ICTP-2026 – VC2 report:
Italy, Triest, ICTP, 20-24 April, 2009

Radiation Damage, Activation and Transmutation of Structural Materials under Long Time Neutron Irradiation (Fusion and Fast Power Reactors)

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The nuclear data base, codes, models and results of investigations of nuclear properties (radiation damage, activation, transmutation and cooling) of metals and based on them structural materials (SMs – steels and alloys mainly for cores) under long neutron exposure (up to 50 years) in the neutron spectra of the RF fast reactor BN-600 and fusion reactor DEMO-RF (the Kurchatov Institute project) are discussed. Two types of the RF SMs are considered: the reduced activation ferritic-martensitic steel (RAFMS) RUSFER-EK-181 (Fe-12Cr-2W-V-Ta-B-C) and low activation (LA) vanadium alloy V-4Ti-4Cr. The analysis of the induced activity in the SMs after their irradiations was carried out for cooling times up to 1000 years. The SMs compositions and neutron spectra used are very typical for the international nuclear community for power nuclear fission and fusion reactors.

The known code FISPACT and the new version of the RF basis library complex ACDAM have been used in the analyses. The RF complex ACDAM includes three parts: (1) ACDAM/ACT – activation/transmutation neutron cross-sections for 704 isotopes from H-1 to Po-210; (2) ACDAM/DEC – decay data library for approximately 1960 radioactive isotopes from H-3 to Cf-252, and (3) ACDAM/DDL – damage data library to calculate the primary radiation damage (dpa) of all compositions of SMs. The complex FISPACT+ACDAM allow to receive all information on nuclear properties of SMs under long time irradiation by neutrons with their energy up to 20 MeV and presented in the endf-6 format.

Primary radiation damages were calculated follow the well known NRT-standard model. In this model the value of the primary radiation damage (displacement per atom - dpa) is the main parameter to compare the radiation damages of SMs under irradiation of different neutron spectra. Nowadays this standard is very popular, but its physical basis is not enough for real applications. The unsolved questions of the NRT-standard are connected with physics of collision cascades under irradiation in real SMs.

Molecular dynamics simulation of the collision cascades and their influence on the generation of radiation damage areas was carried out in vanadium crystals with inner structure (with grain boundaries). Interatomic interactions were described by known many body empirical atomic potential. Developmental character of the displacement cascades is determined in many respects by the presence of extensive interfaces in materials. Grain boundaries act as barrier for expansion of displacement cascades and accumulate considerable proportion of radiation defects.

As conclusion the summary can be made: (1) the complex FISPACT+ACDAM is practically ready for all nuclear calculations (activation-transmutation-cooling-primary damage in NRT-standard (dpa); (2) it is the actual necessity of the development of the new radiation damage standard on the basis of the up to now and nearest future knowledge of physics collision cascades, crystal lattice models with inner structures, the physical properties of SMs under neutron irradiation and the local neutron spectra of advanced power reactors.

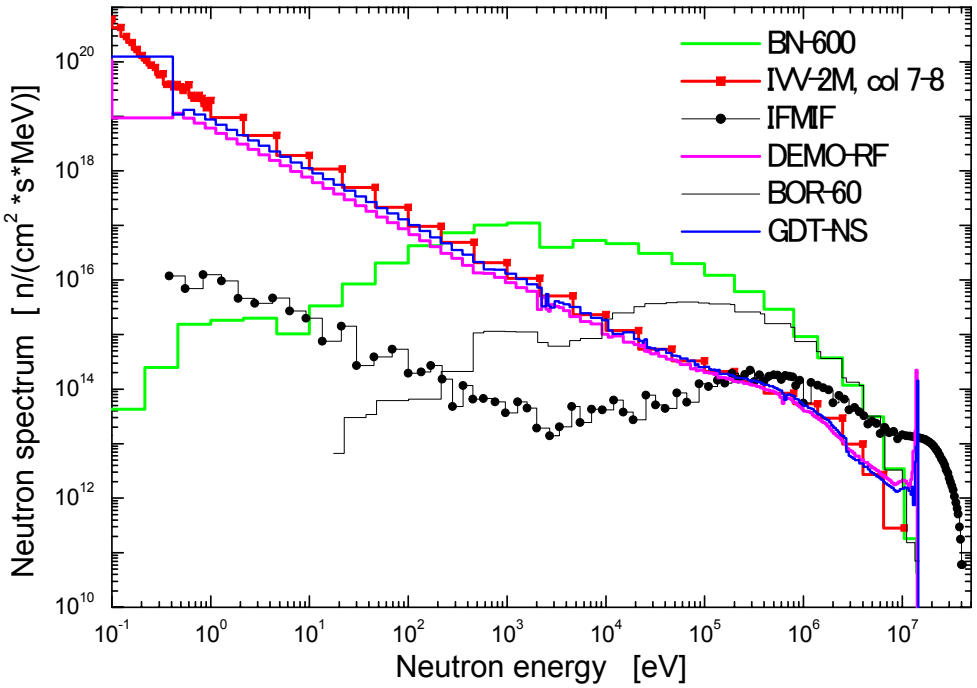
THE RF NUCLEAR FB&FUSION POWER REACTORS – GOALS&REQUIREMENTS

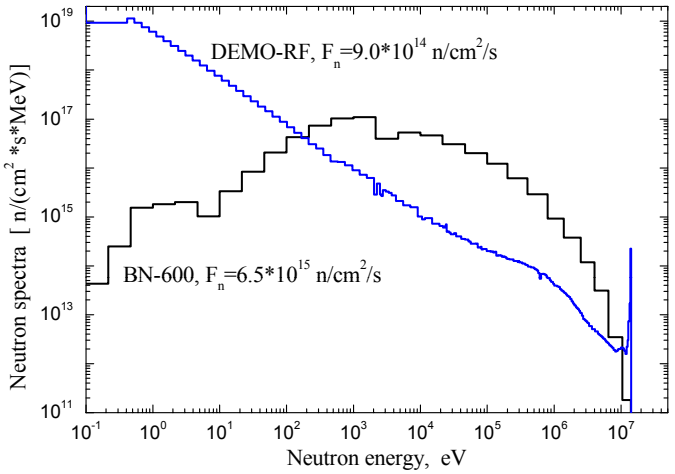
- **Nuclear power reactors:**
  - **F**ast **B**reeder **R**eactors Way (FBRs, Na-Coolant): BN-600 (2020↓), BN-800 (2012↑), BN-K (commercial type BN-1200, 2020↑, under elaboration),
  - Fusion: DEMO (2035↑) and **F**usion **P**ower **P**lant (FPP, 2050↑).

- **Requirements for the Structural Materials (SMs, operation):**
  - FBRs – the fuel burning are (12)17-20-25 % h.a., (80)100-200 dpa,
  - Fusion (DEMO-FPP) - 10-15 MW year/sq.m, 100-200 dpa.

- **Requirements for the SMs (after operation/accident):**
  - Storage, Reprocessing, Low activation, Fast decay of radioactive inventory, Ecology.

Neutron Sources





BN-600 – Fast Sodium Power Reactor,
IVV-2M – Experimental water reactor,
IFMIF – accelerator neutron source (IEA project),
DEMO-RF – Fusion reactor (RF project),
BOR-60 – experimental sodium fast reactor,
GDT-NS – plasma neutron source (RF project).
ITER – under construction (Kadarash, France).

FLUX F_n (n/cm^2/s, E > 0):

BN-600: 6.50* 10^{15} ,
IVV-2M : 5.29* 10^{14},
IFMIF: 6.71* 10^{14} ,
DEMO-RF: 9.00* 10^{14} ,
BOR-60: 3.00* 10^{15} ,
GDT: 5.18* 10^{14} ITER: 3.88* 10^{14}

THE RF SMs FOR POWER NUCLEAR REACTORS

The priorities are the radiation and heat resistance low (reduced) activation SMs . New advanced SMs (mainly for cores) are required for further widening of temperature, mechanical and dose application windows.

The SMs: **→ 100-200 dpa:**

1. **12% Cr RAFMS: type RUSFER-EK-181: Fe-12Cr-2W-V-Ta-B-C (+ technological minimum of impurities).**
   Applications: FBRs: BN-600, BN-800, BN-K (Na). DEMO-FPP (Pb-Li, He).
2. **LA Vanadium alloys type V-4Ti-4Cr (+ technological minimum of impurities).**
   Applications: DEMO-FPP (Li, He). FBRs: BN-K (Na), HTGR (He).

The RF referenced and advanced compositions of the SMs and neutron spectra are sufficiently typical for the international nuclear community for power nuclear fission (FB) and fusion (DEMO) reactors.

THE QUESTIONS ON THE WAY TO THE ADVANCED SMs FOR NUCLEAR POWER REACTORS (mainly for cores of the FB&FUSION reactors)

DIFFERENT:

- NEUTRON SPECTRA.
- NEUTRON FLUXES AND FLUENCES.
- DAMAGE RATES.
- STRUCTURAL MATERIALS AND NUCLEAR TECHNOLOGIES.
- MODELS AND APPROACHES.

HOW TO COMPARE THE RESULTS ?

HOW TO USE THE UP-TO-DATE EXPERIMENTAL RESULTS ?

HOW TO DO THE SCIENCE-BASED RECOMMENDATIONS ?

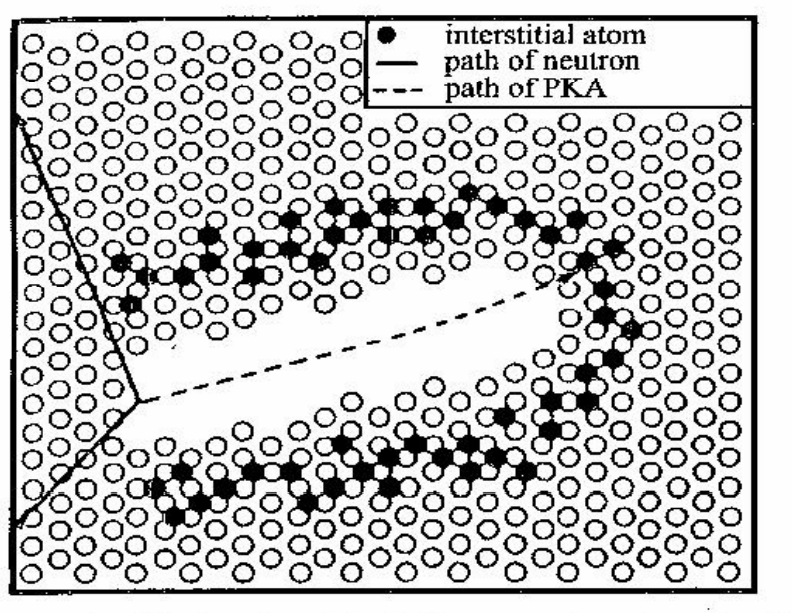
WHAT NEUTRON SOURCES ARE NECESSARY TO PROVIDE ADEQUATE SMs DATABASE FOR THE DESIGN OF INNOVATIVE FISSION AND FUSION POWER REACTORS IN TIME ?

OUR SCIENTIFIC GOALS ON THE WAY TO NEW SMs FOR POWER NUCLEAR REACTORS: PRIMARY RADIATION DAMAGE (PRD)

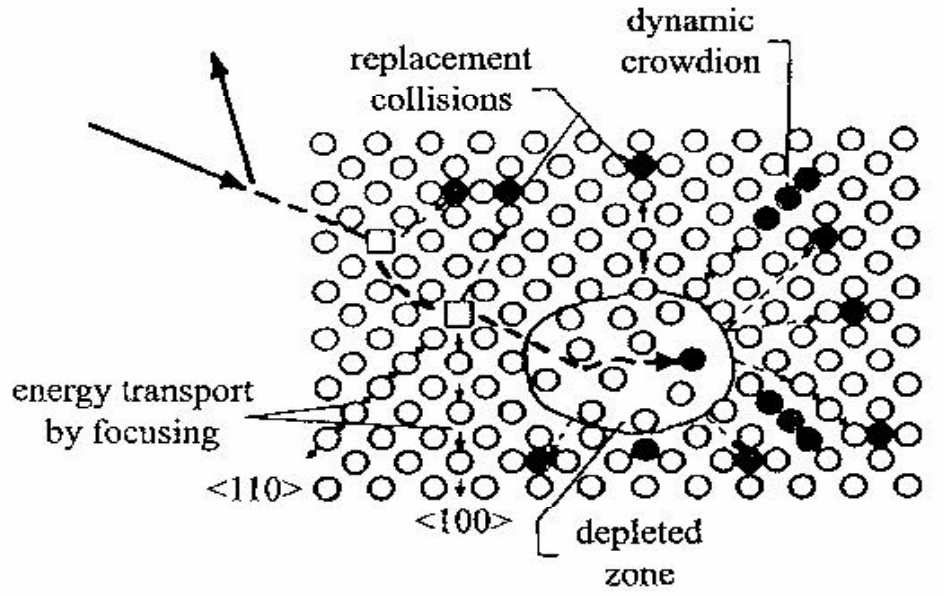
- To determine more detailed the elementary interactions between the radiations and the atoms of solids: elastic collisions, electronic excitations and nuclear reactions.
- To determine the energy of the primary knock-on atom (PKA) and to characterize the recoil spectra produced by the different bombarding particles.
- To prepare the nuclear data bases, codes, models and results of the PRD, activation, transmutation and cooling of SMs during and after irradiation for ensuring the outstripping development of SMs (mainly for cores) for the fission and fusion reactors.
- To calculate NEUTRON TRANSMUTATIONS (burn-in and burn-out of essentially all elements).
- To know a Nuclear Alloyage, especially H and He formations by all (n,p-d-t) and (n,α) reactions.
- To carry out the analysis of the induced activity in the SMs after their irradiation for long cooling time, to suggest the LA compositions with the level of the residual induced activity less than 10^{-2} Sv/h ("remote level") and the possibility of recycling of irradiated SMs for the time not more than 100 years after operation.

