DPA definition and estimates

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A PROPOSED METHOD OF CALCULATING DISPLACEMENT DOSE RATES

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A simple procedure is proposed for calculating the number of atomic displacements produced in a damage cascade by a primary knock-on atom of known energy. The formulae have been chosen to give results in close accord with recent computer simulations of radiation damage phenomena. The proposed new standard is compared with other empirical formulae for estimating the number of atomic displacements in a cascade.

Kingdom Atomic Energy Authority

The NRT (dpa) equation was given in this paper.

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Production of Frenkel pairs

NRT equation: the definition of “dose” (exposure) = an estimate how many defects are produced by the incident neutrons. It assumes that defects are produced as Frenkel (single vacancy + a single self-interstitial) pairs, no defect clustering.

$$N_d(T_d) = \begin{bmatrix} 0 & , & T_d < E_d \\ 1 & , & E_d < T_d < 2E_d/0.8 \\ \dfrac{0.8T_d}{2E_d} & , & 2E_d/0.8 < T_d < \infty \end{bmatrix}$$

The only parameter of the NRT model

Here T_d is the energy available for damage production. For a single neutron or ion it is equal to the energy $F_{D,n}$ deposited into the atomic subsystem = the total energy of the incident particle (neutron or ion) minus the energy lost due to electronic stopping

$$T_D = F_{D,n} = E_0 - F_{D,e}$$

dpa = displacements per atom = $\dfrac{\text{Number of Frenkel pairs in volume from NRT equation}}{\text{Total number of atoms in the same volume}}$

K. Nordlund et al., OECD report «Primary radiation damage in materials» (2013);
M.J. Norgett et al., “A proposed method of calculating displacement dose rates”, Nucl. Eng. Des. **33** (1975) 50-54

Production of defects: threshold effects

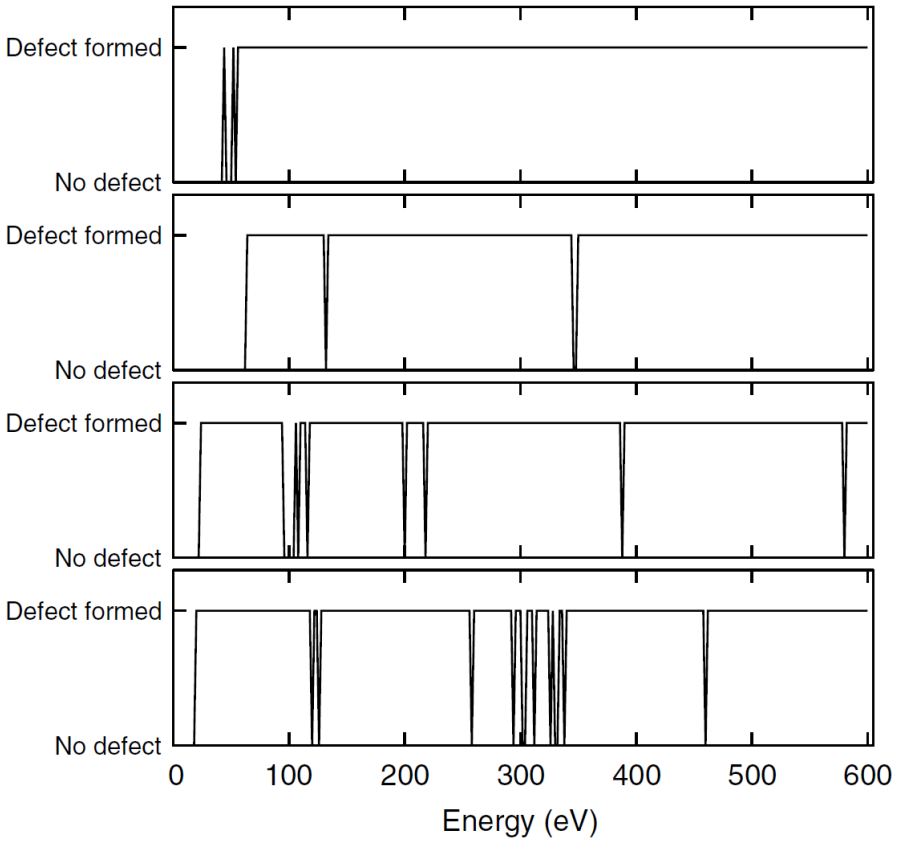


Fig. 1. Probability to form a defect for four recoils in Fe modelled with the ABC potential, as a function of recoil energy. Note that the data illustrates specifically the probability to form *at least* one defect; at the higher energies in many cases more than one defect is formed. In each of the four cases the initial state of the simulation is identical, including identical thermal atom displacements, except for the initial ion energy which is raised in steps of 2 eV.

