DE LA RECHERCHE À L'INDUSTRIE

DART, A BCA CODE TO ASSESS AND COMPARE PRIMARY IRRADIATION DAMAGE IN NUCLEAR MATERIALS SUBMITTED TO NEUTRON AND ION FLUX

L. Luneville, D. Simeone

ECP/CEA

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OUTLINE

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II Primary damage

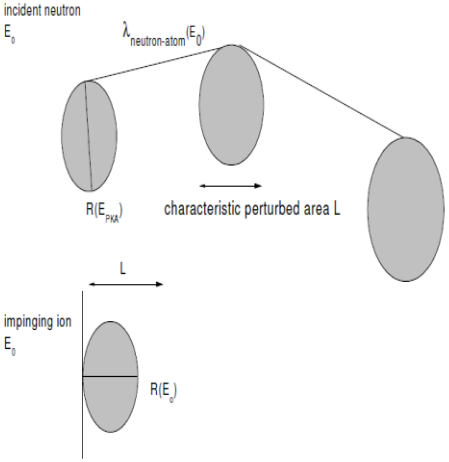
III Results

IV Conclusion

INTRODUCTION

How to characterize damage in materials under irradiation?

Interactions neutron-atoms defined with cross sections



Elastic interactions:

σ=few barns → macroscopic cross section Σ = few cm

The energy is given to the recoil atom : displacement cascades are well separated(> 1 µm)

Inelastic interactions:

❖**Nuclear reaction :** emission of very energetic recoil atoms (H, He) but not only light atoms

ex UO_2 fission U^{235} emission of Kr ions 100 MeV

❖**Transmutation :** modification of chemical species

some parts of the reactor (springs) are composed of inconel containing ^{58}Ni which transmutes in ^{59}Ni with high energy and then creates an increase of damage

INTRODUCTION

Simulating a reactor irradiation with charged particles?

Ion irradiation

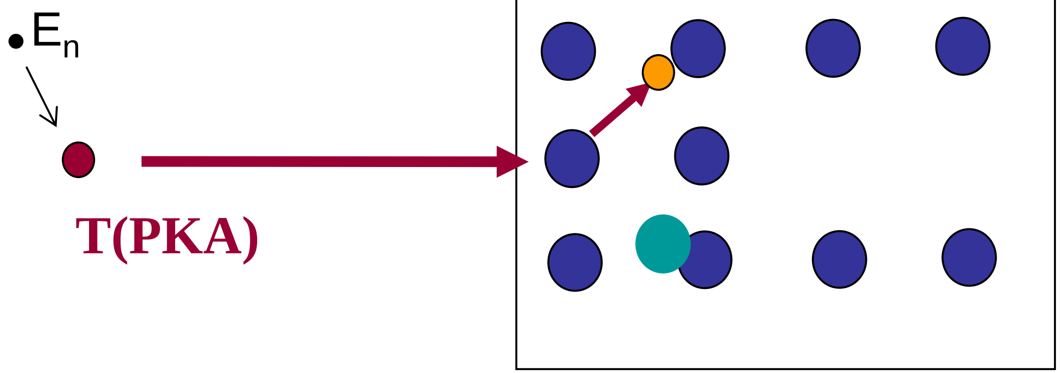
- ❖Simulate elastic collisions neutron-atoms
  - ❖ Creation of displacement cascades
- ❖Modified area under ion irradiation : a few hundred of nanometers
  - ❖ Measurements near the surface (XR glancing incidence) far away from the implantation peak
- ❖Irradiation with light ions : problem of deposited energy due to electronic loss