Materials with the activity level less then $2{,}5*10^{-5}$ Sv/h ("hands on level") is considered as not activated (natural) material.

PRIMARY RADIATION DAMAGE(PRD): COLLISION CASCADE
(history start, 1956)



Original version of the collision cascade from the Primary Knock-on Atom (PKA) as the **displacement spike** with a high core density of vacancies surrounded by an interstitial shell (Brinkman J.A., 1956)



Revised version of the displacement spike from the PKA as a **depleted zone** for the crystallite with the focusons, replacement collisions and channeling (Seeger A., 1958)

COLLISION CASCADES IN CRYSTALS

Direct inside into the displacement process cannot be followed with present experimental techniques and is obtained mostly from computer simulation studies – via supercomputers. Different computer simulation techniques have been used to study the complex process of the slowing down of an energetic ion in a crystal.

Basic algorithms (all largely stochastic in nature):

1. Monte-Carlo method (fa, programs type TRIM).
2. Molecular dynamic simulations (MDS) have been pioneered by G. Vineyard (1963).

The MDS is a technique for computing the equilibrium and transport properties of a classical many-body system.

Many suggested codes permit to research all cascade stages in a unified manner. But in all cases (analytic and numerical) there are many additional approximations (sometimes very questionable):

- many-body problem (electrons and nuclei), long-range forces, 0D-3D defects and its electronic states, effective charges of moving ions, initial state of a model crystallite with inner structure, thermal effects, etc.
- methods of data processing of very massive numerical results to find the general regularities and to estimate and to identify the basic physical mechanisms of the collision cascade and its influence on physical properties of materials.

For reviews see:

(1) D.Frenkel and B.Smit: Understanding MOLECULAR SIMULATION. From Algorithms to Applications. AP, 2002.

(2) Computer Simulation in Materials Science. Nano/Meso/Macroscopic Space&Time Scales. Eds: H.Kirchner, L.Kubin, V.Pontikis. Kluwer AP, 1996.

(3) Gary S. Was. Fundamentals of Radiation Materials Science. Metals and Alloys. Springer, 2007

PRIMARY RADIATION DAMAGE (PRD): DISPLACEMENT PROCESS AND CASCADE

0. **10^{-18} s**: Energy transfer from the incident particle (neutron/ion, including the products of nuclear reactions) – Formation of a primary knock-on atom (PKA).
1. **≈ 10^{-13} s**: Dynamic (ballistic) stage: Slowing down of PKA. Generation of collision cascade as a collection of point defects – vacancy-interstitial (or Frenkel) pairs as the basic elements of radiation damage. No atoms with energy more than material-dependent threshold energy for displacement. The PRD determines by the number of displacement atoms of crystal lattice *dpa* (displacement per atom) as a dose unit.
2. **≈ 10^{-11} s**: Relaxation (recombination) stage – Energy dissipation, spontaneous recombination and clustering – collection of point defects and its clusters in the crystal lattice (maximum temperature of cascade area – thermal spike).
3. **≧ 10^{-8} s**: Diffusion (basic) stage – Defect mobility and reactions by thermal migration, spike core solidification and cooling to ambient temperature.

The PRD event is concluded when the PKA comes to rest in the lattice as an interstitial atom (the end of the diffusion stage).

CASCADE EFFICIENCY = N_{def} (stage 3) / N_{def} (stage 1) < 1 (≈ 0,2 – 0,4).

Subsequent evolution of the radiation defects (after the diffusion stage 3) follows the usual thermodynamic life of real crystal: Kinetic Monte Carlo or Rate Equations codes with parameters from MDS, Quantum Mechanics and Experiments.

PRIMARY RADIATION DAMAGE (PRD): DPA AS A DOSE UNIT - "**NRT – STANDARD**"

The production of point defects (Frenkel pairs) via collision cascades is the dominating cause for property changes in metallic SMs for nuclear reactors.

The level of DPA is the main parameter to compare the radiation damages of SMs under irradiation by different neutron spectra. Up to nowadays the main model to calculate the level of the PRD via DPA units is the "NRT-standard" as the main international convention for real application (**NRT model**: **N**orget, **R**obinson and **T**orrens,1975).

Reliable and user-friendly computer programs for calculating such data for practically all target/irradiation particle-combinations are now generally available. Providing the recoil spectrum would allow to estimate the range of cascade sizes and densities and the number of defects surviving cascade cooling ("cascade efficiency factor"). Although these parameters are in generally not the quantities which finally control the different radiation damage effects (swelling, creep, segregations, strength, etc.), their knowledge would be a further step towards a better correlation of results obtained from different irradiation sources.

Although it is now well established that the dpa-number calculated by the "NRT-standard" does in general not accomplish any correlation of the radiation damage induced by different bombarding particles with irradiation properties of materials, the NRT-convention should be retained.

TRANSMUTATION/ACTIVATION OF SMs

D(t) - Formation of a nuclear product **A** up to irradiation time **t.**

D_0 (t)- Formation rate of a product **A.**

σ(E) – cross sections of all nuclear reactions for a product **A.**

φ(E) dE – the neutron flux in energy interval (E, E+dE),

n – the number of the material components (chemical composition) with the concentrations $\mathbf{x_i}$ (i = 1, 2, …, n) forming a product **A.**

$\mathbf{E_m}$ – minimum energy for nuclear reactions with formation of a product **A.**

$$D(t) = \int_0^t D_0(\tau)\, d\tau$$

$$D_0 = \int_{E_m}^{\infty} \sigma(E)\varphi(E)dE$$

$$\sigma(E) = \sum_{i=1}^{n} x_i \sigma_i ,$$

Low Activation or Reduced Activation Chemical Elements under Neutron Irradiation (FB&DEMO reactors):

RAFMS: **Fe-Cr-W-Ta-V-C,** LA V-alloys: **V-Ti-Cr-C,**

LA Composite: **SiC_f / SiC**

RADIATION RATE DAMAGE K_d , dpa/s, (formation of stable Frenkel's pair):

$$K_d = \int_{E_{\min}}^{\infty} \sigma_d(E)\varphi(E)dE, \quad \sigma_d(E) = \int_{T_d}^{T_{\max}} \nu(T)\frac{d\sigma(E,T)}{dT}dT$$

φ(E) dE– a density of neutron flux in the energy interval (E, E+dE);

$\sigma_d(E)$ – DPA Cross Section;

T – the kinetic energy of the residual nucleus;

T_d - the effective threshold energy needed to shift a nucleus from lattice position;

dσ(E,T)/dT – the spectrum of the recoil residual nucleus (the PKA spectrum) in LAB-system produced via all nuclear elastic, inelastic, (n,2n), (n,p), (n,α), (n,γ) and so on reactions;

v (T) – cascade function, the number of displacement atoms produced by the PKA with energy ***T*** (fa, NRT model + IAEA recommendations).

SMs: TRANSMUTATION/ACTIVATION/COOLING. RADIATION DAMAGE (dpa).

NATIONAL LIBRARIES AND CODES (EXAMPLES)

EU – EASY,

USA – CINDER-90,

JA – TRANSM + RADHEAT-V4,

RF – ACDAM + FISPACT

THE RF NUCLEAR DATA COMPLEX "ACDAM".
The neutron energy in the range (10^{-5} eV - 20 MeV), endf-6 format

1. ACDAM/ACT –

ACtivation/**T**ransmutation neutron Cross Section base to calculate the activation and transmutation (all known nuclear reactions) of materials.

704 target isotopes from H-1 to Po-210.

56 target isotopes from Th-228 to Cf-252.

EVALUATED DATA LIBRA-RIES: FENDL/A-2, EAF-99, BROND-2(3), ENDF/B-VI.3, IRDF-90, JENDL-3 (fission pro-ducts), CENDL-2 (fission products).

Used the RF new evaluations on the basis of experimental and theoretical results and its systematization:

≈ 2600 nuclear reactions were updated and re-evaluated.

2. ACDAM/DeDaL –

DEcay **DA**ta **L**ibrary is based on the EAF-99 and FENDL-2/D Decay Data Libraries.

≈1960 radioactive isotopes from H-3 to Cf-252.

3. ACDAM/DDL –

Damage **D**ata **L**ibrary to calculate the primary radiation damage (dpa-NRT+IAEA recommendations) of all SM-compositions (from H-1 to Au-107).

The DDL library is based on processing of the general purpose data files from the ENDF/B-VI.3 and BROND-2(3) libraries.

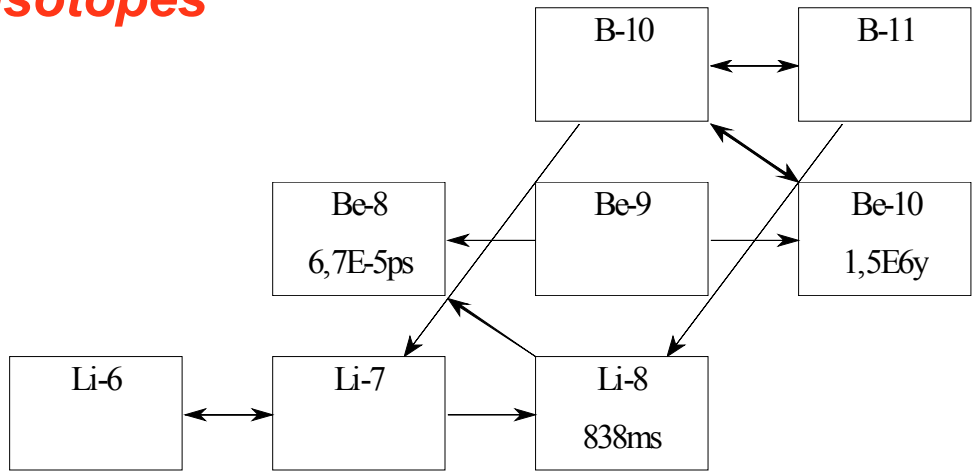
Atomic displacement Cross Sections (DPA) for all shifted nuclei produced via all nuclear elastic, inelastic, (n,2n), (n,p), (n,α), (n,γ) and so on reactions.

DPA Cross Sections were calculated by NJOY-97 package and the evaluated nuclear data files from ENDF/B-VI.8 and BROND-2(3) libraries.

BORON CONTENT AND THE SMs PROPERTIES

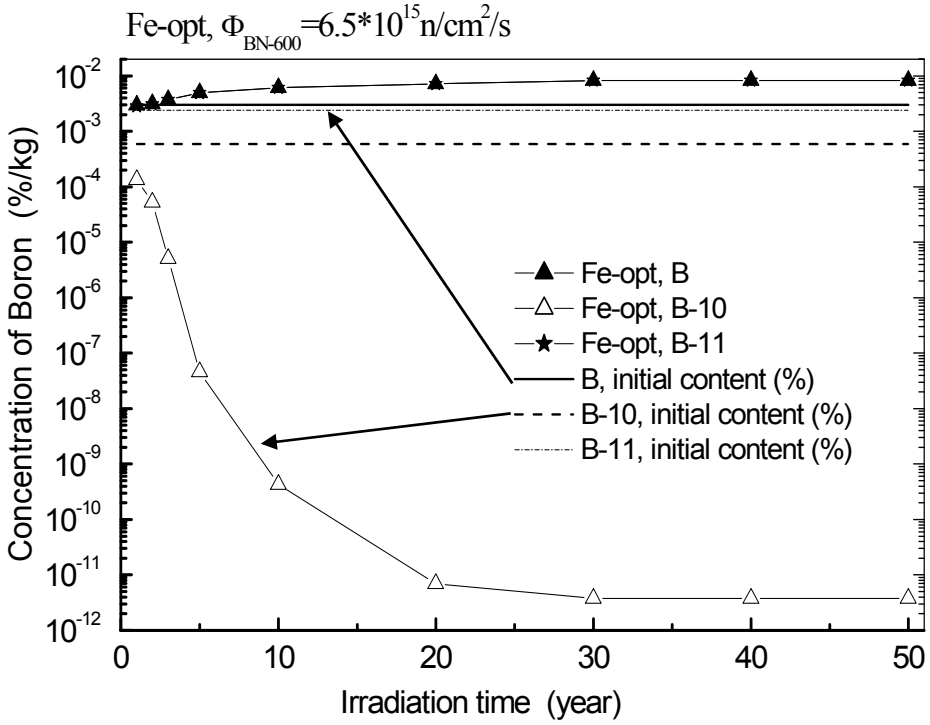
1. B atoms are the principal small addition for all the RF steels to improve their heat-resistance properties (via controlled grain boundaries and inside grains concentrations).
2. He atoms formation by nuclear reaction $B^{10}(n,\alpha)$ (the problem of the He-degradation of the SMs properties). The channel is not dangerous for the neutron spectra of fast and fusion reactors (isotope B-10 transforms to the stable B-11 and other isotopes) and there are others meaning channels for He-formation).

