National Research Center" Kurchatov Institute"

"Development of theoretical modeling of point radiation defects, cascades and sub-cascades formation in diatomic materials (Al_2O_3) irradiated by fast charged paricles on accelarators and fast neutrons in atomic reactors".

A.I. Ryazanov

TM Primary Radiation Damage:
from nuclear reaction to point defects

1 - 4 October, 2012, IAEA, Vienna, Austria

Outline

- **Introduction**
- **Point Radiation Damage Production in Irradiated Materials due to Elastic and Inelastic Processes.**
- **Theoretical Modeling and Numerical Calculations of cascade and sub-cascade formation in irradiated materials.**
- **Formation radiation damage in diatomic materials (Al_2O_3) irradiated by fast charged paricles on accelarators and fast neutrons in atomic reactors.**
- **Conclusions**

Introduction

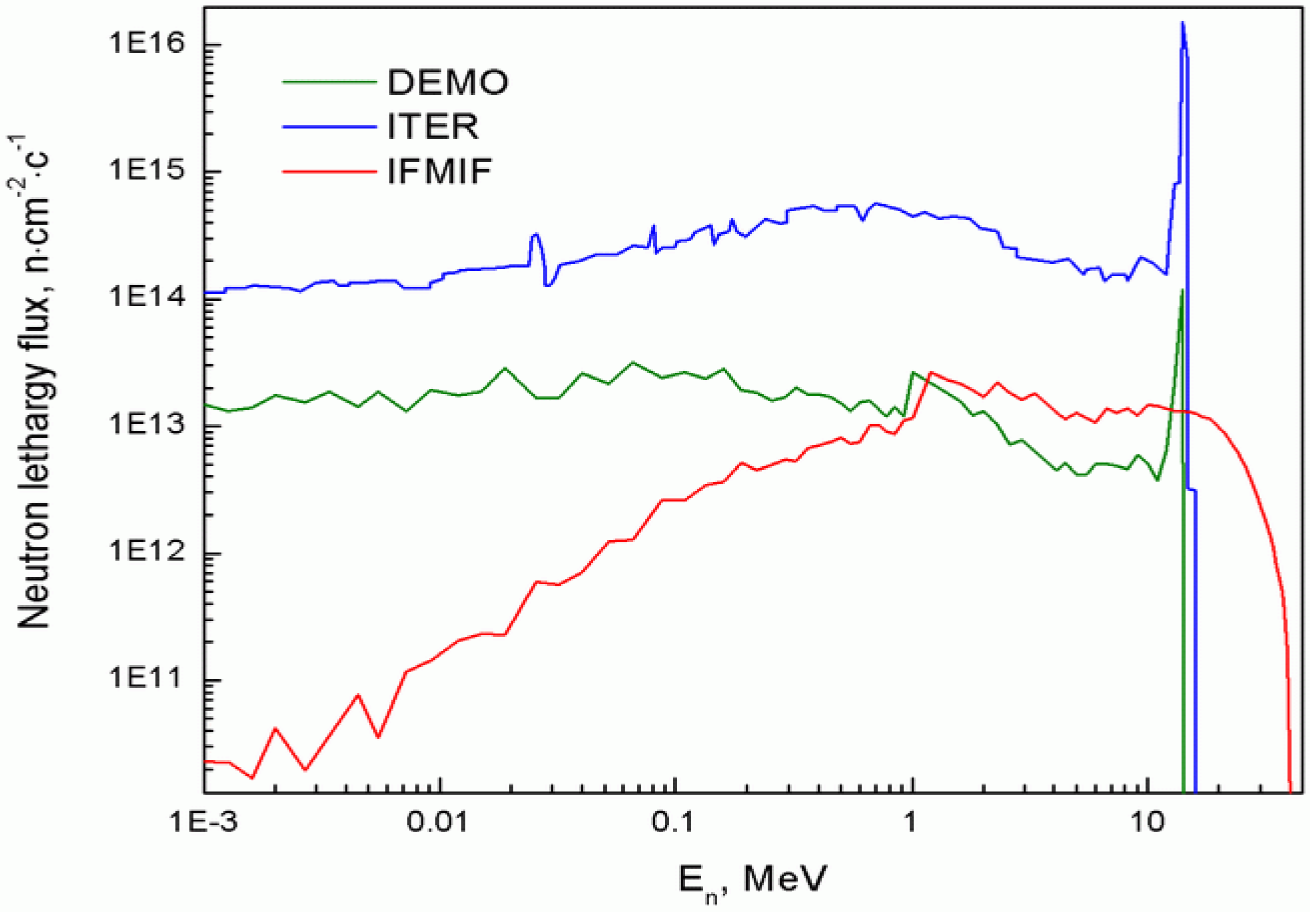
- **Point defect clusters (dislocation loops, voids, bubbles) under fast neutron and ion irradiation in materials are formed into cascades and sub-cascades. DPA value is not enough for the comparison of different types of irradiations. Generation rates of cascades and sub-cascades should be included too.**

- **For description of radiation swelling and creep in different fusion structural materials we have to know the generation rates of sub-cascades in the dependence on fast neutron energy spectra.**

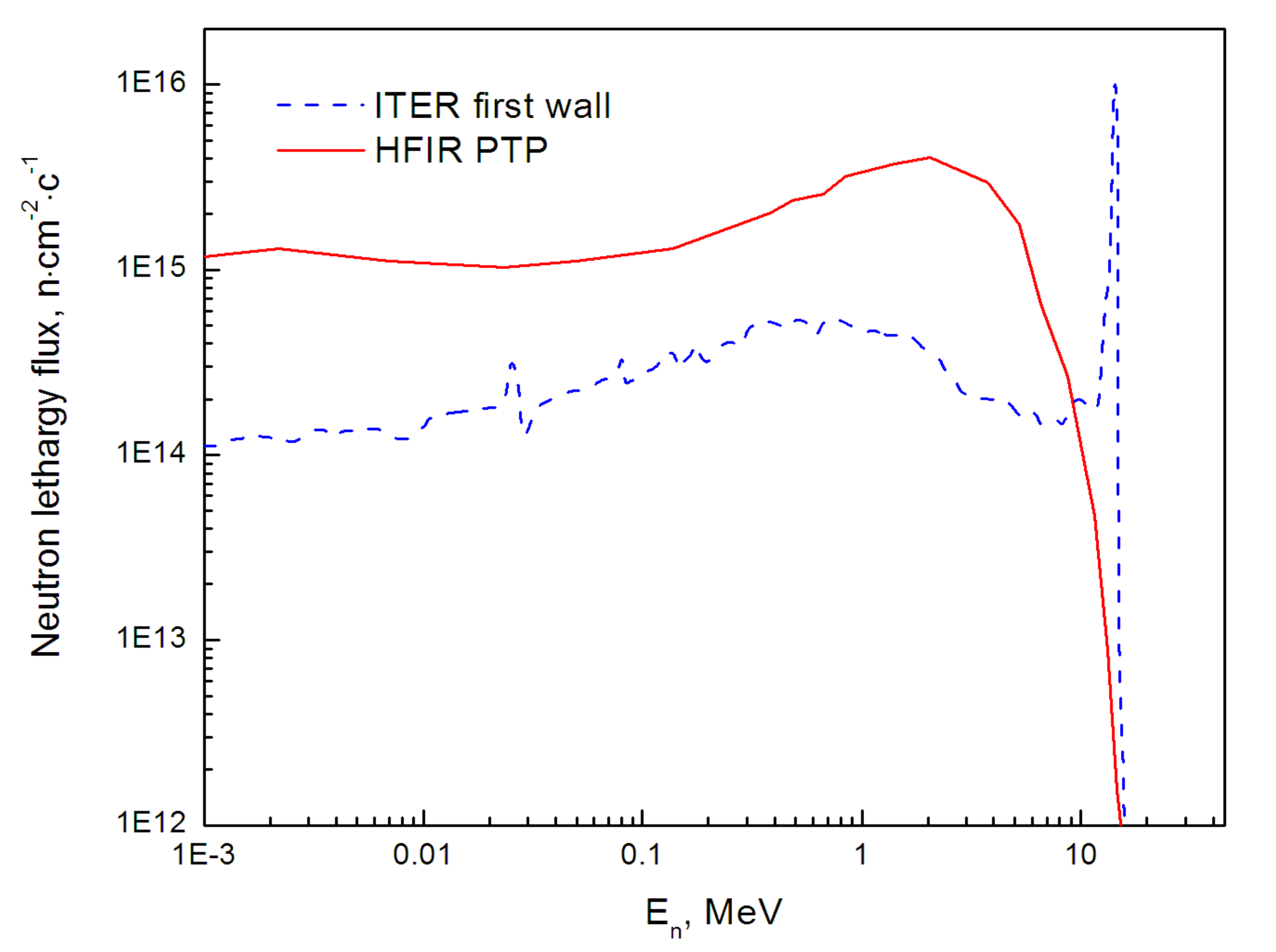
- **In fusion reactors inelastic collisions of fast neutrons with atoms due to different nuclear reaction channels (n,n'; n,γ; n,α; n,p et. al.) should be taking into account for calculations of PKA, recoil atom energy spectra, point defects, cascades and sub-cascades.**

Point Radiation Damage Production in Irradiated Materials due to Elastic and Inelastic Processes

Neutron Energy Fluxes for different Fast Neutron Facilities



Neutron Energy Fluxes for different Fast Neutron Facilities (HFIR, ITER)



Calculations of Point Defects formation in Different Materials

$$\Sigma_D(E_n) = \int_{E_d}^{E_{\max}} \sigma(E_n, T)\nu(T)dT$$

$\Sigma_D(E_n)$ - Displacement cross section as a function of neutron energy ***En***

$\sigma(E_n, T)$ - Differential cross section for scattering of fast neutron with energy ***En*** on atom with the energy transfer ***T*** to atom

