The interest of dpa to handle the microstructure of irradiated materials

[1]L. Luneville, [1]D. Simeone, [1]D. Gosset, [1]G. Baldinozzi, [2]A. Alberman, [3]Y. Serruys, [4]S. Bouffard

[1]CEA/CNRS/ECP LRC CARMEN
2CEA/DEN/DANS/DRSN/DIR
3CEA/DEN/DANS/DMN/SRMP/Jannus
4 CEA/CNRS/ENSICAEN GANIL/CIMAP

Outline

- I Introduction
- II How to compare different irradiations: the DART code
- III Capturing defects on the basis of MD: fractality
- IV Summary-Perspectives

I Introduction

Ultimate goal : how to understand and predict the behavior of materials submitted to irradiation

The notion of dpa : two distinct goals

- **<u>an exposure parameter</u>**

  taking into account both the incident projectile and the material

  able to express in the same "unity" irradiations performed in nuclear plants and accelerators

- **<u>to determine a defect production term</u>**

  to estimate the "damage " induced by irradiation :

  <u>the spatial extension of a displacement cascade is important</u> (at least in some ceramics)

  studies of zirconia : phase transition induced by irradiation

  <u>no longer a universal response :</u> different kinds of defects act on different properties (swelling, creep, diffusion)

  Creep induced by irradiation

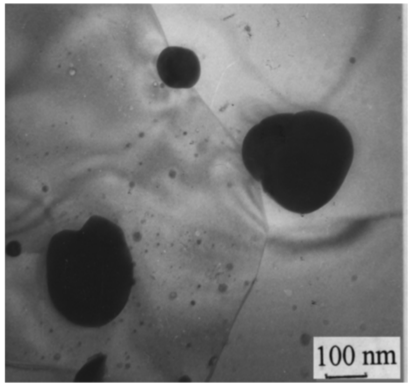
Esterel experiment : the brittle ductile temperature measured did not scale with NRT dpa

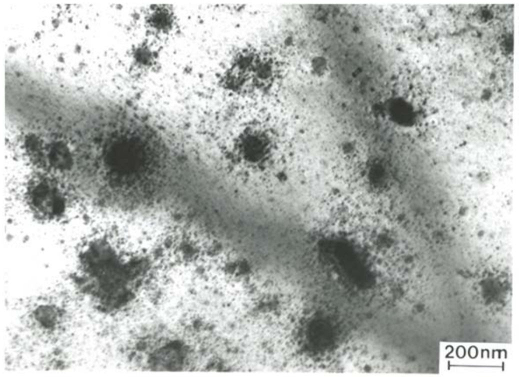
(ASTM symposium , seattle 1999)

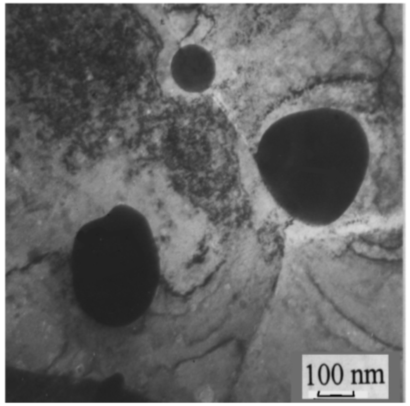
I Introduction

- **An exposure parameter**
  - **Compare different facilities : ion-neutron comparison**
  - **The slowing down of particles from few MeV to few keV can be handled within the BCA approximation : seminal work of Lindhard (1968) notion of displaced atoms …**

TEM patterns of ODS Steel irradiated by different particles at the same dpa value (30 dpa NRT, Ed of 25 eV) : need of better estimators to describe the microstructure







