International Atomic Energy Agency

TM "Primary Radiation Damage: from nuclear reaction to point defects"

Additional Information

http://www-nds.iaea.org/dpa/

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Technical Meeting (F4-TM-43223)
1 - 4 October 2012, IAEA Headquarters, Vienna, Austria

Motivations *(copy from http://www-nds.iaea.org/dpa/)*

The displacement cross section is a reference measure used to characterize and compare the radiation damage induced by neutrons and charged particles in crystalline materials. To evaluate the number of displaced atoms Norget, Torrens and Robinson proposed in 1975 a standard (the so-called NRT-dpa), which has been widely used from that time.

Nowadays this formulation is recognized as suffering from some limitations: it is not applicable for compound materials, does not account for the recombination of atoms during the cascade evolution, cannot be directly validated and has no uncertainties/covarincies as evaluated cross sections usually have now.

Upgrading of the dpa-standard means the inclusion of the results of the Molecular Dynamics (MD), Binary Collision Aproximation (BCA) or other simulations for primary radiation defects (PRD), i.e. Frankel pairs (FP) and Interstitial Clusters, which survive after relaxation of the Primary Knockout Atoms (PKA) cascade.

The essential advantages of the upgraded dpa-standard will be:

- non-dependence on the energy distribution of incident neutrons - this means more correct inter-comparison of radiation damage in the different facilities on the basis of the accumulated dpa-fluence
- it also becomes more feasible for comparison of neutron and charged particles or ion induced damage
- empirical validation against frozen defects at cryogenic temperature (NRT-dpa can never be observed)
- prediction of damage in polyatomic materials and alloys (NRT treats dpa in compounds by mathematical weighting of separated elements)

Purpose of the Meeting *(copy from http://www-nds.iaea.org/dpa/)*

To find ways to overcome the drawbacks of the NRT standard and benefit from the recent developments in primary radiation damage simulations, the Technical Meeting has the objectives to discuss:

- revisiting the NRT standard with the purpose of improving it by the evaluation of uncertainties
- connected with recoil spectra and the energy partitioning model;
- proposal of a new upgraded standard that will capture the annealing of defects in the recoil cascade on the basis of MD, BCA and other models.

As an outcome of discussions the definition of objectives and participating organisations for a new Coordinated Research Project (CRP) on this topic are expected.