Scheme of the B-isotopes transmutatios

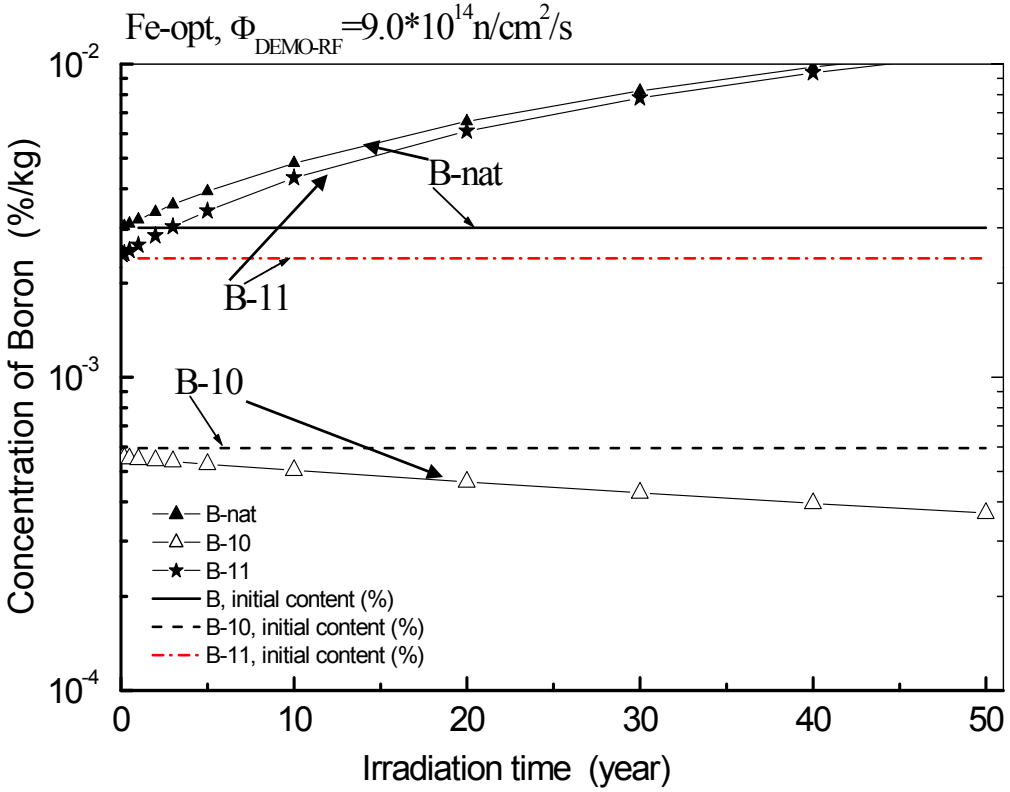


ACDAM: RUSFER-EK-181 (F-opt): Accumulation of Boron and its isotopes after irradiation by BN-600 and DEMO-RF neutron spectra

Horizontal lines are the initial concentrations of boron (B-10, B-11, B-nat) in steel.

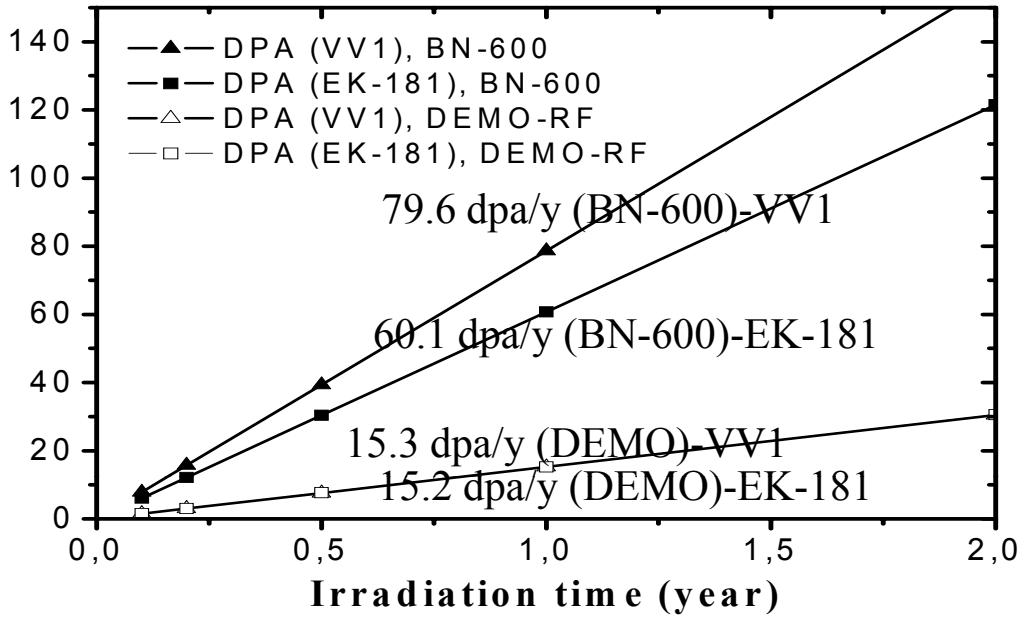


BN-600

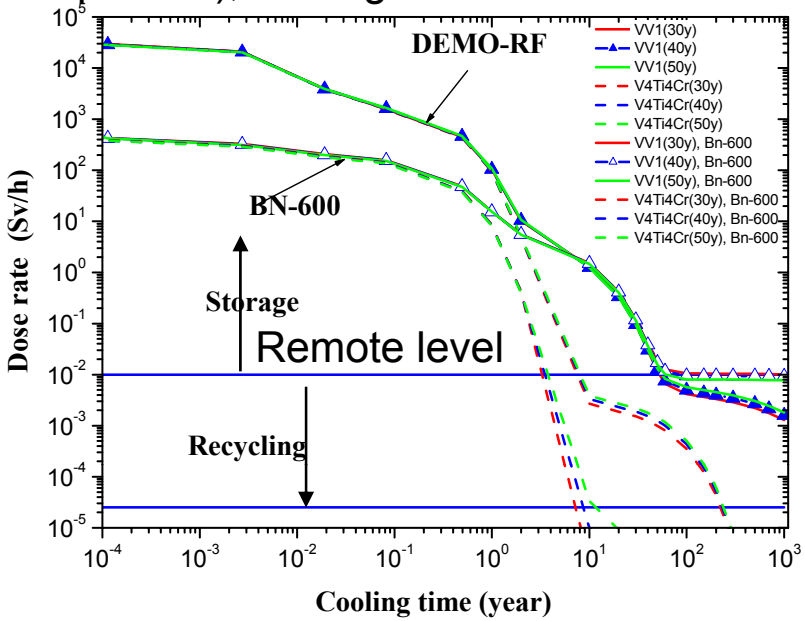


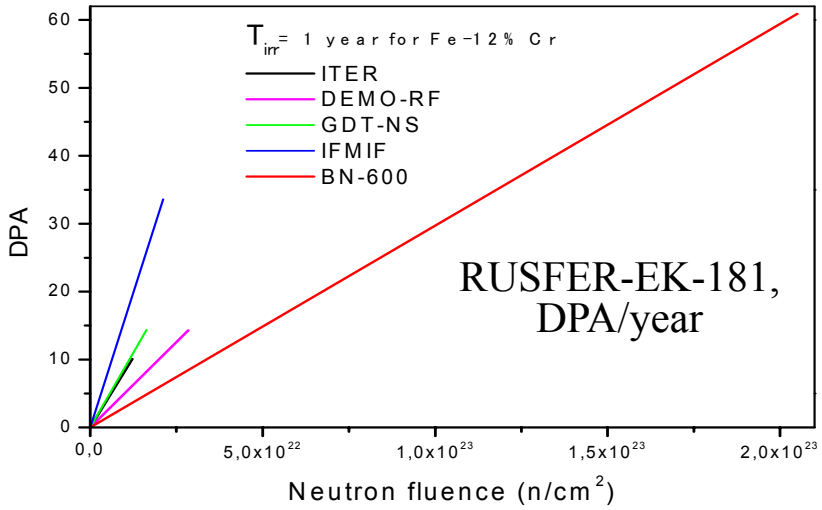
DEMO-RF

ACDAM: V-4Ti-4Cr(VV1)/RUSFER-EK-181 (EK-181): Radiation Damage, Activation, Cooling

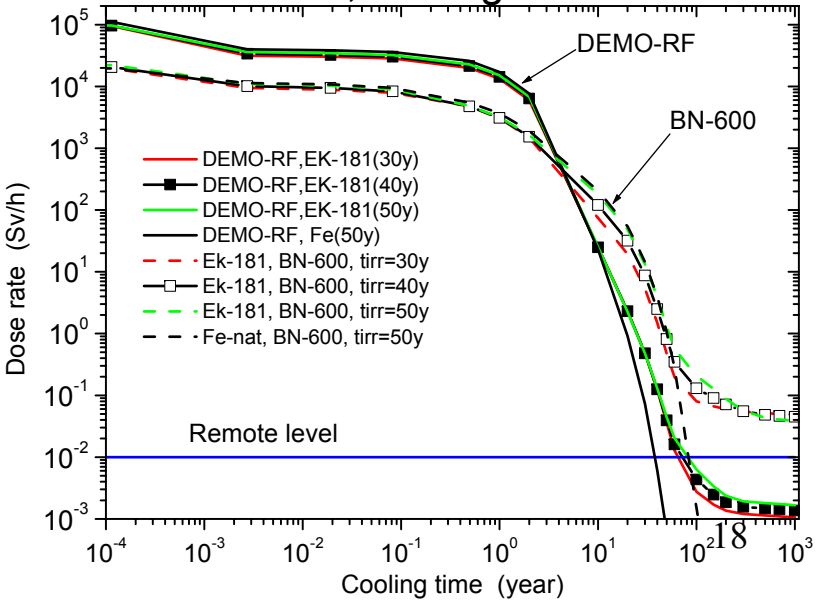


V-4Ti-4Cr (heat VV1) and V4Ti4Cr (no impurities), cooling after Irradiation





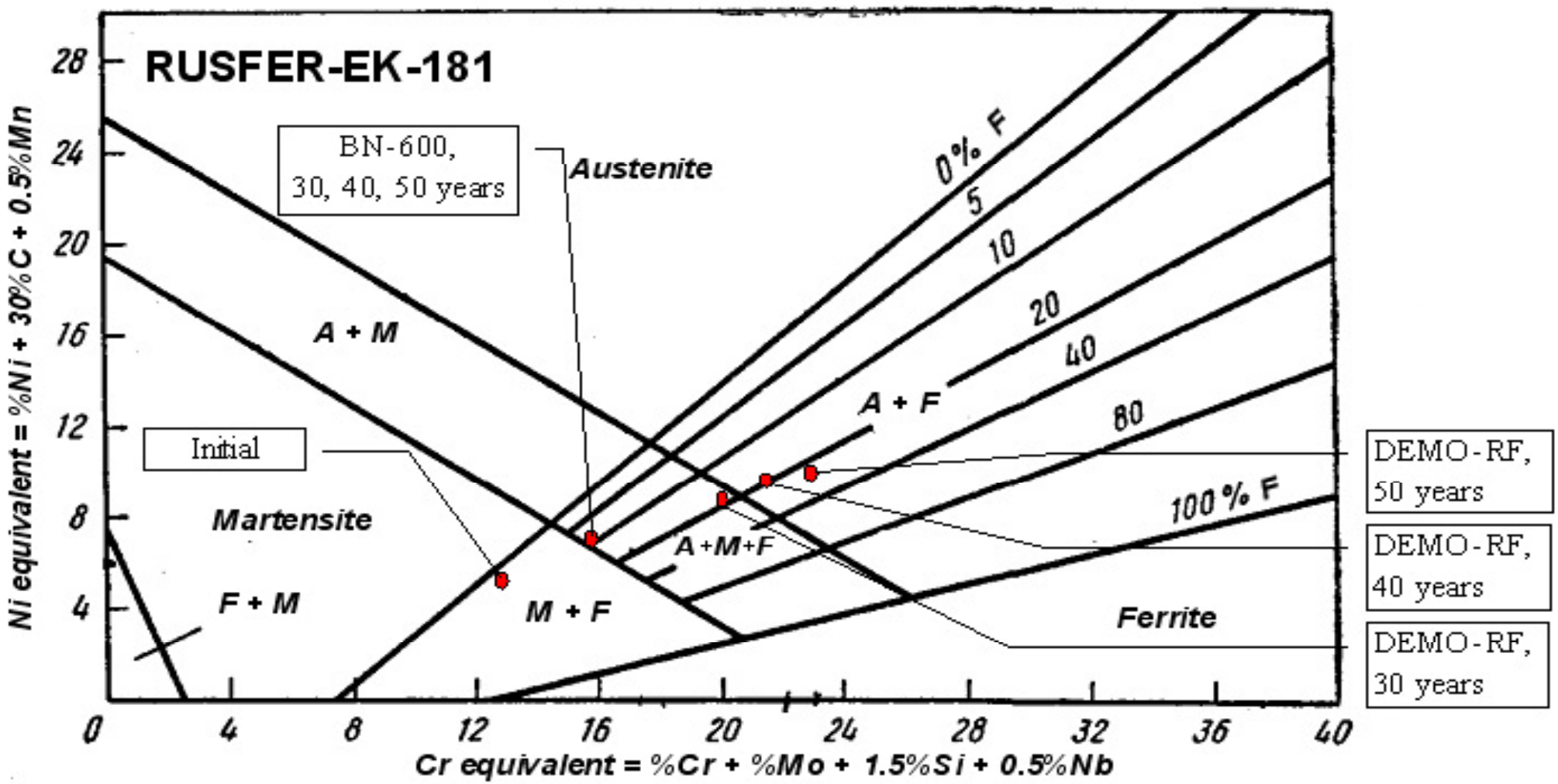
RUSFER-EK-181, cooling after irradiation



