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Primary displacement damage calculation induced by neutron and ion using binary collision approximation techniques (MARLOWE code)

F. Mota, C. J. Ortiz, R. Vila

Laboratorio Nacional de Fusión – CIEMAT, Madrid, Spain, Material group

PROGRAMA

TechnoFusion Program

GOBIERNO DE ESPAÑA

MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

Ciemat

Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

Summary

1. Motive of this work
   a) Fusion Power Reactors
   b) Emulated the Fusion neutron with other neutron sources
   c) Simulation of Neutron Irradiation Effects with Ion irradiation

2. Standard damage dose calculation

   a) Neutron irradiation
   b) Ion irradiation

3. Simulation of defect generated by neutrons and Ions: methodology used

4. Analyses of the displacement damage generation

   a) Simulation of defect formation in materials under irradiation
   b) Description of MARLOWE code
   c) Comparison MARLOWE vs SRIM
   d) Recombination of defects during cascade
   e) Simulation of energy loss of high-energy particles: Modification of MARLOWE
   f) Analyses of damage function induce by monoenergetic Ions (Bragg Peak)
   g) Damage profiles
   h) Damage function and damage dose calculations

5.- Results

6- Conclusions

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The path to Fusion Energy

I+D Tecnología

Structural Materials

Breeder Blankets

Components
- Images SC
- Tritium handling systems
- First wall components
- Diagnostics
- Remote Handling
- etc.

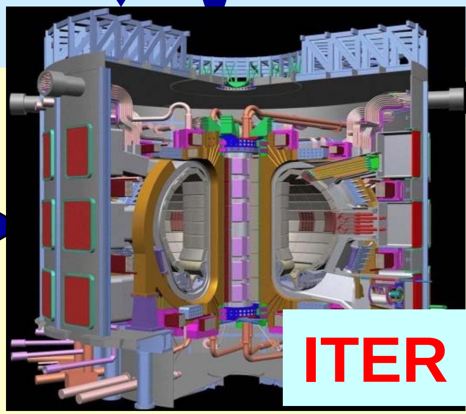
Understanding b... diation effects ... fusion envir... be able to predic... ehaviour

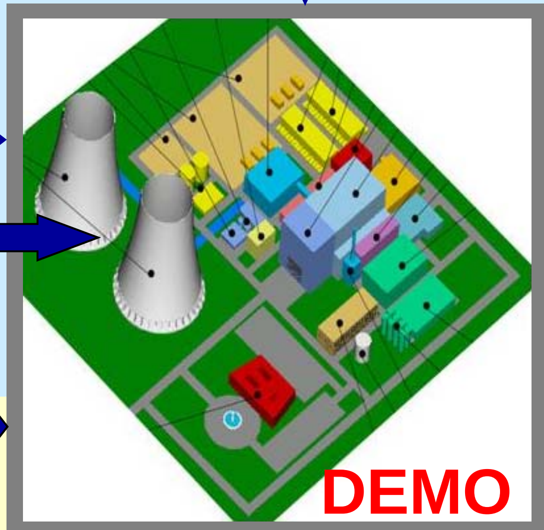
IFMIF, TechnoFusión
Or
Computational simulations

***Blanket* tests in ITER**

I+D Physics

Facilities
- Confinement
- impurities control
- Plasma stability
- etc.



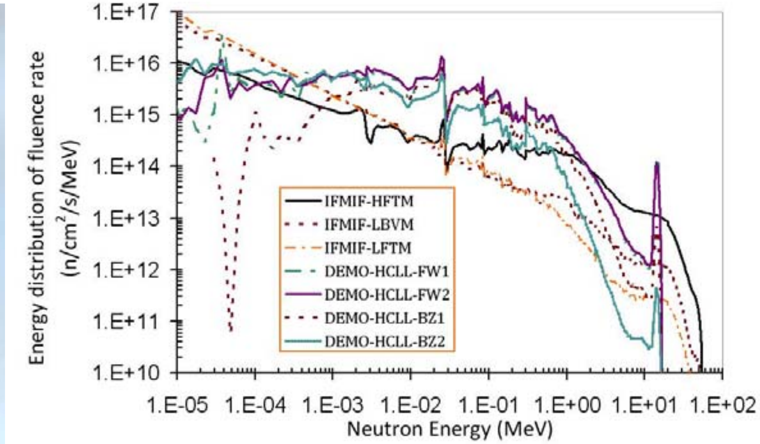


Fusion Power Reactgor

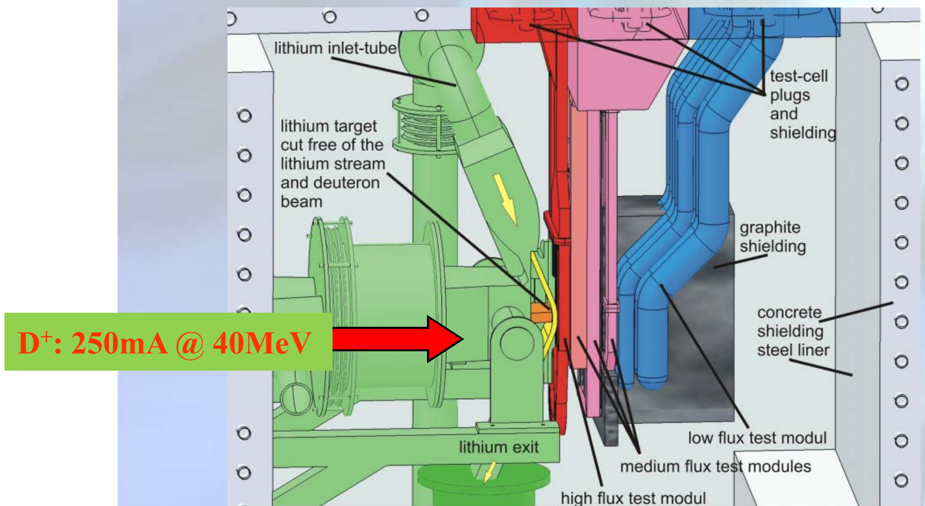
a) Emulated the Fusion neutron with other neutron sources

1.- Exposing the materials to neutronic irradiation conditions similar that the ones in nuclear fusion environments .

- Fission Reactors
- Spallation sources
- Striping sources: IFMIF

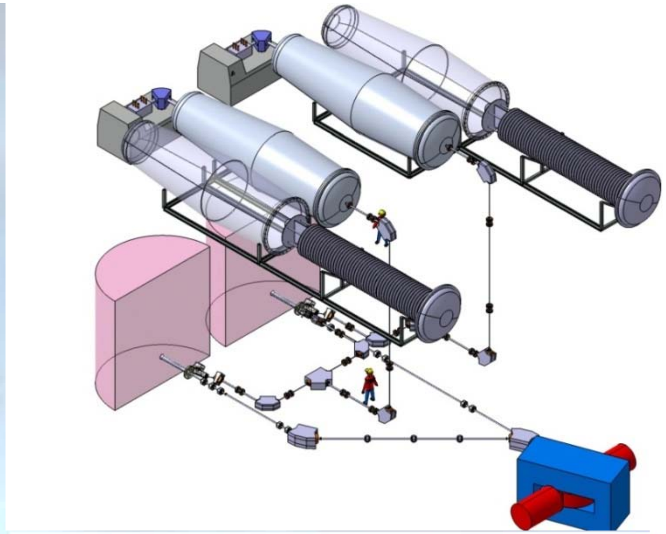


•The objective of the International Fusion Materials Irradiation Facility (IFMIF) is to provide an intense neutron source with adequate energy spectrum to test the suitability of candidate materials for future nuclear fusion power reactor (DEMO). IFMIF will constitute an essential tool in the international strategy towards the achievement of future fusion reactors.



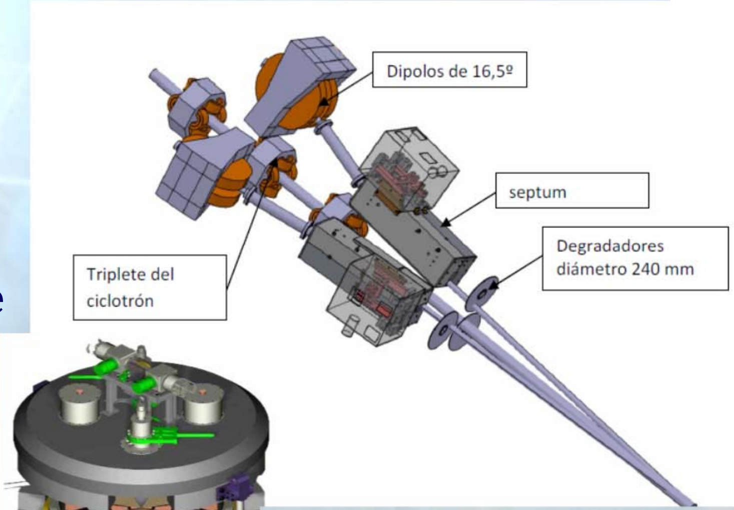
b) Simulation of Neutron Irradiation Effects with Ion irradiation

To avoid all the drawback resulting from neutron irradiation, as for example radiological risk, it is under study to emulate the neutron effects on materials using Ion accelerators

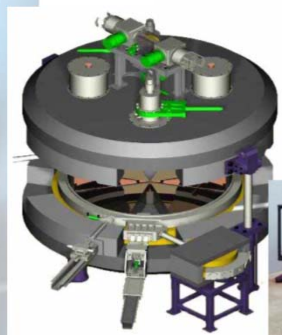


Irradiation Materials area(AIM)

The Material Irradiation Experimental Area of TechnoFusión will emulate the extreme irradiation fusion conditions in materials by means of simultaneously irradiation with three ion accelerators:



- One beam used for self-implanting heavy ions (Fe, Si, C,…) to generate damage.
- Two beams for light ions (H and He) to emulate the transmutation.



Main advantage: Ion irradiation produces little or no residual radioactivity, allowing handling of samples without the need for special precautions.

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2. Standard damage dose calculation for neutron irradition

Currently, two different methods are used to calculate the primary displacement damage induced by neutron irradiation or by ion irradiation:

- Neutron irradiation: the displacement damage doses are calculated considering the NRT model based on the electronic screening theory of Linhard. It is commonly and widely used since 1975.

- Ion irradiation: for experimental research community SRIM code is commonly used to calculated the primary displacement damage dose in order to design irradiation experiment.

2. Standard damage dose calculation for neutron irradition

Displacement Damage Rate caused by neutrons in materials

$$Damage\_Rate\,[dpa/\,fpy] = F[n/cm^2/s] \times \sigma_{dpa}[b] \times 1.E-24[cm^2/b] \times 3.1557E+7[s/\,fpy]$$

where:

F [n/cm^2/s] - neutron flux = F4[n/cm^2]* Source factor [n/s] * 1.E-3 / (e-=1.602177E-19 C)

$\sigma_{dpa}[b] = 0.8 \times DE[b*MeV]/(2 \times E_d[eV])$ - displacement cross section (NRT model)

DE [MeV*b] - damage energy (available in MT=444)

E_d [eV] – threshold energy to displace atoms in lattice (e.g., 40 eV for Fe)

NRT model takes into account the number of initial displacement atoms induced by neutron reactions by mean of effective threshold energy and in order to consider some recombinations an "empirical" factor is used, resolving the Lindhard equation =0.8. But this factor is constant for any materials studied

Table 3. Typical values for the atomic displacement energy E_d needed to compute damage cross sections.