Specific issues to be addressed *(copy from http://www-nds.iaea.org/dpa/)*

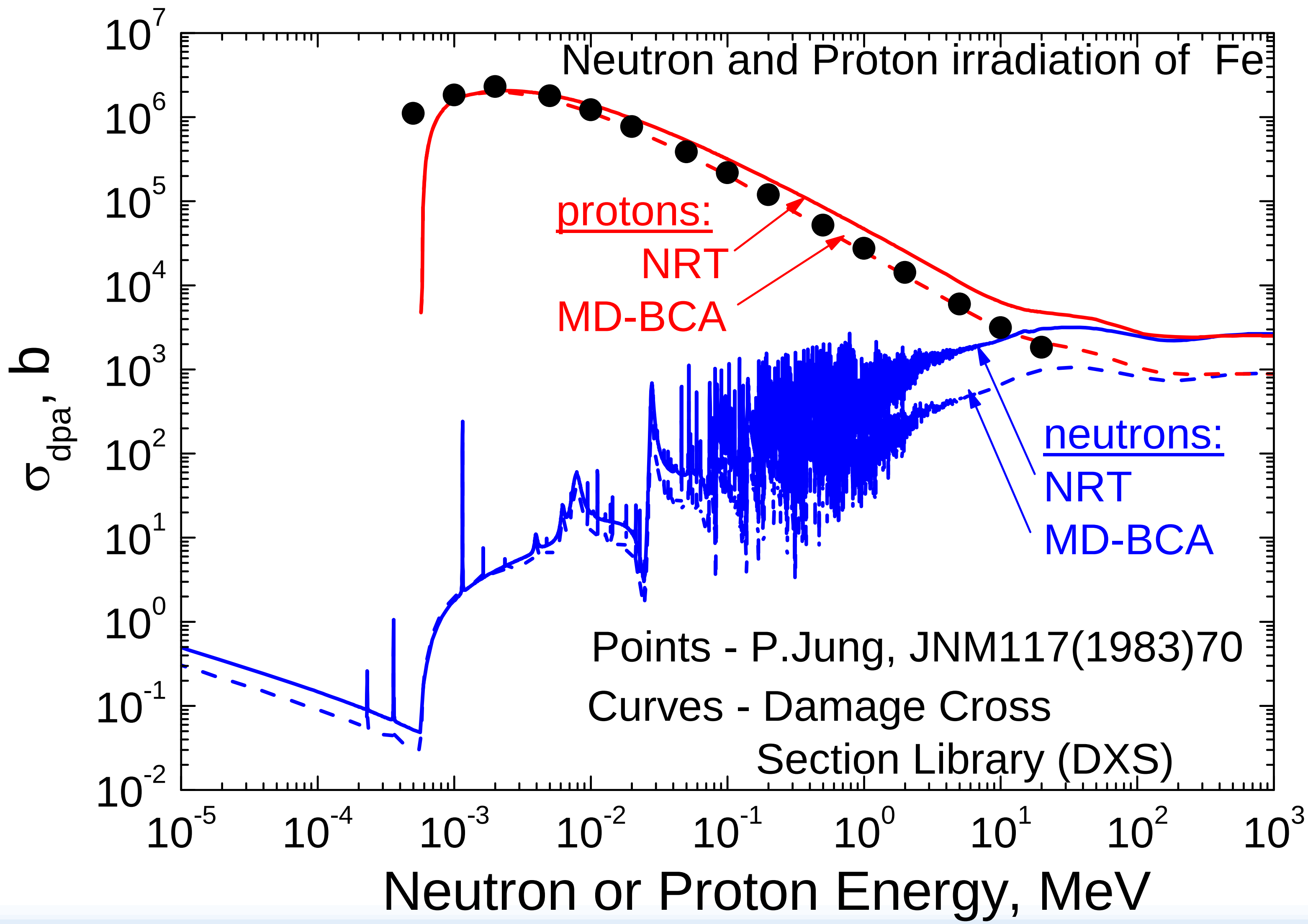
Cross sections, evaluated data libraries and the NRT standard

- PKA spectra - availability in libraries, methods of calculation, agreement and uncertainties
- processing of cross section files to derive KERMA, damage energy and dpa
- gas (helium, hydrogen) production cross sections
- uncertainties/covariances for these quantities