ACDAM: Element concentrations (wt. %) in RAFMS RUSFER-EK-181 after 560 days irradiation in BN-600 and DEMO-RF reactors (influence of B atoms)				
Ele-ment	**Initial concentra-tion**	**BN-600**	**DEMO-RF**	
H	0,0	0.00039 (B=0,0) 0.00039 (B=0,003)	H	0,0041 (B=0,0) 0,0041 (B=0,003))
He **He**	**0,0** **0,0**	**0.000157 (B=0,0)** **0.00027 (B=0,003)**	**He** **He**	**0,0033 (B=0,0)** **0,0033 (B=0,003)**
B **B** **C** **N** Si **Ti** **V** **Cr** **Mn** **Fe** **Zr** **Ce** **Ta** **W**	**0,0** **0,003** **0,160** **0,070** 0,400 **0,050** **0,400** **12,000** **0,600** **84,767** **0,050** **0,050** **0,150** **1,300**	**0,0002** **0,0029** **0,16013** **0,06932** 0,39977 **0,050** **0,402** **12,0046** **0,60733** **84,755** **0,04994** **0,04972** **0,12942** **1,28526**	**B** **B** **C** **N** Si **Ti** **V** **Cr** **Mn** **Fe** **Zr** **Ce** **Ta** **W**	**0,0003** **0,0033** **0,15957** **0,06934** 0,39865 **0,054** **0,436** **12,012** **0,72844** **84,583** **0,04985** **0,0495** **0,15213** **1,29026**

ACDAM: Element concentrations (wt. %) in RAFMS RUSFER-EK-181 after 30, 40 and 50 years irradiation in BN-600 and DEMO-RF reactors

Element	Initial concentrations	BN-600 / DEMO-RF		
		30 y	40 y	50 y
H		0.00728 / 0.07746	0.00949 / 0.10164	0.01161 / 0.12507
He		0.00342 / 0.06376	0.00448 / 0.0845	0.00553 / 0.10499
B	0.003	0.00609 / 0.00822	0.00718 / 0.00977	0.00821 / 0.01124
C	0.16	0.16575 / 0.15517	0.16746 / 0.15353	0.16907 / 0.15188
N	0.07	0.05948 / 0.05963	0.05635 / 0.05653	0.05339 / 0.05360
O		0.00496 / 0.00474	0.00494 / 0.00466	0.00493 / 0.00457
Si	0.4	0.39948 / 0.37819	0.39919 / 0.37107	0.3989 / 0.36407
V	0.4	0.43652 / 1.0839	0.44495 / 1.2984	0.45175 / 1.5072
Cr	12.00	12.257 / 12.87	12.335 / 13.246	12.409 / 13.657
Mn	0.6	0.87624 / 5.2373	0.95865 / 6.7268	1.0297 / 8.1085



Scheffler diagram

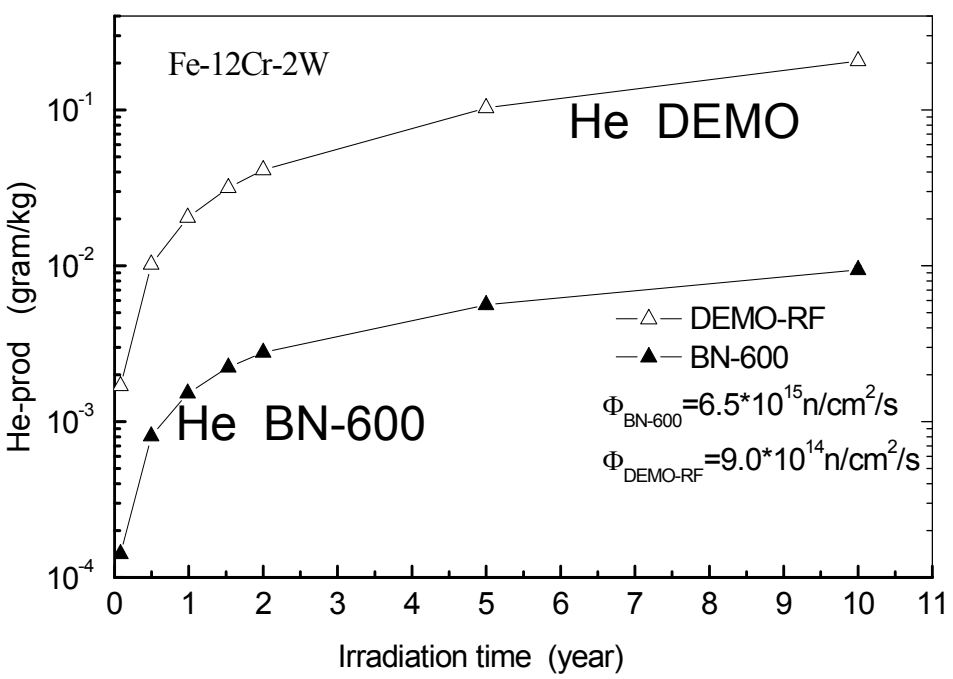
ACDAM: PHYSICS OF THE RADIATION DAMAGE

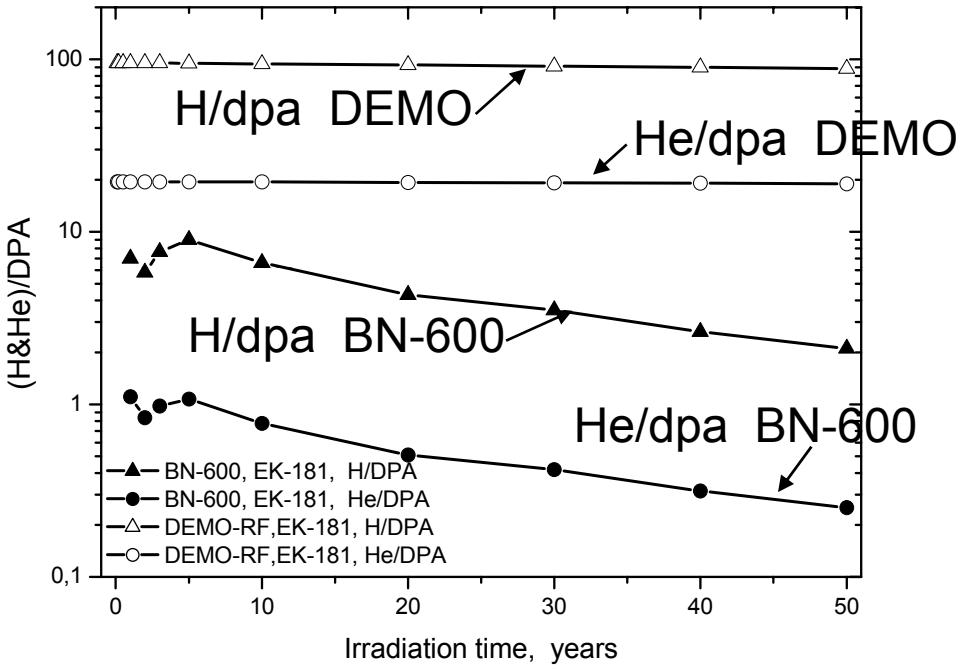
Radiation damage dose $K_d t$, H(t) and He(t) concentrations in V and Fe crystals (**V / Fe**) for BN-600 and DEMO-RF.

Neutron irradiation time is **t = 560** effective days

Flux, n/cm^2/s, E>0	**K_d t, dpa** V / *Fe*	**H, appm** V / *Fe*	**He, appm** V / *Fe*	**H / K_d t** V / *Fe*	**He / K_d t** V / *Fe*
DEMO-RF 9.00x10^{14}	23.49 / *23.32*	580.6 / *1084.0*	97.43 / *286.1*	24.72 / *46.19*	4.15 / *12.19*
BN-600 6.50x10^{15}	122.1 / *92.20*	19.59 / *241.5*	1.09 / *3.65*	0.16 / *2.62*	0.01 / *0.15*

ACDAM: He, H/DPA and He/DPA ratio for the RAFMS RUSFER-EK-181 irradiated in the BN-600 and DEMO-RF reactors.





How to compare and to predict the degradations of the radiation properties via H, He and dpa formations ?

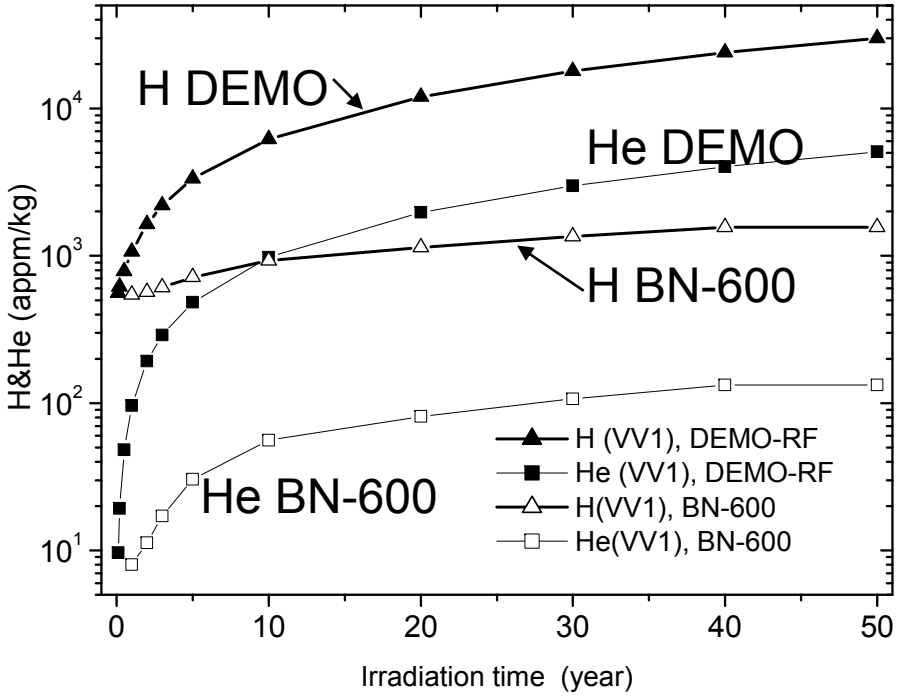
ACDAM: Element concentrations (wt. %) in V-4Ti-4Cr alloy (VV1) after 560 days irradiation in BN-600 and DEMO-RF reactors (influence of B atoms)

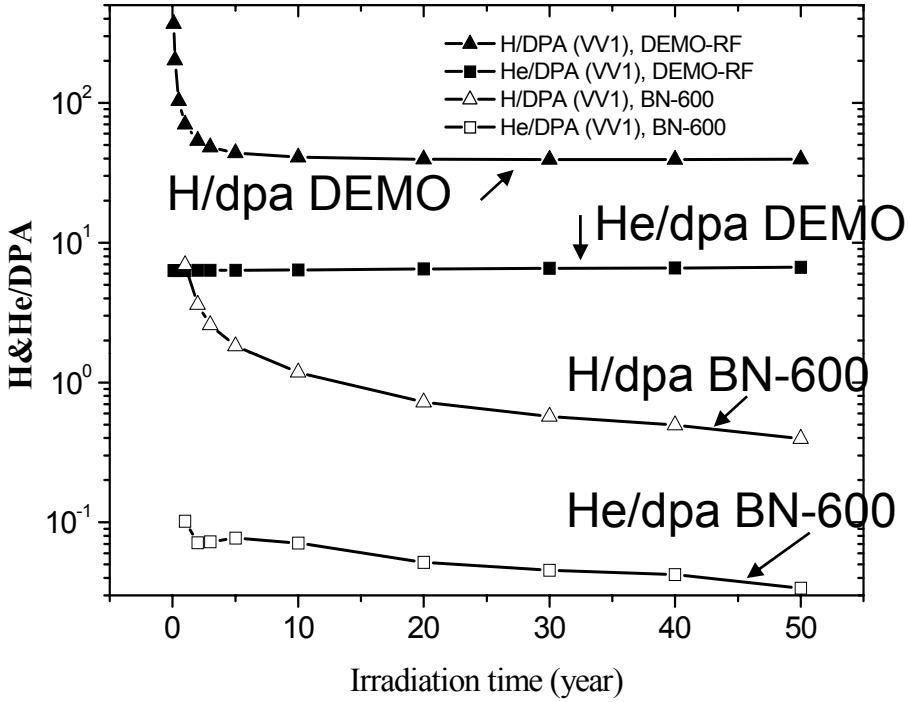
Element	Initial concentration	BN-600 (560 days)	DEMO-RF (560 days)	
H	0.001	0,001 (B=0,0) 0,001 (B=0,0005)	H	0,0028 (B=0.0) 0,0028 (B=0.0005)
He He	0,0 0,0	0.000031 (B=0,0) 0.000050 (B=0.0005)	He He	0,00116 (B=0,0) 0,00116 (B=0,0005)
B **B** C N O **Ti** **V** **Cr** **Fe** **Nb** **Mo**	**0,0** **0.0005** 0.02 0.015 0.040 **4.000** **91.834** **4.000** **0.025** **0.001** **0.001**	**0.000043** **0.000494** 0,02006 0,01485 0,03995 **3,999** **91,25302** **4,58183** **0,025** **0.001** **0.001**	**B** **B** C N O **Ti** **V** **Cr** **Fe** **Nb** **Mo**	**0.000064** **0.000561** 0,02005 0,01486 0,03986 **4,054** **91,78421** **3,99118** **0,025** **0.001** **0.001**