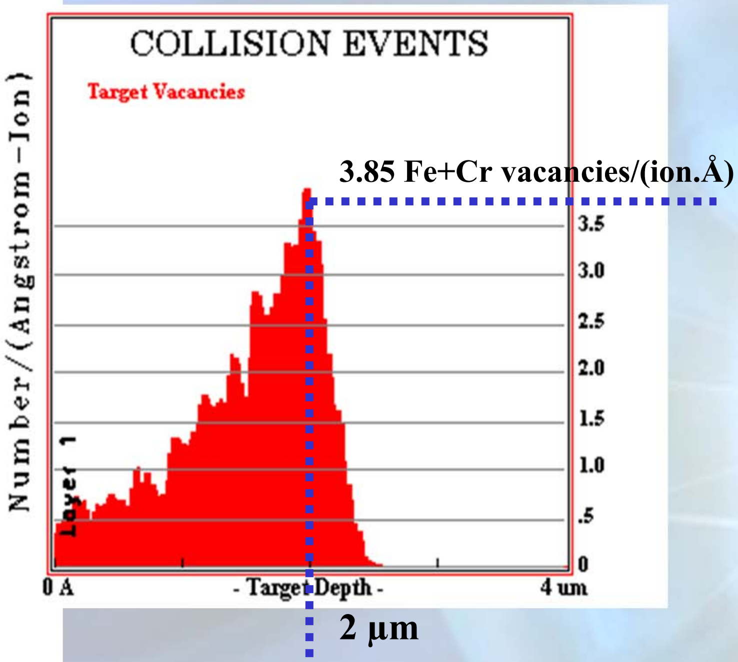
Element	E_d, eV	Element	E_d, eV
Be	31	Co	40
C	31	Ni	40
Mg	25	Cu	40
Al	27	Zr	40
Si	25	Nb	40
Ca	40	Mo	60
Ti	40	Ag	60
V	40	Ta	90
Cr	40	W	90
Mn	40	Au	90
Fe	40	Pb	25

In addition, NRT suffers from several limitations in most materials analysed. For example:

- it is not applicable for compound materials and
- It is not good for covalent materials.
- it does not account for the recombination of atoms during the cascade evolution

Calculation of displacements per atom induced by ions at Bragg peak:

- If the transferred energy is < Ed , then the atom remains in its lattice site (phonon energy)



- If it is > Ed , then the new recoil has this transferred energy, minus the displacement Energy (taking into account that SRIM ignore the crystal lattice
- Expanded for the special case of the displacement being caused not by the ion but by a recoiling target atom
- If the recoiling atom knocks out a target atom, and the incoming atom does not have enough energy to go on, then it will fall into the lattice site emptied by the recoiling lattice atom

$$dpa(vac/atoms) = \frac{total\ dose(ions/cm^2)\cdot\left(\frac{vac}{ion\cdot \text{Å}}\right)\cdot 10^8}{atomic\ density(atoms/cm^3)}$$

The main shortcoming:

- It does not consider lattice structure, therefore, it is good methodology to emulate the displacement damage in amorphous system but it is not appropriate to study crystalline structure.
- In addition, the displacement damage is considered by mean of the effective displacement threshold energy.

Summary

we can realize that both methodologies previously described do not have anything in common. Hence, it is very difficult to compare both kinds of calculations in order to design irradiation experiments to emulate neutron fusion irradiation conditions.

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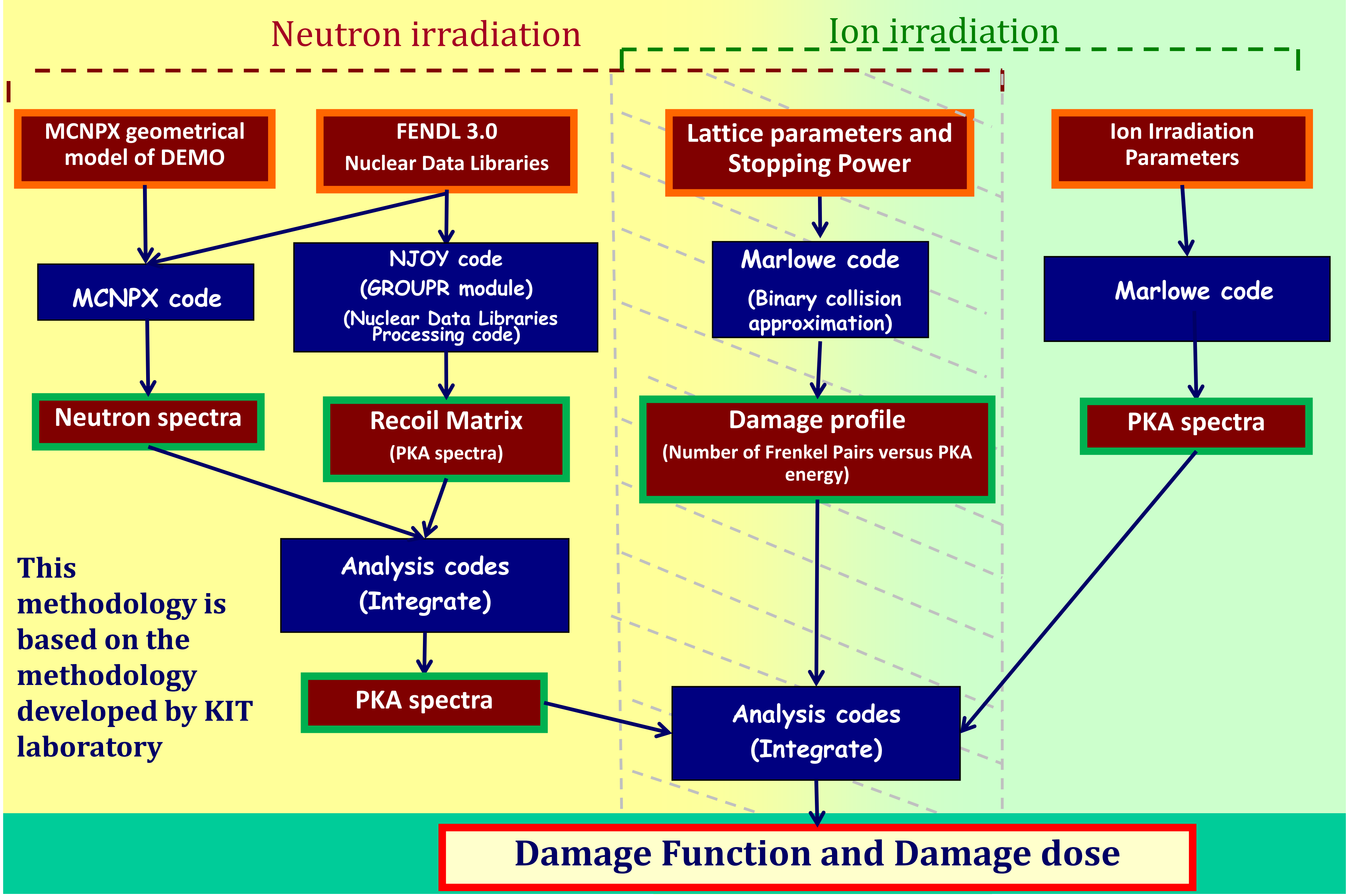
Methodology objectives

- we can realize that both methodologies previously described to calculate the primary displacement damage have nothing in common.
- Our objective were to find the way to calculate the primary displacement damage induced by neutron irradiation or by Ion irradiation starting from the same point, that is, using something common to both kind of irradiation.
- To develop a methodology to be able to unify the criteria of displacement damage calculations for both kinds of radiations assessed, hence, using a common element of both radiations to calculate it.
- This Methodology would allow to design irradiation experiments with ions to be able to emulate neutron fusion effects on materials

3.- Simulation of defect generated by neutrons and Ions: methodology CIEMAT



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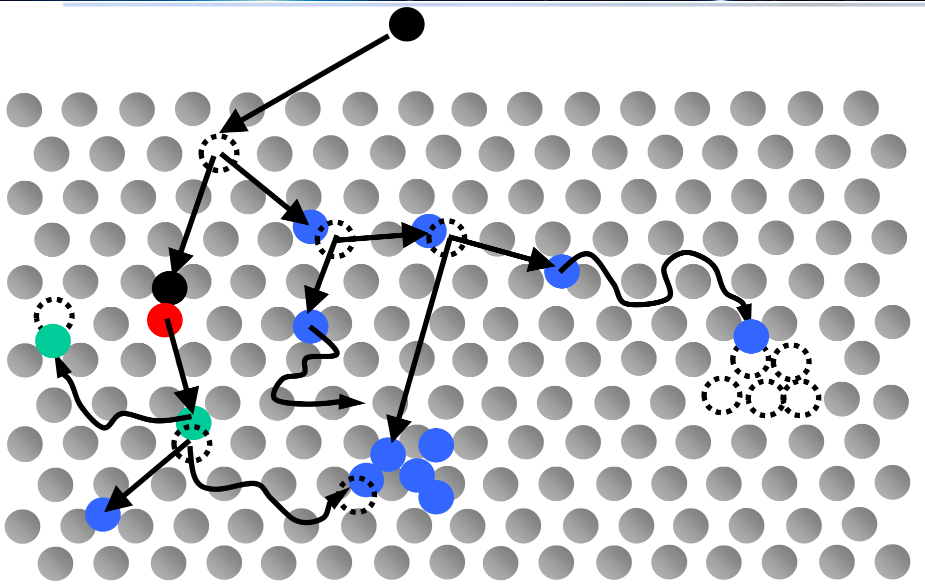
4. Analyses of the displacement damage generation:
a) Simulation of defect formation in materials under irradiation



•Neutron irradiation induces Elastic and Inelastic nuclear reaction. The displacement of ions (PKA spectrum) are generated with both elastic and inelastic reactions, although the elastic reaction contribute, more or less, in more than of a 90 %, depending on the isotope analyze.

•Heavy Ion (PKA spectrum) irradiation mainly induces elastic reactions producing displacements damage

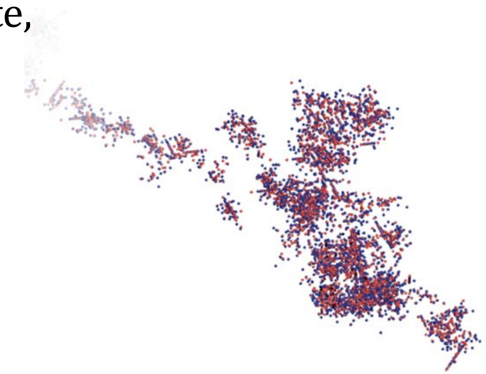
•Neutron/Ion irradiation produces different types of defects: I, V, He, H, clusters…

• It is essential to predict/simulate:
- Defects created by neutron/ion irradiation
- Long-term evolution of defects and impurities

• After they are created, defects can:
- Migrate,
- Agglomerate,
- Recombine,
- Dissociate,
- etc…

• The prediction of defect evolution can be achieved by means of OKMC or Rate Theory models.

• Defects formed during cascade are required as input. However, high-energy neutrons generate PKA with high energy (~MeV), which implies a very large amount of displacements. This is not computationally achievable with Molecular Dynamics.



• **We propose to tackle this problem using MARLOWE code, based on the Binary Collision Approximation (BCA).**

4. Analyses of the displacement damage generation:
b) Description of MARLOWE code

- MARLOWE is a Monte Carlo code based on the Binary Collision Approximation (BCA).

- It allows simulating displacement of atoms in materials, much faster than Molecular Dynamics (due to BCA) and exploring much higher energies (GeV).

- Allows very good statistics: 10^4-10^6 cascades, typically in hours.

- Allows defining the lattice structure and accounts for effects such as channeling, replacements, linear collision sequence, recombination of I-V, etc….