$\nu(T)$ - Total number of point defects produced by PKA with energy ***T***

E_d - Displacement energy

$$E_{\max} = E_n \frac{4m_n M_{PKA}}{(m_n + M_{PKA})^2}$$

Norgett-Robinson-Torrens (NRT) model for radiation point defect formation

$$\nu(T) = 0.8\frac{\hat{T}(T)}{2E_d}$$

$$\hat{T}(T) = \frac{T}{1 + k(3.4008\varepsilon_i^{1/6} + 0.40244\varepsilon_i^{3/4} + \varepsilon_i)}$$

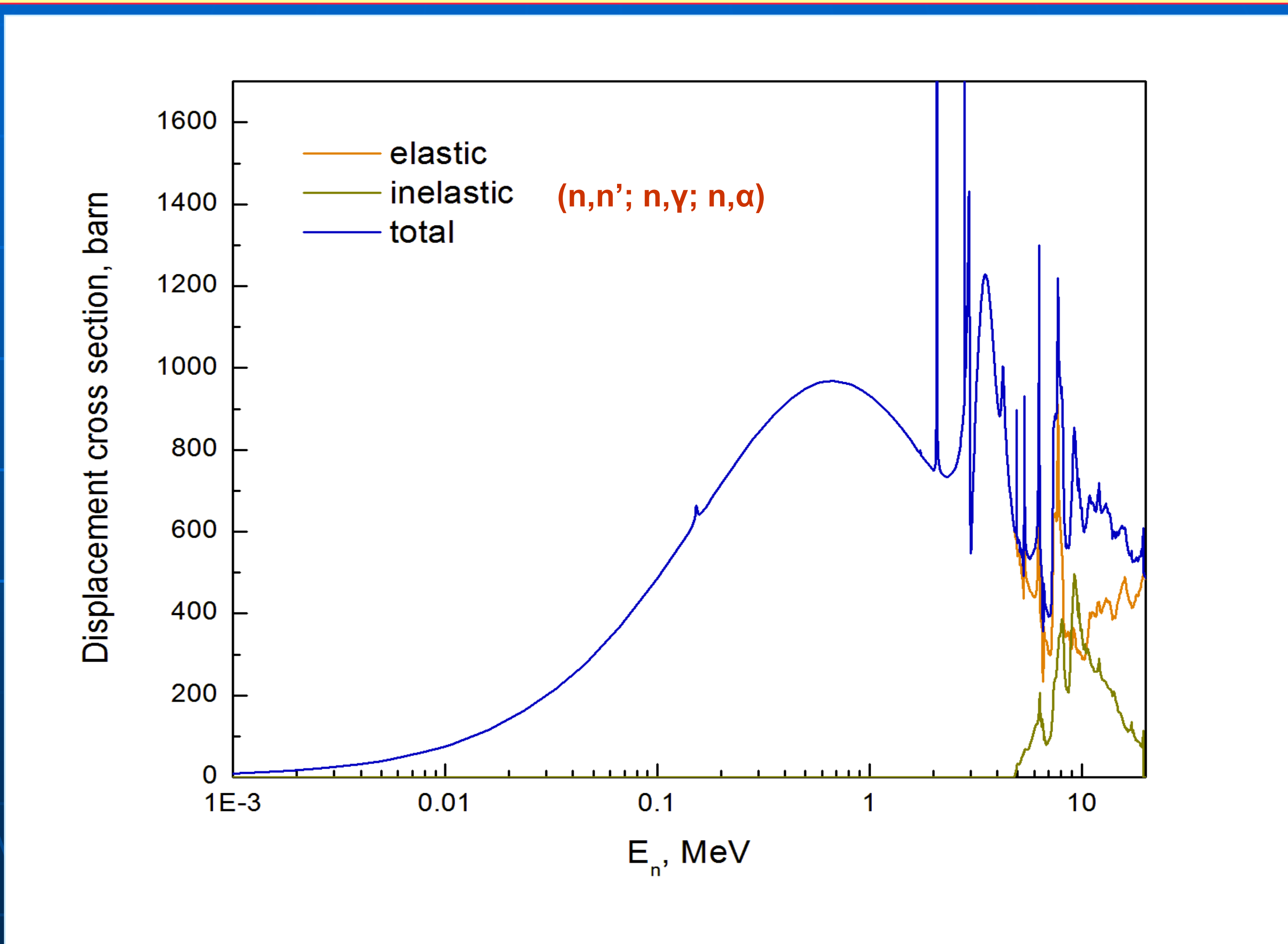
$$\varepsilon_i = \frac{A_T T}{(A_i + A_T)}\frac{a}{Z_i Z_T e^2}$$

$$k = \frac{32}{3\pi}\left(\frac{m_e}{M_T}\right)^{1/2}\frac{(A_i + A_T)^{3/2} Z_i^{2/3} Z_T^{1/2}}{A_i^{3/2}(Z_i^{2/3} + Z_T^{2/3})^{3/4}}$$

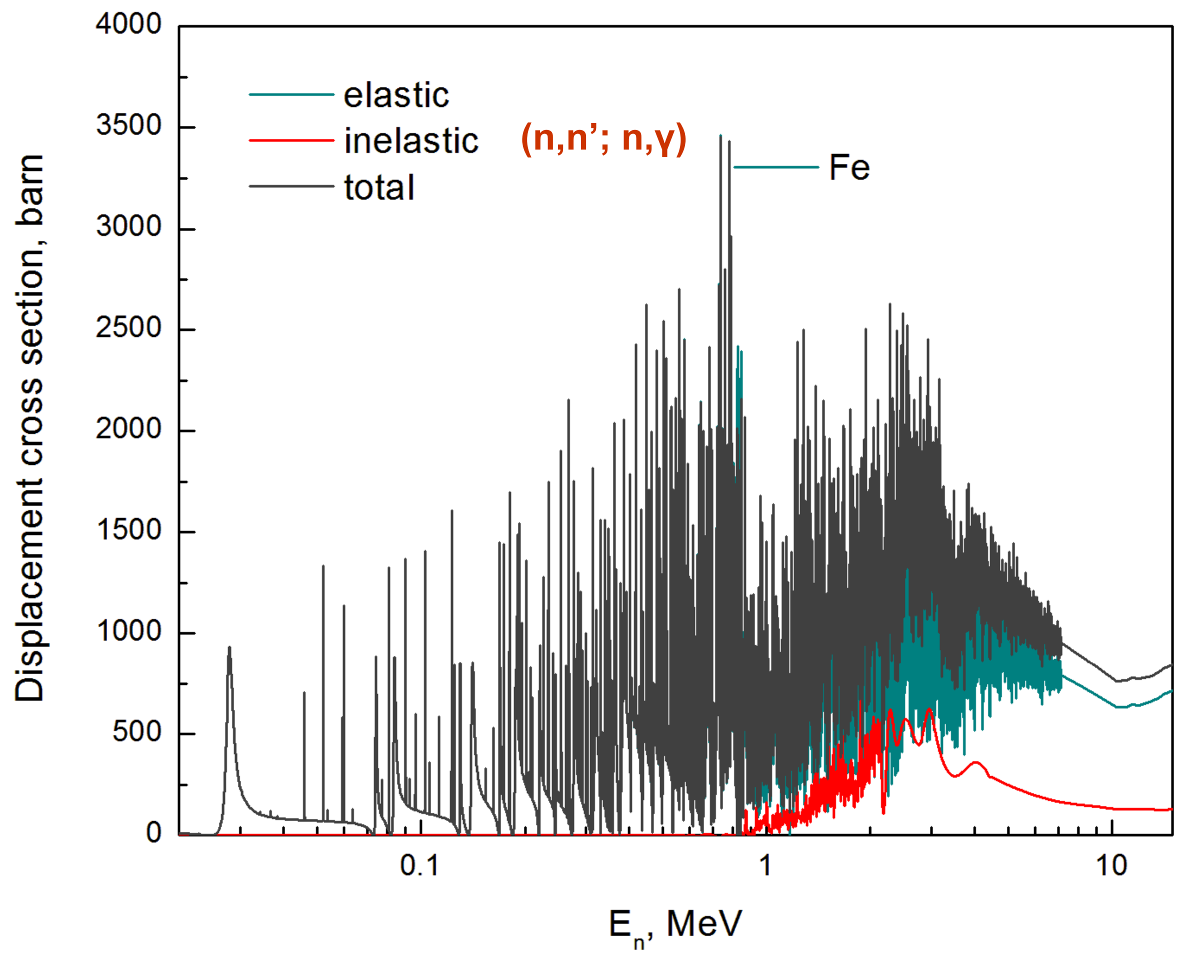
$$a = \frac{a_0(9\pi^2/128)^{1/3}}{(Z_i^{2/3} + Z_T^{2/3})^{1/2}}$$

a - is the Bohr radius, m_e - is the electron mass, M_T - is the mass of the target atom, e - is the electron charge, E_d is the displacement energy, A_i and A_T are atomic masses of the incident (recoil) and target atoms respectively, Z_i and Z_T are atomic numbers of the incident (recoil) and target atoms respectively