ACDAM: Element concentrations (wt. %) in V-4Ti-4Cr alloy (VV1) after 30, 40 and 50 years irradiation in BN-600 and DEMO-RF reactors

Element	Initial concentrations	BN-600 / DEMO-RF		
		30 y	40 y	50 y
H	**0.001**	**0.00225 / 0.03706**	**0.00267 / 0.04945**	**0.00309 / 0.06202**
He		**0.00064 / 0.02355**	**0.00084 / 0.03172**	**0.00105 / 0.04003**
B	**5.00E-04**	**0.00119 / 0.00163**	**0.00142 / 0.00196**	**0.00164 / 0.00228**
C	**0.02**	**0.02152 / 0.02126**	**0.02198 / 0.02165**	**0.02242 / 0.02201**
C14		**0.0012 / 0.00037**	**0.0016 / 0.00047**	**0.002 / 0.00057**
N	0.015	0.01275 / 0.01284	0.01208 / 0.0122	0.01144 / 0.01159
O	**0.04**	**0.03967 / 0.03791**	**0.03956 / 0.03723**	**0.03944 / 0.03657**
Si	0.025	0.02543 / 0.02388	0.02556 / 0.0235	0.02569 / 0.02313
Sc		0.00015 / 0.02554	0.00018 / 0.03337	0.00021 / 0.04091
Ti	**4.0**	**4.0126 / 5.1608**	**4.0154 / 5.5811**	**4.0182 / 6.0169**
V	**91.8342**	**81.375 / 90.75**	**78.131 / 90.32**	**75.016 / 89.873**
Cr	**4.0**	**14.779 / 3.8188**	**18.09 / 3.7592**	**21.271 / 3.7007**
Mn		**0.0023 / 0.00144**	**0.00331 / 0.0019**	**0.00451 / 0.00232**
Fe	**0.025**	**0.02513 / 0.02337**	**0.02527 / 0.0228**	**0.02548 / 0.02224**

ACDAM: H, He concentrations and H/DPA and He/DPA ratios for V-4Ti-4Cr (VV1) alloy irradiated in the BN-600 and DEMO reactors

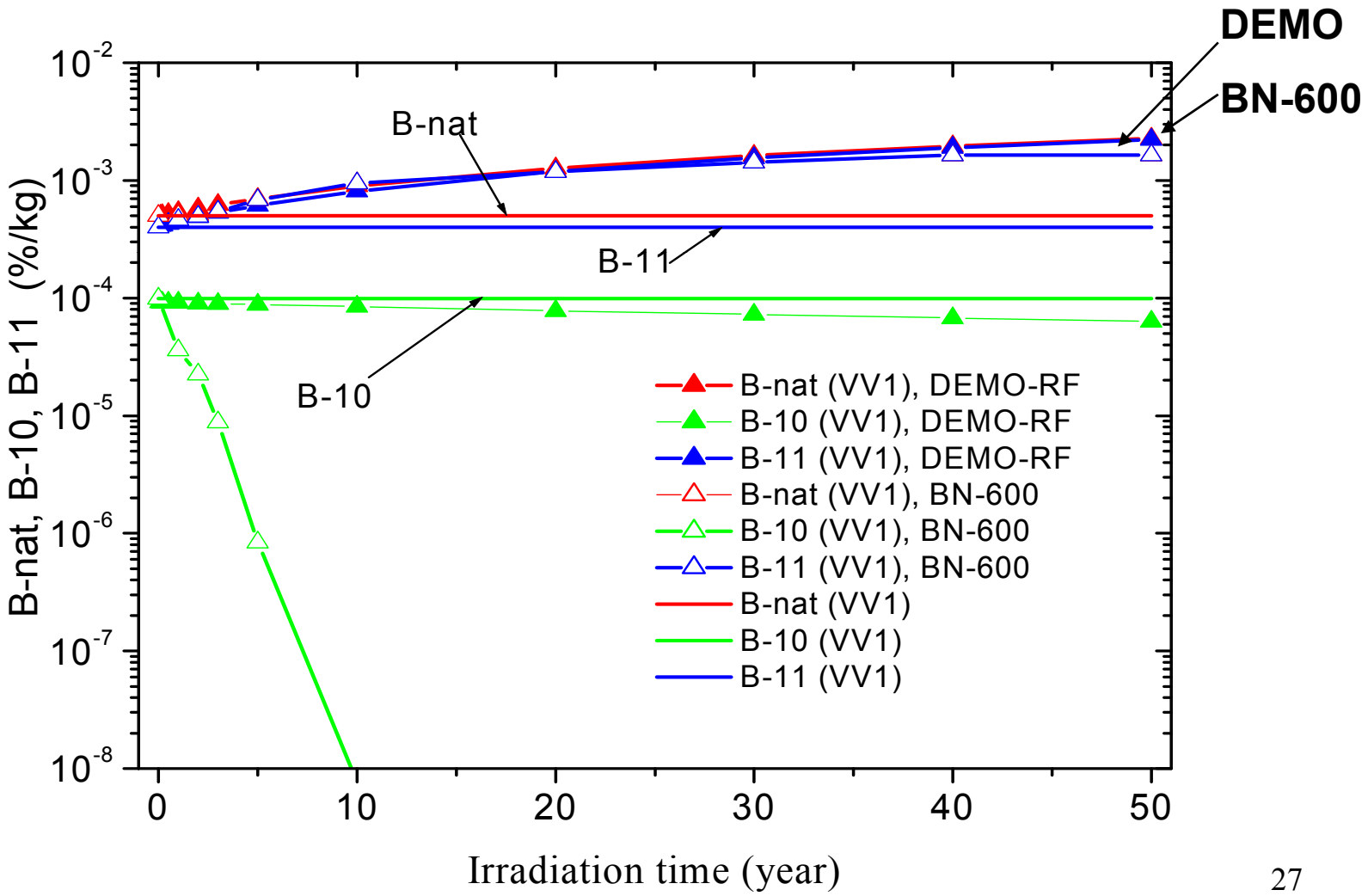




How to compare and to predict the degradations of the radiation properties via H, He and dpa formations ?

ACDAM: **Accumulation of Boron and its isotopes after irradiation of the V-4Ti-4Cr (VV1) alloy in BN-600 and DEMO-RF.**

Horizontal lines are the initial concentrations of B-10, B-11 and B-nat in alloy.



THE MDS OF ATOMIC COLLISION CASCADES IN DIFFERENT METALL CRYSTALLITES ARE THE VERY EXTENSIVE AREA OF SCIENTIFICAL ACTIVITY (mainly with the ideal initial crystal lattice structure, the results are very similar):

For reviews see Gary S. Was. Fundamentals of Radiation Materials Science. Metals and Alloys. Springer, 2007.

THE MDS OF ATOMIC COLLISION CASCADES IN VANADIUM CRYSTALLITE WITH INTERNAL STRUCTURE (GB)

S.G.Psakhie, K.P.Zolnikov, D.S.Kryzhevich, A,V.Zheleznyakov, V.M.Chernov: Physical Mesomechanics, 2008, v. 11(4), p. 3-13.

MDS: Lammps code: http:/lammps.sandia.gov

VANADIUM CRYSTAL: BCC STRUCTURE. *FS potential by M.I. Mendelev*

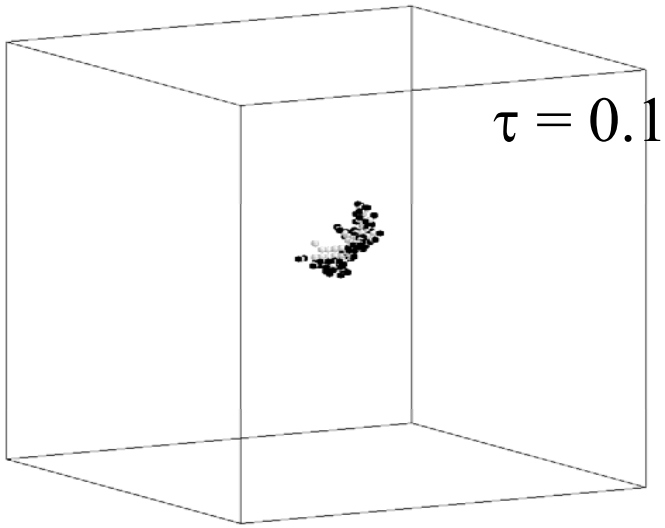
THE GRAIN BOUNDARY (GB) TYPE: **Σ13 or Σ17**

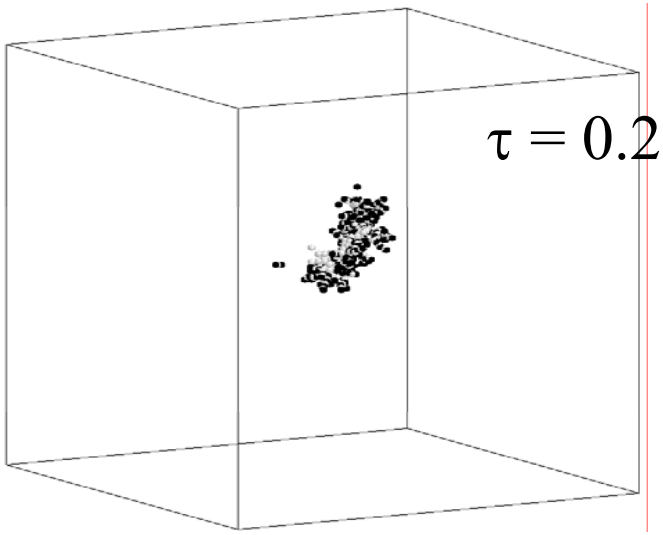
The atoms number: 65 000 (E_{PKA} < 500 eV),

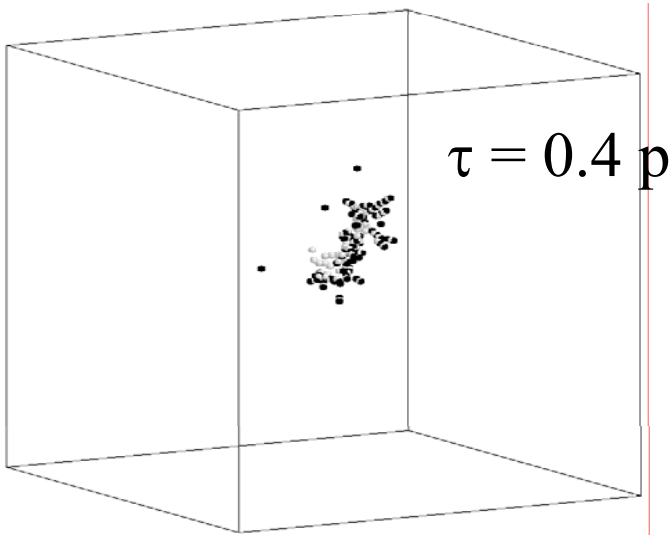
450 000 (E_{PKA} > 500 eV).

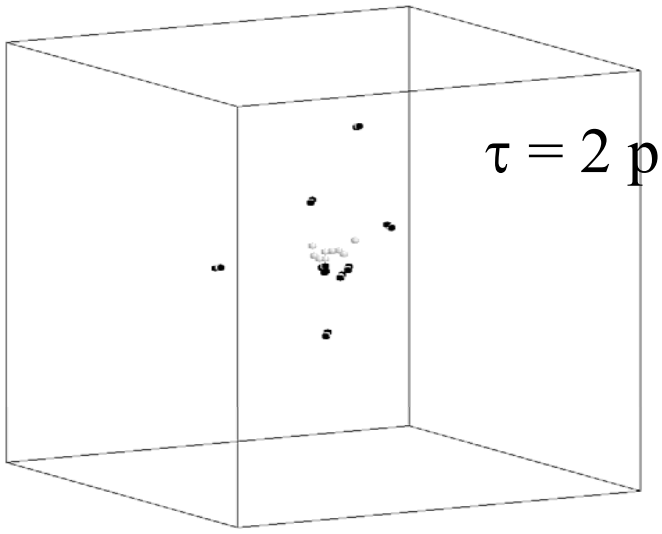
VANADIUM (450 000 atoms): MD simulation of cascades in vanadium crystal with the ideal initial lattice structure.

