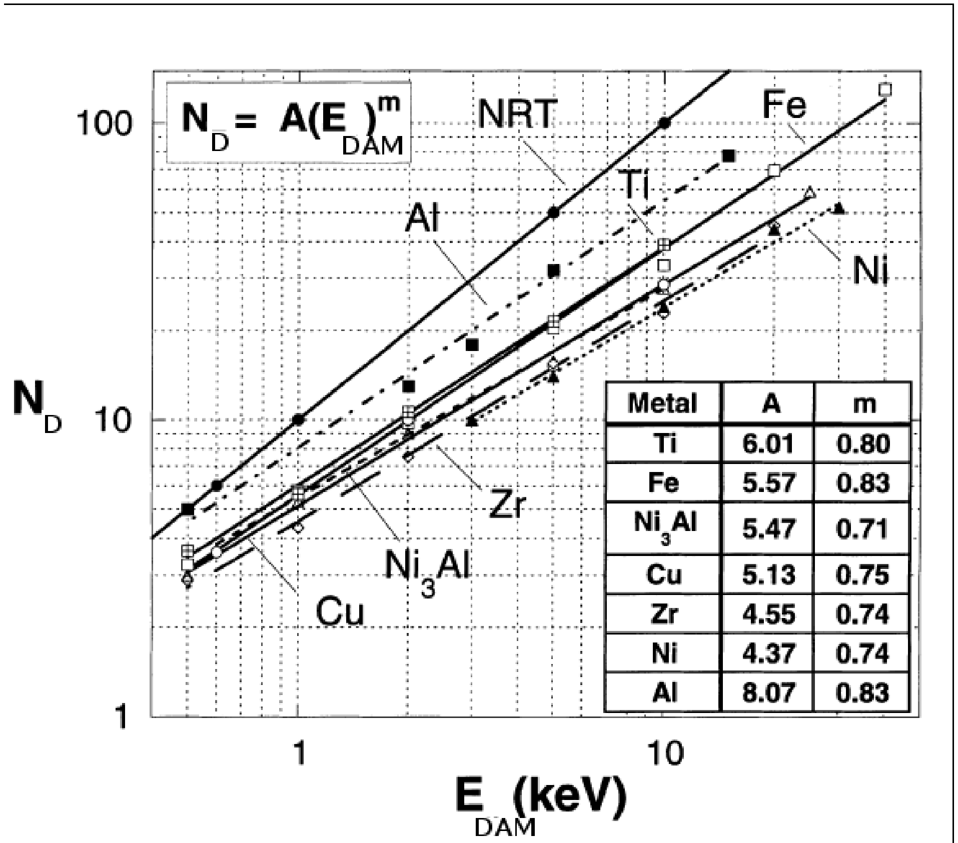
$$N_D = k_d E_{dam} / 2E_d$$

- **In NRT the quantity k_d is the damage efficiency for which has a constant value of 0.8**

- Now accepted that k_d is dependent on PKA energy
  - Extensive experimental work on displacement production by high energy PKA (cascades)
  - Molecular dynamics simulation of cascade events, and monitoring of point defects surviving the damage event
  - Experiment and modelling confirm that k is energy dependent and decreases to a level of approximately 0.3