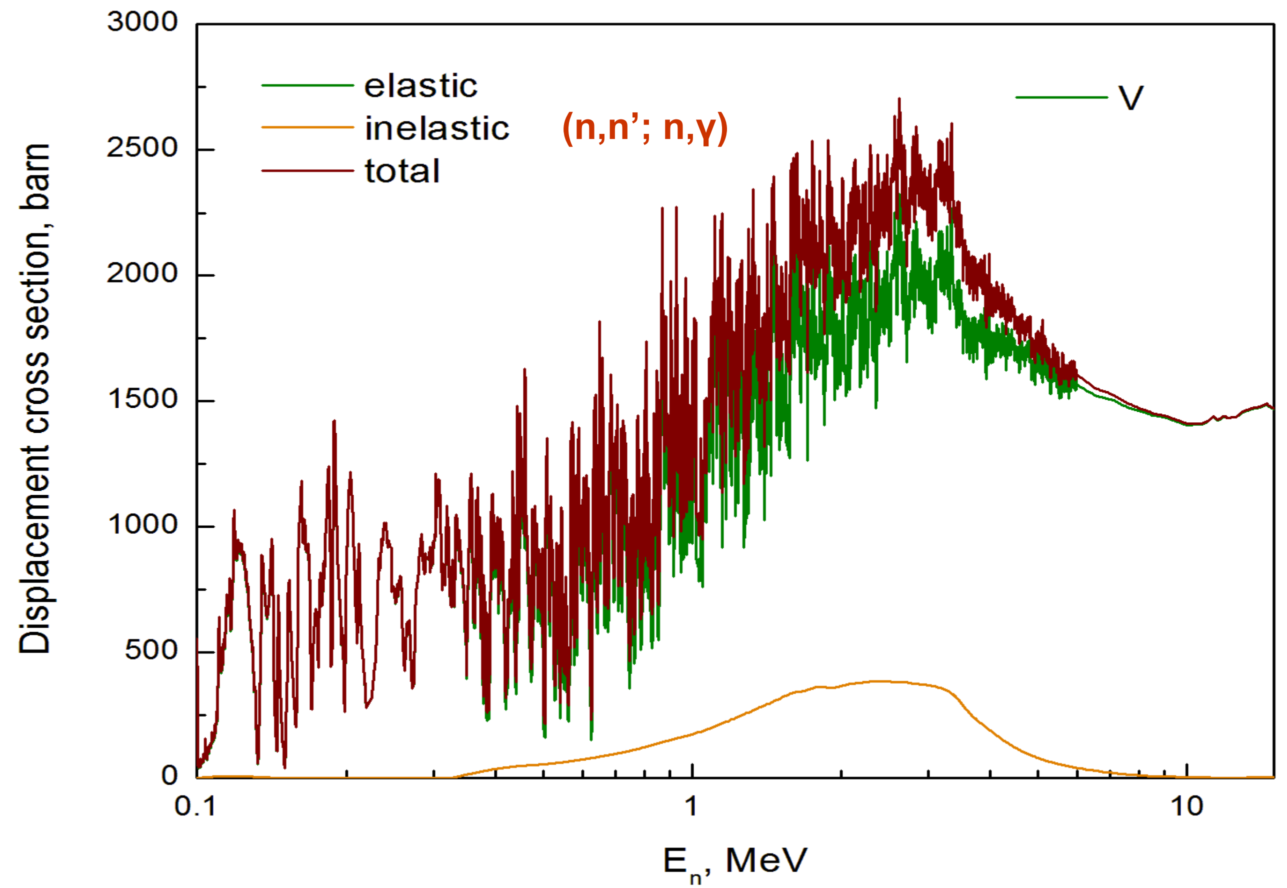
Cross Section of Point Defect Formation in C as a Function of Neutron Energy



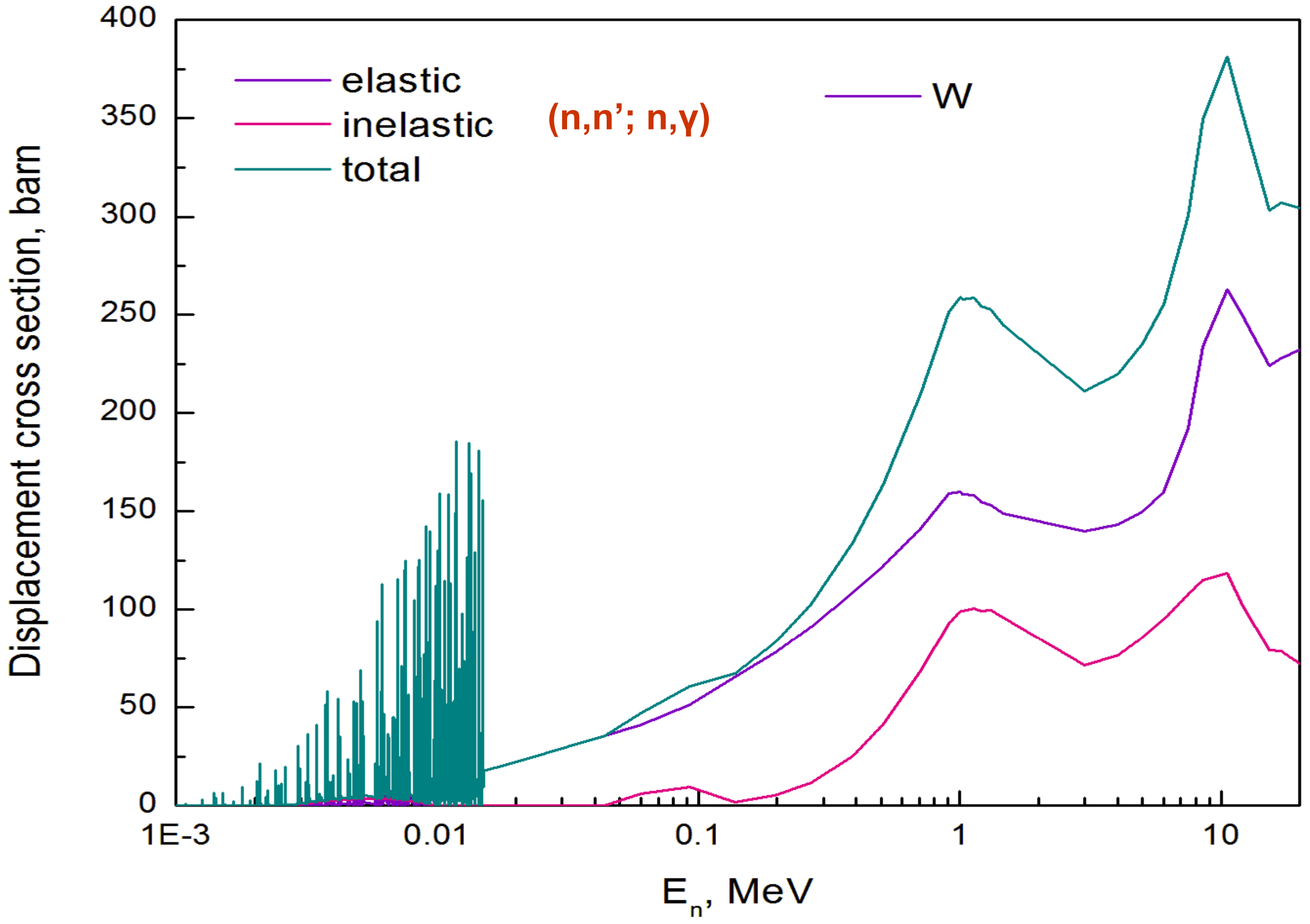
Cross Section of Point Defect Formation in Fe as a Function of Neutron Energy



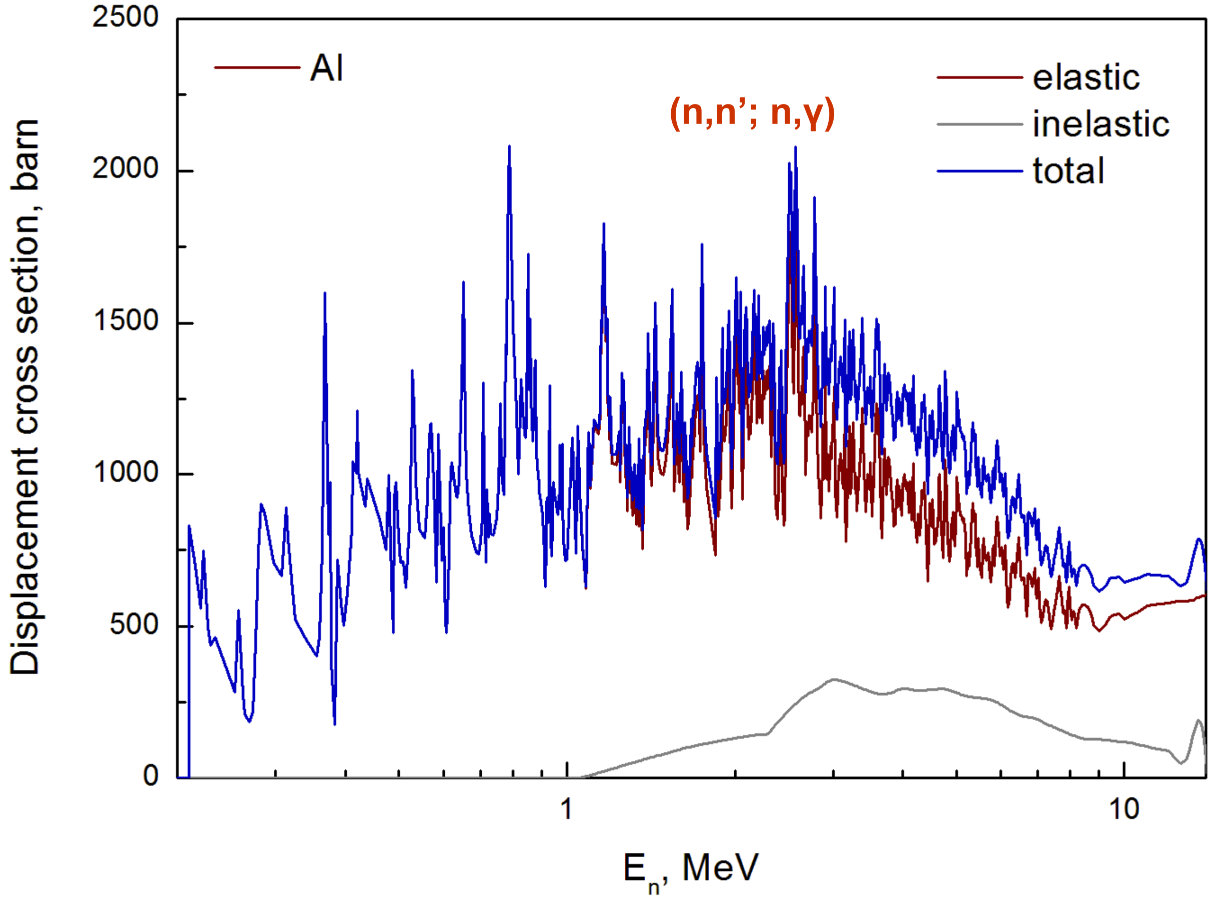
Cross Section of Point Defect Formation in V as a Function of Neutron Energy