[320] E_{PKA} = 1 keV

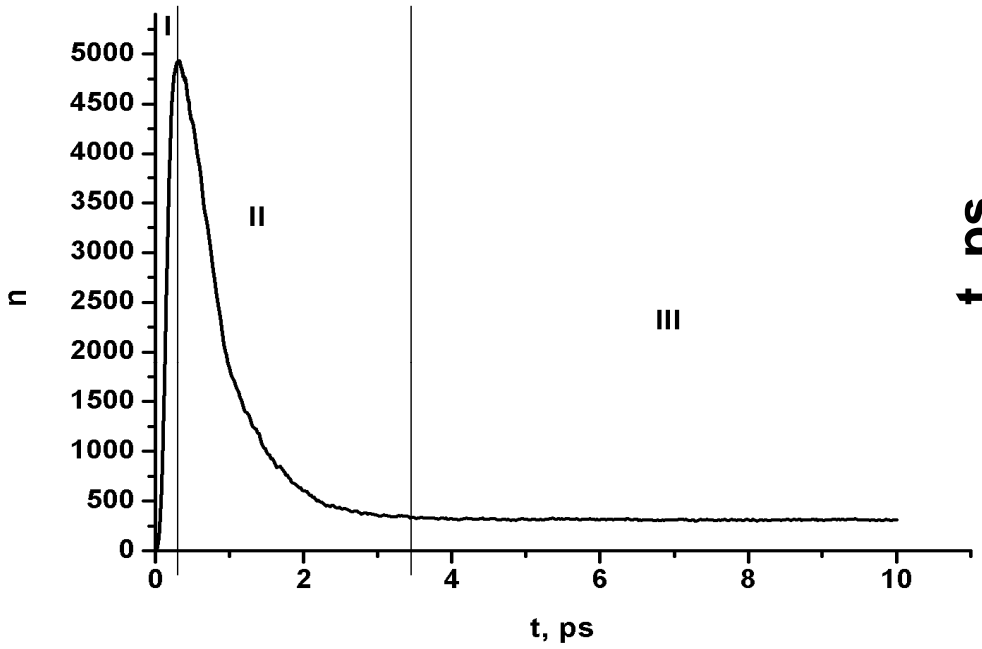


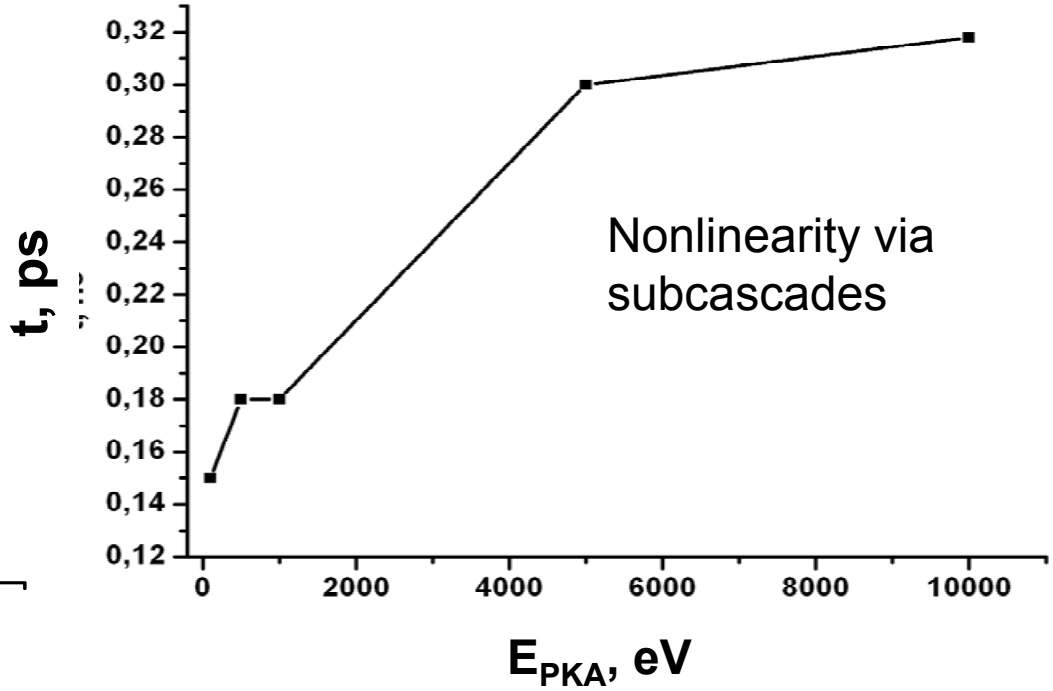






THE STAGES OF THE COLLISION CASCADE IN VANADIUM CRYSTAL WITH THE IDEAL INITIAL LATTICE STRUCTURE





The time dependence of the Number of the point defects **n(t)** (Frenkel pairs). [100] E_{PKA} = 10 keV.

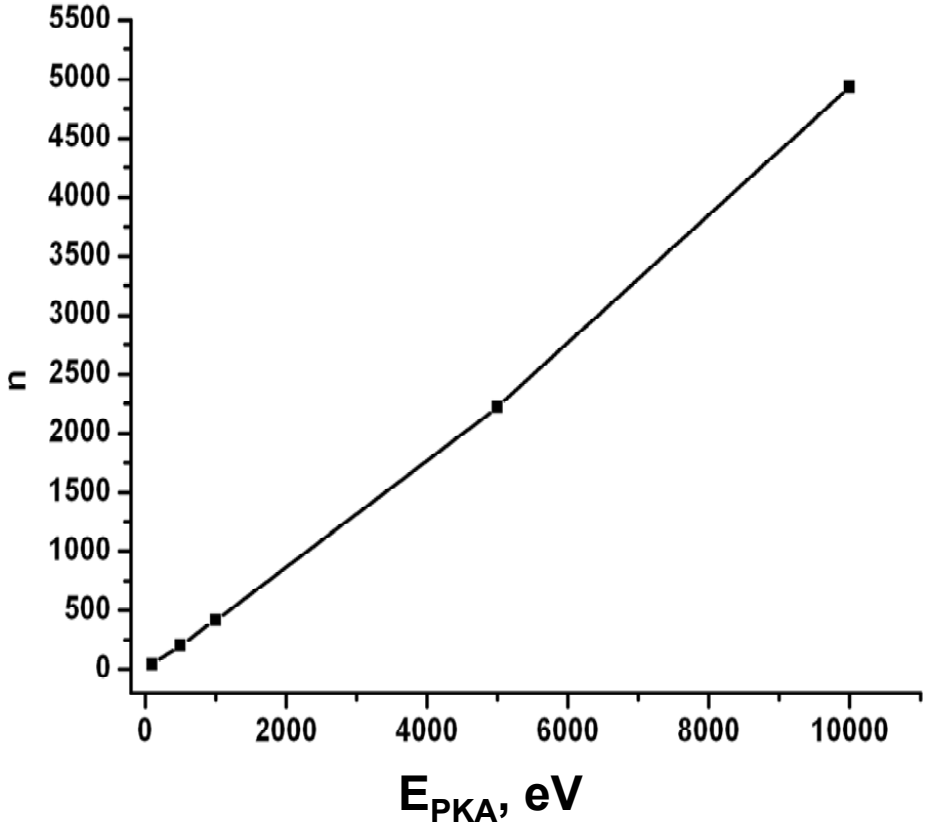
I – dynamic (ballistic) stage (max number of the defects),

II – Relaxation (recombination) stage.

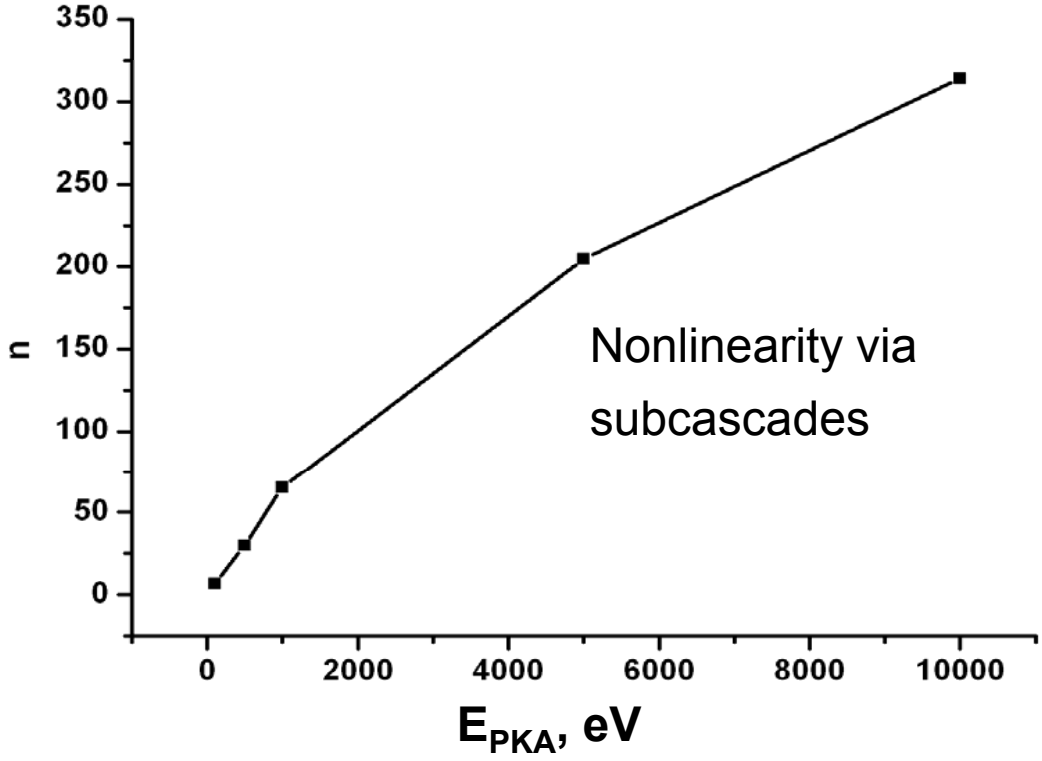
III - Diffusion (basic) stage.

Dependence of the time "peak" **t** (ps) from the PKA Energy ([100] E_{PKA} , eV)

The dependence of the point defects number (n) from [100] PKA energy (E_{PKA}, eV) for the cascade stages I and III in vanadium crystal with the ideal initial lattice structure.

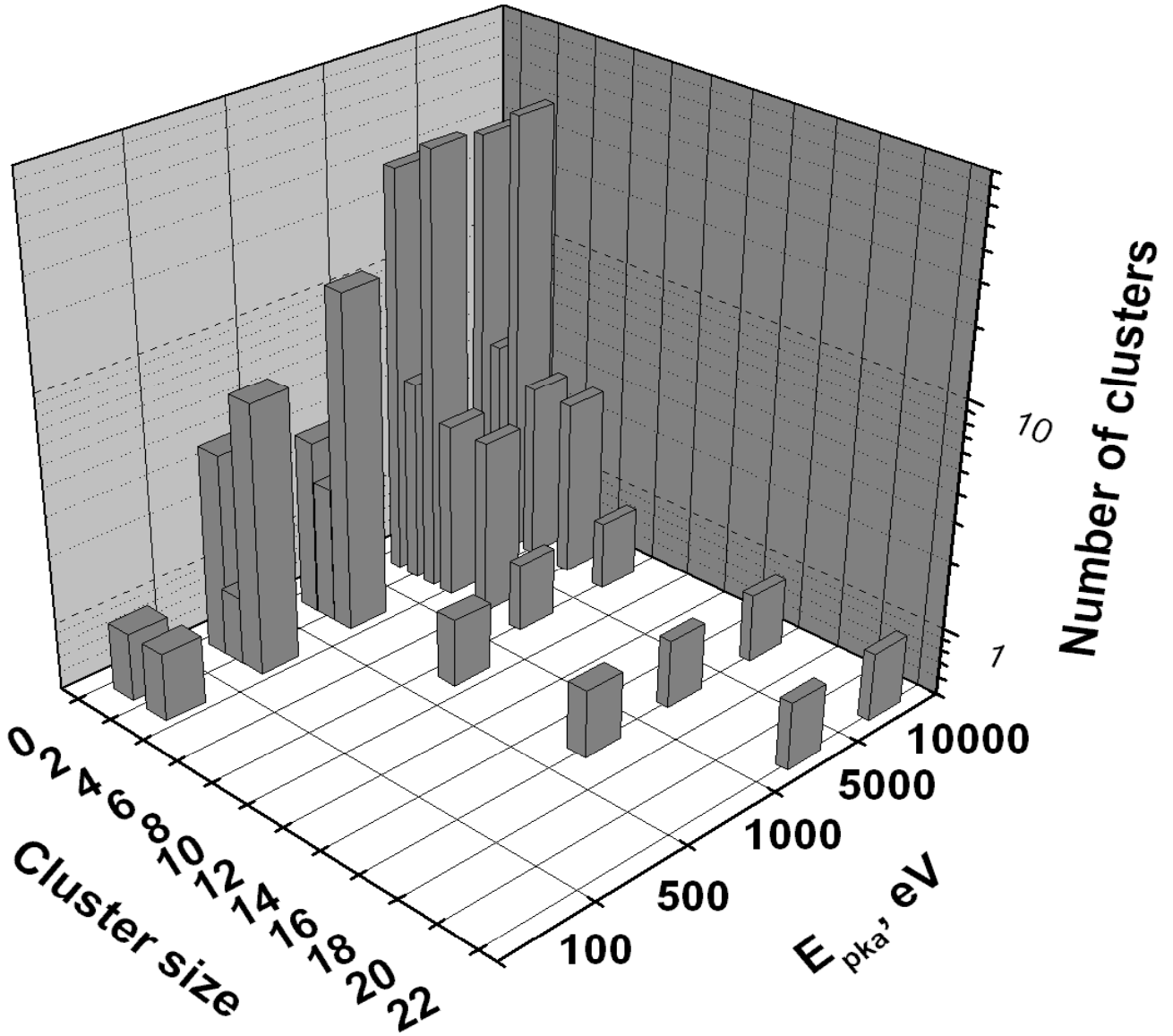


The number of the point defects **n(t)** to the end of the dynamic stage I - time “peak”