- Can be used to simulate displacements in monocristal, polycristal and amorphous materials.

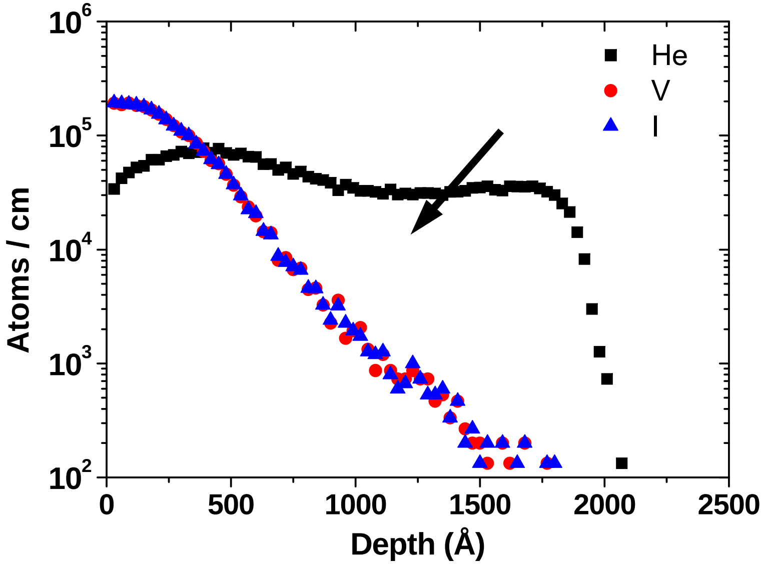
- The binding energies used to calculate the energy of displacement atoms is obtained from first-principles calculations or molecular dynamics calculations.

- Accounts for the recombination of defects that takes place during thermal spike (like MD) by means of an effective capture radius I-V. This capture radius is adjusted on experiment or MD.

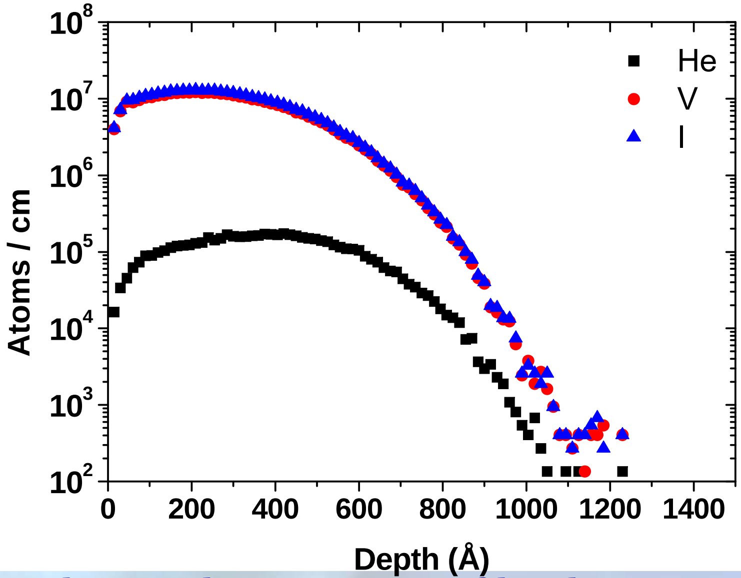
4. Analyses of the displacement damage generation: c) Comparison MARLOWE vs SRIM

- MARLOWE code
 - allows to define the lattice structure and thus accounts for effects such as channeling, replacements, focusons, stenons,…
 - Simulations can be performed in monocrystal, polycrystal or amorphous (SRIM amorphous only).

He 8 keV in PolyFe: MARLOWE



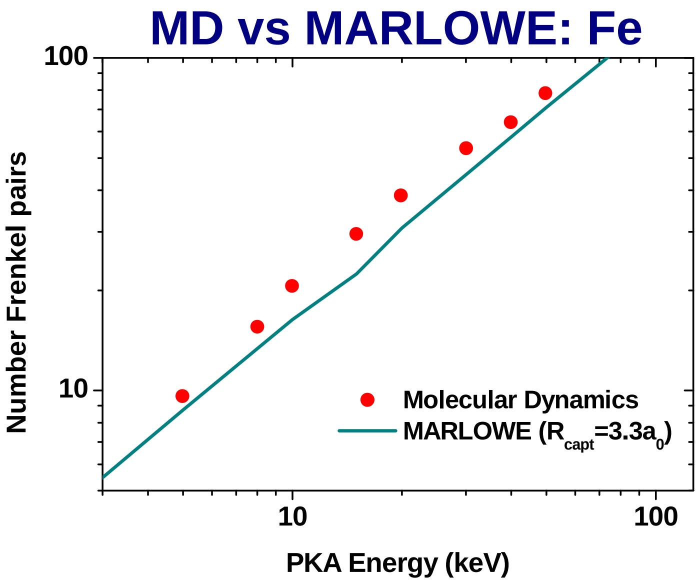
He 8 keV in amorphous Fe: SRIM

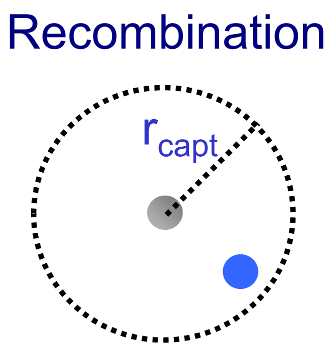


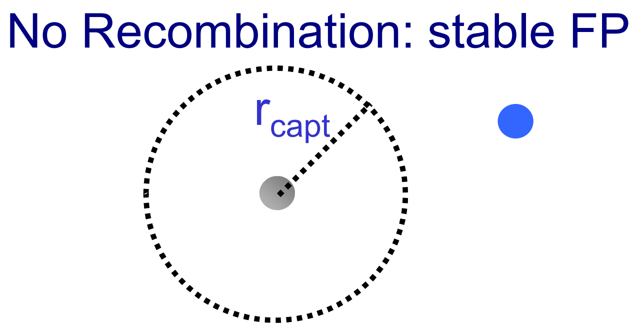
- MARLOWE predicts a long penetration tail in the implantation profile, due to channeling effects, which is not possible with SRIM.
- The number of defects predicted by MARLOWE is significantly different than the one predicted by SRIM since MARLOWE accounts for a possible recombination of defects during irradiation (emulating thermal spike with a capture radius).

4. Analyses of the displacement damage generation:
d) Recombination of defects during cascade

- It is well-known that the materials experiment the phenomenon of thermal-spike during which a very hot phase is reached, sometime leading to a local melting of the material.
- During the cooling phase, a significant amount of defects recombine.
- MARLOWE can account for the recombination of defects that takes place during thermal spike (like MD) by means of an effective capture radius I-V.
- After each cascade, defect positions are analysed. If two defects are found to lie within a distance smaller than the capture radius, then we consider the defects would recombine during the thermal spike.
- The capture radius is usually adjusted on experimental data or MD results.







4. Analyses of the displacement damage generation:
e) Simulation of energy loss of high-energy particles: Modification of MARLOWE

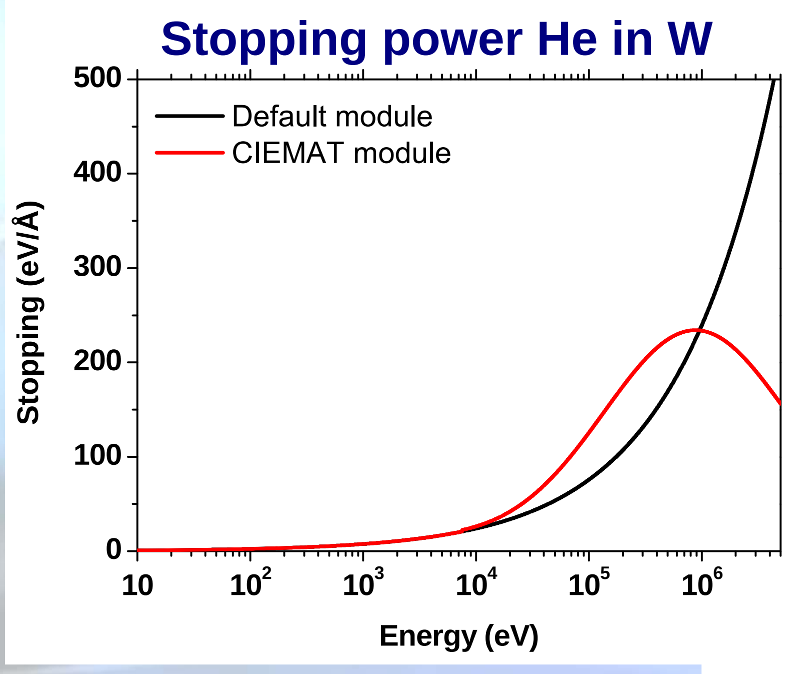
● The energy-loss model implemented by default in MARLOWE is based on the LSS theory (Lindhard, Scharff and Schiøtt). According to this theory, the stopping power is proportional to velocity.

● For $v_{ion} \geq v_{Bohr}$ ($E \approx 25$ keV/amu) this is no longer the case.

● MARLOWE code was recently modified at CIEMAT to account for the energy loss of ions in materials at energies higher than 25 keV/amu (MeV-GeV).

● To do so, the so-called heavy ion scaling rule can be used to calculate the stopping power of atoms with energies above 25 keV per amu. However, a more efficient way was found and that consists in using directly the stopping power data found in SRIM code. The typical stopping powers in nuclear materials (Fe, W, …) are available.

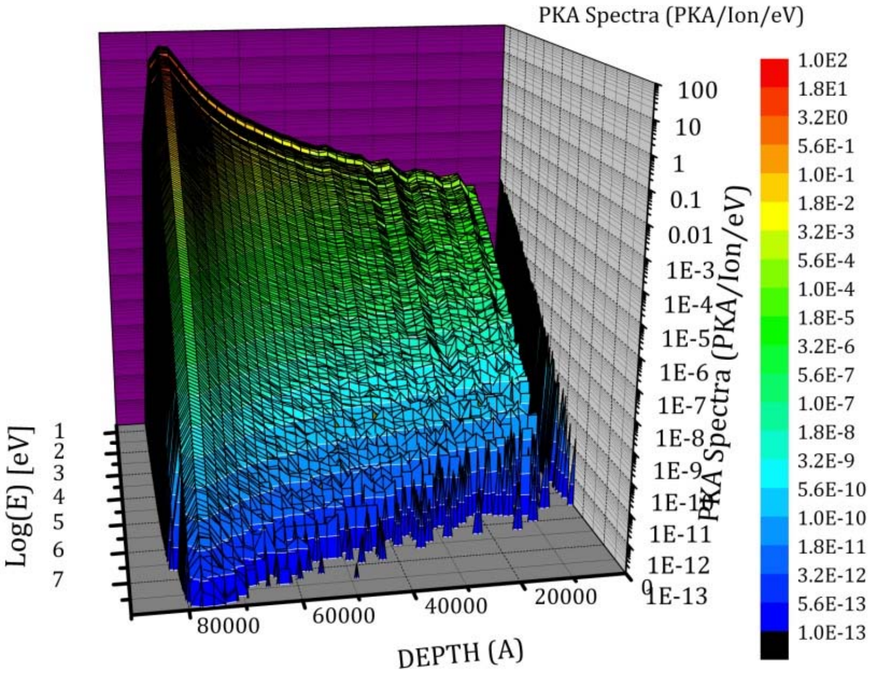
● MARLOWE now allows to simulate the stopping of ions in materials with energies of MeV (or even GeV), such as those formed by fusion or transmutation reactions.

