International Atomic Energy Agency

TM “Primary Radiation Damage: from nuclear reaction to point defects”

Short Overview of Objectives

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

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

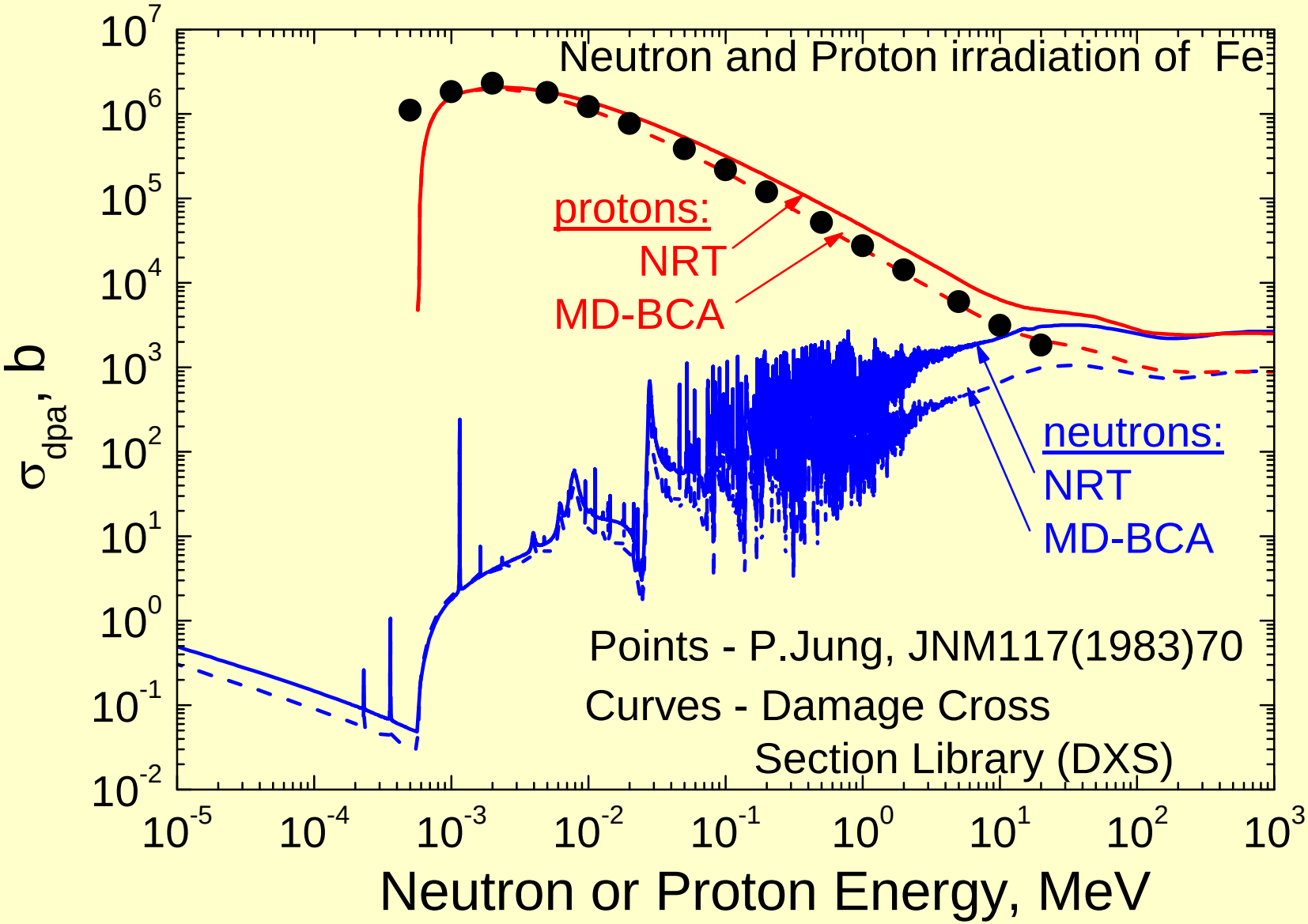
Objectives/Motivation

- **Recently one expert rose a question "What does 1 dpa really mean ?"**
- **"It means that every atom is shifted by the incident particle or reaction product one times from its rest position."**
- **"How you may know this ?"**
- **"… by performing following calculations:**
  - **the incident particle spectrum is known as input,**
  - **computing spectra of reaction Recoils (nuclear reaction models),**
  - **subtraction of ionization losses (Lindhard partitioning model)**
  - **division by 2 binding energy of atom in crystalline lattice and multiplication by 0.8**
  - **finally coming up with NRT-dpa standard"**
- **"You rely on modelling, how can you prove and qualify accuracy ?"**
- **" … at the moment – direct experimental proofing looks impossible, dpa cross sections have not uncertainty"**