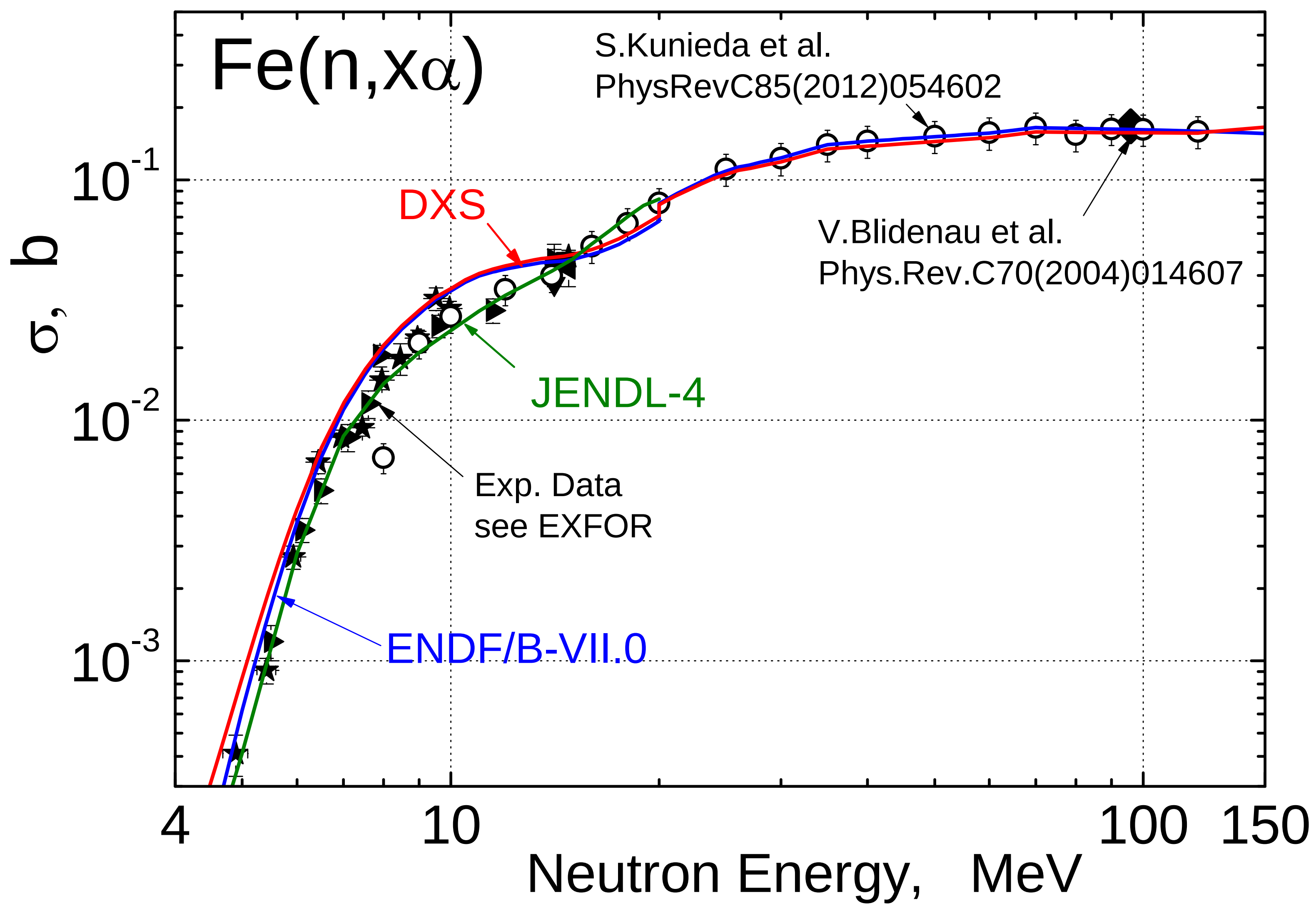
MD, BCA and other simulations of survived primary point defects in mono- and poly-atomic materials and thermal-spike-enhanced recombination

- scope of materials - pure metals, Fe-xC, semiconductors (Si, Ge), insulators and ceramics (Al2O3, SiC ...)
- PKA energy range covered by different simulation methods
- calculation outputs - survived Frankel Pairs (FP), simple interstitial clusters
- dependence on temperature and material composition
- incorporation of MD/BCA results in processing codes (NJOY) or storage in a separate cross section database
- empirical validation
- applications
- others