Electron irradiation

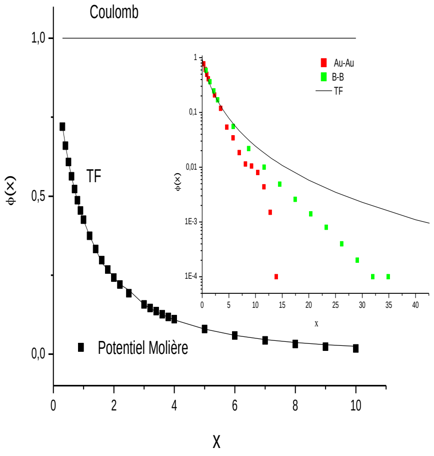
- ❖No displacement cascades : isolated defects
- ❖Measurements of displacement energies of an atom
- ❖Measurements of the mobility of defects
- ❖Impact of electronic loss

PRIMARY DAMAGE

Description of the displacement cascade induced by neutrons



Binary Collision Approximation (SRIM,DART,MARLOWE)
PKA : Primary Knocked-on Atom



❖Ion-ion interactions are described only using the repulsive part of the interatomic potential (different from MD simulations)

❖Calculation of a damage energy $E_D(E)$ and a number of displaced atoms : $\kappa E_D(E)\ /2E_d$ but not a number of defects !!!

Interest : universal Thomas-Fermi potential (no need to define a specific potential for each material)

Limitation : no defect calculation

PRIMARY DAMAGE

Two elements to calculate the damage function (in the Binary Collision Approximation)

$\chi(E_n,T)$: cross section neutron-atom : gives the energetic distribution (T) of the recoil atoms displaced by a neutron of energy E_n

$E_D(T)$: deposited energy by the ion : energy available for displacements i.e.when substrating the electronic loss

Calculating the damage energy $E_D(T)$

DART : numerical resolution of Lindhard equations (polyatomic material)

electronic stopping power : the same as used by SRIM 2013 (based on measurements)

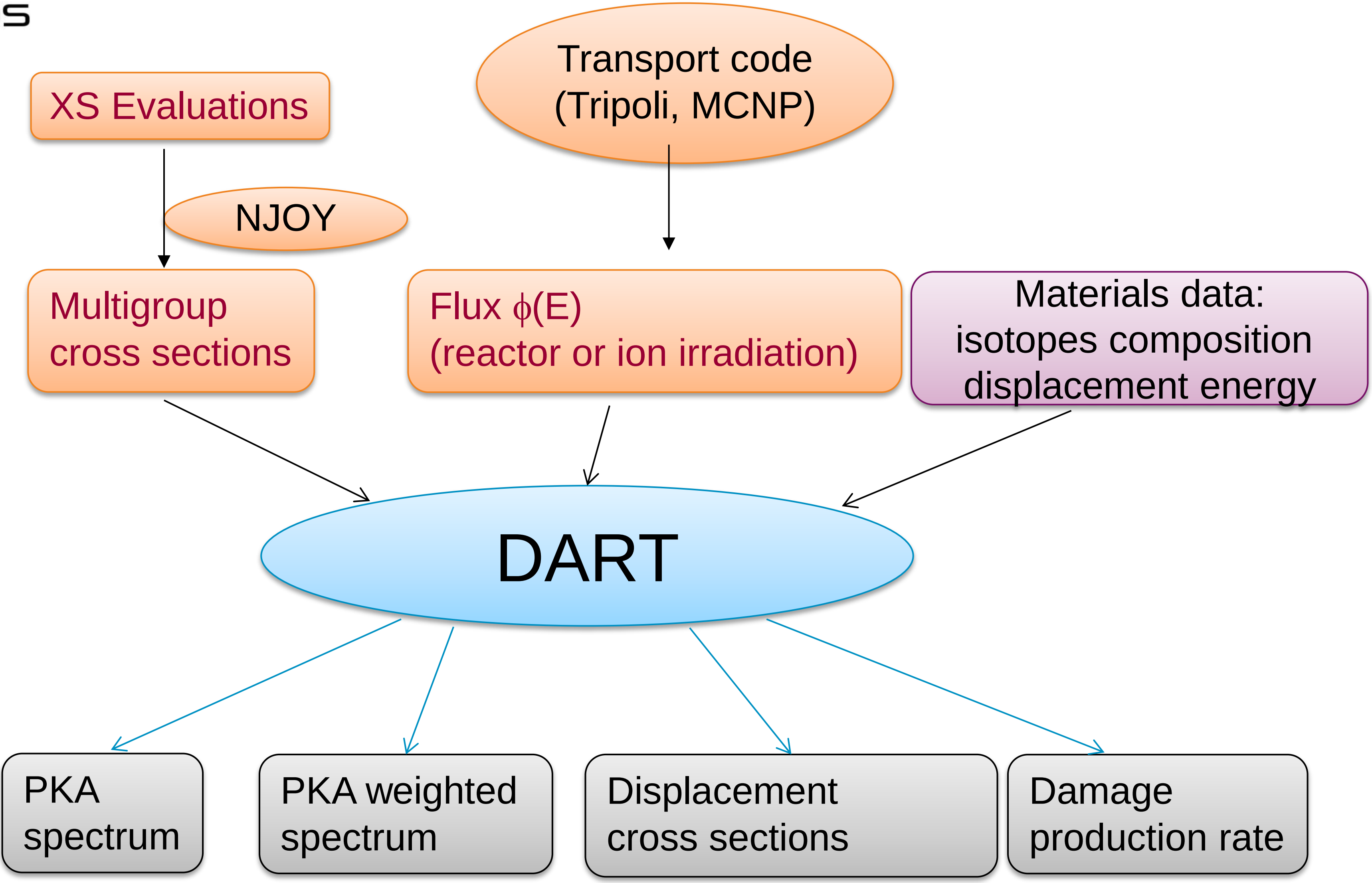
SRIM : Monte Carlo resolution of Lindhard equations (spatial description)