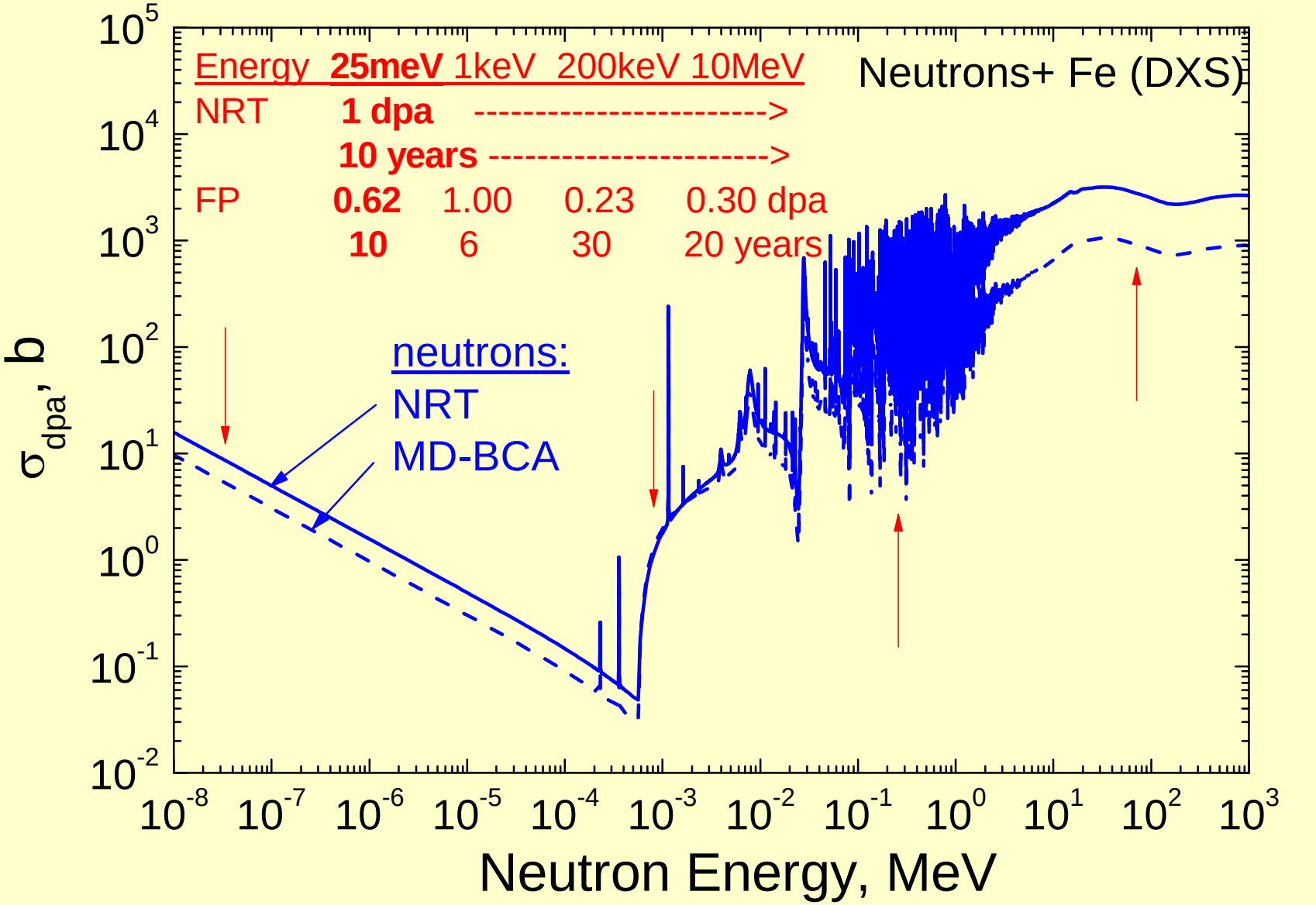
Objectives/Motivation (cont.)

- **“Shifting of every atom at least once likely will destroy a lattice**
  - how you can explain rather long life of materials in reactors ?”
- **“… indeed, many knocked atoms return back to their normal positions”**
- **“Could you also model this ?“**
- **“ … such modelling involves:**
  - **simulating of PKA cascade evolution by MD, BCA …**
  - **now taking into account polyatomic structure and temperature of material**
  - **and eventually estimation of the number of atoms not returned back = the interstitial-vacancies pairs survived after cascade relaxation (primary radiation defects - PRD)**
- **”Is it possible experimentally validate PRD calculations?”**
- **“… such survived primary defects could be measured, e.g. at cryogen T”**
- **“How large are differences between NRT and PRD estimates?”**

Objectives/Motivation (cont.)



Objectives/Motivation (cont.)



Technical Meting' Objectives

- **revisiting the NRT standard to look for possible improvements (e.g., evaluation of uncertainties resulted from recoil spectra and energy partitioning model)**
- **considering a new upgraded standard that will capture defects annealing in the recoil cascade on the basis of MD, BCA and other models** (*we have to be still rather close to the cross sections, like T dependent CS in resonance or cold neutron CS for compounds*)
- **the results of Expert Group on Primary Radiation Damage (PRD) – part of Working Party "Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems" hosted by NEA**
- **formulation of objectives of a new Coordinated Research Project**

  proposal for new CRP was approved by:

  - 29th Meeting of International Nuclear Data Committee (8-11 May 2012)

  - Long-term Needs for Nuclear Data Development (2 - 4 Nov 2011)

Damage Library – dpa and gas production XS hosted by NDS

(could be regarded as starter library for CRP)

- **DXS (A. Konobeev):**
  - dpa-cross section (both **NRT & PRD**):
    - **8 pure metals Al, Ti, V, Cr, Fe, Ni, Cu, Zr**
    - neutron and proton energies: **10^{-5} eV - 3 GeV**
  - gas {**^{1,2,3}H, ^{3,4}He**} production cross-section:
    - **4 elements Cr, Fe, Ni, W**
    - neutron and proton energies: **< 3 GeV**

- **IRDF-2002/Electronics Materials:**
  Si, Ga in Ga-As (ASTM E722)
  Ga-As specific feature:
  empirical efficiency factor
  depending on PKA energy
  to account for
  property changes
  when exposed to different fields