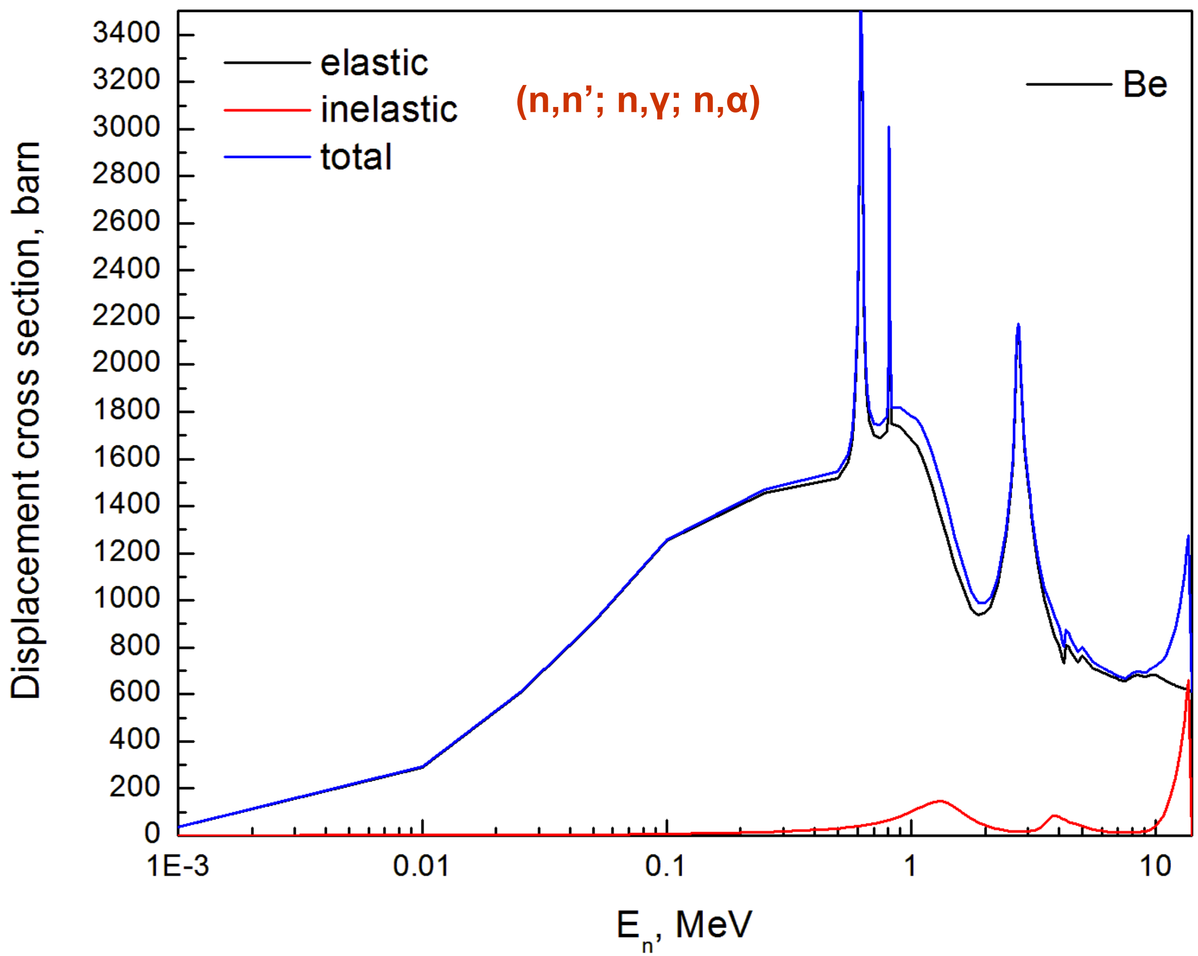
Cross Section of Point Defect Formation in W as a Function of Neutron Energy



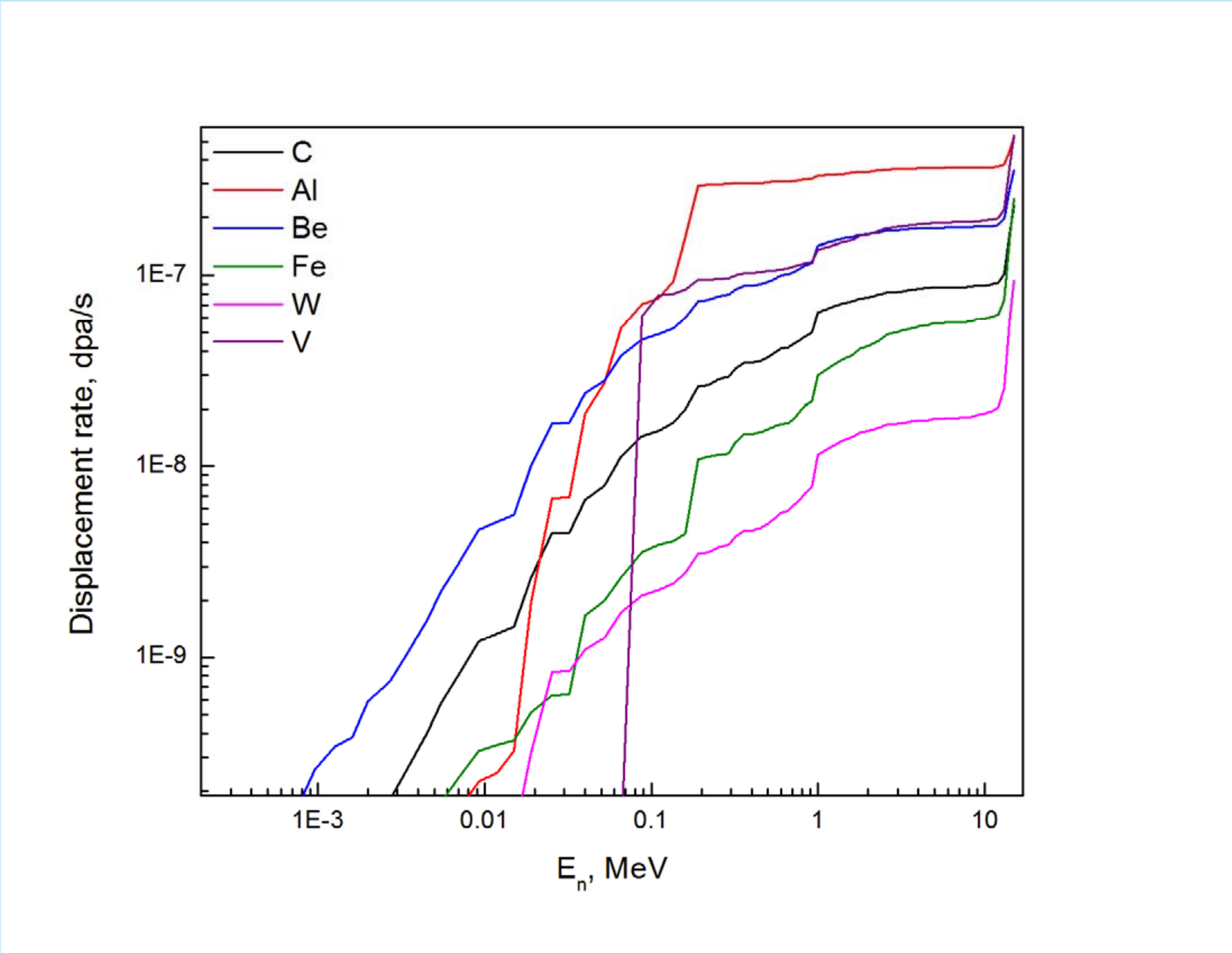
Cross Section of Point Defect Formation in Al as a Function of Neutron Energy



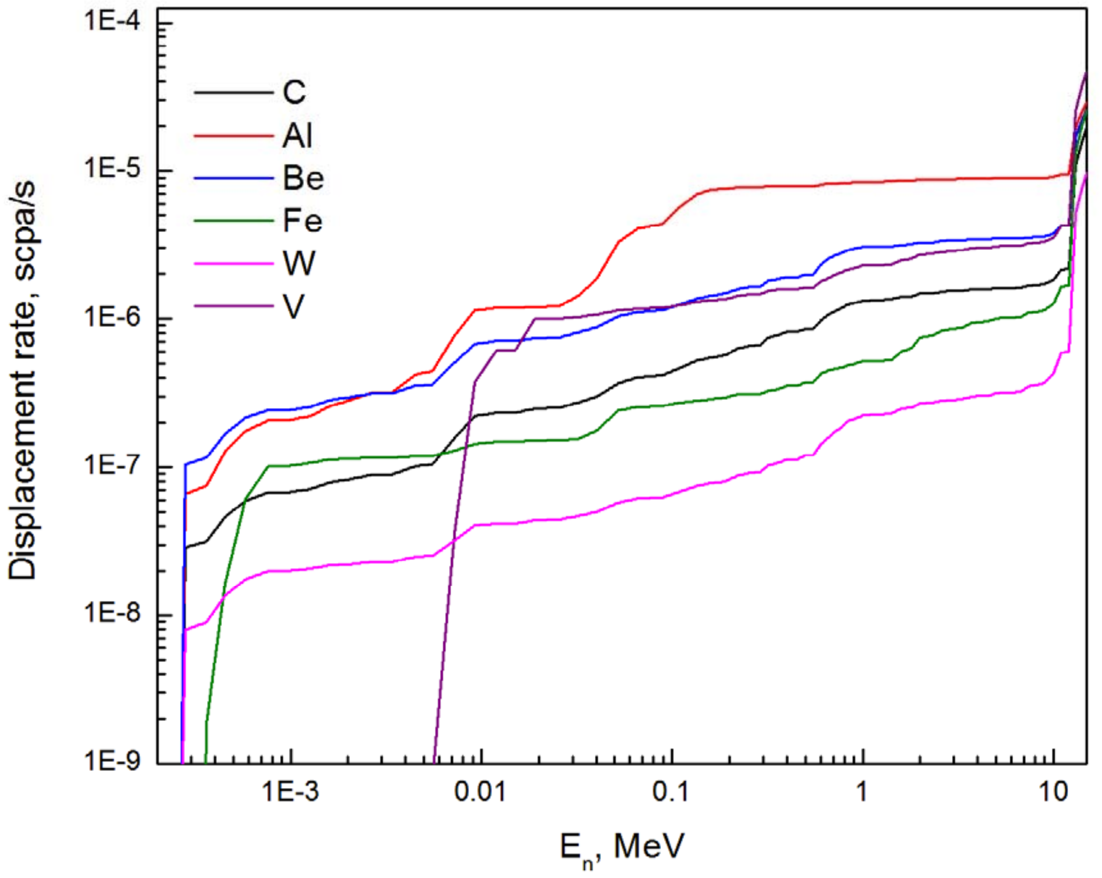
Cross Section of Point Defect Formation in Be as a Function of Neutron Energy