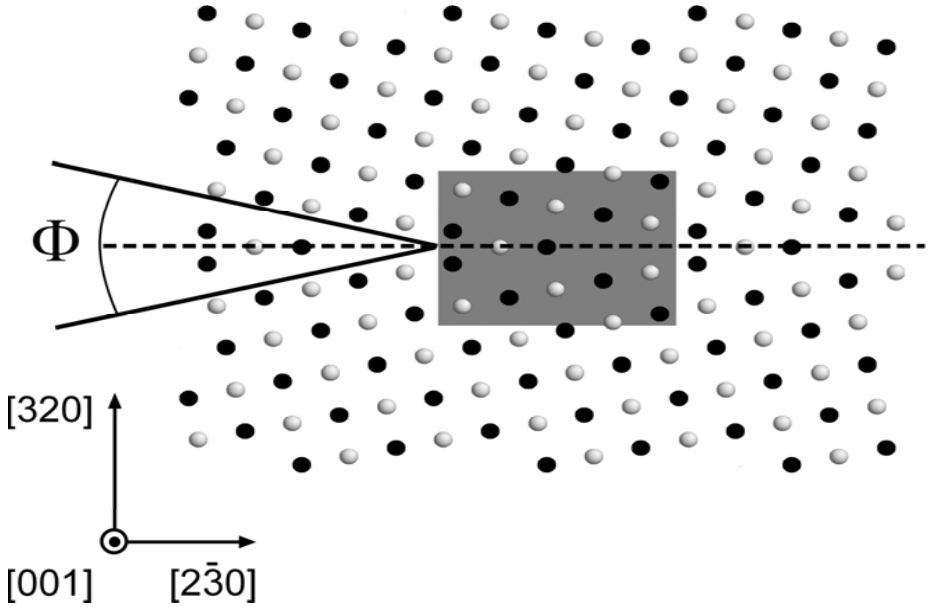
The number of the point defects **n(t)** to the end of the basic (diffusion) stage III

Number of clusters as a function of their sizes and [100] PKA energy in V crystal with the ideal initial lattice structure (basic stage 3)

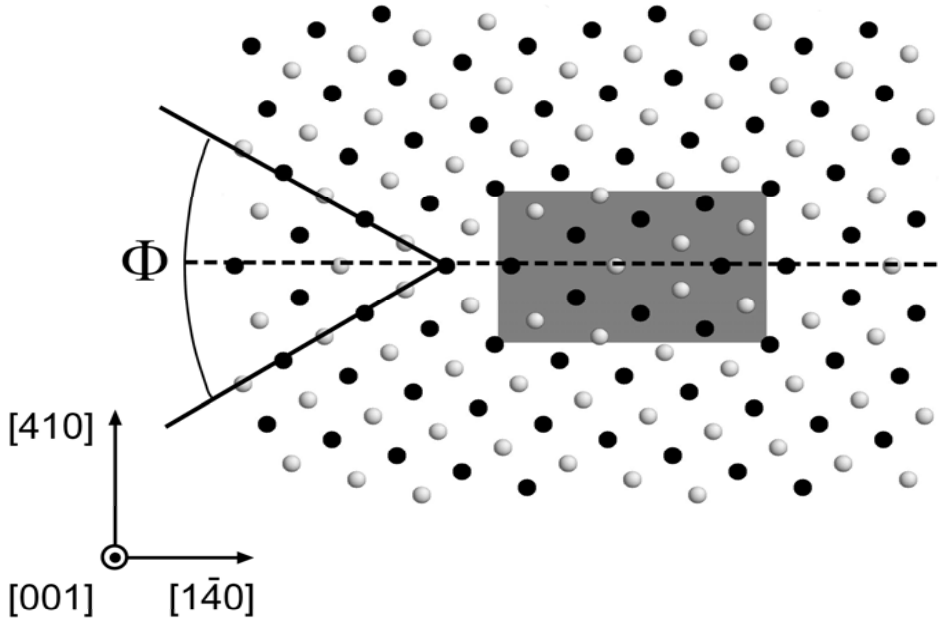


VANADIUM: MD Simulation of cascades in the vicinity of grain boundaries

Σ13 and Σ17 GRAIN BOUNDARY MODELS: Projections of atoms on (001) plane.



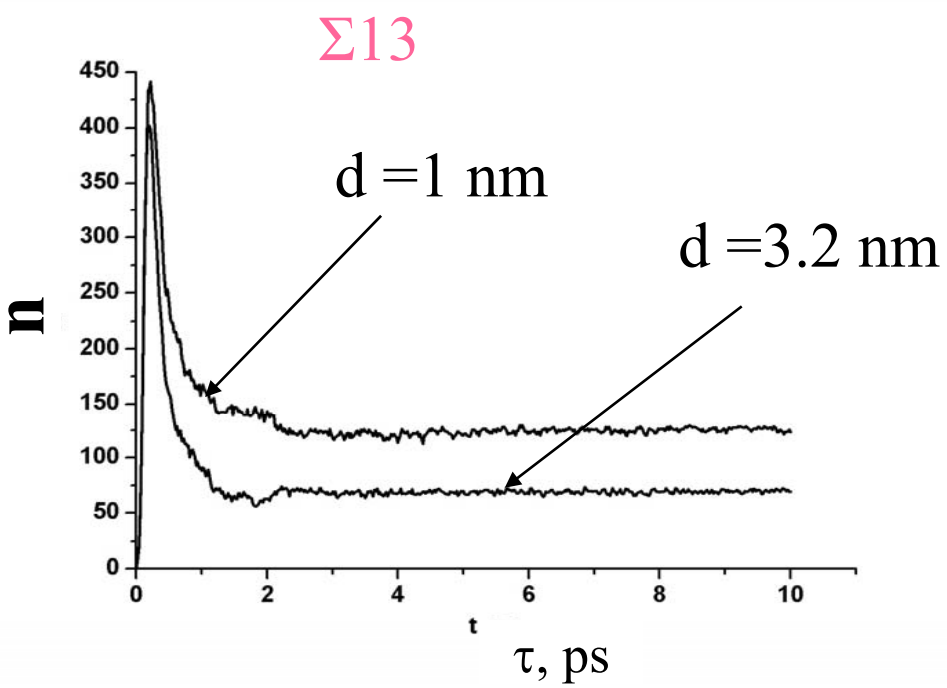
Σ13 (320)[001] Φ = 22.62°

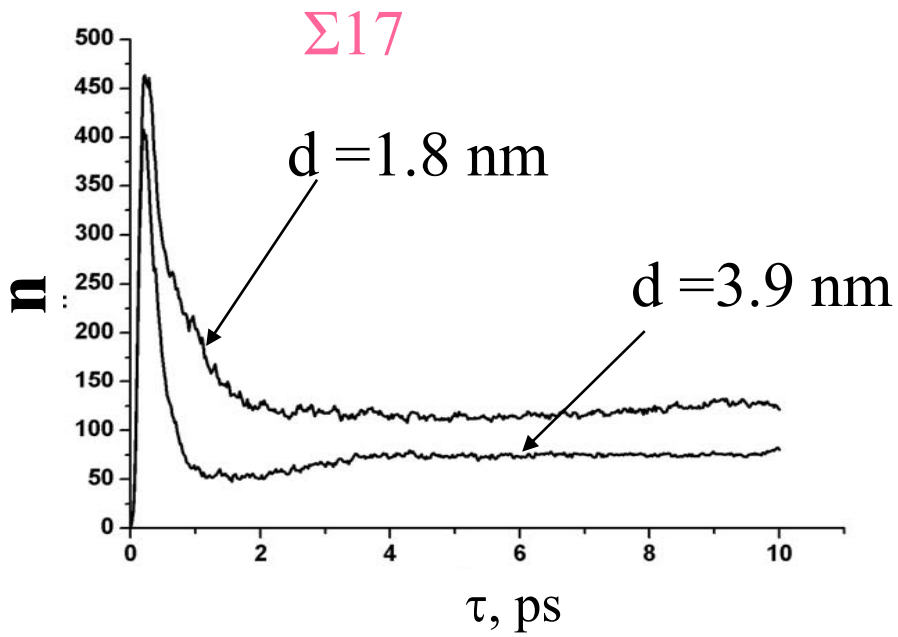


Σ17 (410)[001] Φ = 28.07°

Black area – the distance period along the boundary.

VANADIUM: MD Simulation of cascades in the vicinity of grain boundaries





E_{PKA} = 1 keV

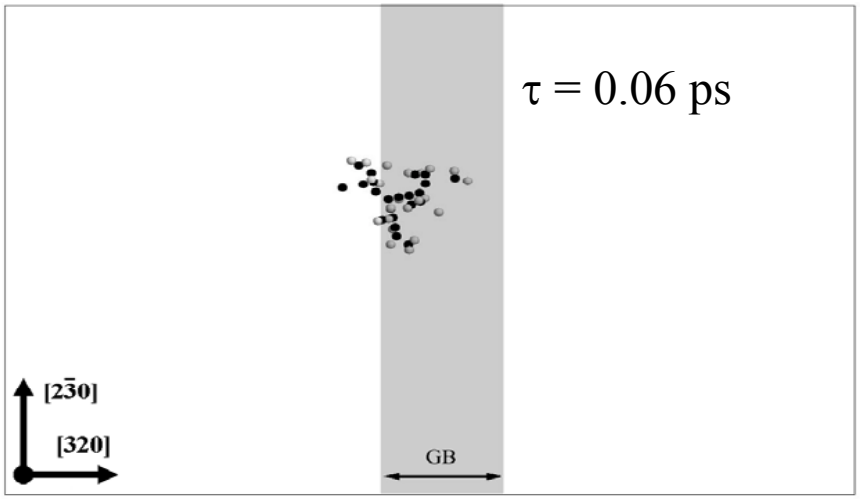
⊥ to the GB

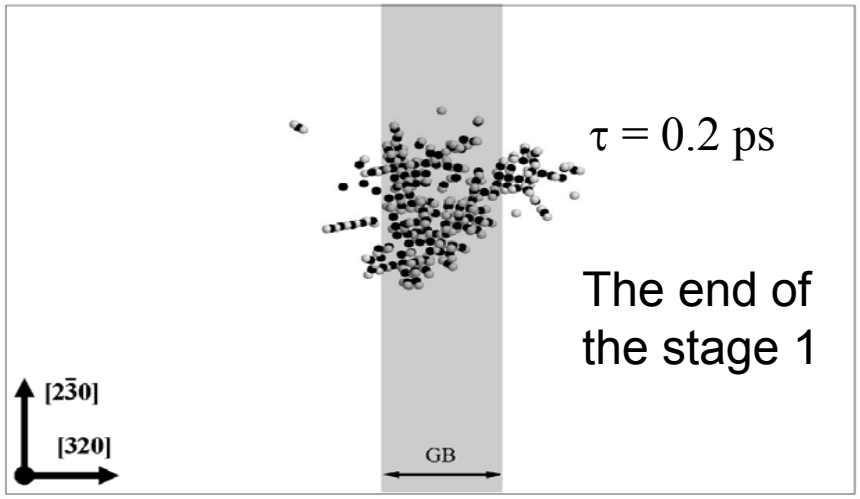
Time dependence on the number of point defects n (τ).

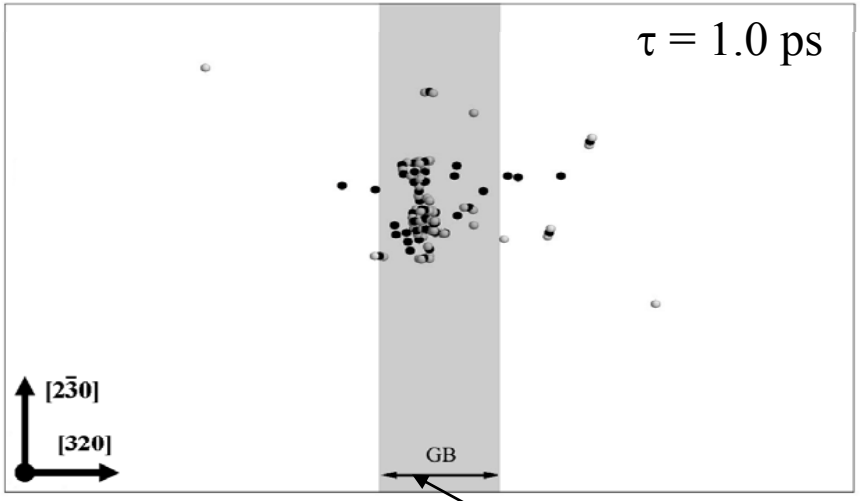
d - the distance from the PKA initial position to the GB

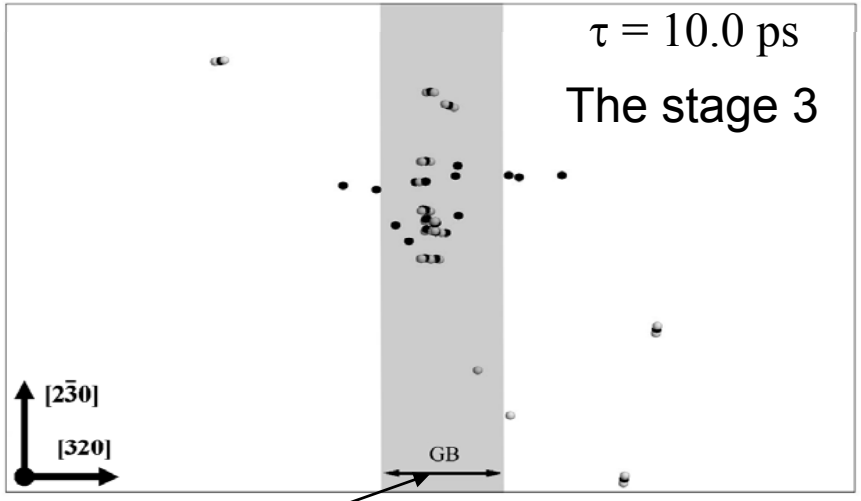
VANADIUM CRYSTAL: THE CASCADE SIZE (THE PROJECTIONS OF POINT DEFECTS ON (001) PLANE) IN DIFFERENT TIME.