He 1 MeV @ 700K

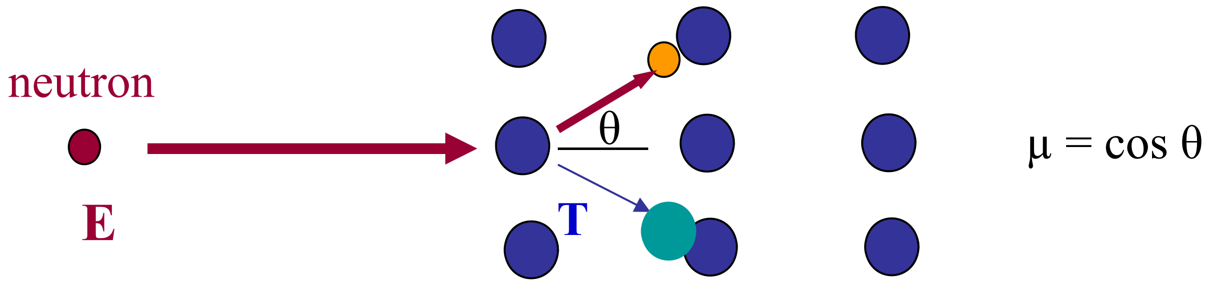
Phenix FBR @ 750K

Ar 600 keV @ 700K

Different microstructures (I Monnet, JNM 335, 311 (2004))

II How to compare different irradiations: the DART code

Accurate description of neutron-atom interactions beyond the Isotropic Emission Compound Nucleus model (used in SPECTER version 1998) using ENDFB-VI



The PKA production cross section is obtained from nuclear cross sections

$$\chi(E,T) = \sigma(E)\int \frac{1}{\partial T / \partial \mu} f(\mu, E, E')dE'$$

Total cross sections and angular distributions are now clearly taken into account from nuclear evaluations (ENDFB-VI) (JNM 353, 89 (2006))

- **Treatment of angular anisotropy for all elastic interactions**

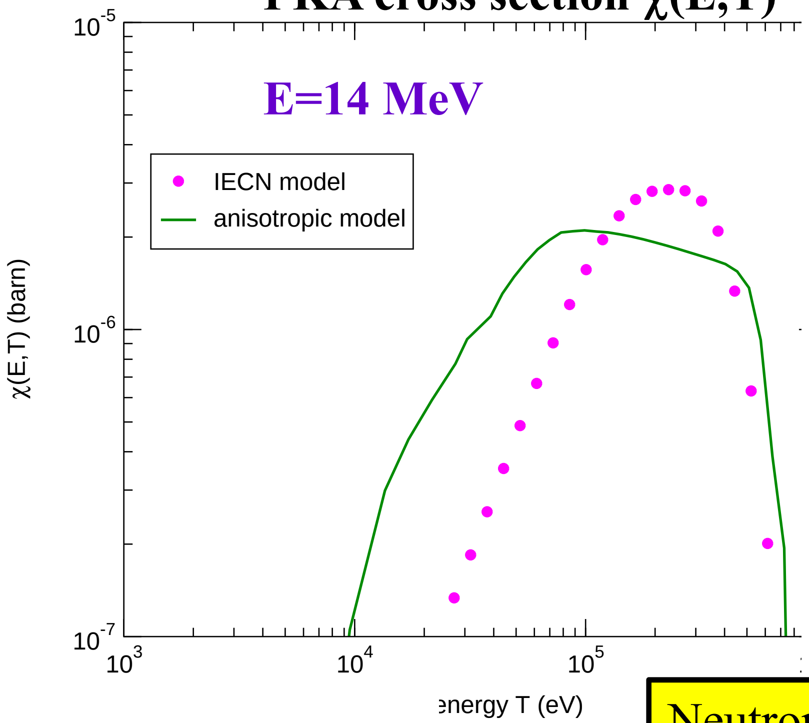
II How to compare different irradiations: the DART code

- The production rate of displacements (dpa/s)