Treatment of Damage Production





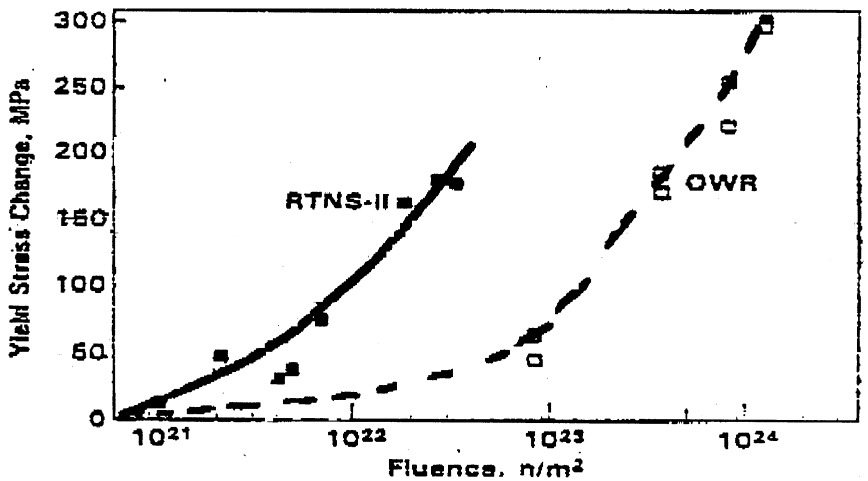
Metal	A	m
Ti	6.01	0.80
Fe	5.57	0.83
Ni_3Al	5.47	0.71
Cu	5.13	0.75
Zr	4.55	0.74
Ni	4.37	0.74
Al	8.07	0.83

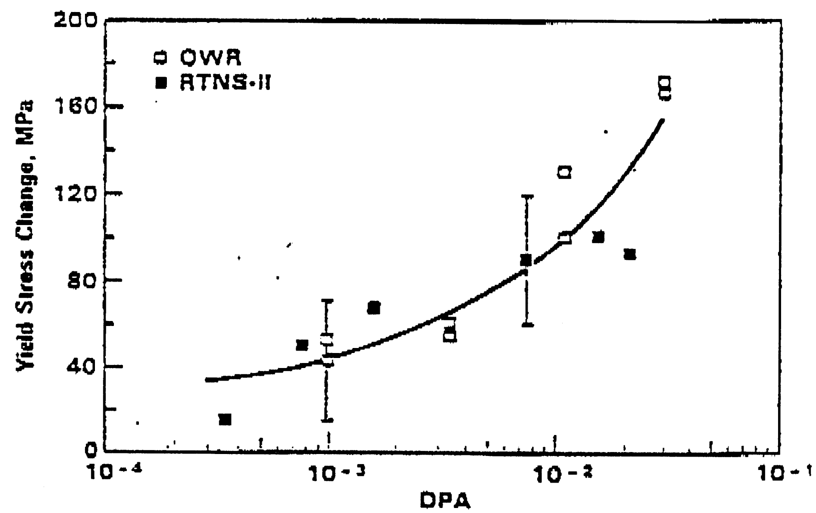
Modelling data for Fe on the energy dependence of k_d (Stoller and Greenwood)

Modelling data on a number of metals (Bacon and co-workers)

Implications of energy dependent k_d

- Existing NRT formalism will provide a good correlation (or exposure parameter) for environments where the dpa is generated by high energy recoils (say > 5keV)