GB Σ 13. [320] E_{PKA} = 1 keV. The distance between PKA and GB = 1,81 nm.





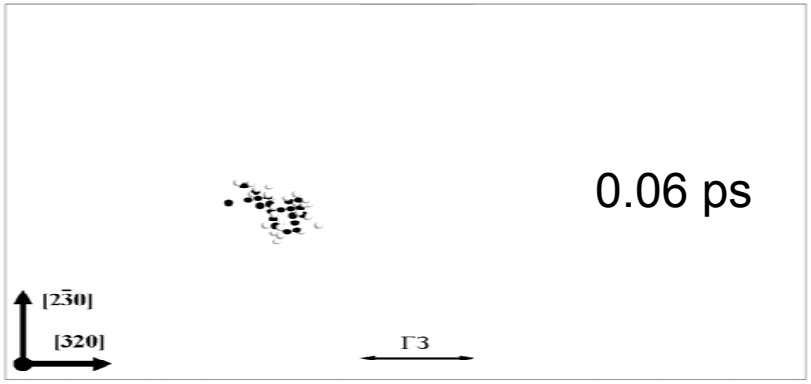


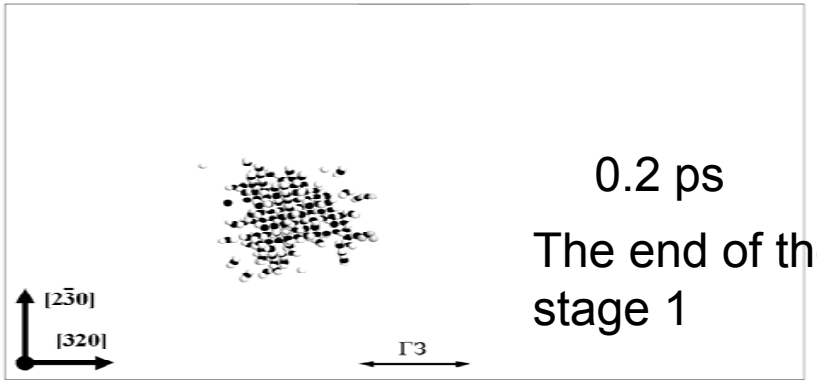


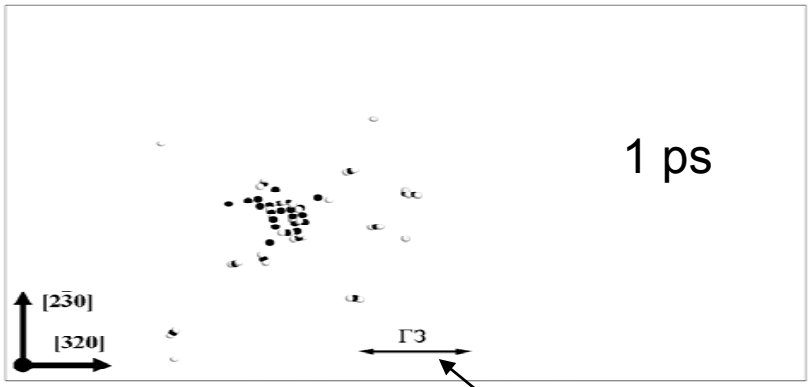
Grain Boundaries

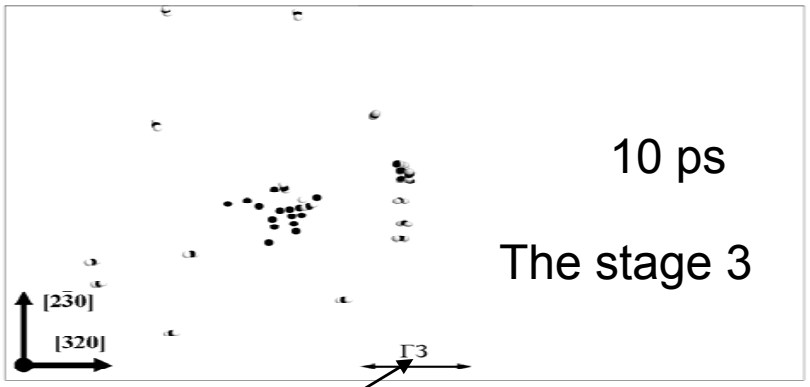
VANADIUM CRYSTAL: THE CASCADE SIZE (THE PROJECTIONS OF POINT DEFECTS ON (001) PLANE) FOR DIFFERENT TIMES.

GB Σ 13. [320] E_{PKA} = 1 keV. The distance BETWEEN PKA AND GB = 3,87 nm.







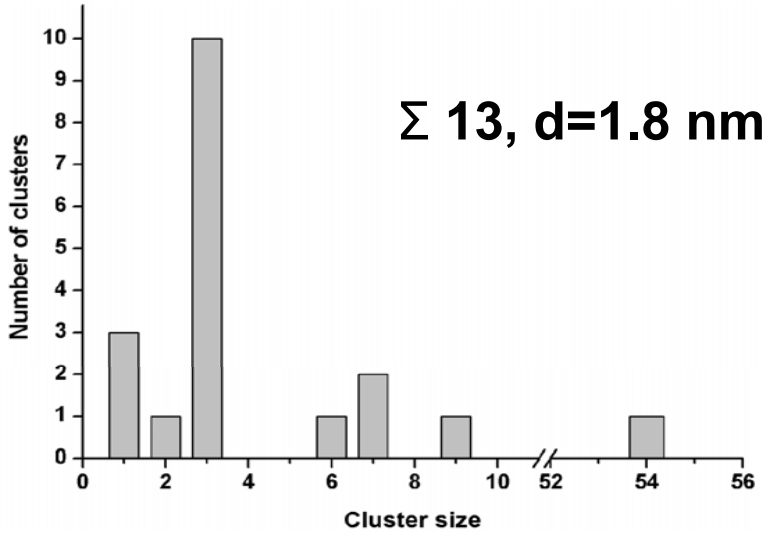


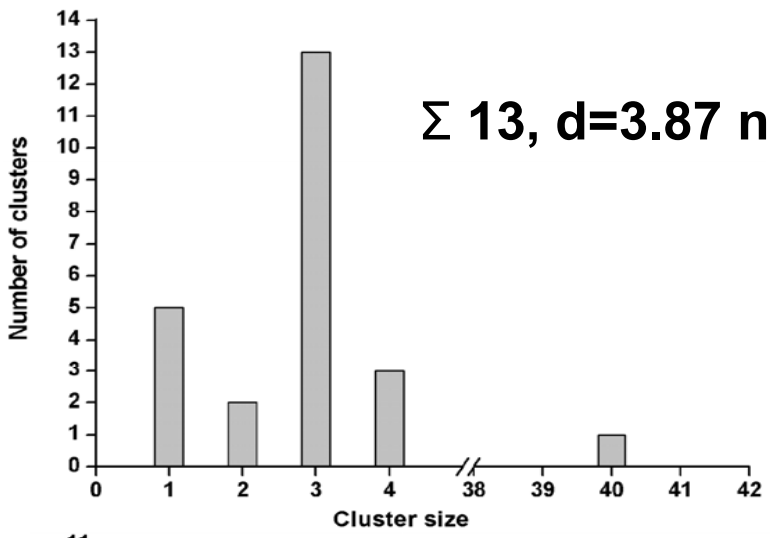
Grain Boundaries

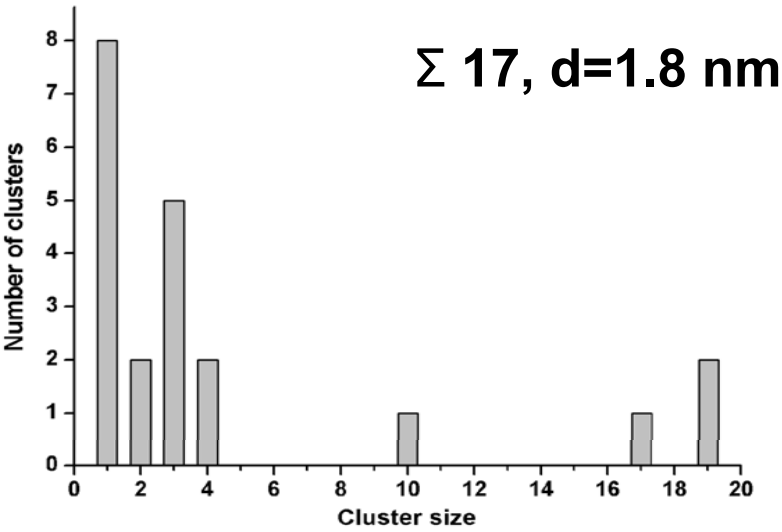
THE INFLUENCE OF GRAIN BOUNDARIES ON THE CASCADE FORMATIONS

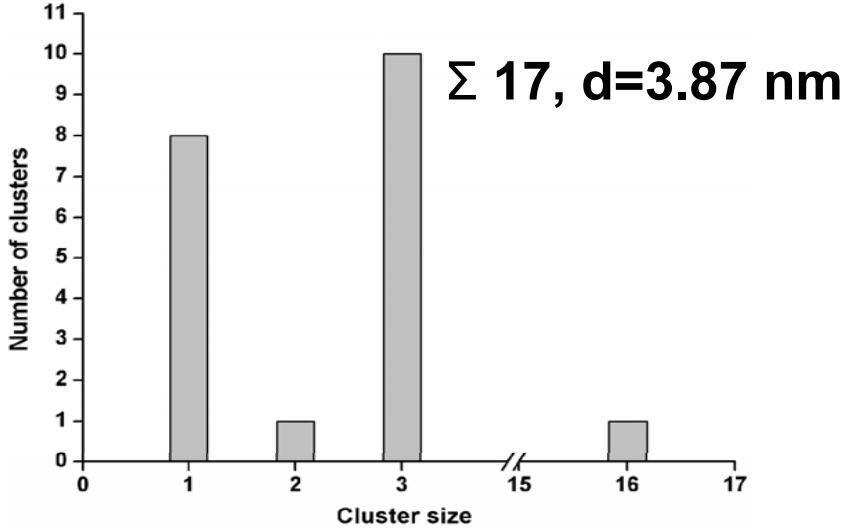
Boundary type	Distance between PKA and GB	The part of point defects inside the GB to the end of the relaxation stage of cascade (stage II)
Σ13	1.8 nm	89 %
	3.9 nm	54 %
Σ17	1.8 nm	86 %
	3.9 nm	55 %

DEPENDENCE OF THE CASCADE STRUCTURES (THE CLUSTERS SIZES AND NUMBERS) ON THE BASIC (DIFFUSION) STAGE 3 FROM THE DISTANCE BETWEEN PKA AND GB (d, nm)









THE INFLUENCE OF GRAIN BOUDARY (GB) ON CASCADE EVOLUTION:

1. THE GB EXERTS THE ESSENTIAL INFLUENCE ON THE CASCADE EVOLUTION (IN VANADIUM CRYSTAL).

2. THE GB ACCUMULATES THE CONSIDERABLE PART OF POINT DEFECTS. THE LARGE SIZE CLUSTERS ARISE INSIDE THE GB AREA.

3. DEVELOPMENTAL CHARACTER OF THE DISPLACEMENT CASCADES IS DETERMINED IN MANY RESPECTS BY THE PRESENCE OF EXTENSIVE INTERFACES IN MATERIALS.

4. THE GB HINDERS THE CASCADE PROPAGATION ON ITS OTHER SIDE.
   THE GB IMPENETRABILITY DEPENDS FROM ITS TYPE, PKA ENERGY AND DISTANCE BETWEEN PKA AND GB.

Summary:

1. The National Models, Nuclear Libraries and Codes types:

RF – ACDAM + FISPACT; EU – EASY; USA – CINDER-90;

JA – TRANSM + RADHEAT-V4

for the Calculations of the Radiation Damage (DPA-NRT), Activation, Transmutation and Cooling seem to be appropriate for the SMs R&Ds for Nuclear Power Reactors.

2. THE RF NUCLEAR ESTIMATED DATA LIBRARY ACDAM (+ FISPACT) allows to calculate all radiation characteristics for any materials (704 target isotopes from H-1 to Po-210), for any type of neutron spectra (fission and fusion) with energy up to 20 MeV, for any irradiation and cooling time:

radiation damage (dpa-NRT-IAEA) & activation & transmutation & cooling.

3. Although it is now well established that the dpa-number calculated by the "NRT-standard" does in general not accomplish an correlation of the radiation damage induced by different bombarding particles with irradiation properties of materials, the NRT(+IAEA)-convention should be retained.

4. There is the necessity of the R&D of the new radiation primary damage model for the all cascade stages (to modify the "NRT-model") on the basis of the up to date and nearest future knowledge of atomic and solid states physics and physics of collision cascades in real crystal lattice models with internal structures (0D-3D initial crystal lattice defects).

“OUR NEAR FUTURE IS NUCLEAR FISSION & FUSION JOULE-POWER”

MY GRATITUDE TO THE IAEA & ICTP

Thanks for your Attention & Patience