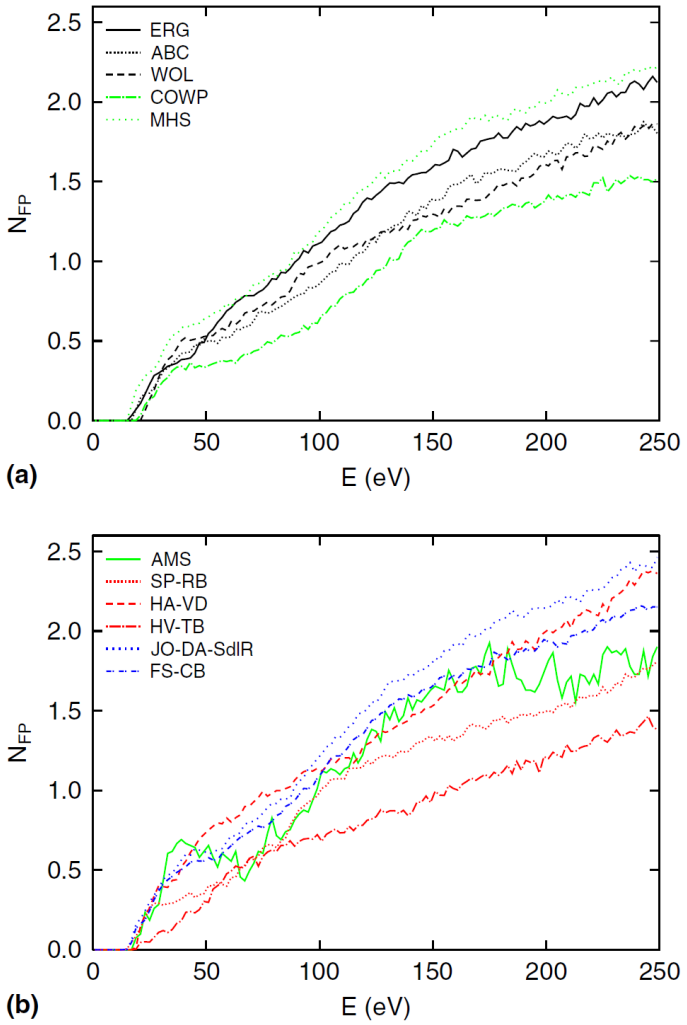
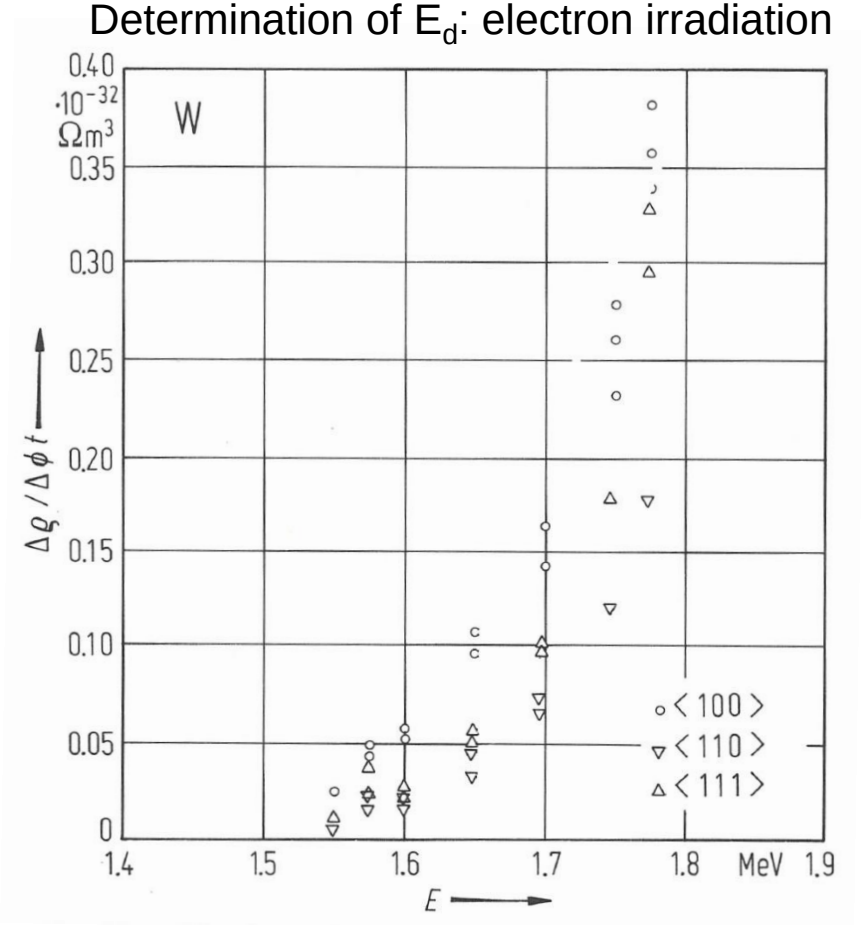