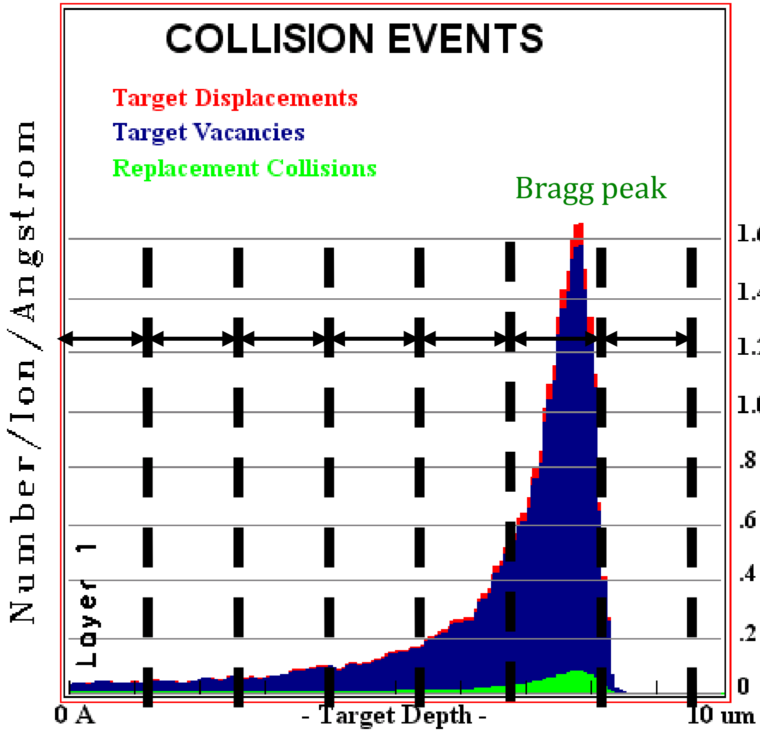


4. Analyses of the displacement damage generation:
f) Analyses of damage function induce by monoenergetic Ions (Bragg Peak)

- A subroutine was implemented into MARLOWE code to calculate the PKA spectrum on different depth bins of the implantation profile.

- PKA Spectra Fe Ion impinging upon iron with energy 100 MeV as a function of Depth.



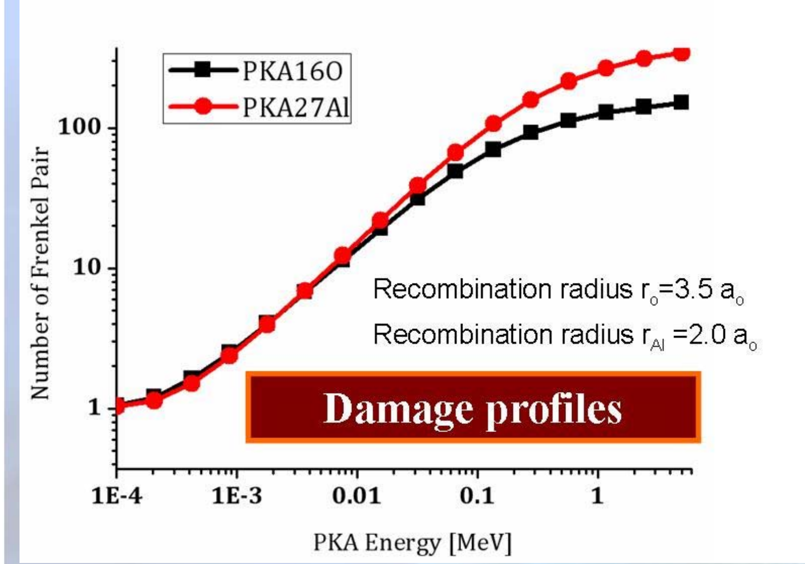


- It give us capability to calculate the displacement damage dose rate for each length bins

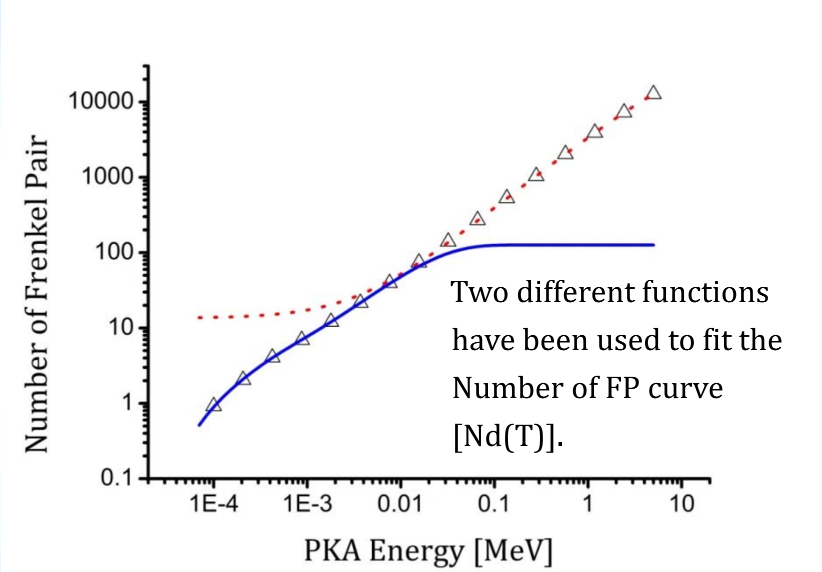
Mainly, Two kinds of results are obtained from MARLOWE

1.- Damage profiles, that is, Number of Frenkel pair versus PKA energy

For example :Al_2O_3



For example :Tungsten



2.- PKA spectra induced by ion irradiation

3.- Coordinates of defects of each displacement cascade can be recorded in order to be used as input in OKMC models

4. Analyses of the displacement damage generation: h) Damage function and damage dose calculations

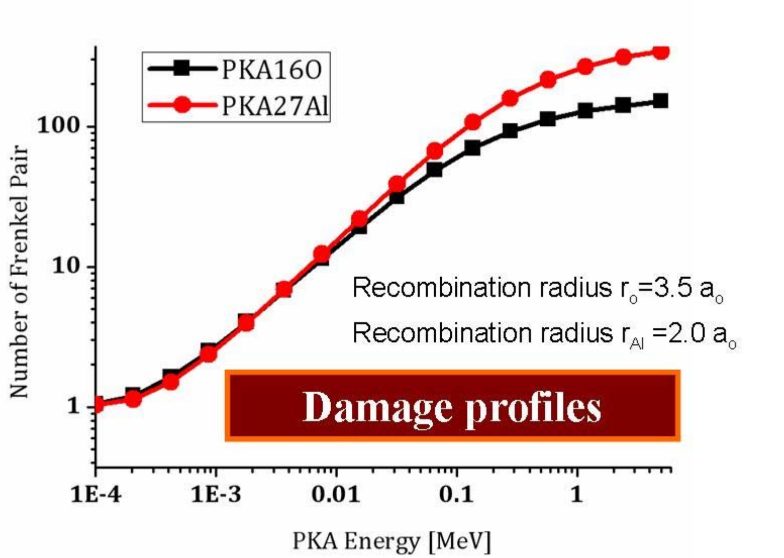
The PKA spectrum describes how the damage is actually produced and the damage function W(T) converts this PKA spectrum to the total damage in the material

$$W(T) = \frac{1}{D/t}\int^{T}\sigma_{PKA}(T')N_d(T')dT'$$

- σ_{PKA} (T) PKA spectrum
- N_d(T) number of Frenkel pairs
- T PKA kinetic energy

The W(T) is calculated to each isotope separately and after it is weighted

N_d(T) number of Frenkel pairs



Damage profile for W ions (PKA) in W calculated with Marlowe code

The damage dose, that is, the concentration of oxygen vacancies as a function of neutron dose

$$dpa = \sum_i \sigma_{PKA}(T_i)N_d(T_i)\Phi_{Total}t$$

where Φ_{Total} is the total neutron fluence rate and t is the exposition time

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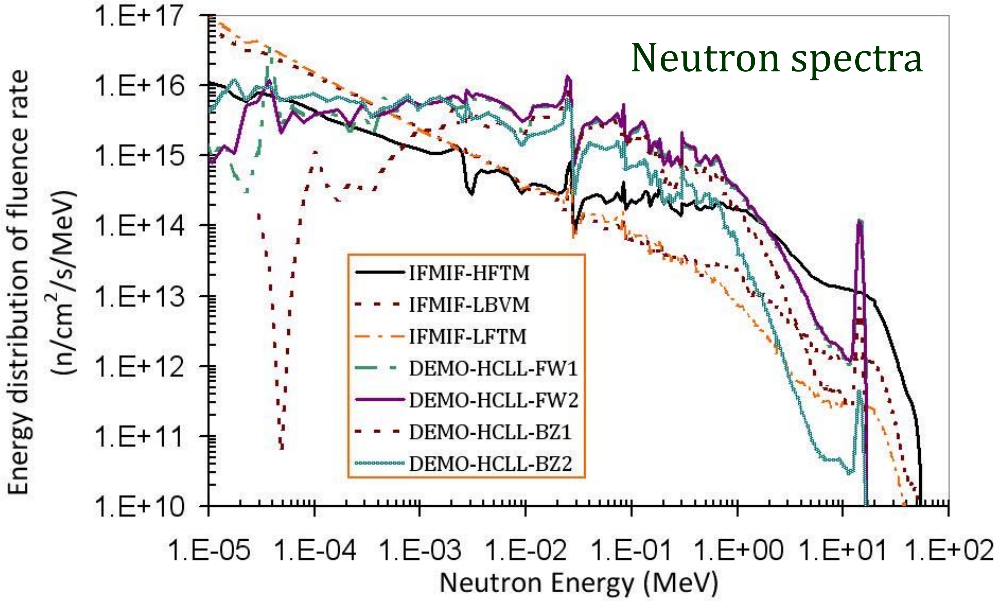
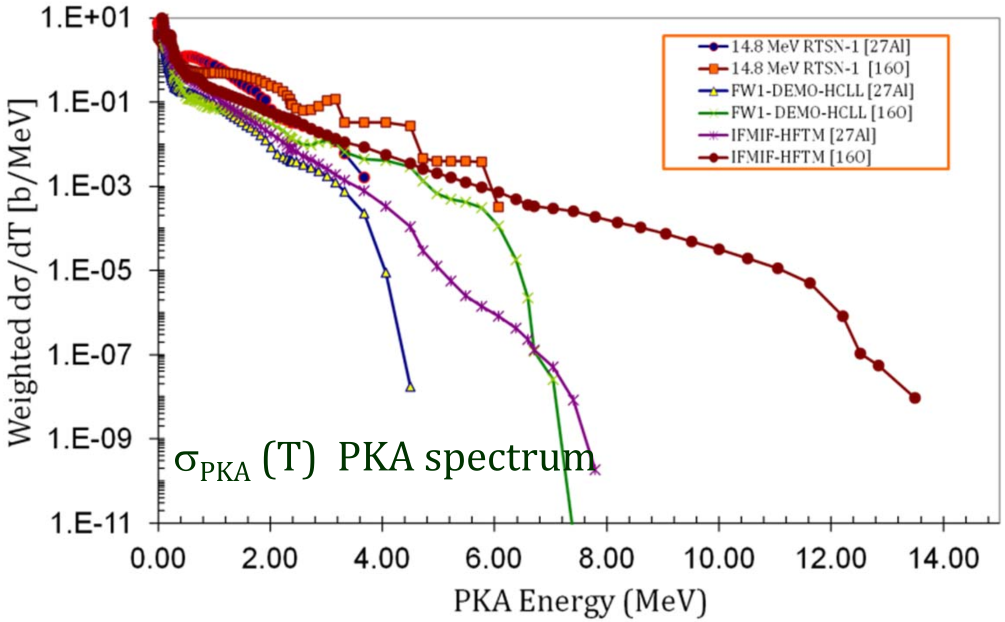
5. Results: a) Simulation of damage function of Al2O3 in irradiation facilities for fusion reactor applications