DXS Damage Library

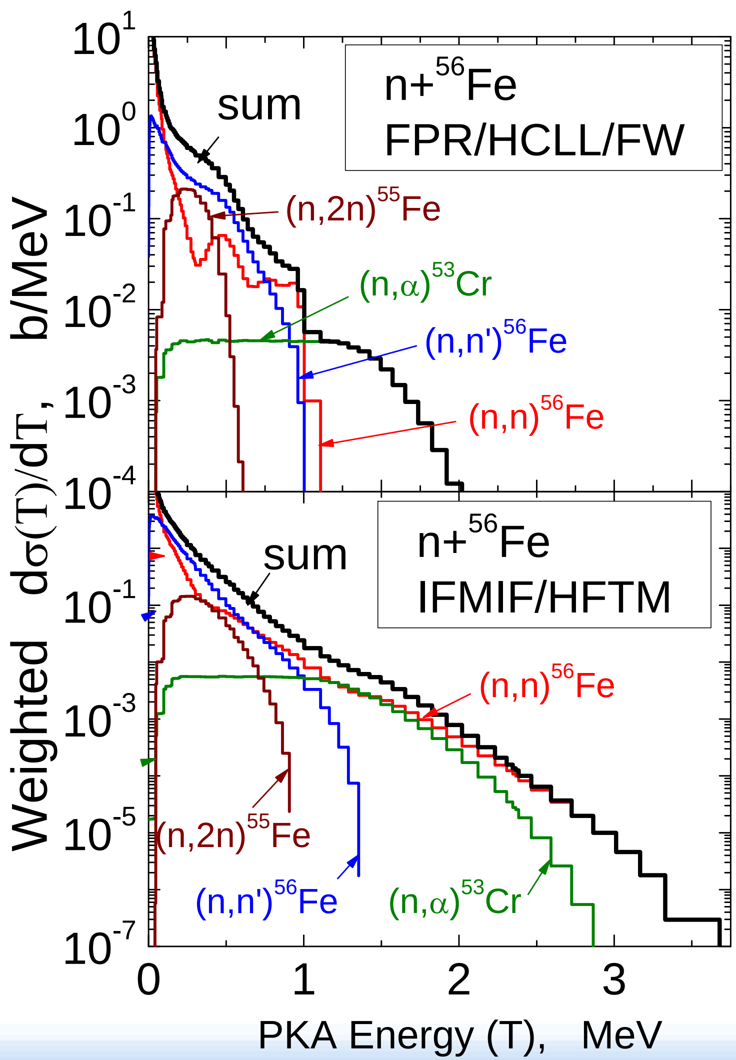


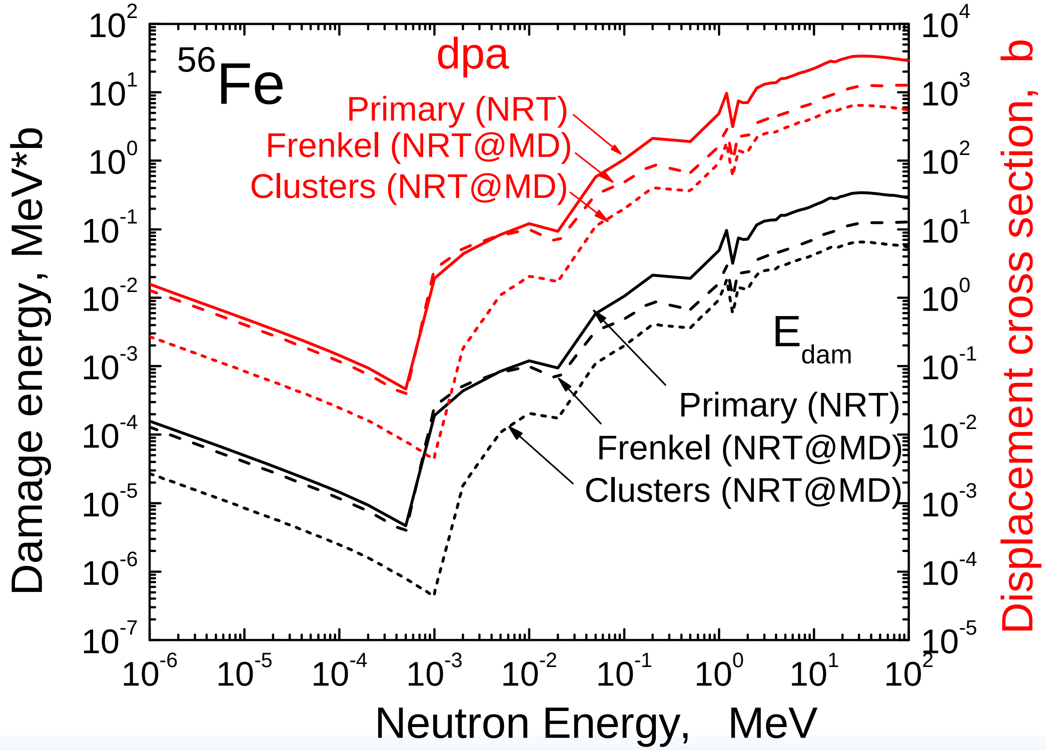
Gas production cross section



PKA spectra and Damage energy from ENDF/B-VII

PKA spectra





Current status: NRT-standard for dpa assessment

For crystalline materials NRT-dpa calculations rely on:

- Primary Knock-on Atoms (PKA) energy spectra $\frac{d\sigma(E,T)}{dT}$ — Nuclear Reaction
- Robinson-Lindhard model for partitioning $P(T_i)$ of Recoils Energy into Ionization and Damage Energy $E_a(E)$ that will be available to knock out Atom (*without cascade consideration*) — Ions Stopping
- Norgertt-Robinson-Torrens (NRT) model for conversion of damage energy E_a in *dpa*-Cross-Section regarding lattice knock-out threshold energy E_d — Solid Physics