Fig. 4. Average number of defects produced as a function of recoil energy $N_{FP}(T)$ for the different potentials. For clarity the figure is split in two parts.

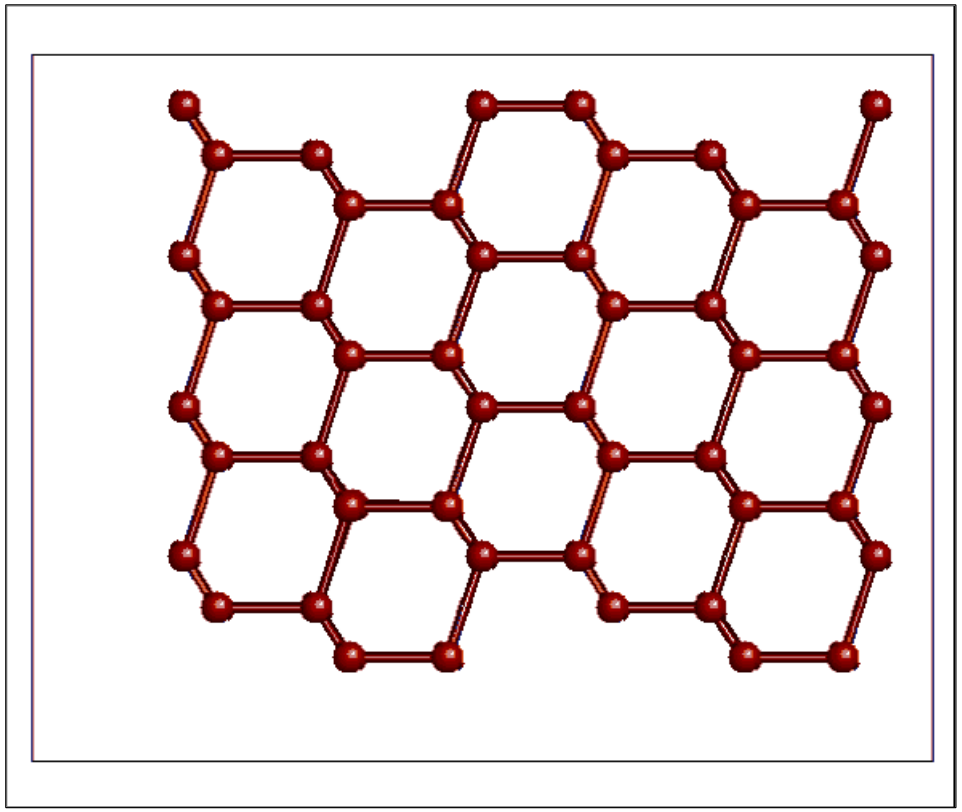
K. Nordlund et al., Nucl. Instr. Meth. B**246** (2006) 322-332

Production of defects: threshold effects

Determination of E_d: electron irradiation



The determination of threshold displacement energies in tungsten: $E_d(100)$=42 eV, $E_d(111)$= 44 eV, $E_d(110)$=70 eV.



A DFT simulation of a low energy collision event in Si, 20 eV initial recoil. Defects do not form if the energy of the initial recoil is below Ed.