Marlowe : same as SRIM but taking into acount the cristalline structure of the material

Calculating the number of displaced atoms

$\nu(T) = \kappa E_D(T) / 2E_d$ where E_d is the displacement energy (NRT approximation)

PRIMARY DAMAGE : DART



XS Evaluations

Transport code (Tripoli, MCNP)

NJOY

Multigroup cross sections

Flux $\phi(E)$ (reactor or ion irradiation)

Materials data: isotopes composition displacement energy

DART

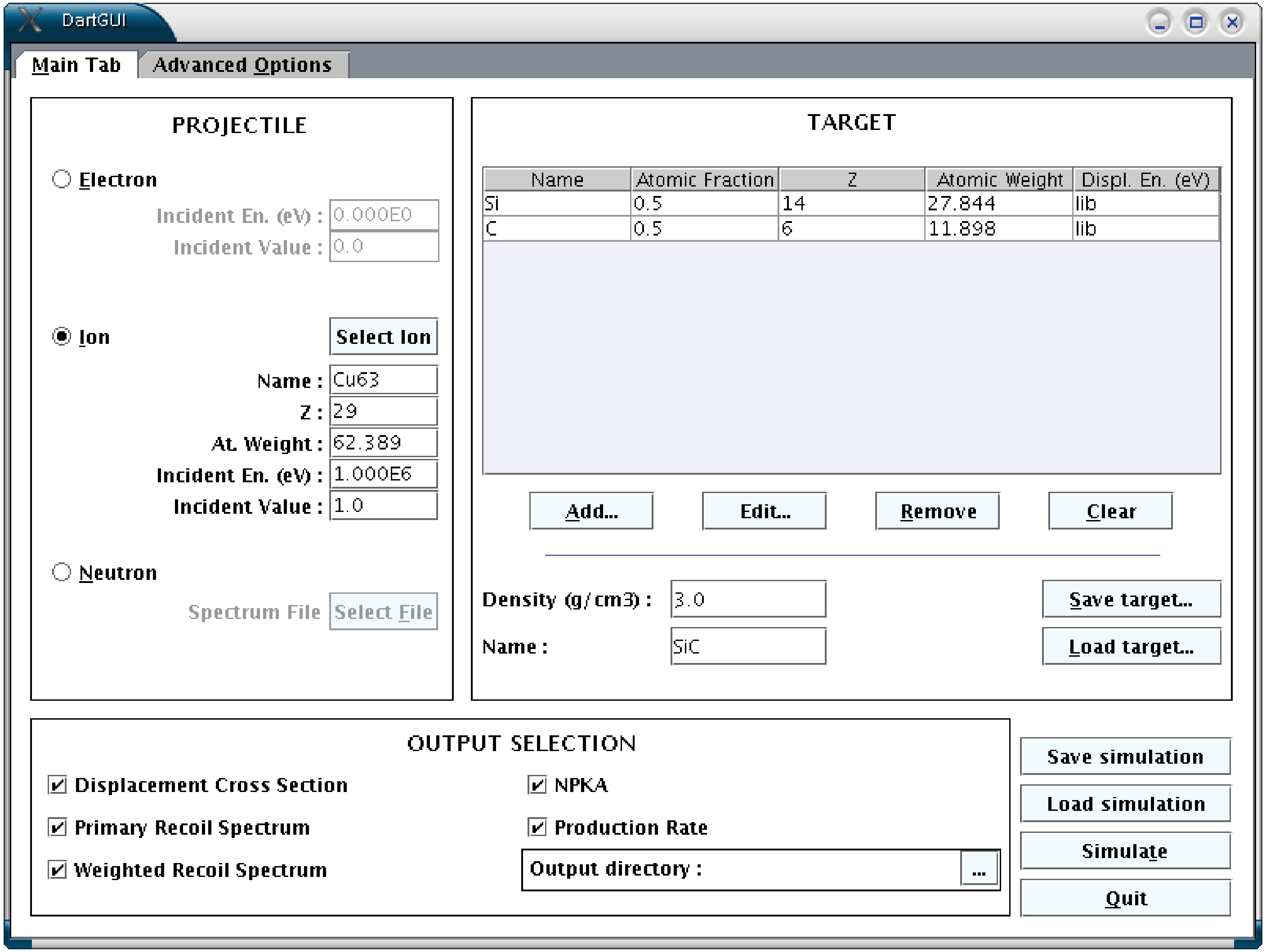
PKA spectrum

PKA weighted spectrum

Displacement cross sections

Damage production rate

PRIMARY DAMAGE : DART GRAPHIC USER INTERFACE