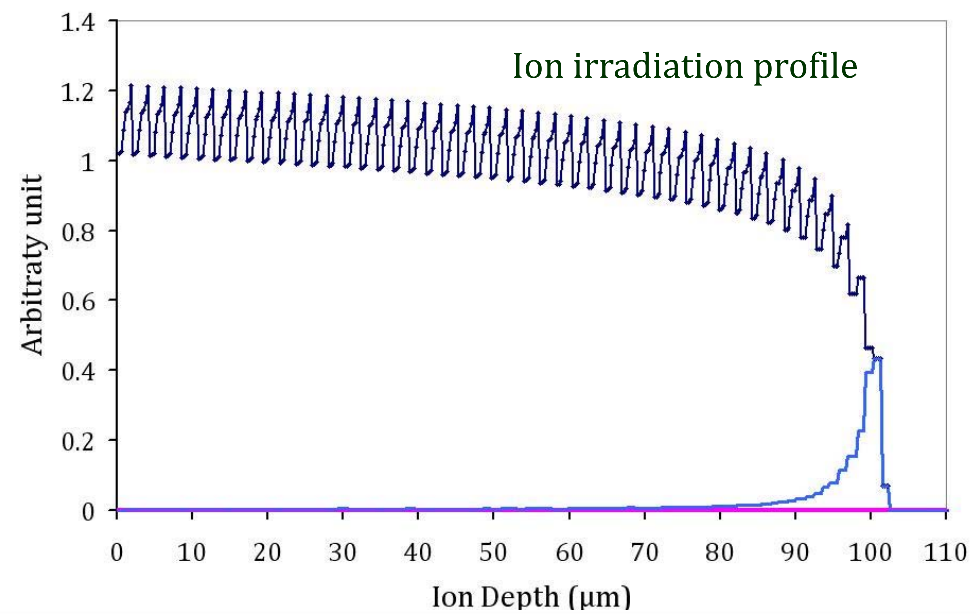


- PKA spectra calculation: induced by neutron irradiation

Neutron spectra for different facilities and irradiation spot

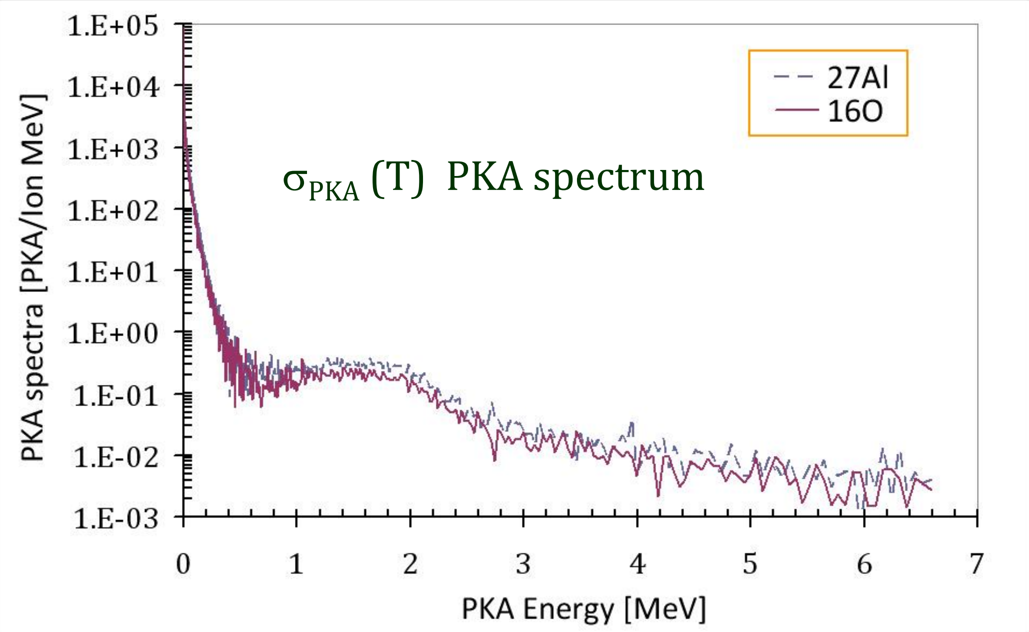
Neutrons spectrum-weighted total PKA's differential cross sections for all the isotopes studied (n + Isotope) in A) HFTM and B) DEMO-HCLL-FW1

5. Results: a) Simulation of damage function of Al2O3 in irradiation facilities for fusion reactor applications



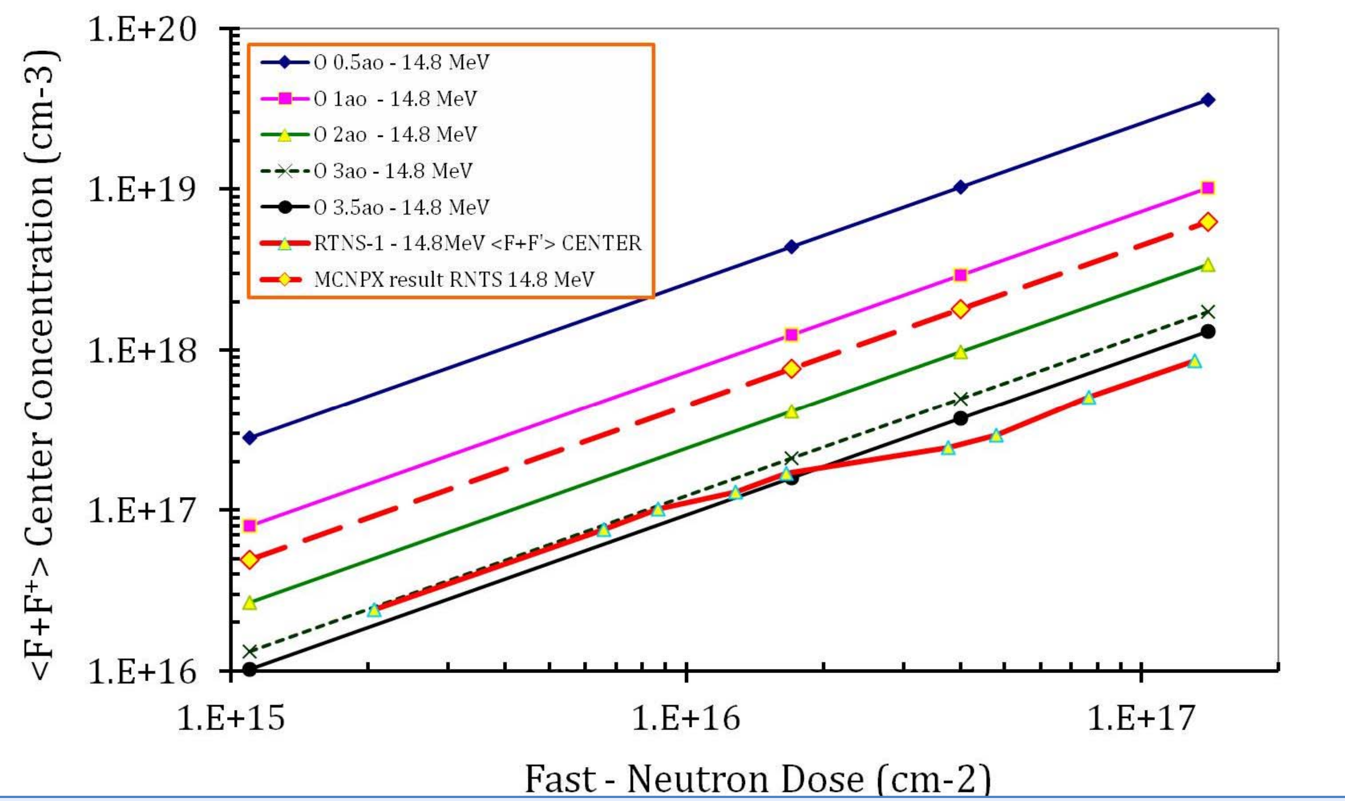
PKA spectra calculation: induced by Ion irradiation with beam degrader

Depth homogeneous profile generated by 27Al Ion irradiation on Al_2O_3 using beam degrader with maximum Ion energy of 300 MeV



27Al and 16O PKA's differential spectra induced by Depth homogeneous profile by 27Al Ion irradiation on Al_2O_3.

5. Results: a) Simulation of damage function of Al2O3 in irradiation facilities for fusion reactor applications: Choice of athermal recombination radius using Marlowe code

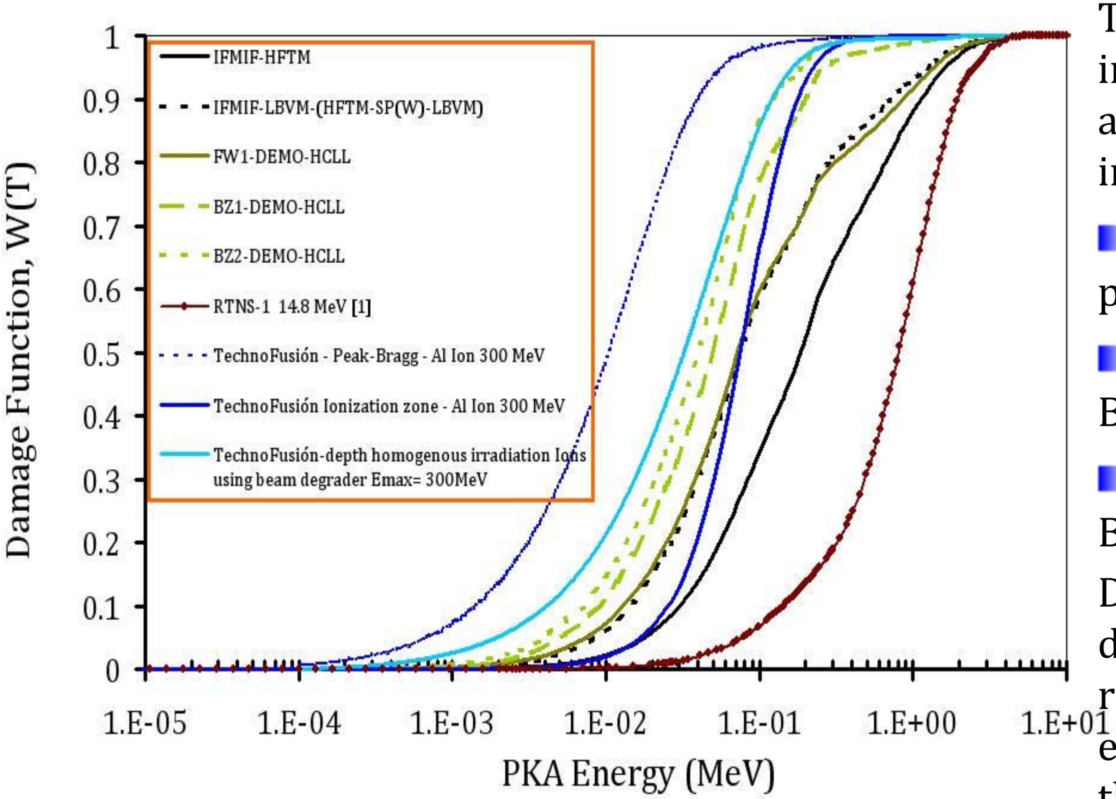


- **The capture radius was fitted to experimental data since nowadays it was not possible to find MD calculations on alumina useful for this issue. But It is important to select experiments with low neutron dose in order to avoid long term evolution of defect events.**