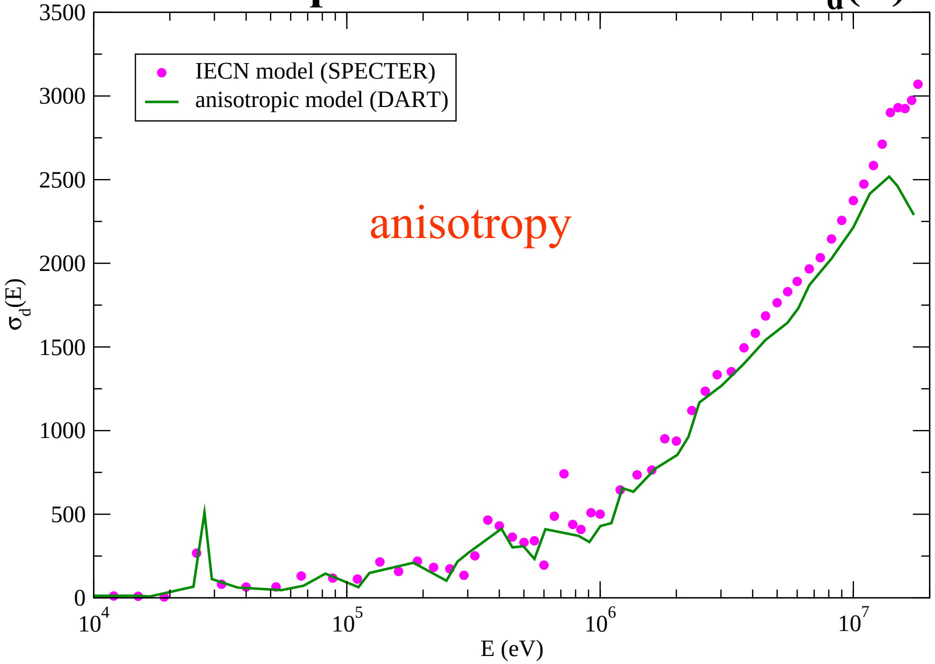
$$K = \int \phi(E)\sigma_d(E)dE$$

We also calculated the PKA cross section $\chi(E,T)$ and the displacement cross section $\sigma_d(E)$ within the BCA pointing out the anisotropy of the neutron cross section

PKA cross section $\chi(E,T)$



Displacement cross section $\sigma_d(E)$



Neutron 14 MeV in Iron

(JNM 2006, NIMB2007)

II How to compare different irradiations: the DART code

- **Different estimators**

  How to handle the evolution of the microstructure with surrogates (i.e. ions !)

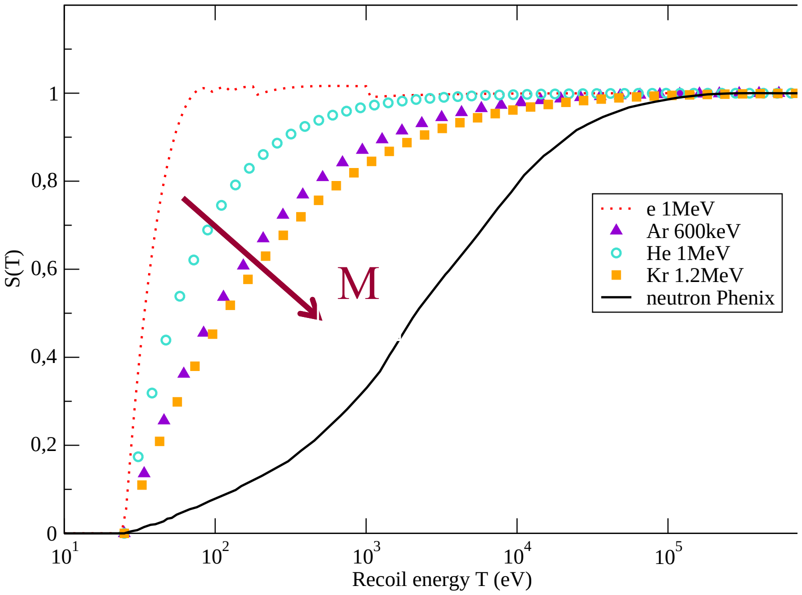
  - **Need to define energetic distributions**
    - PKA spectrum
      - Defines the energetic distribution of the PKA
    - Recoil spectrum
      - Defines energetic distribution of all recoil atoms (calculated within BCA)

- **DART was developed to give these estimators (pka, recoil spectra) in polycristalline materials**
  - **Neutrons (neutron-atom cross sections from nuclear evaluations ENDFB-VI)**
  - **Ions (ion-atom cross sections derived from the Thomas Fermi potential (BZL), Lindhard formalism for polyatomic compounds)**
  - **Electrons (e-atom Mott cross sections)**