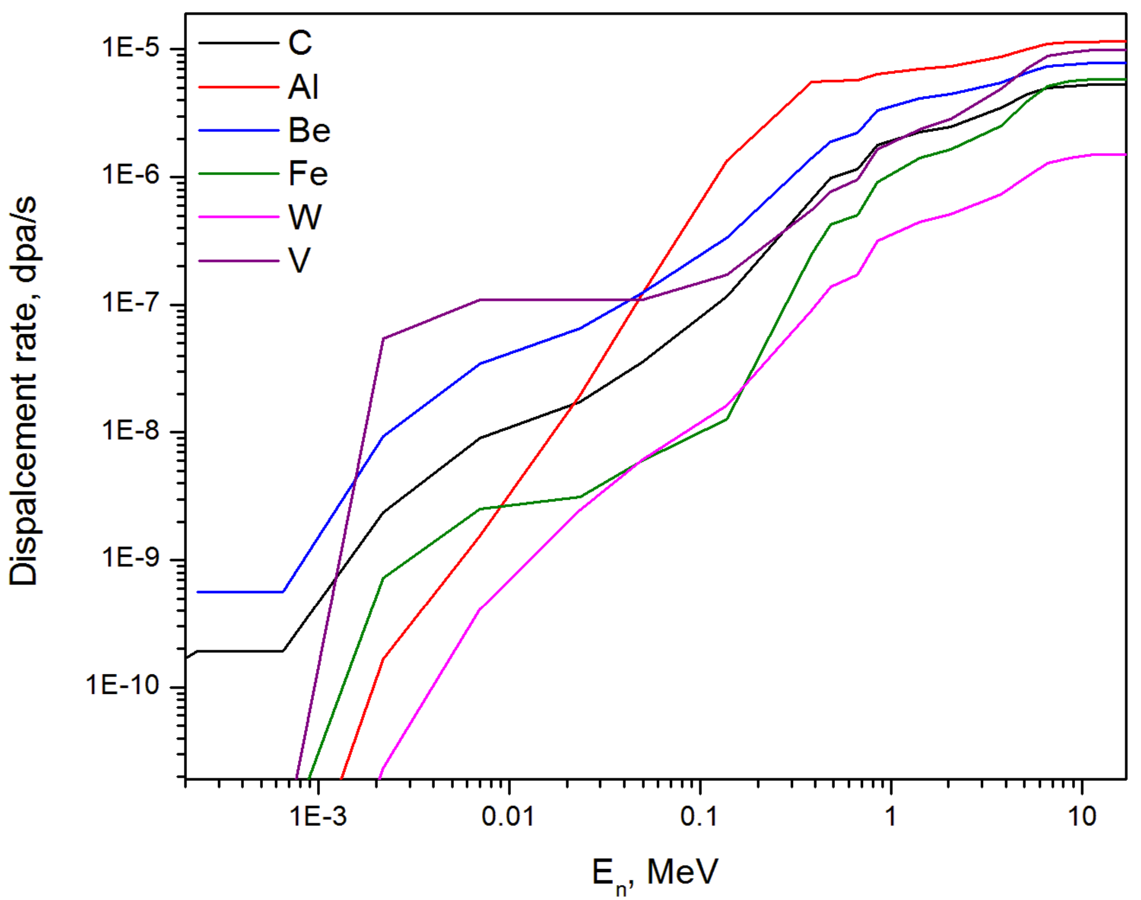
Displacement Rate of Point Defects in different Materials under Neutron Irradiation in DEMO



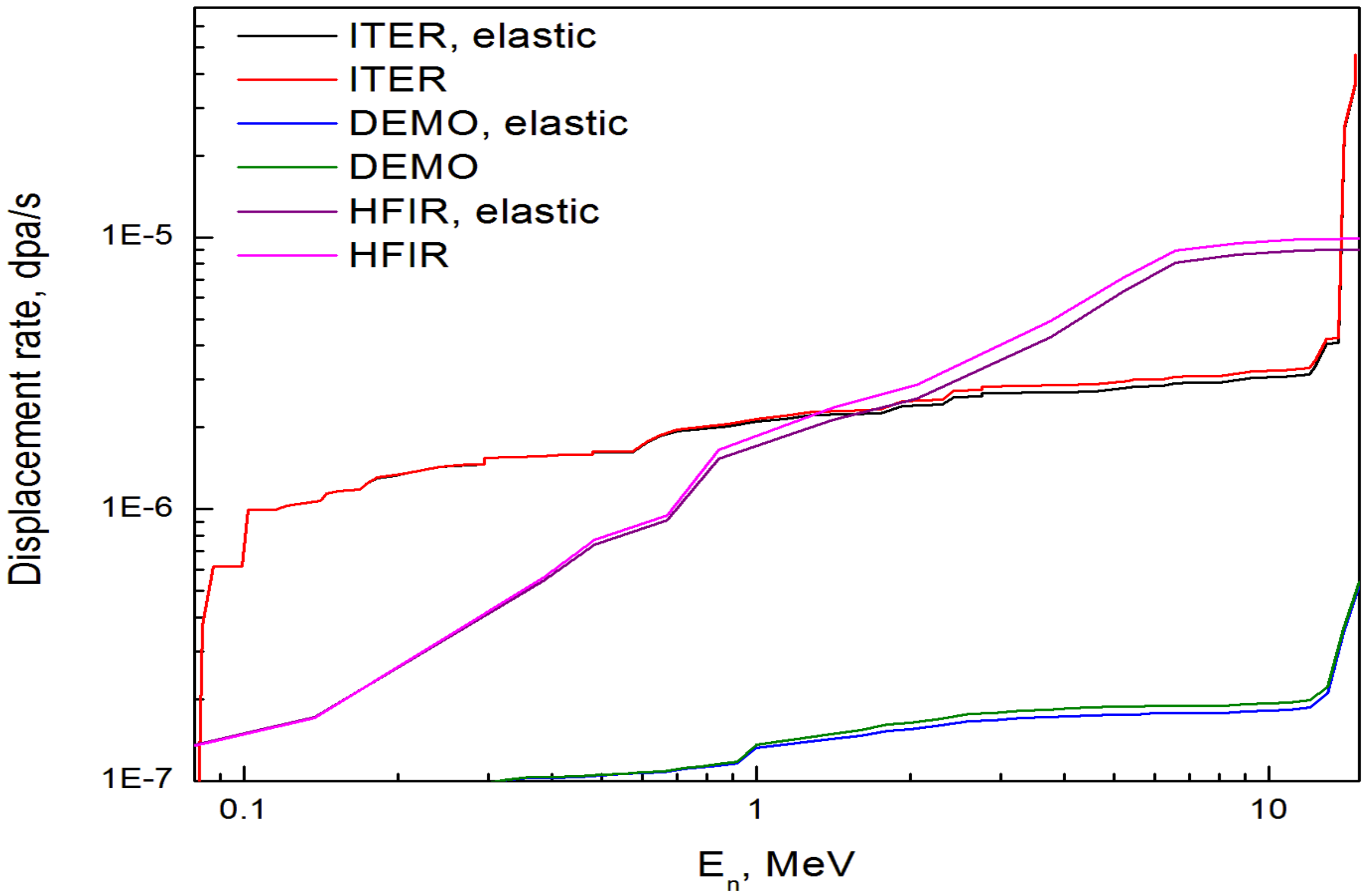
Displacement Rate of Point Defects in different Materials under Neutron Irradiation in ITER