F. Maury et al. Radiation Effects **38** (1978) 53-65

Production of defects in tungsten: experiment

Radiation Effects
1978, Vol. 38, pp. 53–65

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FRENKEL PAIR CREATION AND STAGE I RECOVERY IN W CRYSTALS IRRADIATED NEAR THRESHOLD

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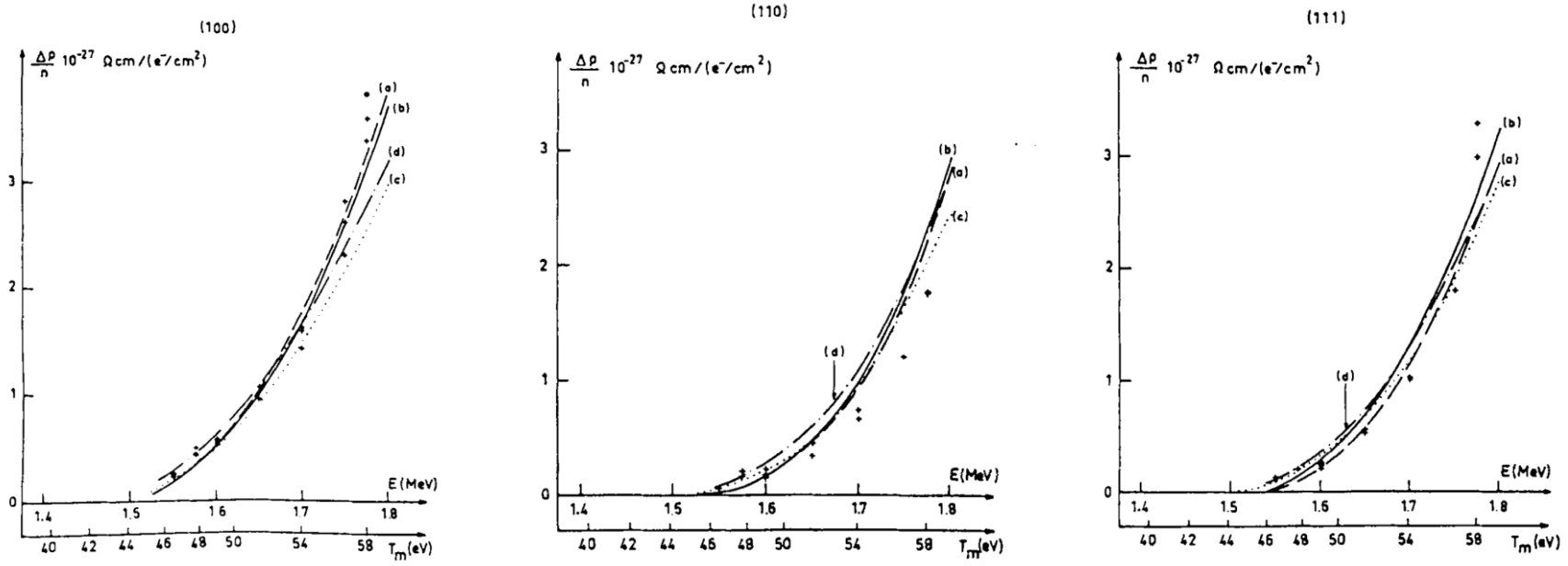
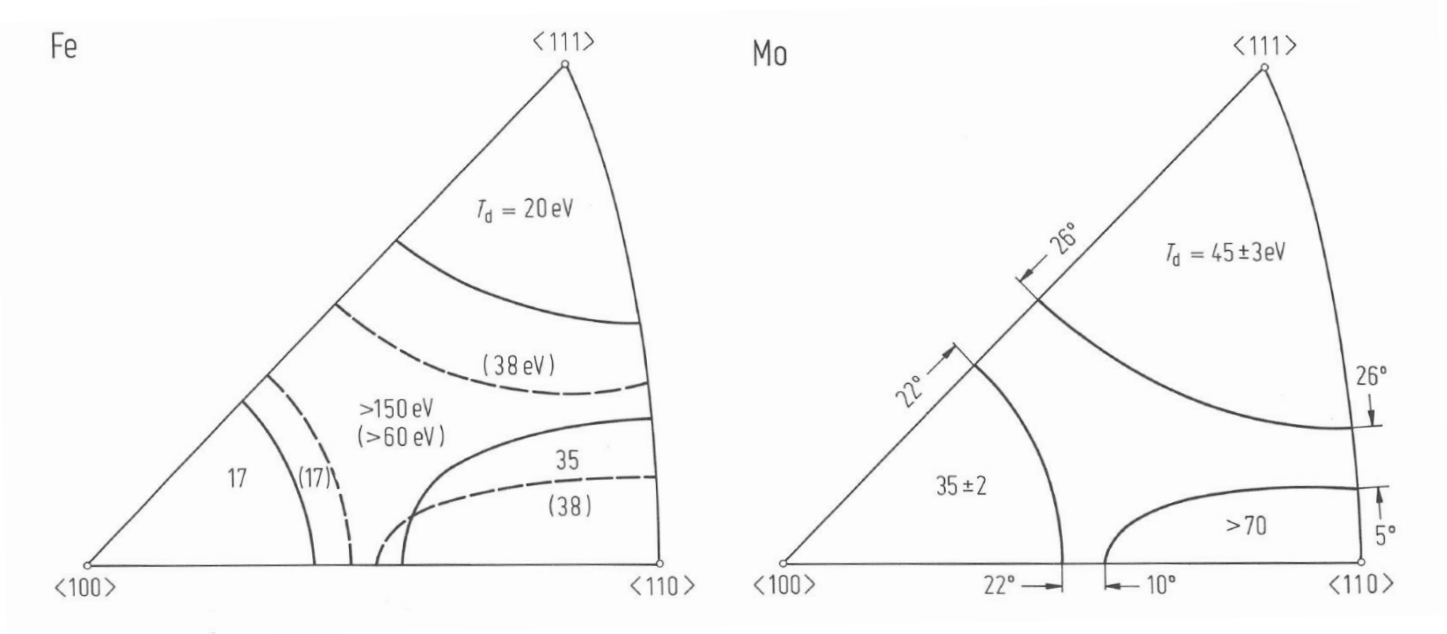