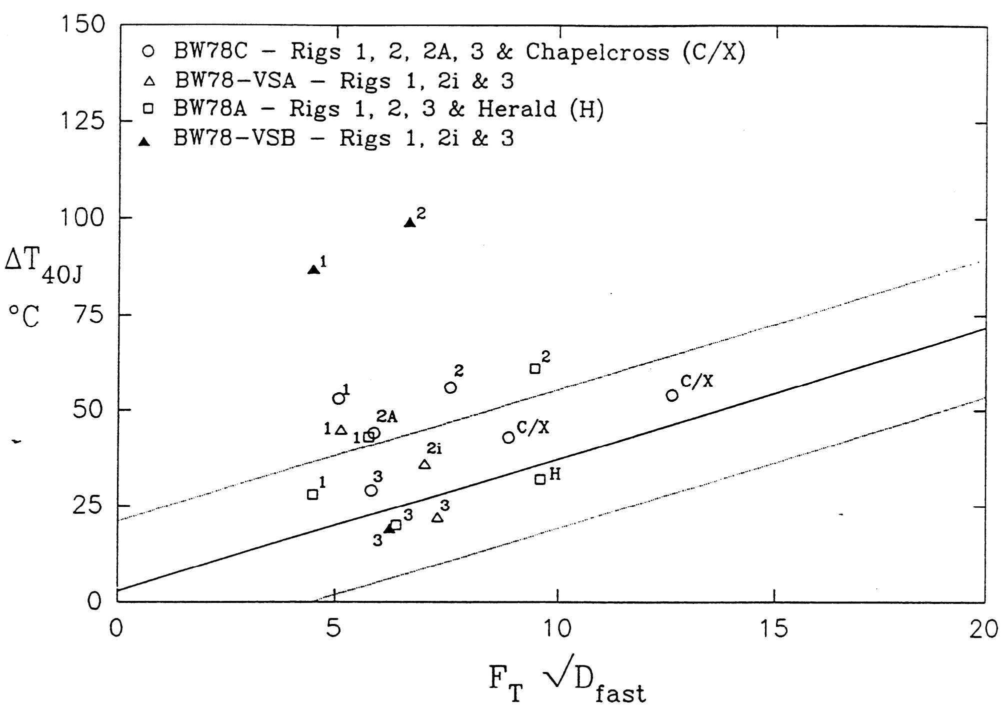




- RPV steel irradiated in 2 different irradiation environments at 60°C
  - RTNS-II 14 MeV neutrons, OWR Fission spectrum (Heinisch)

Implications of energy dependent k_d

- Existing NRT formalism will **not** provide a good correlation (or exposure parameter) for environments where the dpa is generated by different energy recoils (low vs high).



Damage from thermal neutrons is more effective at creating embrittlement than NRT allows

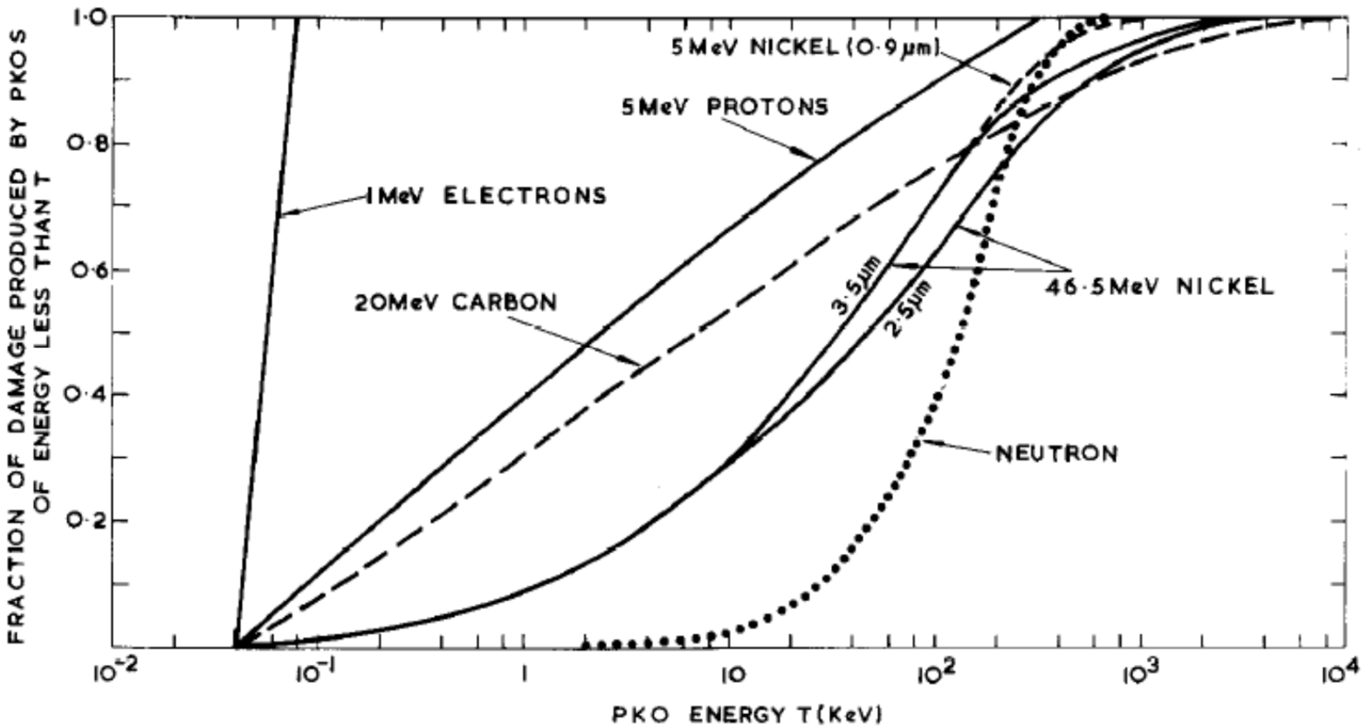
Thermal neutrons in Fe create PKA ~ 400eV