PROJECTILE

○ Electron

Incident En. (eV) : 0.000E0

Incident Value : 0.0

● Ion

Name : Cu63

Z : 29

At. Weight : 62.389

Incident En. (eV) : 1.000E6

Incident Value : 1.0

○ Neutron

Spectrum File

TARGET

Name	Atomic Fraction	Z	Atomic Weight	Displ. En. (eV)
Si	0.5	14	27.844	lib
C	0.5	6	11.898	lib

Density (g/cm3) : 3.0

Name : SiC

OUTPUT SELECTION

☑ Displacement Cross Section

☑ Primary Recoil Spectrum

☑ Weighted Recoil Spectrum

☑ NPKA

☑ Production Rate

Output directory :

RESULTS

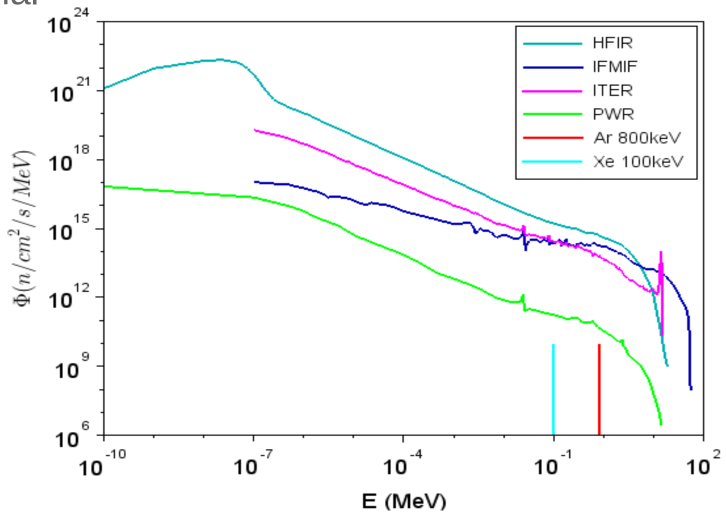
How to compare different irradiations? Which estimators?