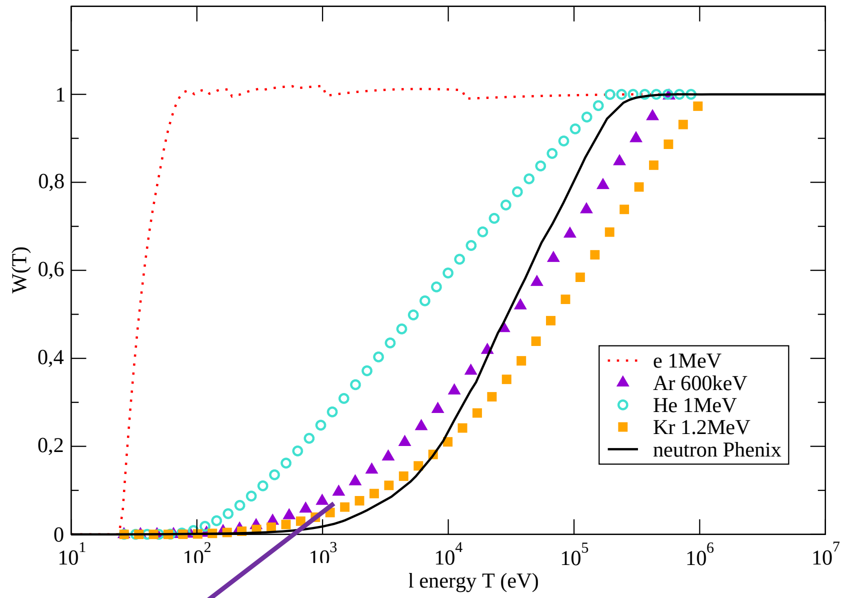
II How to compare different irradiations: LRC CARMEN

the DART code

- ❑**Simulation of ODS steels microstructures in a particles accelerator**
  - ➢ **Choice of the impinging particle: mass, energy**



PKA spectrum



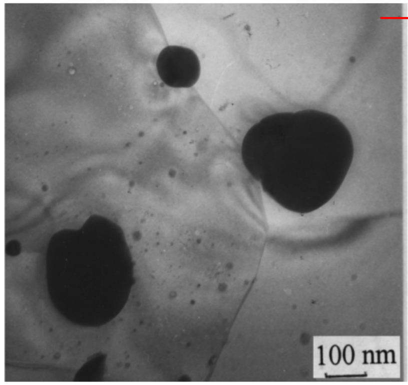
Recoil spectrum

Choice of 600 keV Argon ion beam

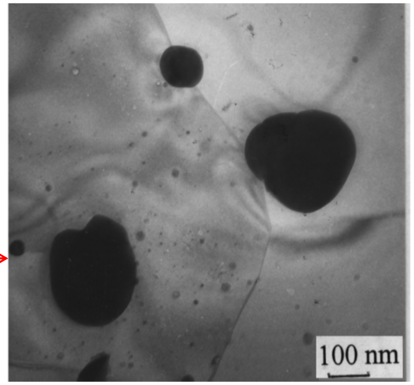
II How to compare different irradiations: the DART code

Microstructure study of ODS Steel by TEM observations

Before irradiation



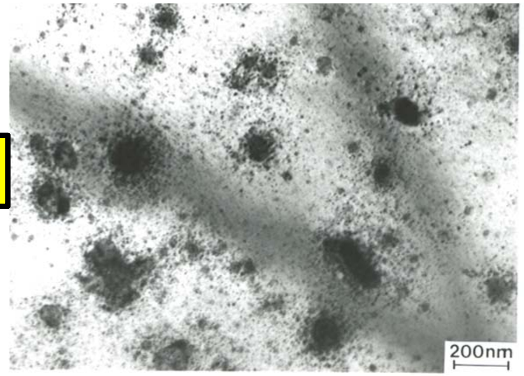
After irradiation 30 dpa NRT



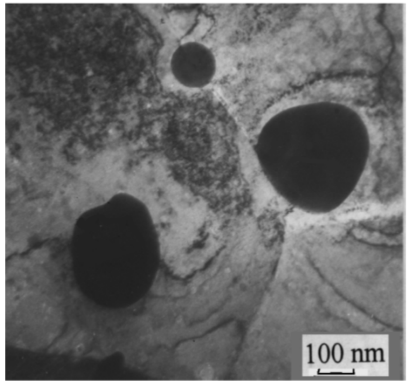
He 1 MeV
(W ≠W(FBR))