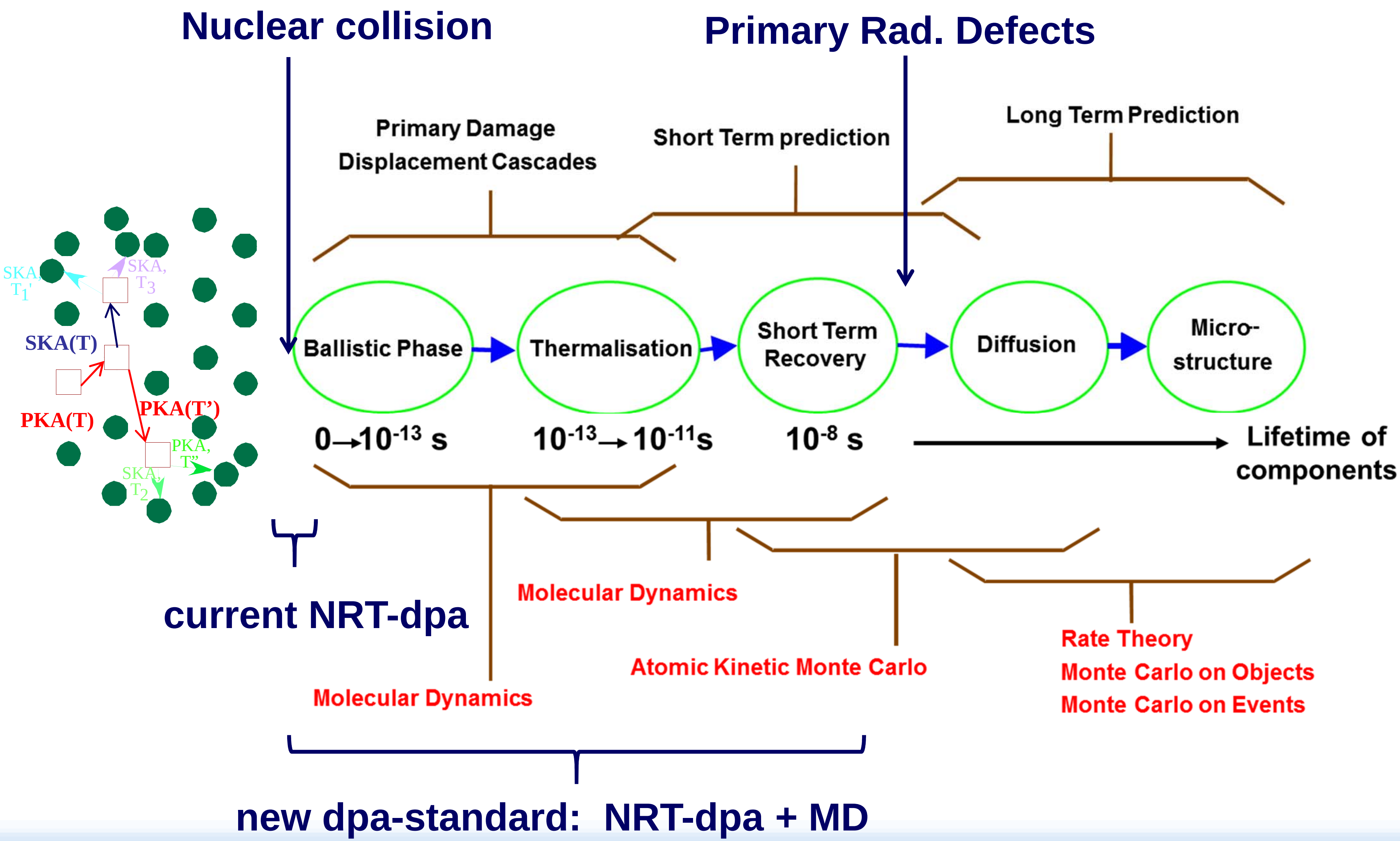
NRT formalised approach:

*Damage Energy [MeV*b]* → *dpa-Cross Section [b]*

$$E_a(E) = \sum_i \int_{E_d}^{T} \frac{d\sigma(E,T_i)}{dT_i} P(T_i)\ dT_i$$

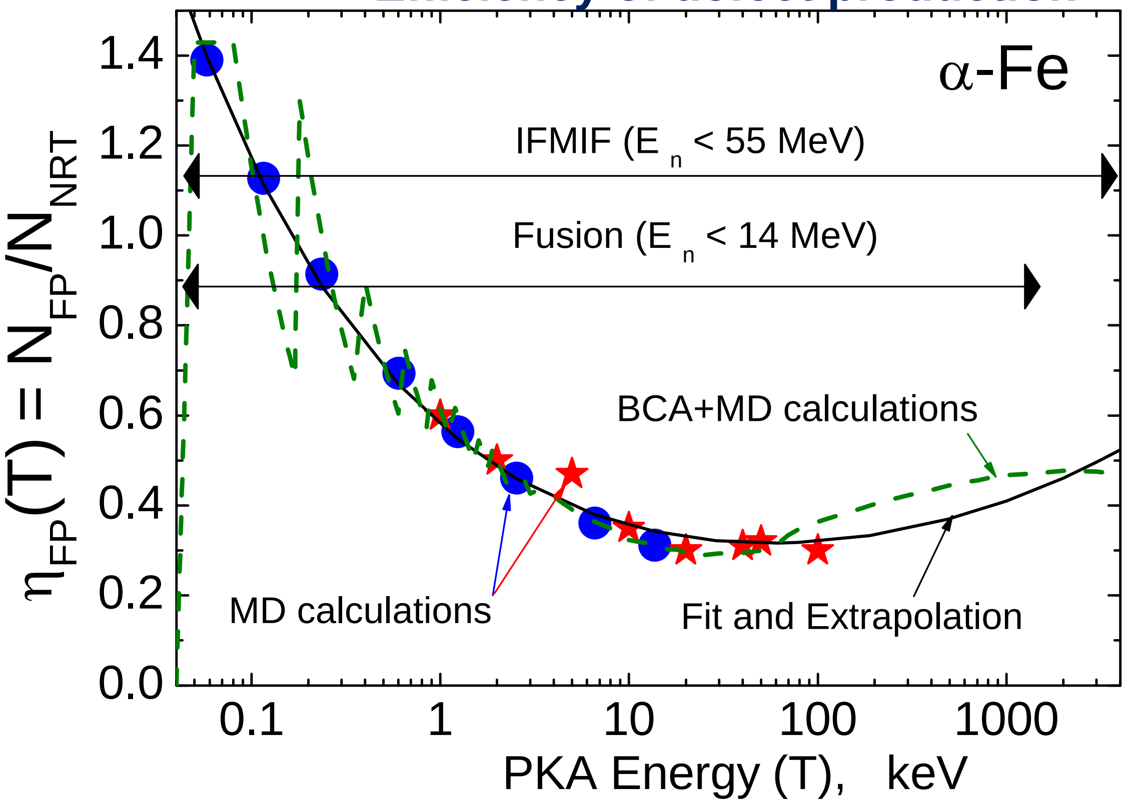
$$\sigma = \frac{0.8}{2E_d} E_a$$

Radiation Damage time evolution and dpa-assessment stages



Replacing of NRT standard
by Primary survived Radiation Defects (PRD =Frankel pairs)