- **The simulation were compared with experimental data carried out with RTNS 14.8 MeV neutron source. In that experiment they calculated the concentration of (F and F^+) centers (*) K. Atobe and M. Nakagawa, Cryst. Latt. Def. and Amorph. Mat. 17 (1987) 229-233**

- **In addition, the experimental and computational data are also compared with calculation carried out using MCNPX code considering the NRT model. They are far from the experimental results.**

5. Result : a) Simulation of damage function of Al2O3 in irradiation facilities for fusion reactor applications



The damage function for different irradiation spots of DEMO HCLL or IFMIF are compare with the damage function induced by

- Depth homogeneous ion irradiation profile.
- Ionization area of monoenergetic Ion Beam
- Bragg Peak area of monoenergetic Ion Beam

Depth homogeneous Ion irradiation (beam degrader) is a good option to perform relevant irradiation experiments to emulate the neutron effects for the back of the breeder zone of DEMO

Facility and irradiation spot		Neutron Source IFMIF		DEMO-HCLL				Ion Source TechnoFusión	
		HFTM	LBVM	FW1	FW2	BZ1	BZ2	Al+ ION irradiation (beam degrader): Emax= 300 MeV	
Thermal power		10MW		4000MW					
n-flux total [n/cm2 s]		6.8E+14	1.7E+14	1.5E+15	1.6E+15	8.3E+14	3.9E+14	Ion intensity	112 nA
MCNPX-NRT (Ed-Al=34 eV, Ed-O=83 eV) [dpa/fpy]		15	2.6	19	20	9	3		
Displacement damage production assuming recombination [dpa/fpy]	Recombination radii r0=3.5 ao							Irradiation depth	100 µm
	rAl= 1.0 ao	7.9	1.6	13.5	13.8	6.1	2.4	[dpa/fpw] assuming recombination	2.1
	rAl= 2.0 ao	3.5	0.7	6.0	6.1	2.7	1.1		1.0
	rAl= 3.0 ao	2.5	0.5	4.3	4.4	2.0	0.8		0.7

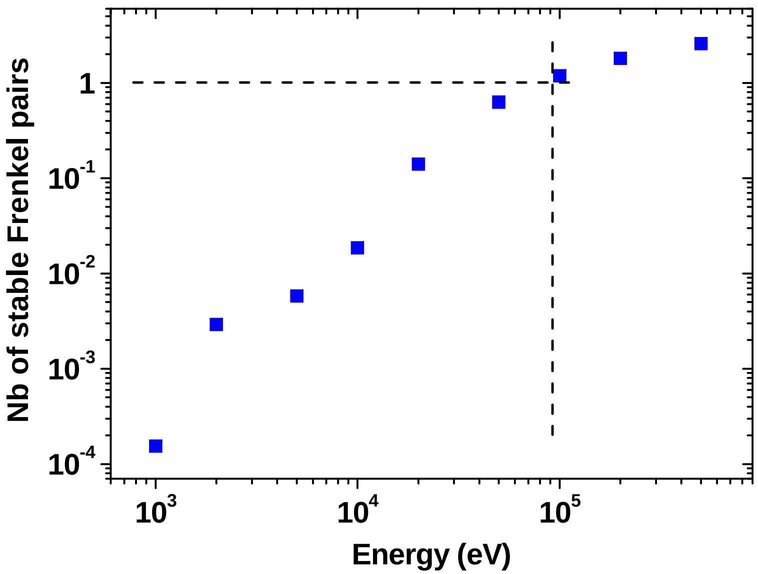
4. 5. Result : b) Formation of stable Frenkel pairs in W

● The formation of Frenkel pairs was simulated for W PKA ranging from 100 eV to 5 MeV. The irradiation of W by H was also simulated for energies ranging from 1 keV to 1 MeV in W polycristal.

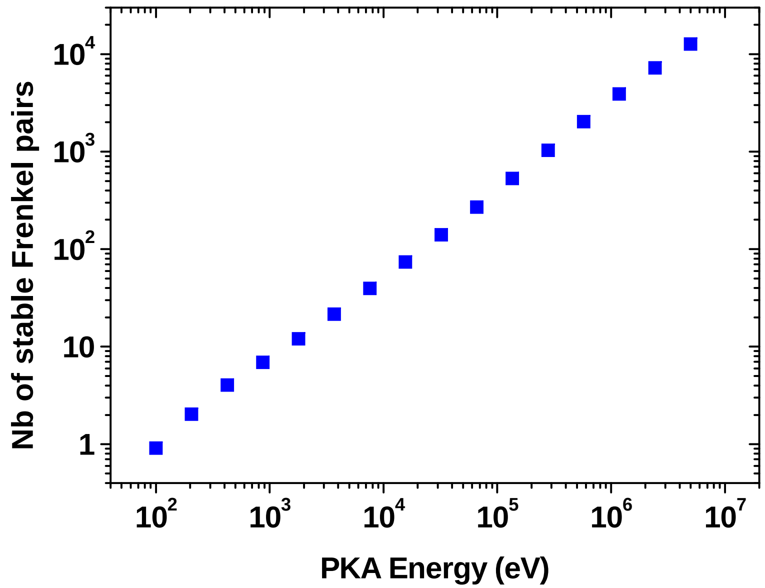
● The capture radius used in the simulations to account for the recombination of defects during cascade is $1.20a_0$, adjusted to reproduce Seidman's experiments*.

● During simulations, coordinates of defects of each cascade can be recorded in order to be used as input in OKMC models (see work in W-Walloys EFDA and LAKIMOCA code).

H irradiation



W PKA



● Statistically, high energies are necessary for H to create a stable Frenkel pair. Expected due to its light mass.

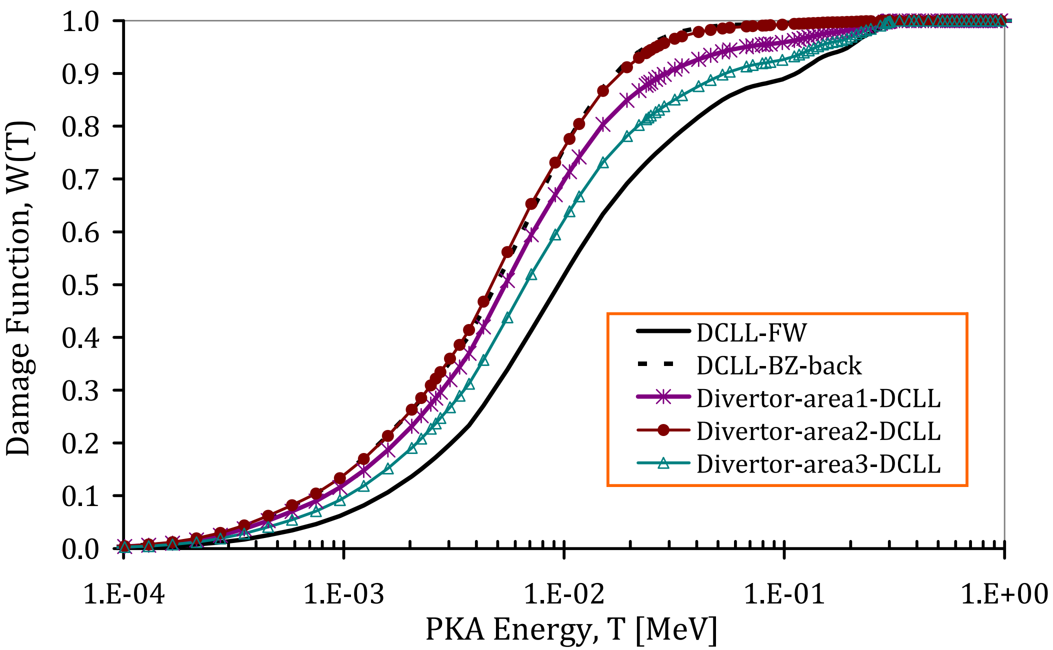
● On the other hand, W only requires a small amount of energy to displace an atom from its lattice site.

*Seidman et al. Phys. Stat. Solid. (b) 144, 85 (1987)

5.- Result : c) Damage Functions of Tungsten in several locations of DEMO

- First: Damage function for Tungsten submitted to the neutron spectra of two locations of the DEMO DCLL, First Wall and Back of the Breeder Zone of DEMO in order to delimitate the extreme irradiation area.

- Second: The damage function for tungsten on the divertor for three different areas.



- Depending on the area of the divertor studied the damage function change considerably.

- For all divertor areas studied the Tungsten suffer less neutron damage than in the first wall of DEMO.

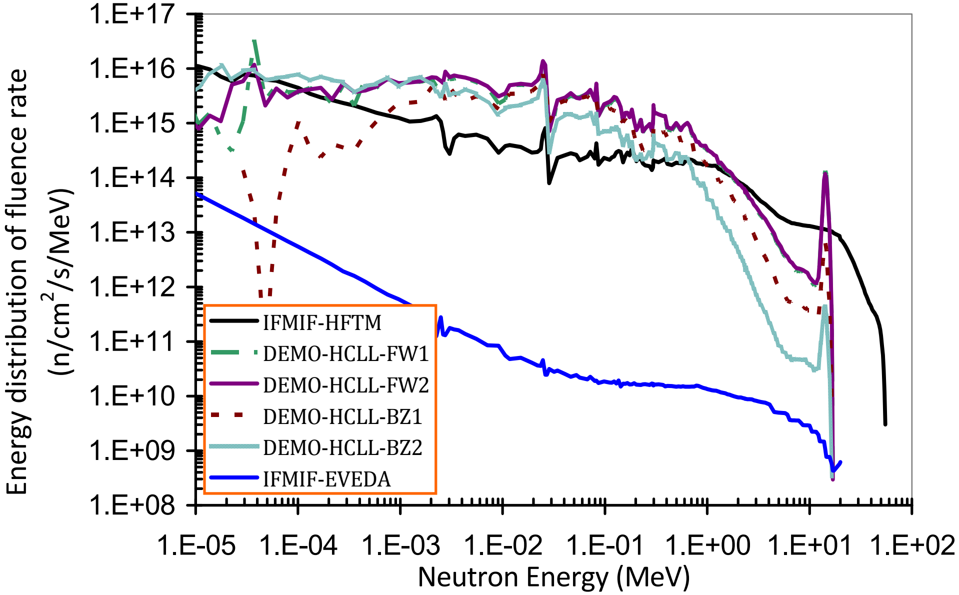
- Regarding neutron irradiation, the dose damage experimented by the tungsten components is similar or lower than that observed in the middle of the BZ of DEMO

Dpa values for tungsten for the divertor and for several inboard blanket locations of the DEMO DCLL