Experimental defect production curves can also be fitted using a range of threshold displacement energies (a) 60.7 eV; (b) 58.1 eV; (c) 55.3 eV; (d) 55.0 eV, all <90 eV.

Production of defects in crystalline metals

The crystallographic anisotropy of defect production



$$E_d(\theta,\varphi) = (2E_{110} - E_{100}) + 2(E_{100} - E_{110}) \times [\sin^4\theta(\cos^4\varphi + \sin^4\varphi) + \cos^4\theta]$$
$$+ 9(E_{100} - 4E_{110} + 3E_{111}) \times \sin^4\theta \cos^2\theta \sin^2\varphi \cos^2\varphi$$

Interpolation formula: For tungsten $E_d(100)$=42 eV, $E_d(111)$= 44 eV, $E_d(110)$=70 eV, and θ and φ are the polar and azimuthal angles of the spherical system of coordinates.

R. v Jan, A. Seeger, phys. stat. sol. **3** (1963) 465-472;
F. Maury et al. Radiation Effects **38** (1978) 53-65

Production of defects in tungsten

Crystallographic anisotropy of defect production in the NRT model can be eliminated by averaging $E_d(\theta,\varphi)$ over the entire solid angle of 4π, i.e. over all the directions of the initial velocity of the primary knock-on atom (PKA)

$$E_d = \overline{E_d(\theta,\varphi)} = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} E_d(\theta,\varphi)\sin\theta d\varphi d\theta =$$

$$\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} \sin\theta d\varphi d\theta\left[(2E_{110}-E_{100})+2(E_{100}-E_{110})\times[\sin^4\theta(\cos^4\varphi+\sin^4\varphi)+\cos^4\theta]+9(E_{100}-4E_{110}+3E_{111})\times\sin^4\theta\cos^2\theta\sin^2\varphi\cos^2\varphi\right]$$

The result is

D.R. Mason *et al.*, Journ Physics Cond Matter **26** (2014) 375701

$$E_d = \overline{E_d(\theta,\varphi)} = (2E_{110}-E_{100})+\frac{6}{5}(E_{100}-E_{110})+\frac{9}{105}(E_{100}-4E_{110}+3E_{111})$$

Substituting $E_d(100)$=42 eV, $E_d(111)$= 44 eV, $E_d(110)$=70 eV, we arrive at the average threshold value of

$$E_d = 55.3\,\text{eV}$$

This value is 40% lower than the often used threshold displacement energy of 90 eV. What is remarkable is that the (obviously incorrect) threshold energy of 90 eV was proposed in 1981 – in a conference paper based on inaccurate data derived from MD simulations - already *after* the experimental data had been published (in 1978).