Factor of 2 consistent with experimental and modelling data on the energy dependence of k in NRT formalism

(Jones and co-workers)

$$\text{dpa} = \text{dpa}_{fast} + \kappa\ \text{dpa}_{thermal} \quad \kappa = 2 \pm 0.5$$

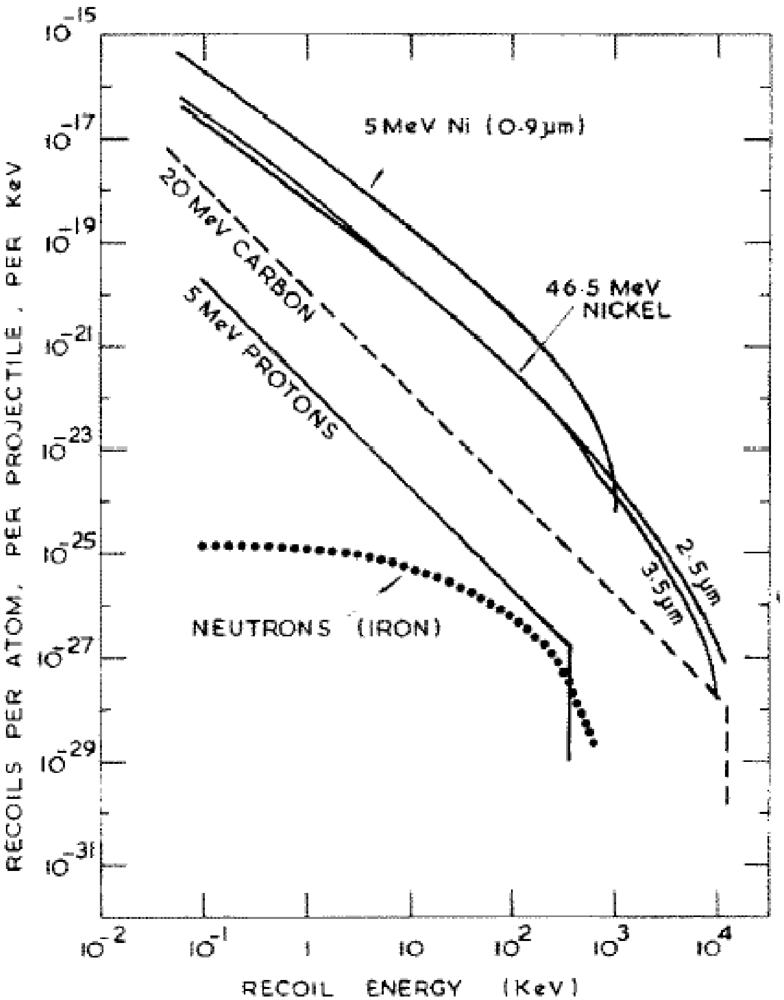
Ion beams: Importance of energy dependent k_d



- Damage from high energy cascades is more important in fast neutron irradiation (fusion even stronger)

- 1 MeV electrons – no cascades

Ion beams: Importance of energy dependent k_d



Marwick

Table 1
The proportion of total damage produced by primary knock-ons with more than 5 keV energy (%).