No evolution

After irradiation 30 dpa NRT



FBR 750K 576 Days

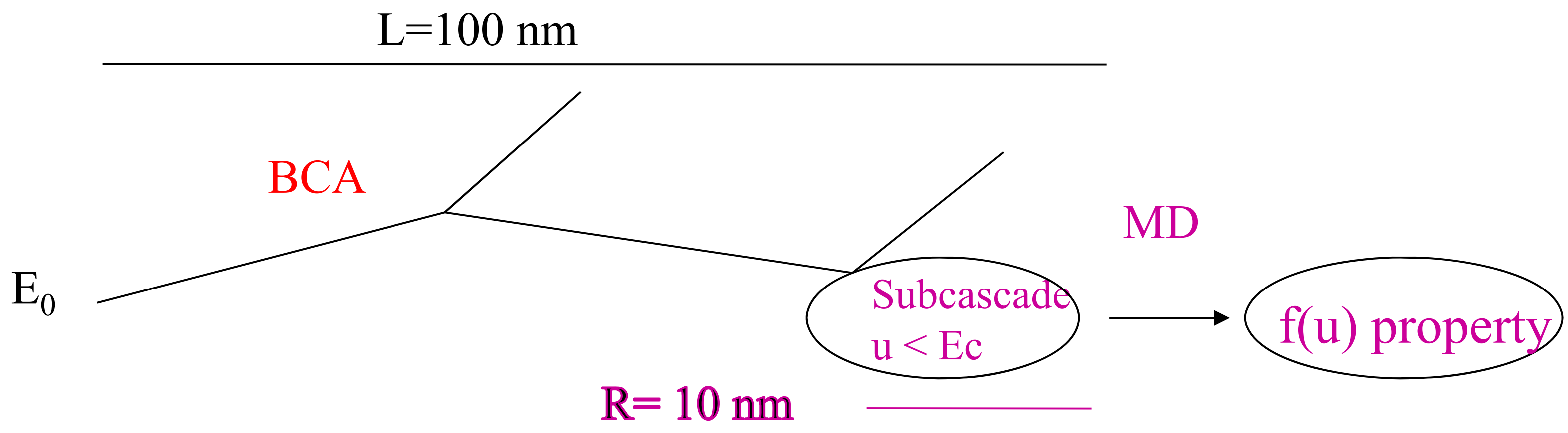


Ar 600keV 673K
(W similar W(FBR))

Reduction of oxide size

III Capturing "defects" on the basis of MD: fractality

- Idea : **integrate information of cascade fragmentation in sub cascades**



For each subcascade of energy u generated, the number of defects in this subcascade is obtained with a MD simulation -> fragmentation energy threshold

$$NF(E_0) = N_{sc}(E_0) \int_{Ed}^{Ec} p_{sc}(u)\ du\ f(u)$$

What you need from MD

Link MD simulations to BCA : the Fractal approach of a displacement cascade allows to **calculate the threshold formation energy for a sub cascades E_c**