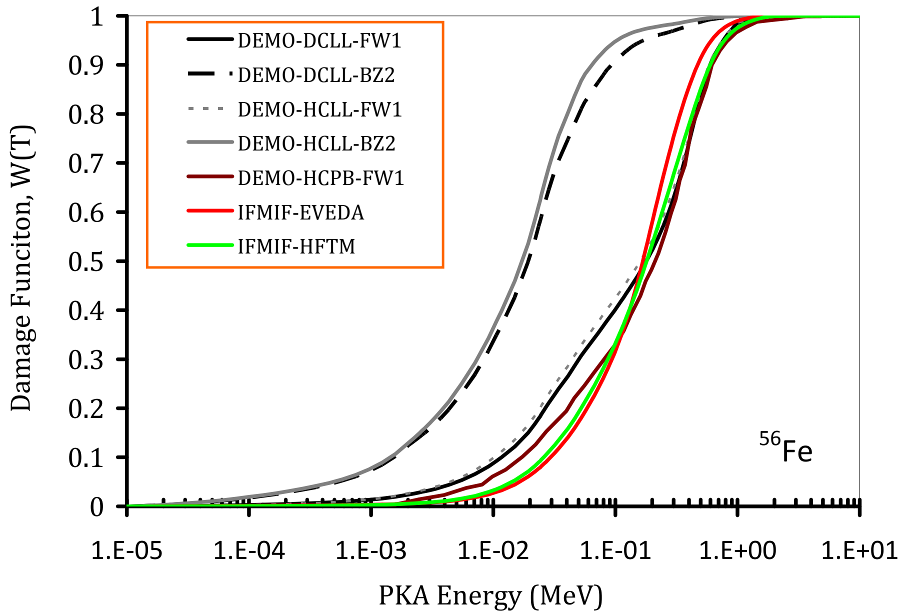
Dpa/year	Blanket of DEMO DCLL				Divertor DEMO DCLL		
	FW (front)	FW (back)	BZ (middle)	BZ (back)	Area 1	Area2	Area 3
Tungsten (19.35 gr/cm^3)	8.1	7.1	4.1	1.5	3.2	2.6	4.6

5.- Result : d) Possible experiments in IFMIF-EVEDA

Neutron spectrum in IFMIF-EVEDA Beam Dump compared with DEMO and IFMIF



Damage Functions of Iron in DEMO, HFTM-IFMIF and in LIPAc Beam Dump



Facilities and irradiation spots		Neutron Fluence Rate [n/cm²s]	MCNPX dpa calculation [dpa/fpy]	Methodology calculation [dpa/fpy]
DEMO-HCLL	FW1	1.52762E+15	30	6.8
	FW2	1.58466E+15	29	6.6
	BZ1	8.29694E+14	8	1.8
	BZ2	3.91556E+14	2	0.5
IFMIF-EVEDA	Beam Dump	9.3971E+10	6.5E-03	7.2E-04
IFMIF	HFTM	6.79149E+14	31	6.5

Summary

1. Motive of this work
   a) Fusion Power Reactors
   b) Emulated the Fusion neutron with other neutron sources
   c) Simulation of Neutron Irradiation Effects with Ion irradiation

2. Standard damage dose calculation
   a) Neutron irradiation
   b) Ion irradiation

3. Simulation of defect generated by neutrons and Ions: methodology used

4. Analyses of the displacement damage generation
   a) Simulation of defect formation in materials under irradiation
   b) Description of MARLOWE code
   c) Comparison MARLOWE vs SRIM
   d) Recombination of defects during cascade
   e) Simulation of energy loss of high-energy particles: Modification of MARLOWE
   f) Analyses of damage function induce by monoenergetic Ions (Bragg Peak)
   g) Damage profiles
   h) Damage function and damage dose calculations

5.- Results

6- Conclusions

6.- Conclusions

- A methodology was developed to calculate the damage due to fusion neutrons in Materials (monocristal, polycristal and amorphous systems). This methodology is based on the methodology developed by KIT laboratory. It consists of a combination of Nuclear Data Libraries Processing, Neutronic transport and Monte Carlo Binary Collision codes.

- This Methodology allows to design irradiation experiments with ions to emulate neutron fusion effects in materials. It is possible because the displacements damage generation have been calculated using the same methodology for both neutron and ion irradiations (starting from PKA spectra)

- The resulting damage profile used to calculate damage function and damage dose was calculated using MARLOWE code.

  - A dedicated module developed at CIEMAT was used to account for energy loss of Ions in materials at energies in the Bethe regime (>> 25 keV / amu).

  - Allows defining the lattice structure and accounts for effects such as channeling, replacements, linear collision sequence, etc….

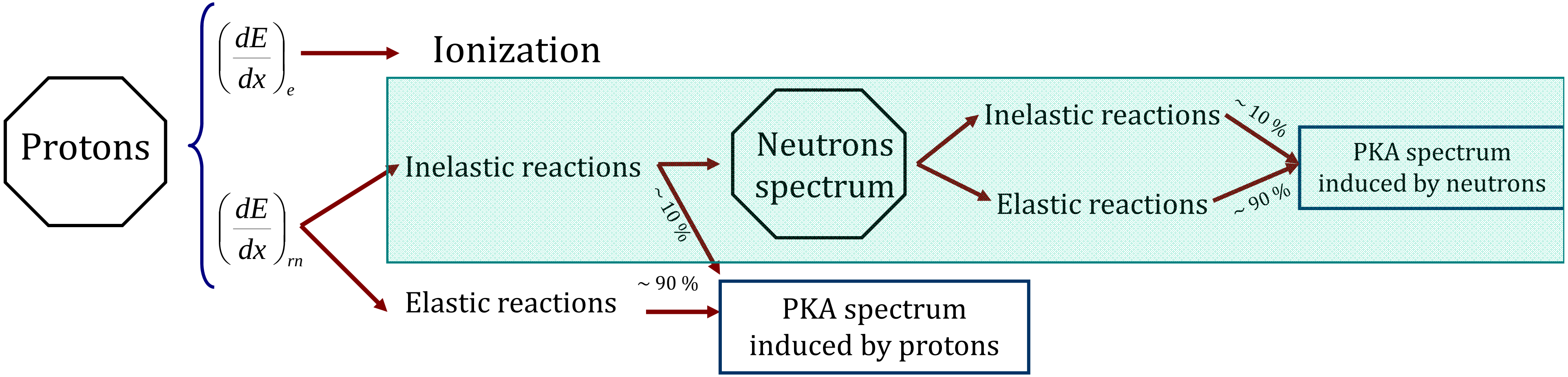
  - In order to take into account the recombination of defects, the capture radius is generally adjusted on experiments or MD calculations.

  - A subroutine was implemented to calculate the PKA spectrum on different depth bins of the implantation profile.

- Mainly, a methodology to develop displacement damage data libraries using the MARLOWE code is proposed in order to standardize the calculation of primary displacement damage on compound materials.

Future Works

- Extend this methodology to proton irradiation



To develop

Thank you
for your attention

3. Simulation of defect generated by neutrons and Ions: methodology used

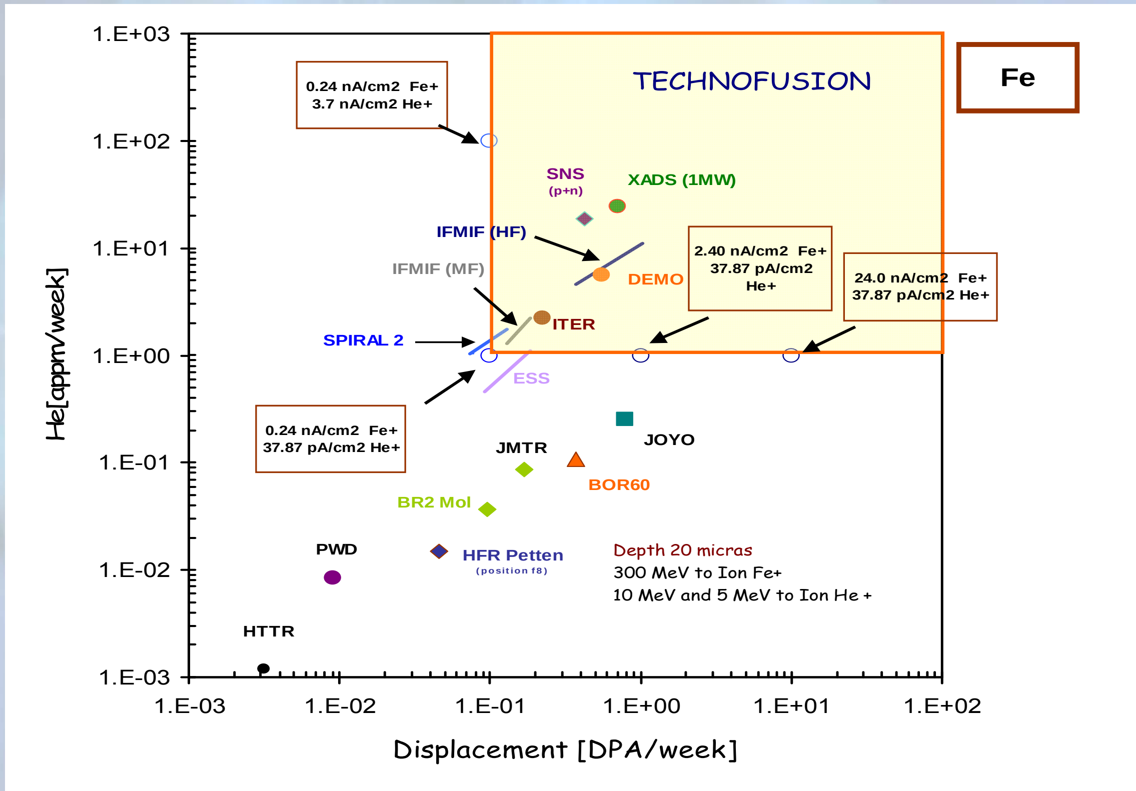
- The level of damage expected in fusion conditions is such that the performance of materials and components under these extreme irradiation conditions is still unknown. It is very important to predict the generation of the displacement damage.

- * Neutron irradiation induces Elastic and Inelastic nuclear reaction. The displacement of ions (PKA spectrum) are generated with both elastic and inelastic reactions, although the elastic reaction contribute, more or less, in more than of a 90 %, depending on the isotope analyze.

- Heavy Ion (PKA spectrum) irradiation mainly induces elastic reactions producing displacements damage.

- Neutron/Ion irradiation produces different types of defects: I, V, He, H, clusters…

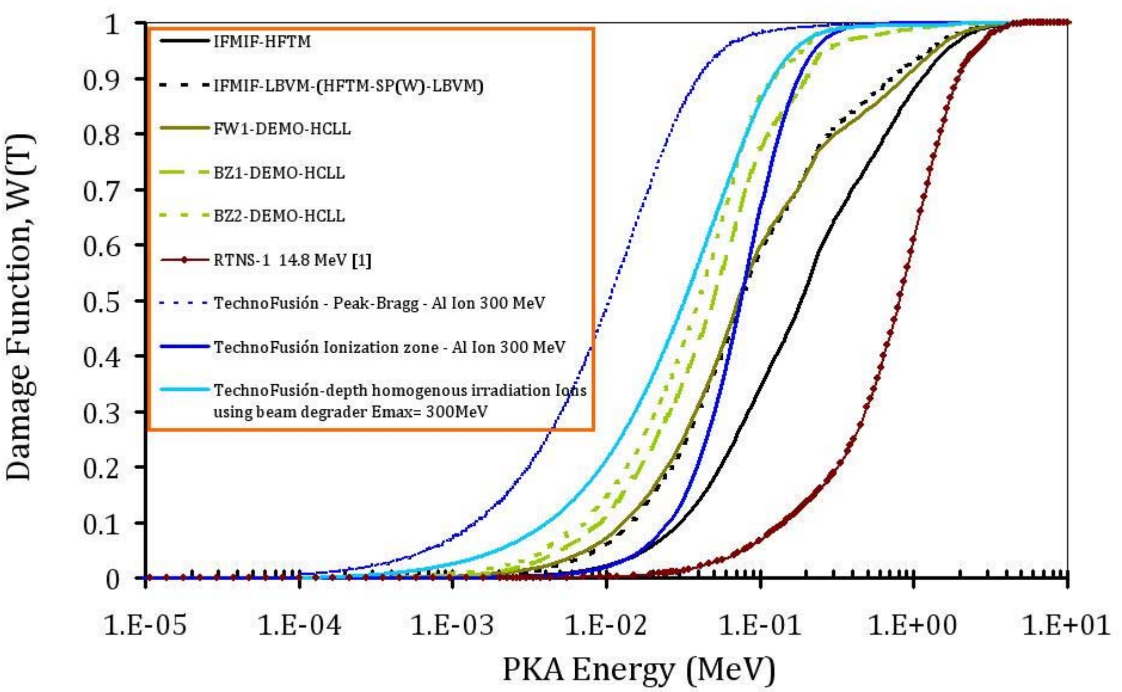
- The calculation of damage generated by fusion neutrons requires a dedicated methodology since, in principle, available codes only simulate the stopping of ions, not neutrons which are not subject to a coulombic potential.