Surviving ratio = Frankel pairs to NRT
= Efficiency of defect production

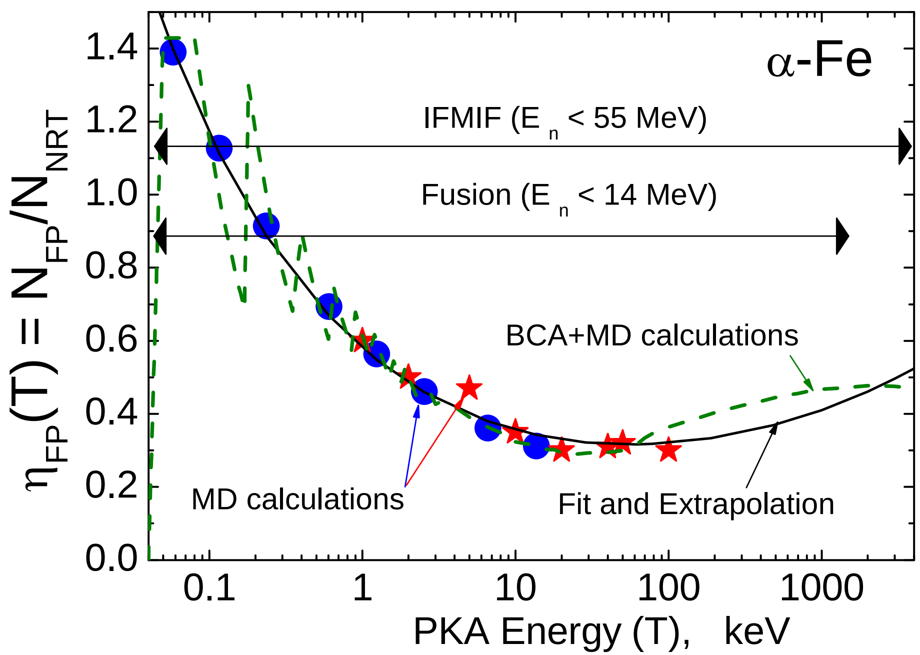


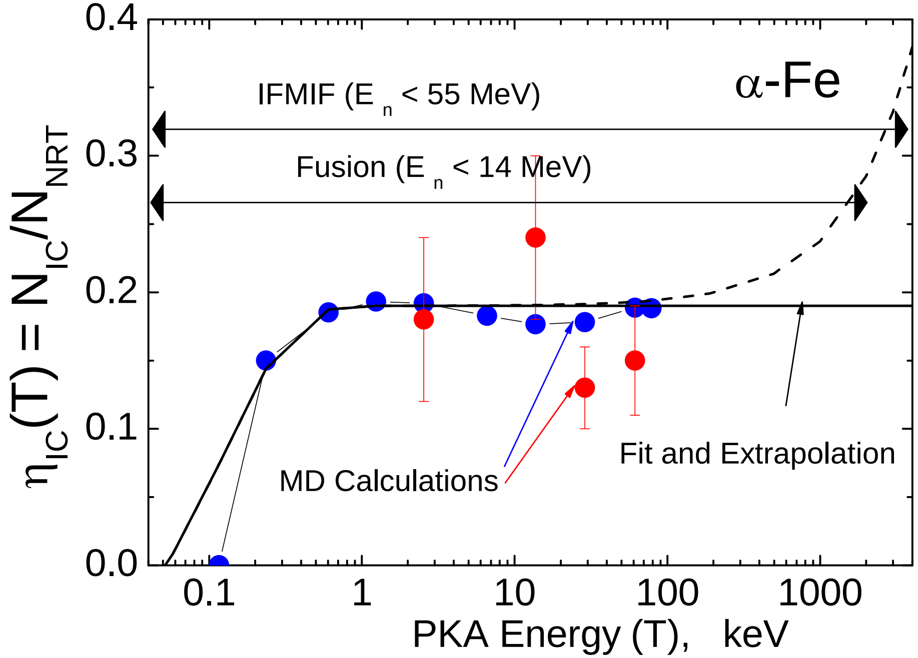
Reference:
MD : R.E. Stoller et al., JNM 271(1999)57
D.J. Bacon et al., JNM 323(2003)152
BCA : C.H. Broeders et al., JNM 328 (2004)197

- probability to survive depends on PKA energy and
- number of primary defects survived after cascade relaxation may be essentially less than those initially displaced from lattice by nuclear reactions

Replacing of NRT standard to evaluate primary survived defects (Frankel pairs and Interstitial Clusters)

Frankel pairs $\eta_{FP}(T) = \frac{N_{FP}}{N_{NRT}}$ or $\eta_{IC}(T) = \frac{N_{IC}}{N_{NRT}}$ Interstitial Clusters





MD taken from: R.E. Stoller and L.R.Greenwood, JNM 271(1999)57 and D.J. Bacon, Yu.N. Osetsky et al., JNM 323(2003)152
BCA calculated by: C.H.M. Broeders, A.Yu. Konobeyev, JNM 328 (2004)197