IV Capturing defects on the basis of MD: LRC CARMEN

fractality

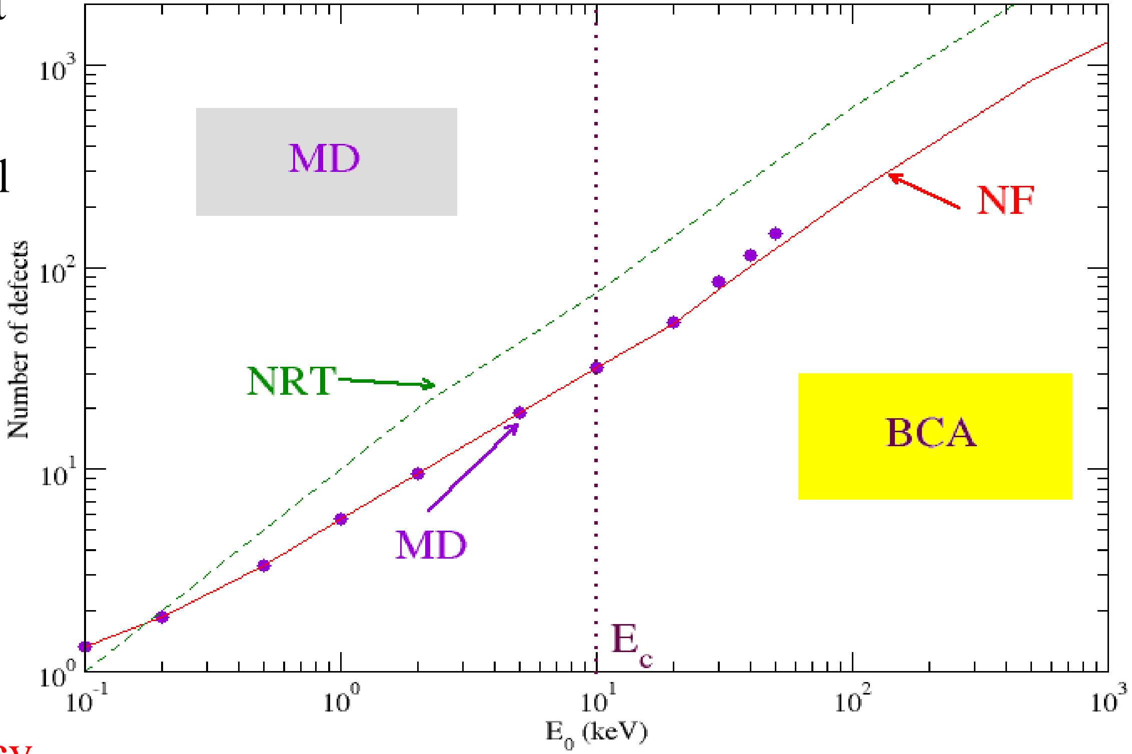
Application : number of defects in iron irradiated by Fe ions

- ❑ MD simulations of defects in iron for incident energy < 50 keV (Stoller)

- ❑ NRT formulation for all incident energies
  Large discrepancy

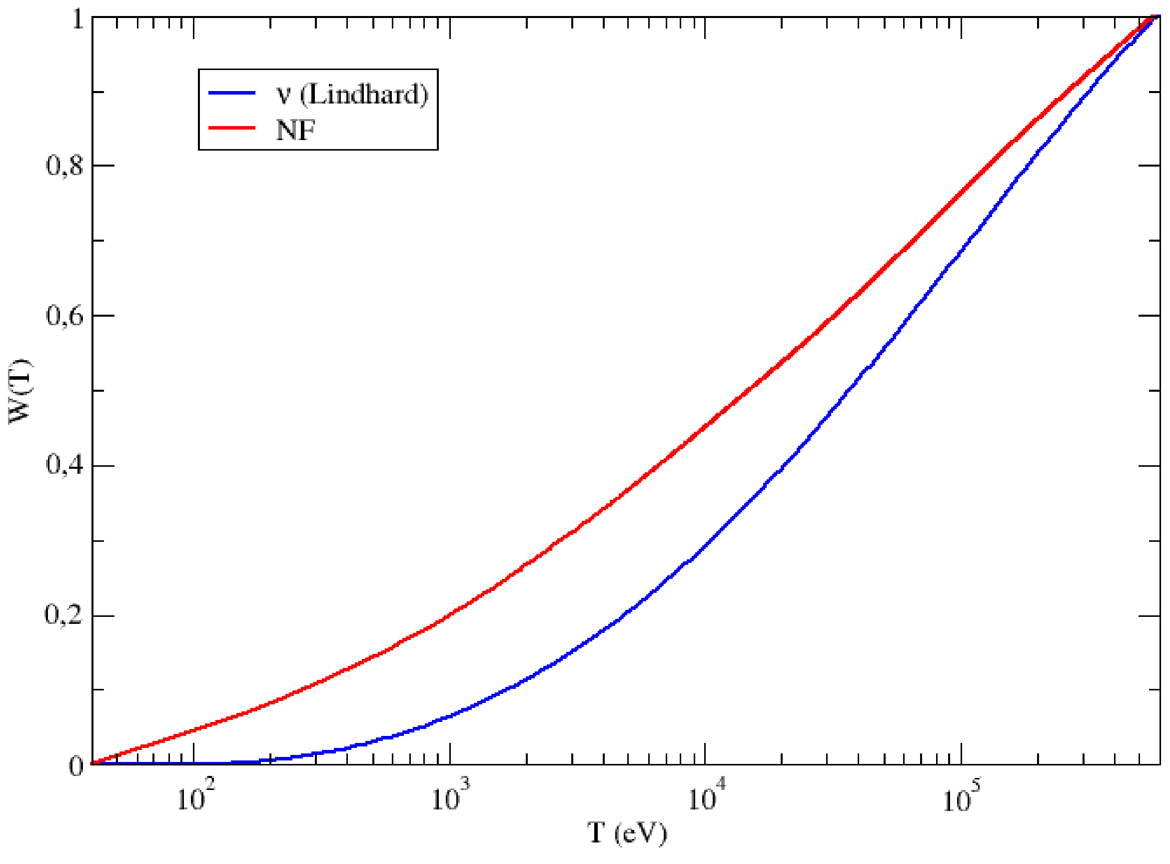
- ❑ Subcascade formation energy : Ec = 10keV