TECHNOFUSION
Fe
0.24 nA/cm2 Fe+
3.7 nA/cm2 He+
0.24 nA/cm2 Fe+
37.87 pA/cm2 He+
2.40 nA/cm2 Fe+
37.87 pA/cm2
He+
24.0 nA/cm2 Fe+
37.87 pA/cm2 He+
SNS
(p+n)
XADS (1MW)
IFMIF (HF)
IFMIF (MF)
DEMO
ITER
SPIRAL 2
ESS
JOYO
JMTR
BOR60
BR2 Mol
PWD
HFR Petten
(position f8)
HTTR
Depth 20 micras
300 MeV to Ion Fe+
10 MeV and 5 MeV to Ion He +
He[appm/week]
Displacement [DPA/week]
1.E+03
1.E+02
1.E+01
1.E+00
1.E-01
1.E-02
1.E-03
1.E-03
1.E-02
1.E-01
1.E+00
1.E+01
1.E+02

5. Result : a) Simulation of damage function of Al2O3 in irradiation facilities for fusion reactor applications

- Damage function and damage dose

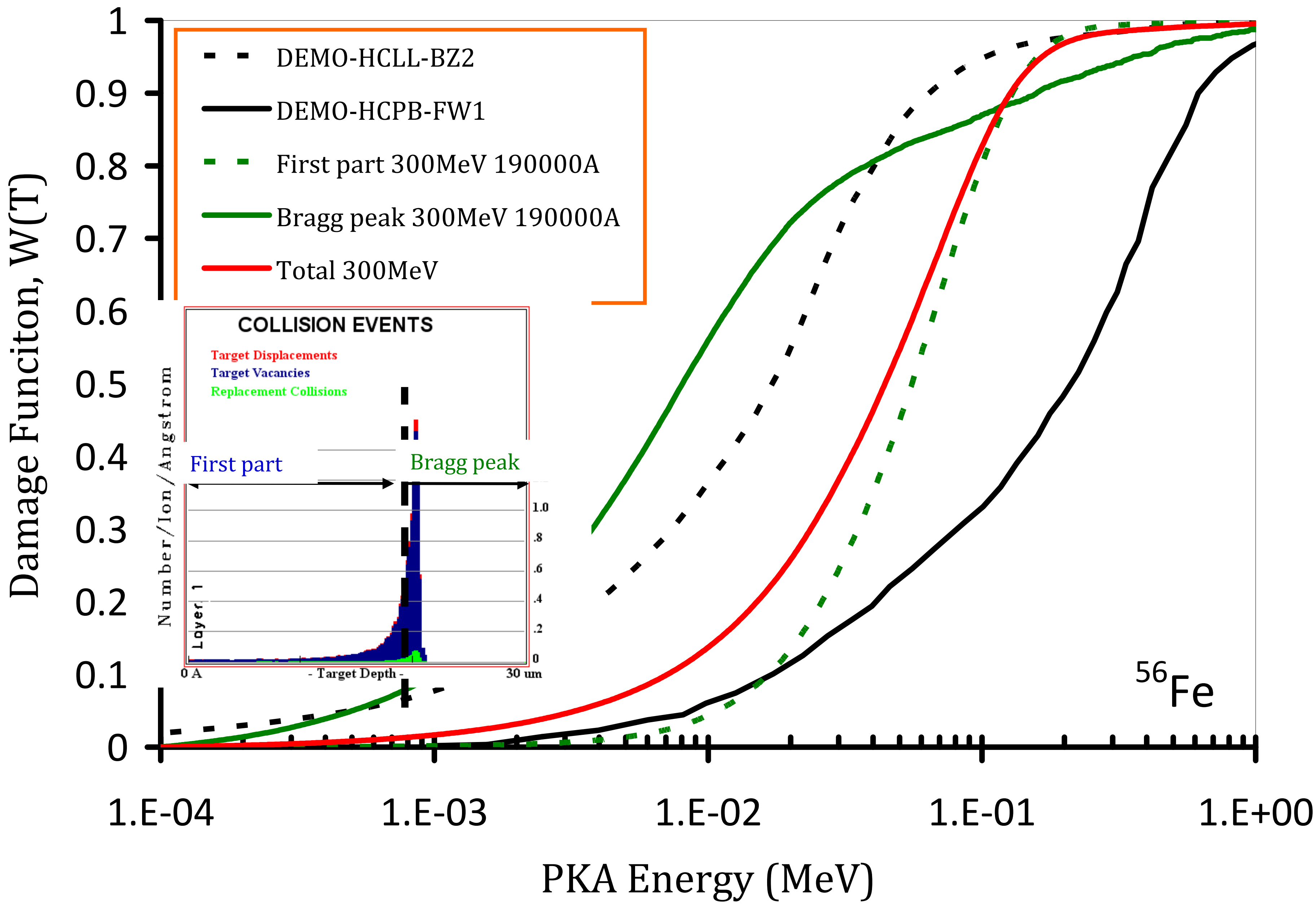


- The damage function for TechnoFusión considering depth homogeneous irradiation (beam degrader) is a good irradiation spot to perform relevant irradiation experiments for the back of the breeder zone of DEMO. Ionization area of the TechnoFusión monoenergetic Ion Beam is a good area to reproduce the level of damage expected in the breeder zone of DEMO. This configuration is recommended to have an accelerated testing.

- The LBVM gives a damage function that fits with the expected for the beginning of the breeder zone of DEMO, but the dose damage is closer to expected in the back of the breeder zone of DEMO.

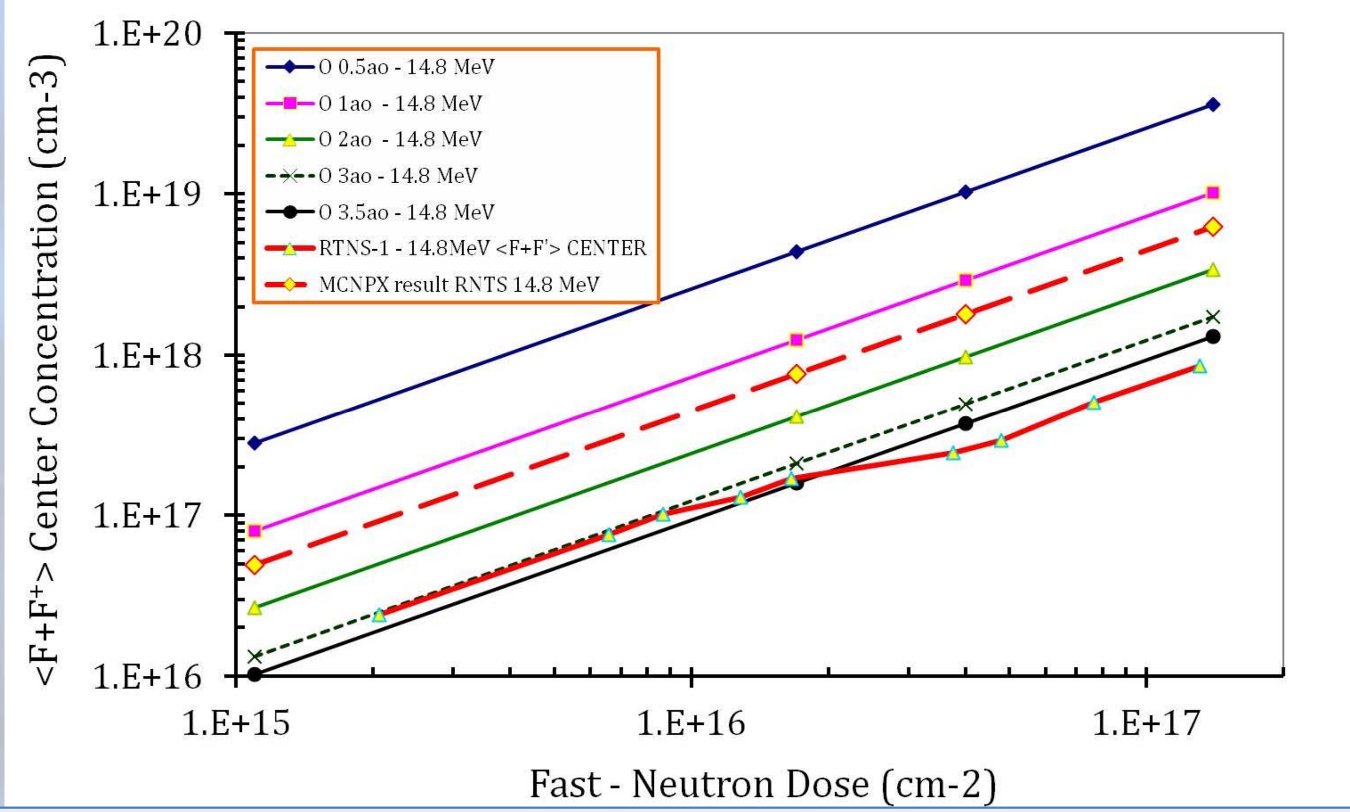
Facility and irradiation spot		Neutron Source IFMIF		DEMO-HCLL				Ion Source TechnoFusión	
		HFTM	LBVM	FW1	FW2	BZ1	BZ2	Al+ ION irradiation (beam degrader); Emax= 300 MeV	
Thermal power		10MW		4000MW					
n-flux total [n/cm2 s]		6.8E+14	1.7E+14	1.5E+15	1.6E+15	8.3E+14	3.9E+14	Ion intensity	112 nA
MCNPX-NRT (Ed-Al=34 eV, Ed-O=83 eV) [dpa/fpy]		15	2.6	19	20	9	3		
Displacement damage production assuming recombination [dpa/fpy]	Recombination radii r0=3.5 ao							Irradiation depth	100 μm
	rAl= 1.0 ao	7.9	1.6	13.5	13.8	6.1	2.4	[dpa/fpw] assuming recombination	2.1
	rAl= 2.0 ao	3.5	0.7	6.0	6.1	2.7	1.1		1.0
	rAl= 3.0 ao	2.5	0.5	4.3	4.4	2.0	0.8		0.7

5. Result: b) Analyses of damage function induce by monoenergetic Ions (Bragg Peak)



5. Results: a) Simulation of damage function of Al2O3 in irradiation facilities for fusion reactor applications

Choice of athermal recombination radius using Marlowe code



Computational and experimental results of the oxygen vacancies concentration depending on the fast neutron dose induced by the neutron source (14.8 MeV) RTNS-1. For experimental data the oxygen vacancies was determined by the sum of F and F+ center. The simulation results, are represented with the legend "O [0.5, 1.0, 2.0, 3.0, 3.5]aO – 14.8 MeV" for each recombination radius value. The experimental data is shown with the legend "RTNS-1 14.8 MeV <F+F+> CENTER". In addition, the data are also compared with calculation carried out using MCNPX code considering the NRT model