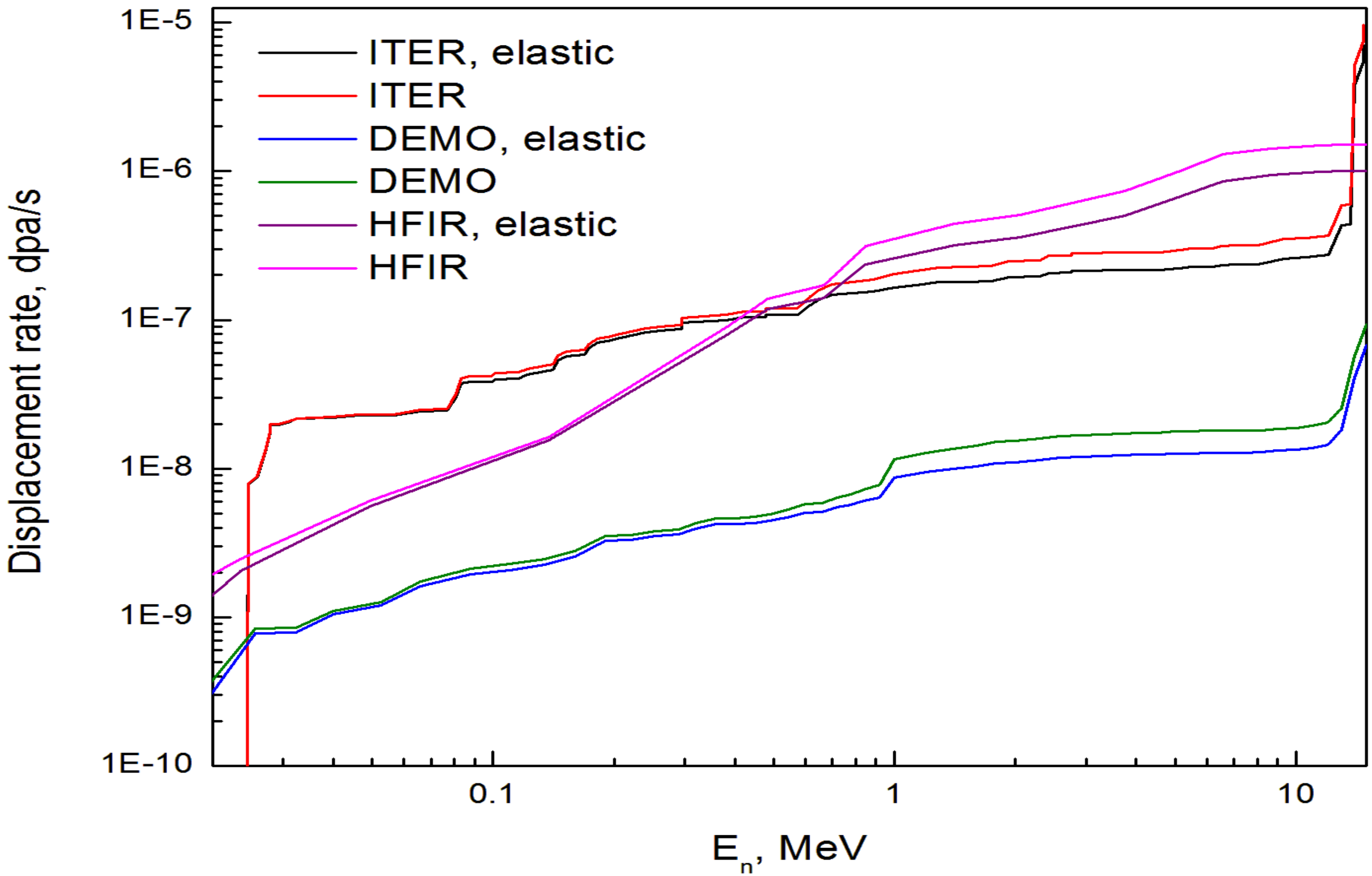
Displacement Generation Rate of Point Defects in different Materials under Neutron Irradiation in HFIR



Displacement Rate of Point Defects for V in different Fusion and Fission Facilities

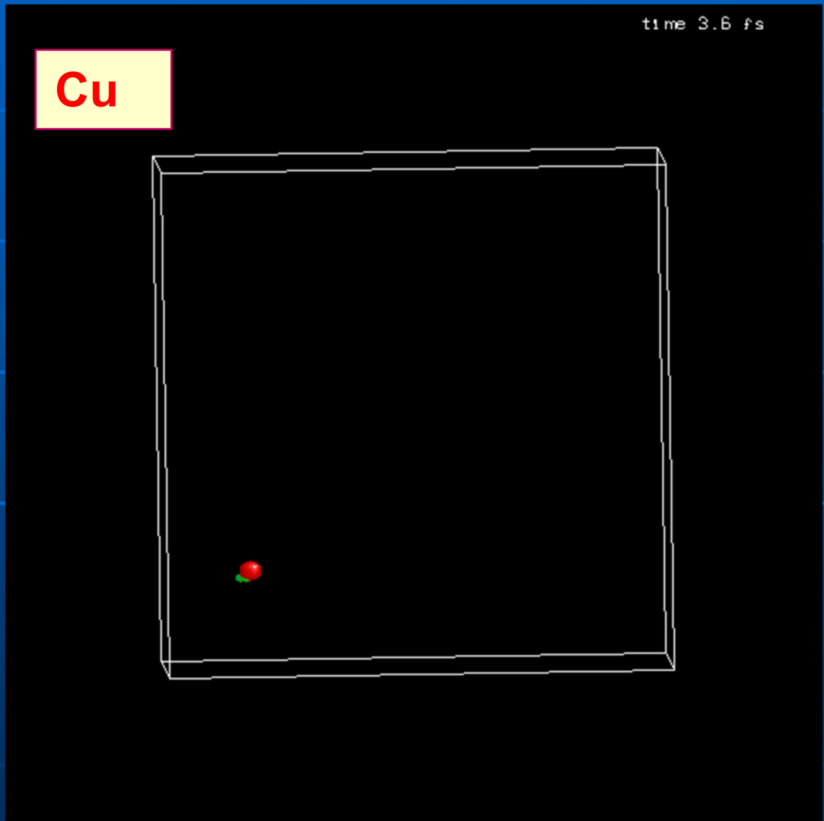


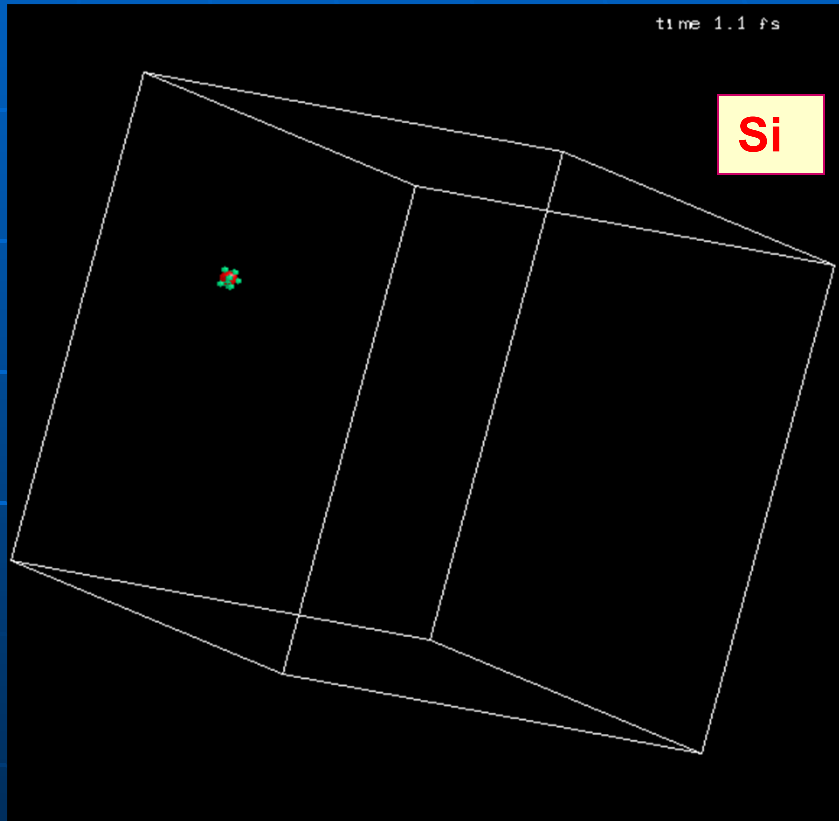
Displacement Rate of Point Defects for W in different Fusion and Fission Facilities



Theoretical modeling and numerical calculations of cascade and sub-cascade formation in irradiated materials

Comparison of cascade and sub-cascade formation in light and heavy materials.

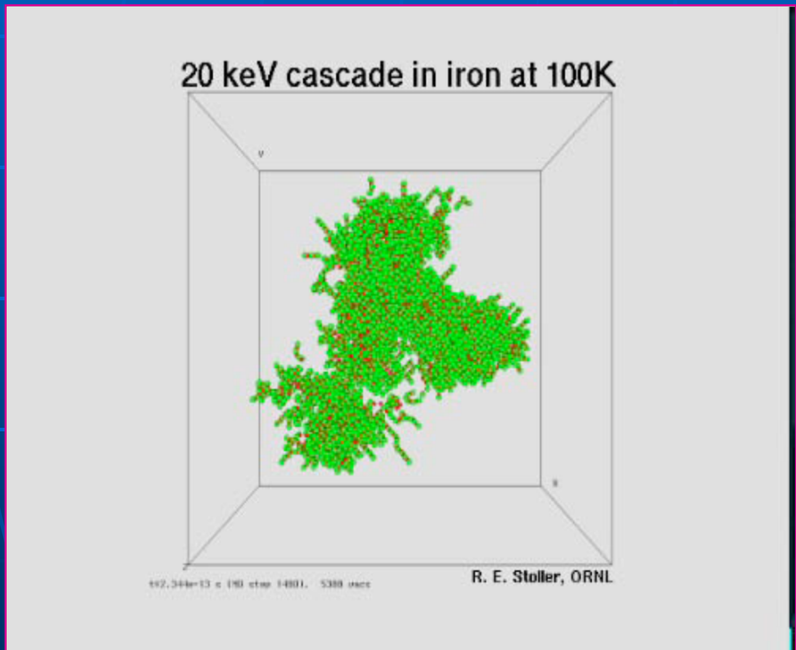


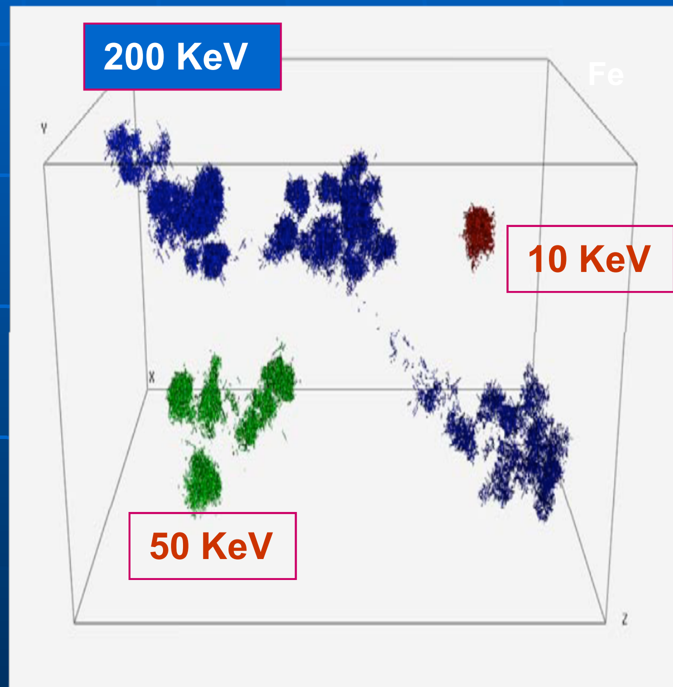


K. Nordlund (1998)

Molecular Dynamics simulations have found the primary damage formation is similar for fission and fusion neutrons

- Subcascade formation leads to asymptotic behavior at high energies
- Agrees with experimental data (TEM, etc.) (S. Zinkle, 2004)





R.E. Stoller, 2004

Theoretical Model

First idea was suggested by M.Kiritani:

Y. Satoh, S. Kojima, T. Yoshiie, M. Kiritani, J. Nucl. Mat., 179-181, (1991) 901.
Y. Satoh, T.Yoshiie, M.Kiritani, J.Nucl.Mat., 191-194, (1992), 1101.