- ❑ Number of defects NF using the subcascade decomposition
  Less than 15 % discrepancy from MD



IV Capturing defects on the basis of MD: fractality

Calculating W(T) using NF : a way to stiff W(T)



V Summary-Perspectives

Summary

- **DPA does not allow to predict by himself the microstructure**
- **From accurate nuclear data, it becomes possible to calculate PKA spectrum..(anistropy, nuclear reactions..)**
- **Introducing a recoil spectra, it becomes possible to select surrogate to minic the microstructure induced by neutron irradiation**

Perspectives

- **How to handle the spatial distribution of defects (and their lifetime) to predict the microstructure ??**
- **For fission products and spallation (ions with E of around few hundreds of MeV), "damages" induced by the "electronic stopping power" is not taken into account (cf experiments performed at GANIL)** (H Dammak et al. PRL 74, 1135 (1995))

IV Capturing defects on the basis of MD: fractality

- <u>Why do we need to link BCA and MD ?</u>

  Introducing MD in the calculation of a new dpa estimator

- **sensitivity of interatomic potentials?**

- **how to handle the electronic stopping power in these simulations?**

We need to go beyond the dpa notion to describe the spatial spreading of defects in order to compare different microstructures (irradiation ions-neutrons)

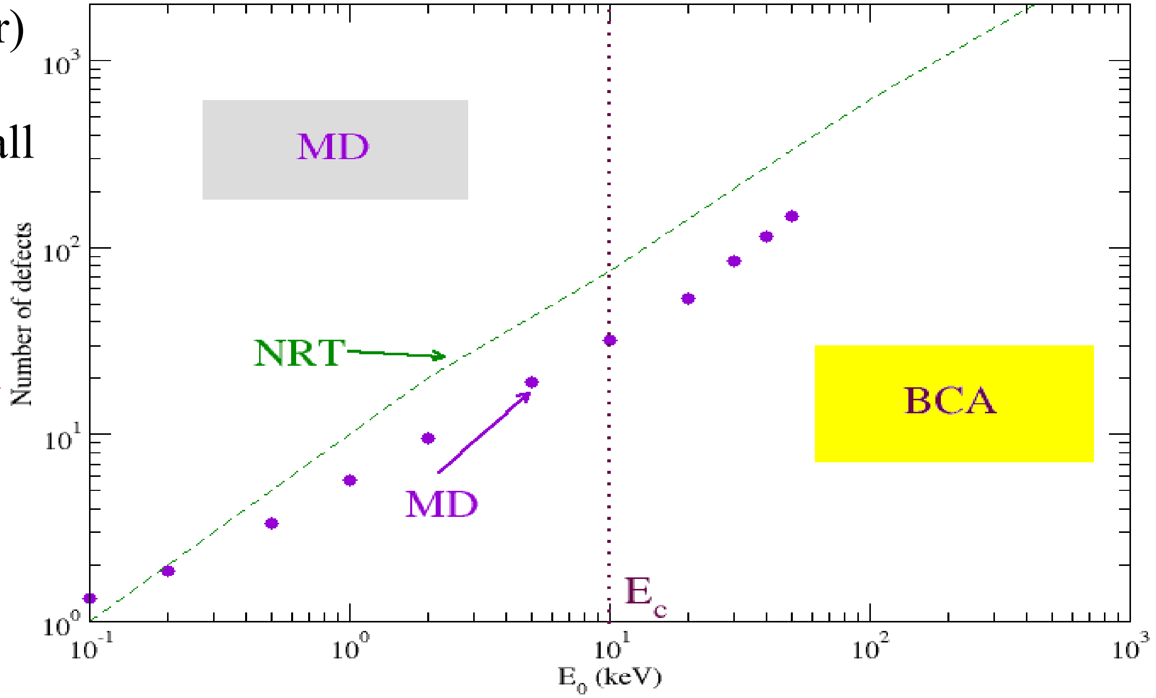
IV Capturing defects on the basis of MD: LRC CARMEN
fractality