Damage production rate (dpa/s)

number of displaced atoms per second in the material

$$R^{Mat} = \int \sigma_d^{Mat}(E)\phi(E)dE$$

Irradiation	Total flux (n/cm²/s)	R in Fe (dpa/s)	Time to reach 0.1 dpa in Fe
HFIR	$5\ 10^{15}$	$1.4\ 10^{-6}$	20 h
IFMIF	$7\ 10^{14}$	$1.2\ 10^{-6}$	23 h
ITER	$4\ 10^{4}$	$5\ 10^{-7}$	55 h
PWR	$3\ 10^{11}$	$9.8\ 10^{-11}$	280000 h
Ar 800 keV	10^{12}	$4.9\ 10^{-4}$	200 s
Xe 100keV	10^{12}	$5.6\ 10^{-3}$	18 s



Flux for different reactors

Dpa rate is much higher for ion irradiation than in reactor. The time to obtain the same dpa must be reduced (factor 1000) in ion accelerators.

RESULTS

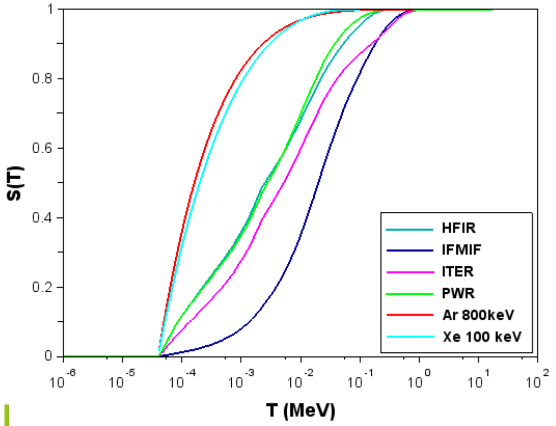
How to compare different irradiations? Which estimators?

PKA spectrum for monoatomic material

S(T) proportion of PKA having an energy <T

- ❖Strong dependence of the incident spectrum
- ❖Same PKA spectrum means same distribution of energy in the material

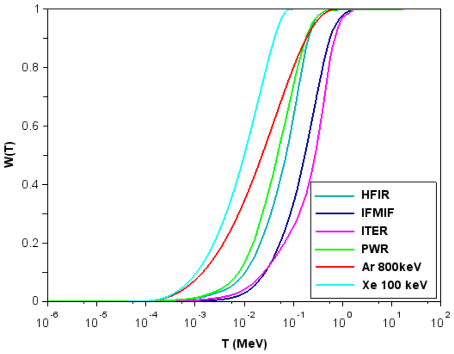
PKA spectra in iron



PKA weighted spectrum for polyatomic material

The energy given to the recoil gives different number of displacements in each sublattice of the material. The recoil energy is then weighted by the number of displaced atoms to define the PKA weighted spectrum

PKA weighted spectra in Fe-10%^{58}Ni

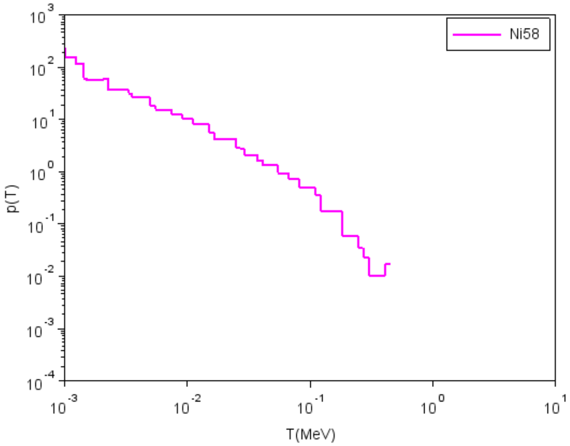


Comparison of PKA spectra for different irradiations

Impact of XS evaluations (ENDF-BVII)