Some first results from:

H.L.Heinisch, B.N.Singh , Philosophical Magazine A, vol. 67(1993) 407.
H.L.Heinisch, B.N.Singh , J.Nucl.Mat., 251 (1997) 77.
R.E.Stoller, Mat. Res. Soc. Symp. Proc. Vol. 373 (1995) 21.
R.E.Stoller, Proc. ICFRM-8, J.Nucl.Mat. 555 (1998) 10.

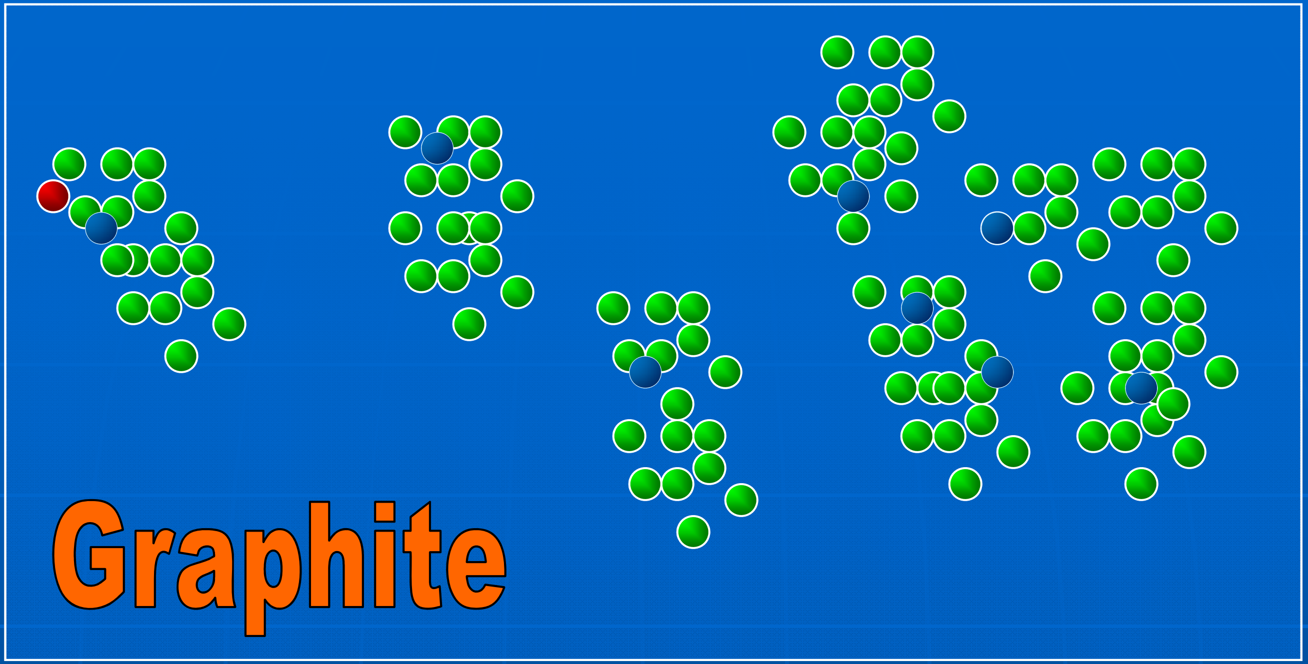
Following development of theoretical model:

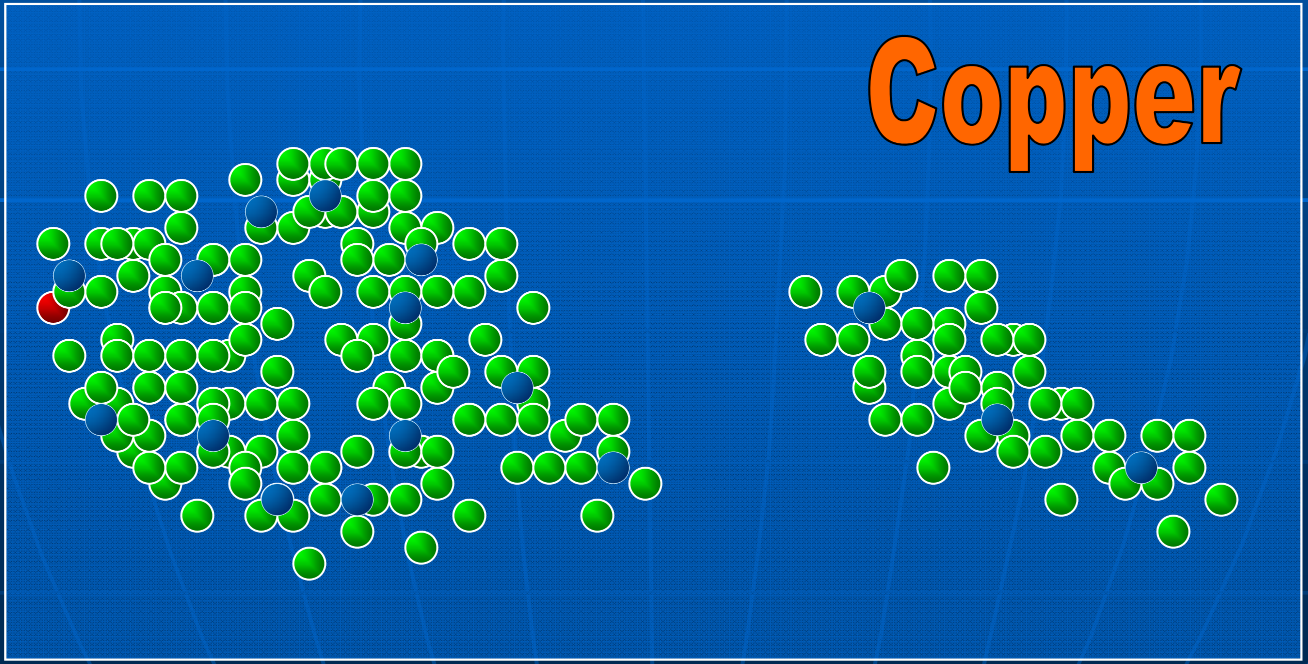
A.I. Ryazanov, E.V.Metelkin, Atomic Energy, v.83, No 3, (1997), 653.

Binary elastic collision model is used for moving atoms with real interatomic potential.

New criterion for sub-cascade formation is suggested.

Sub-cascade formation cross - sections and generation rates of sub-cascades are calculated for different neutron energy spectra in fusion facilities.