Application : number of defects in iron irradiated by Fe ions

- ❑ MD simulations of defects in iron for incident energy < 50 keV (Stoller)

- ❑ NRT formulation for all incident energies
  Large discrepancy

- ❑ Subcascade formation energy : Ec = 10keV



II Calculating « dpa » in compounds within the BCA framework

- **Dpa in compounds within the Lindhard formalism: DART**

Assumptions : neglect the crystalline structure (polycristalline materials)

(no crowdion, i.e. MARLOWE …)

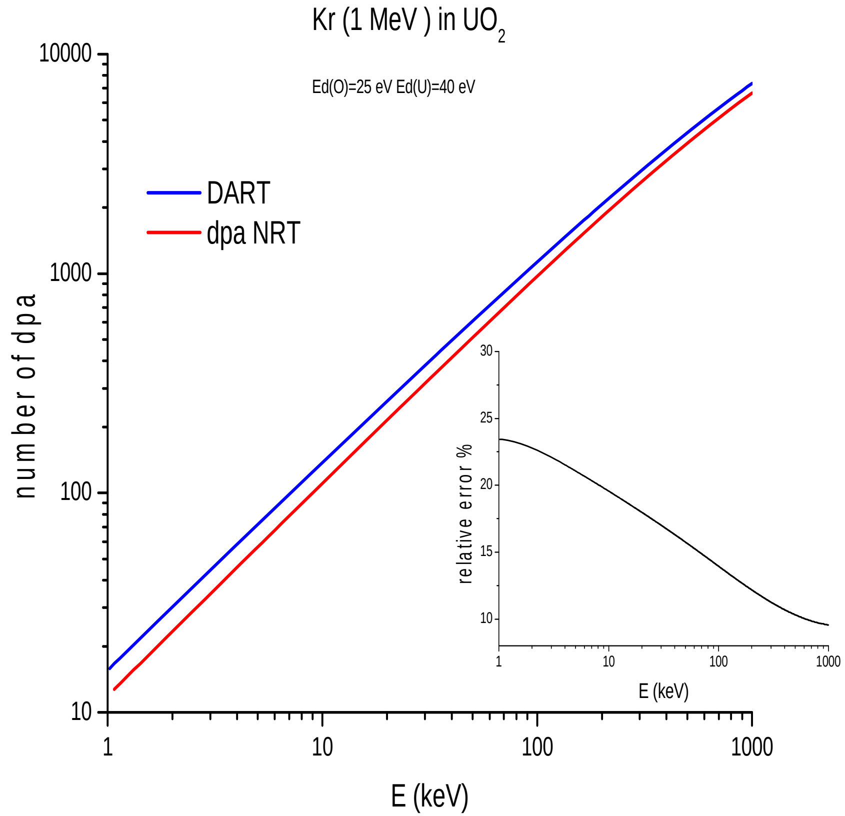
For a compound of N elements,

N equations (different from a simple weighting used in dpa NRT)

Comparison between dpa NRT and dpa calculated using the Lindhard formalism (DART).

The ratio is not a constant

(JNM 246, 206 (1997),JNM 353, 89 (2006))



III How to compare different irradiations: the DART code

FBR (phoenix) neutron spectrum and iron target
100 groups