Importance of Ni alloys (Inconel springs in Candu reactors)

^{58}Ni is the most abundant isotope in natural Ni



Energetic distribution of PKA after the collision between a neutron and a ^{58}Ni atom in the HFIR reactor

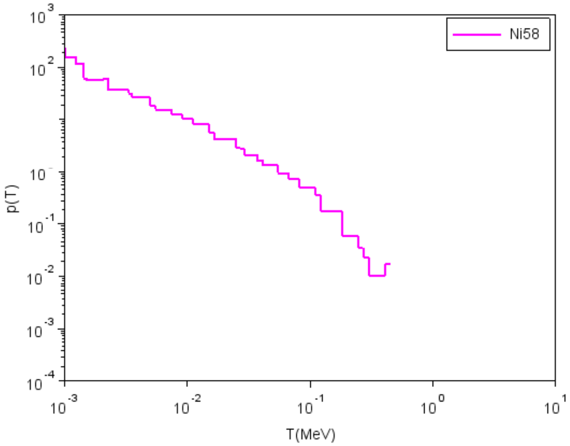
Impact of XS evaluations (ENDF-BVII)

Importance of Ni alloys (Inconel springs in Candu reactors)

^{58}Ni is the most abundant isotope in natural Ni

Under neutron irradiation a transmutation of ^{58}Ni occurs ^{58}Ni + n → ^{59}Ni

→ apparition of ^{59}Ni not present in natural Ni



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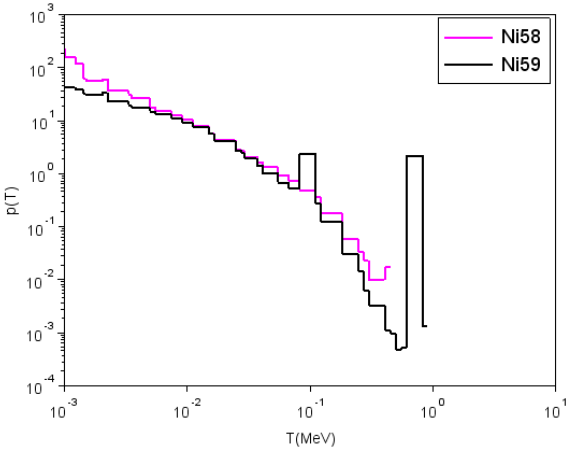
Transmutation

^{58}Ni + n → ^{59}Ni



Energetic distribution of PKA after the collision between a neutron and a ^{59}Ni atom in the HFIR reactor

Impact of XS evaluations (ENDF-BVII)

Importance of Ni alloys (Inconel springs in Candu reactors)

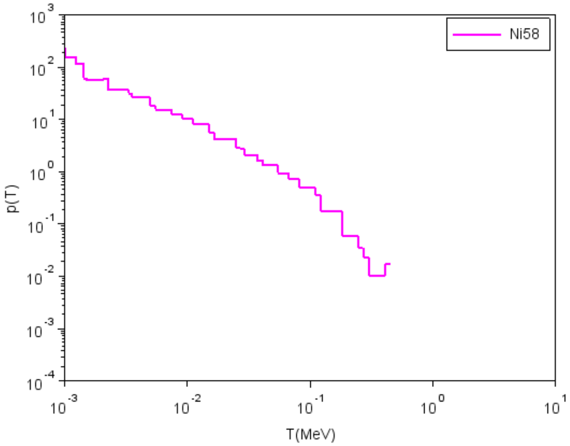
The reaction of thermal neutrons on ^{59}Ni generates very energetic Fe ions (>500 keV) [Griffiths AECL Nucl. Rev 2 (2013)]