F. Maury et al., Radiation Effects **38** (1978) 53-65

Production of Frenkel pairs

dpa = displacements per atom = $\frac{\text{Number of Frenkel pairs in volume from NRT equation}}{\text{Total number of atoms in the same volume}}$

Example: Samples of W in a tokamak are exposed to the flux of 14 MeV neutrons of 10^{14} neutrons/(cm^2•s). Estimate NRT dpa's accumulated in the samples over (i) one hour, (ii) one day, (iii) one year. The average total cross-section of scattering of a neutron by W is ~$6•10^{-24}$ cm^2. The average threshold defect formation energy in tungsten is 55 eV. Assume that approximately 30% of energy of atomic recoils is absorbed by electronic excitations that do not contribute to defect production.

Solution:

How many times neutrons hit an atom, per second

dpa *rate* W = (0.8/2) •(0.7)• 10^{14} • $6•10^{-24}$ × (150000 eV / 55 eV) = $0.46•10^{-6}$ 1/s

Average PKA energy transferred in a collision between a 14 MeV neutron and a tungsten atom.

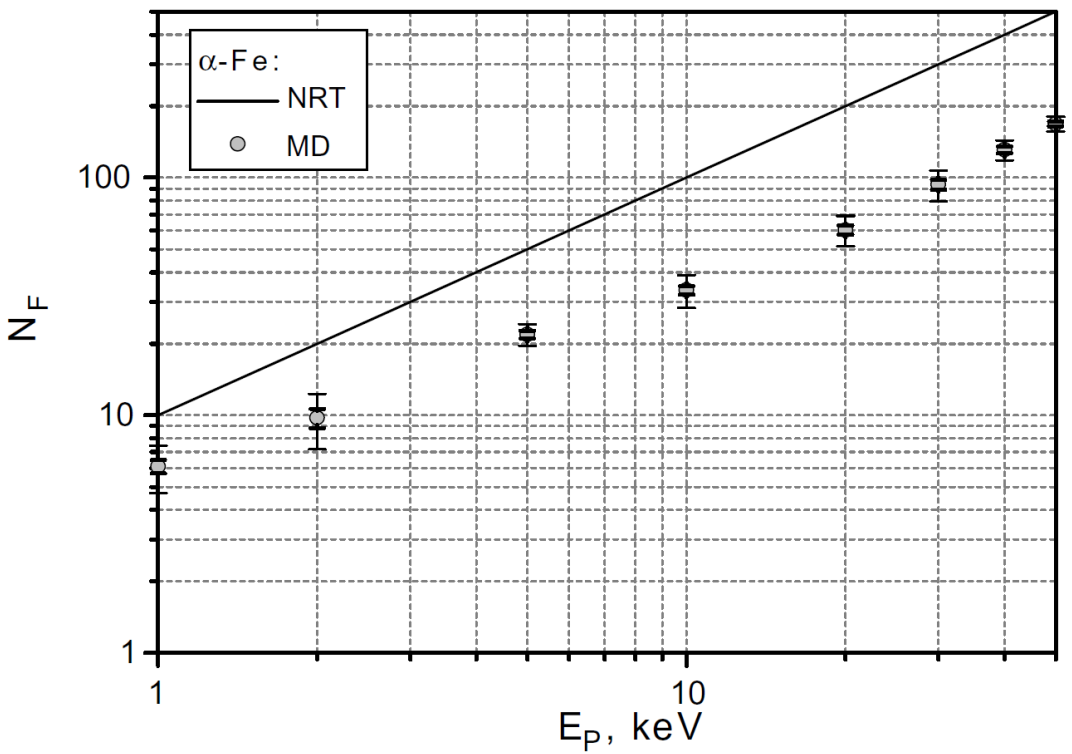
$$N_d(T_d) = \begin{bmatrix} 0 & , & T_d < E_d \\ 1 & , & E_d < T_d < 2E_d/0.8 \\ \frac{0.8T_d}{2E_d} & , & 2E_d/0.8 < T_d < \infty \end{bmatrix}$$

United Kingdom Atomic Energy Authority

How accurate is the NRT dpa model?

The number of Frenkel pairs produced by a PKA with energy T, and calculated using the Norgett-Robinson-Torrens equation is “NRT dpa”.

Cascade simulations show (see the figure) that the number of Frenkel pairs actually produced in collision cascades is much lower than the estimate derived from the NRT equation.



D.J. Bacon *et al*., Journ. Nucl. Mater. 323 (2003) 152