- probability to survive depends on PKA energy and
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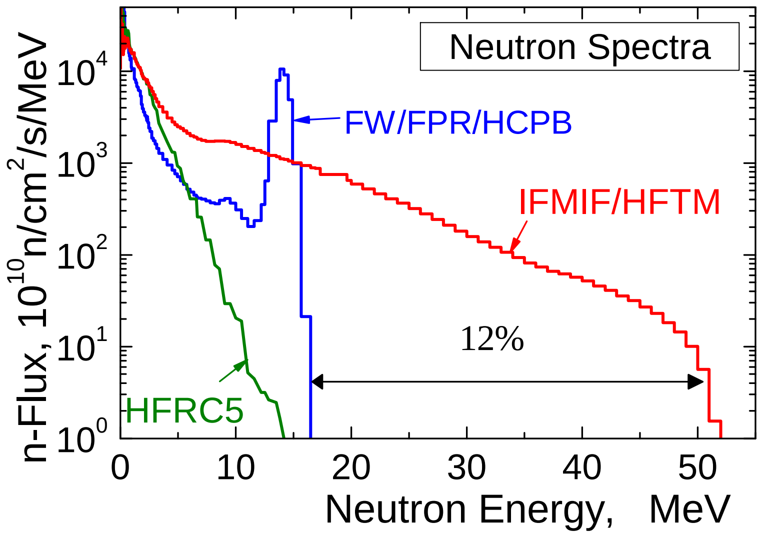
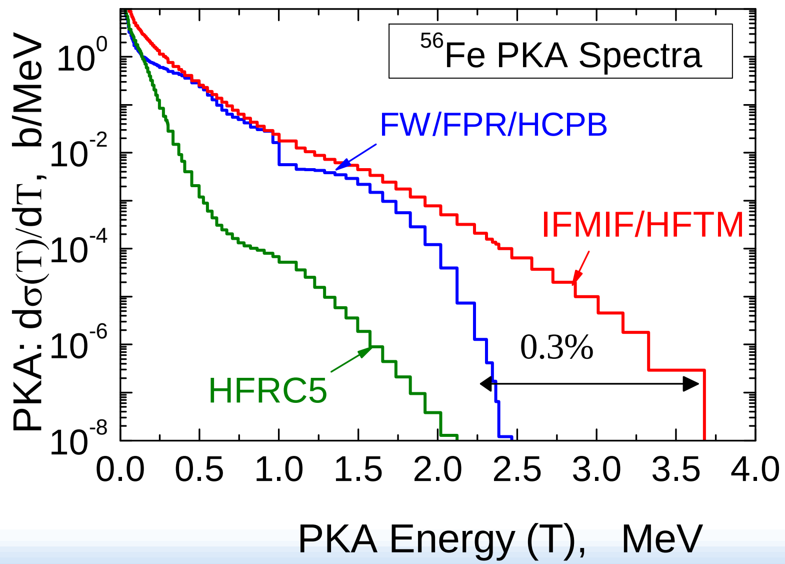
Replacing of NRT dpa-standard by survived primary defects: applications for different neutron environments





Facility	**IFMIF HFTM**	**FPP FW**	**HFR Col. 5**
Thermal Power, MW	10	3400	45
n-Flux, 10^{+14} n/cm^2/s	7.3	11	12
dpa (NRT), 1/fpy	**30**	**20**	**10**
dpa (MD: Frankel Pairs)	**9.7**	**6.7**	**3.3**
dpa (MD: IS Clusters)	**5.6**	**3.8**	**1.9**

replacing NRT (= recoils created by nuclear reaction) by MD+BCA (= primary defects survived after PKA cascade relaxation) will take into account
(i) difference in PKA spectra and will allow
(ii) reliable inter-comparison of dpa fluence in facilities with different neutron spectra

S.P. Simakov et al. JNM 386(2009)52

NDS Damage Libraries: NRT-dpa as a part of IRDF-2002

- **3 Structural Materials:**
  Cr in steel -1985 W.L. Zijp Petten
  Fe in steel - ASTM Standard E693
  - EURATOM Standard
  Ni in steel - 1985 W.L. Zijp Petten

- **2 Electronics Materials:**
  Si in Si and Ga in Ga-As - ASTM Standard E722
  Ga-As specific feature: empirical efficiency factor depending on PKA energy was implemented to account for property changes when exposed to different fields

- **Source of ASTM Standards:**
  ENDF/B-VI and NJOY97 (NRT),
  E_d = 40 eV(Fe) = 25 eV(Si) =10 eV(GaAs)

- **Data Format:**
  ENDF-6, 640 groups (1.E^{-10} – 20)MeV for SAND-II