$^{59}Ni + n \rightarrow {}^{56}Fe + \alpha$

$^{59}Ni + n \rightarrow {}^{59}Co + H$

Transmutation

$^{58}Ni + n \rightarrow {}^{59}Ni$



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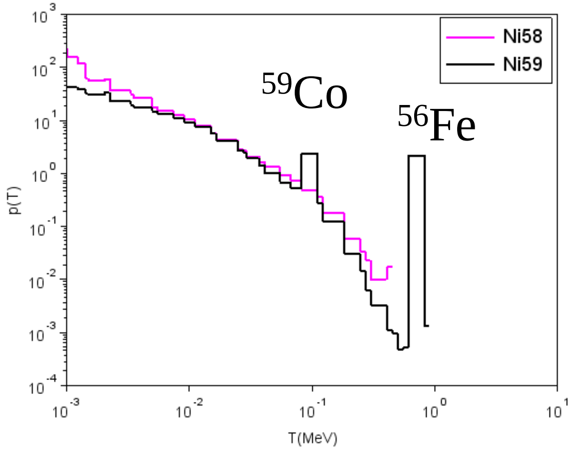

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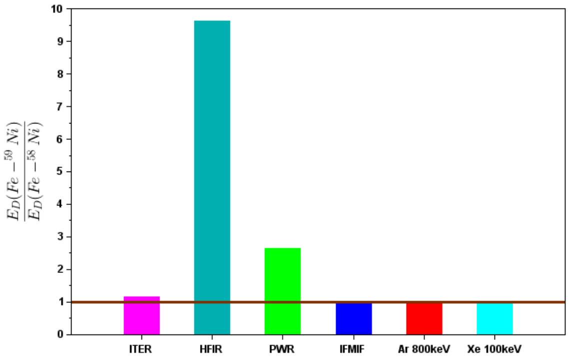
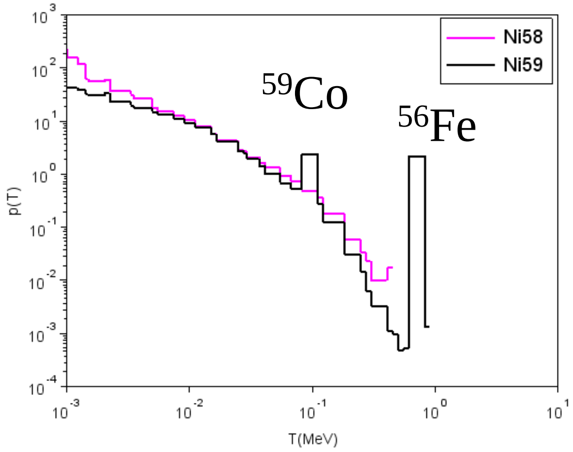


Ratio of the production rate between Fe-10%^{59}Ni and Fe-10%^{58}Ni

Increase of the production rate

x3 in PWR
x10 in HFIR



Energetic distribution of PKA after the collision between a neutron and a ^{59}Ni atom in the HFIR reactor

Importance of

- good neutron cross sections
- calculations with isotopes and not natural elements

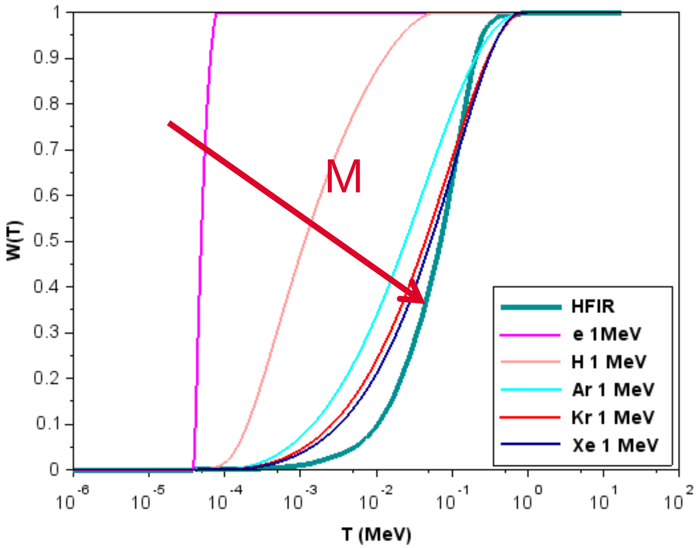
CONCLUSION

How to compare different irradiations?