Fast neutron spectrum	99
46.5 MeV nickel (rocked)	79
5 MeV nickel	79
20 MeV carbon	54
5 MeV protons	42
1 MeV electrons	0

Table 2
The density of damage produced by one particle·cm^{-2} (dpa) assuming E_d = 40 eV.

Fast-neutron spectrum		9.4×10^{-22}
46.5 MeV Ni.	4.4 μm a)	1.0×10^{-15}
46.5 MeV Ni (rocked)	2.5 μm	1.0×10^{-16}
	3.5 μm	7.4×10^{-17}
5 MeV Ni	0.9 μm	1.1×10^{-15}
20 MeV carbon	(surface)	1.3×10^{-18}
5 MeV protons	(surface)	1.2×10^{-20}

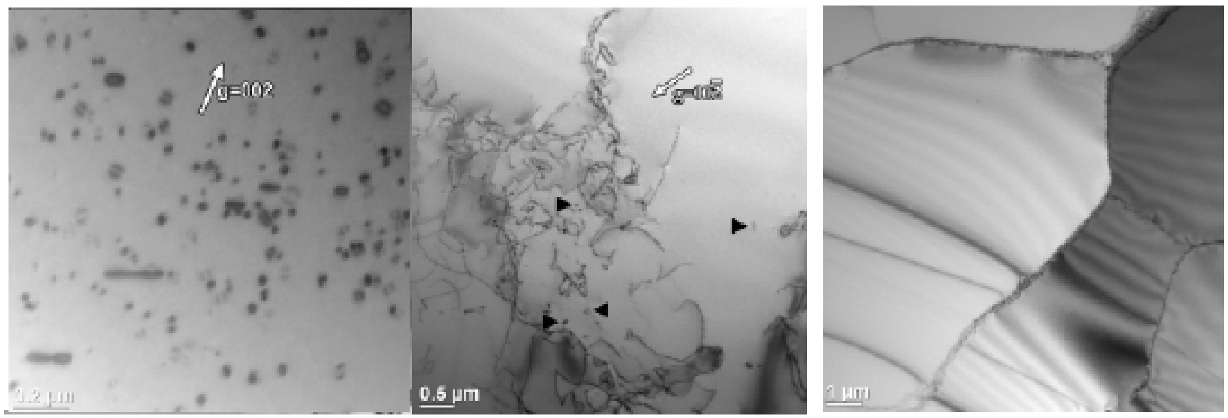
a) Peak.

Conclusions: Damage Production

- Methodology for evaluating dpa has been established for ~40 years.
- Has been used extensively in the literature as an indicator of the damage level a component/test piece experiences in service or in an irradiation experiment .
- Limitations if data are to be compared from environments where the damage is produced by predominantly low energy PKAs vs one where the damage is produced from predominantly high energy PKAs (<keV vs 10's keV)
- Suggest that if an energy dependent damage efficiency k_d is employed to calculate dpa then this has to be indicated and comparison to the results from employing the NRT standard (k_d=0.8) should be given.
  - Read across to 'historic' dpa estimates

Comment I

- Methodology for evaluating dpa assumes that in metals no damage is created by electronic loss
- At very high values of electronic loss evidence that damage can be produced by electronic loss (or defect annealing may occur)
    - Threshold for damage depends on metal (Duffy and co-workers)



0.5mm 2mm unirradiated

122MeV/nucleon ^{76}Ge into Al at < 100^{o}C

keV nm^{-1}	Metal (threshold)
30–35	Zr (30)
	Bi (31)
35–40	Fe (40)

- RaDIATE??

N Itoh, D M Duffy, S Khakshouri and A M Stoneham. "Making tracks: electronic excitation roles in forming swift heavy ion tracks" J. Phys.: Condens. Matter **21** (2009) 474205.

Comment II

- When using dpa as to correlate data from different irradiation environments it is also critical to note whether there are differences in gas/dpa ratios

- High He and H levels can cause a significant change in a material's irradiation response