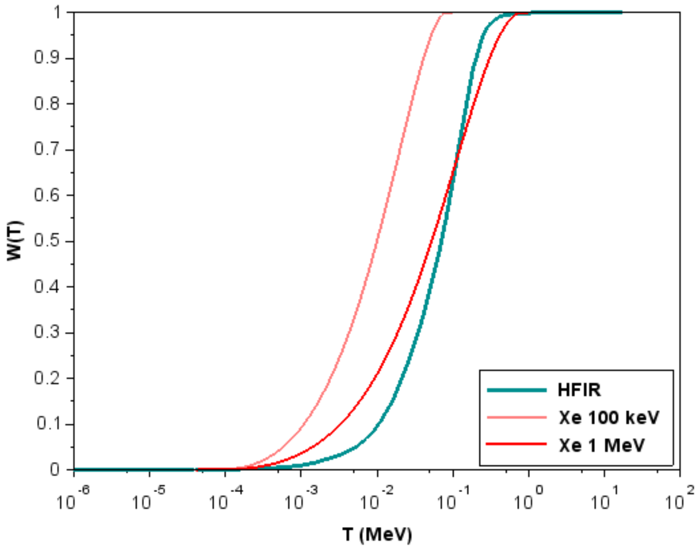
DART code in the BCA approximation allows calculating for ion and neutron irradiation :

❖PKA spectra → choose ion and energy with the PKA spectrum as close as possible to the PKA spectrum with neutrons

Choose ion



Choose energy



PKA weighted spectra in Fe-10%^{58}Ni

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DART code in the BCA approximation allows calculating for ion and neutron irradiation :

❖PKA spectra → choose ion and energy with the PKA spectrum as close as possible to the PKA spectrum with neutrons

❖Damage production rate (dpa/s) and damage (dpa) → choose time of ion irradiation to have the same dpa than with neutrons

❖Validation with other codes

- Neutrons : SPECTER and HEATR (NJOY module)
- Ions : SRIM and MARLOWE

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How to compare different irradiations?

DART code in the BCA approximation allows calculating for ion and neutron irradiation :

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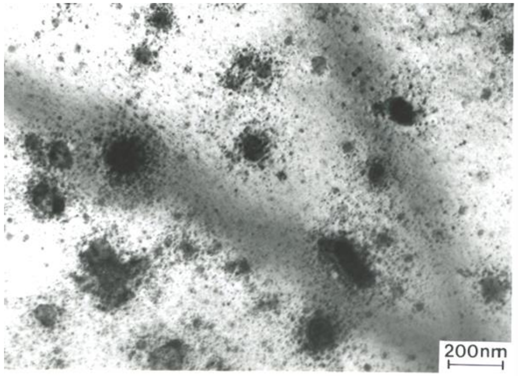
(http://www.oecd-nea.org/tools/abstract/detail/nea-1885/)



ODS irradiated in Phenix 750K,1.5 10^{-6} dpa/s, 30dpa *(I. Monnet, Ph. D.)*

BUT

❖BCA approximation (damage and not defects) → DM ?

❖Even if the dpa is equal for ions and neutrons, the time of irradiation is 1000 times lower for ions → impact of time and flux ?

❖Simulation of primary damage (time of the displacement cascade 10^{-12}s)

❖Validation ? Measurements of microstructure after several hours

TO GO FURTHER

Predict a microstructure : flux and T effects

Stationnary state induced by 1 MeV Ar ions in AgCu at 450 K(Cu precipitates) Phase Field simulation*(G. Demange Ph D.)*