Graphite

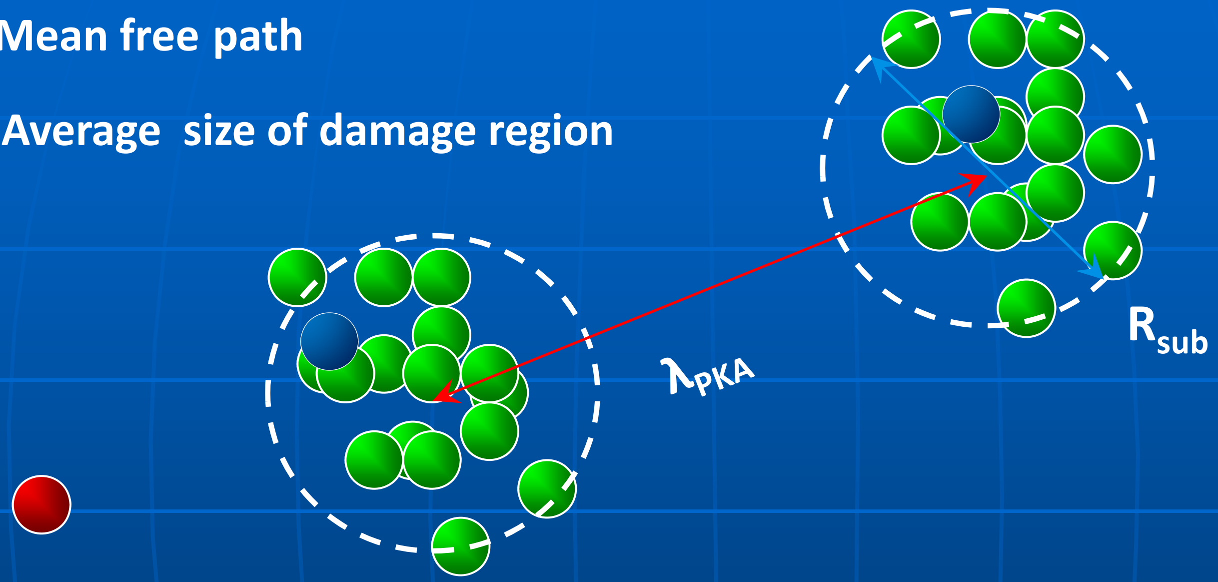

Copper

PKA

SKA

λ_{PKA} **Mean free path**

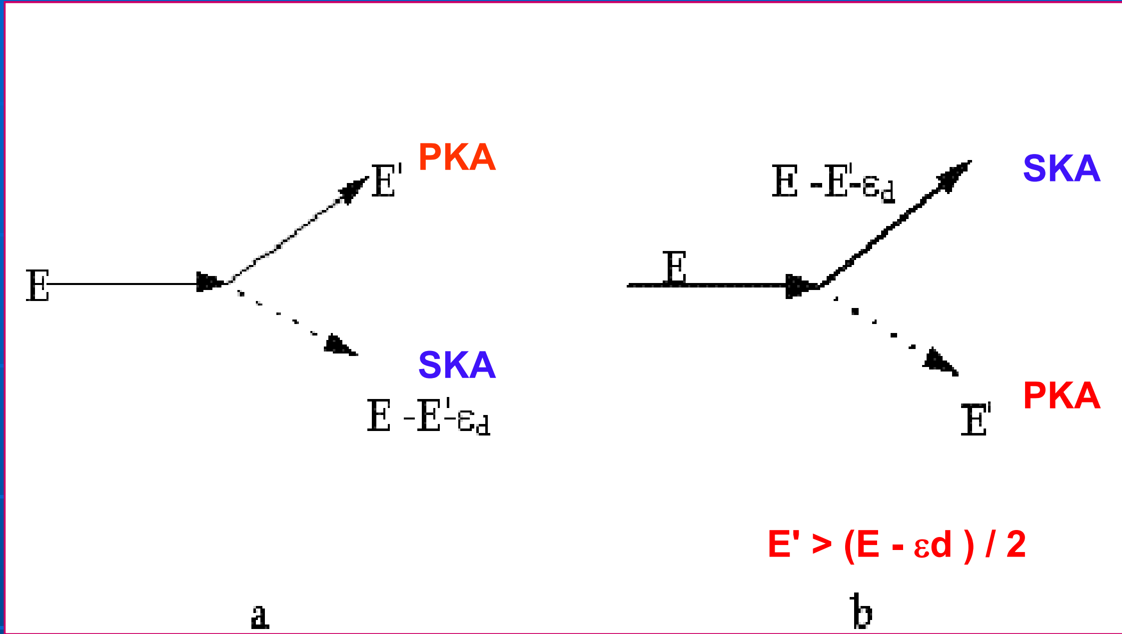
R_{sub} **Average size of damage region**



Sub-cascade formation criterion:

$$\lambda_{PKA} \geq R_{sub}$$

Binary Collision Model



Σ(E→E') **- the differential cross-section for incident atom with initial energy *E* to get after elastic collision energy *E'***

The cross-section $\Sigma(E, E_{sf})$ **characterizing the collision with transfer energy higher than *Esf***

$$\Sigma(E, E_{sf}) = \int_{E_{sf}}^{(E-\varepsilon_d)/2} dT\,[\Sigma(E \rightarrow E' - T - \varepsilon_d) + \Sigma(E \rightarrow T)] = \int_{E_{sf}}^{(E-\varepsilon_d)/2} dT P(E, T) \Sigma(E)$$

$\lambda_{PKA}(E)$ - the distance between two collisions

$$\lambda_{PKA}(E) = \frac{1}{N_a \Sigma(E, E_{sf})}$$

$R_{sub}(E, E_{sf})$ – the average size of damage zone produced by *SKA*

$$R_{sub}(E, E_{sf}) = \int_{E_{sf}}^{(E-\varepsilon_d)/2} P(E,T) R(T) dT$$

P(E,T) the probability density for *SKA* with initial energy ***E*** to have a kinetic energy ***T*** after collision

R(T) the displacement depth of *SKA* with an initial kinetic energy ***T***

$$R(T) = \int_0^T \frac{dT}{(dT / dx)_{tot}}$$

where $(dT/dx)_{tot} = (dT/dx)_n + (dT/dx)_e$ - the total stopping power including the elastic stopping power $(dT/dx)_n$ and inelastic (electronic losses) stopping power $(dT/dx)_e$

$$\lambda_{PKA} \geq R_{sub}$$

Threshold Energy for Sub-cascade Formation

	Cu	Ag	Au
Suggested Model	**20 KeV**	**62 KeV**	**210 KeV**
Monte Carlo Method	**26 KeV**	**48 KeV**	**172 KeV**

$$E_{sf}(KeV) = 0,0056Z^{2.415}$$

A.I.Ryazanov, E.V.Metelkin,

Atomic Energy, v.83, No 3, 1997, 653.

Number of Sub-cascades as a Function of PKA Energy

$$N_{sc}(E) = 1 + \int_{2E_{sf}}^{E} \frac{N_a \Sigma_{sf}(T)\,dT}{\left(\frac{dT}{dx}\right)_{tot}}$$

$\Sigma_{sf}(T)$ **is the energy cross section for sub-cascade formation,**

N_a **is the density of target atoms,**

$$\left(\frac{dT}{dx}\right)_{tot} = \left(\frac{dT}{dx}\right)_n + \left(\frac{dT}{dx}\right)_e$$

$$\left(\frac{dT}{dx}\right)_n = \frac{N_a \varepsilon}{T} \int_0^{T^2/\varepsilon^2} \left(\frac{\pi a^2}{2t^{1/2}}\right) \frac{\lambda t^{1/2-m}\,dt}{(1+(2\lambda t^{1-m})^q)^{1/q}}$$

$$\left(\frac{dT}{dx}\right)_e = N_a \left(S_L(T)^{-1} + S_{BB}(T)^{-1}\right)^{-1}$$

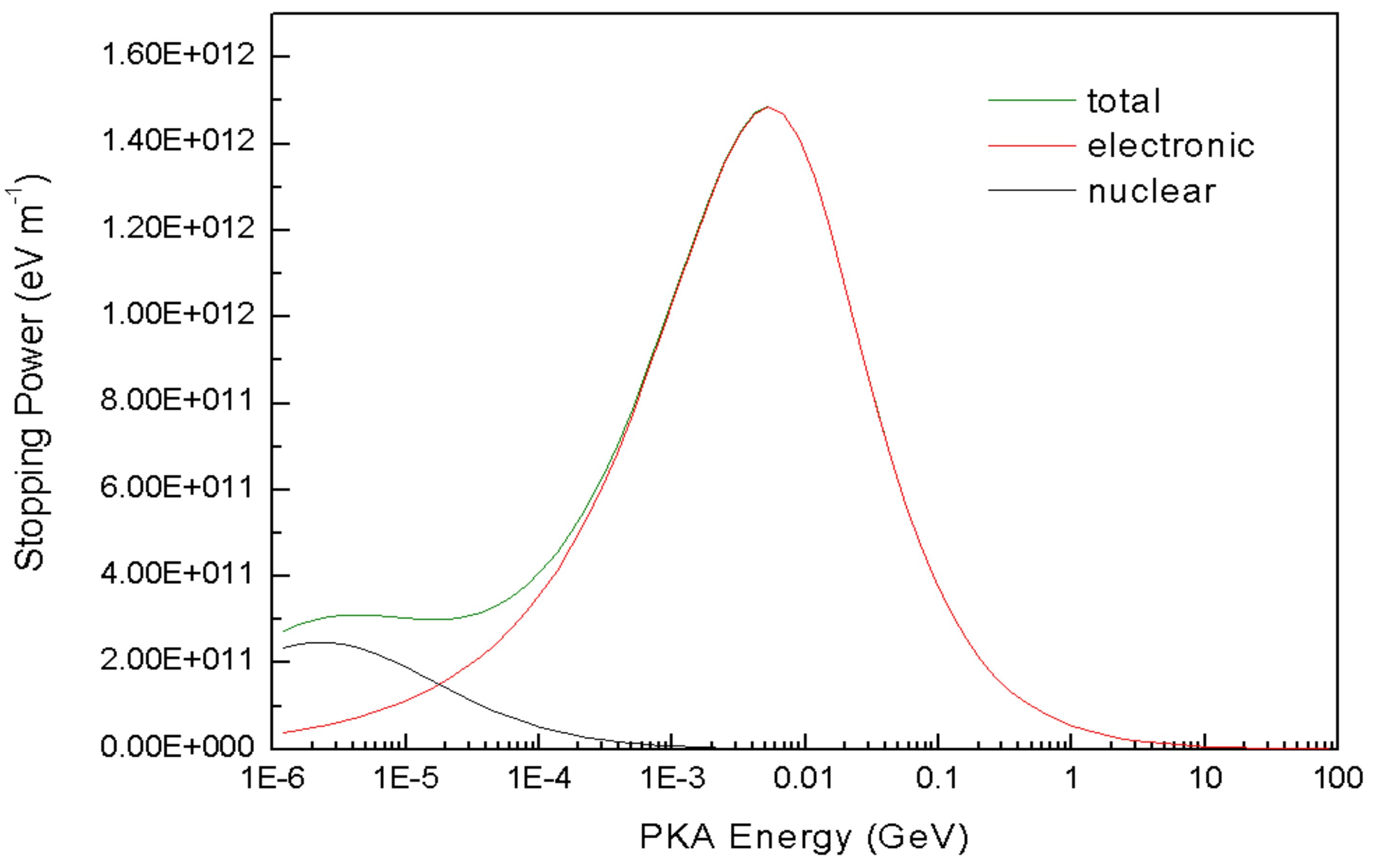
$$S_L(T) = k_L T^{1/2}$$

$$k_L = \frac{4 a_0 h \sqrt{2} Z_i^{7/6} Z_T}{(Z_i^{2/3} + Z_T^{2/3})^{3/2} \sqrt{M_i}}$$

$$S_{BB}(T) = \frac{8\pi Z^2 e^4}{I \varepsilon_b} \ln\left(\varepsilon_b + 1 + \frac{5}{\varepsilon_b}\right)$$

$$\varepsilon_b = \frac{4 T m_e}{Z_T I \cdot M_i}$$

Total Energy Loss for Moving Atoms in Graphite



Calculations of Cross Sections of Sub-cascade Formation in Different Materials

$$\Sigma_{sf}(E_n) = \int_{E_{sf}}^{E_{\max}} \sigma(E_n, T) N_{sc}(T) dT$$

$\Sigma_{sf}(E_n)$ - Cross section of sub-cascade formation as a function of neutron energy ***En***

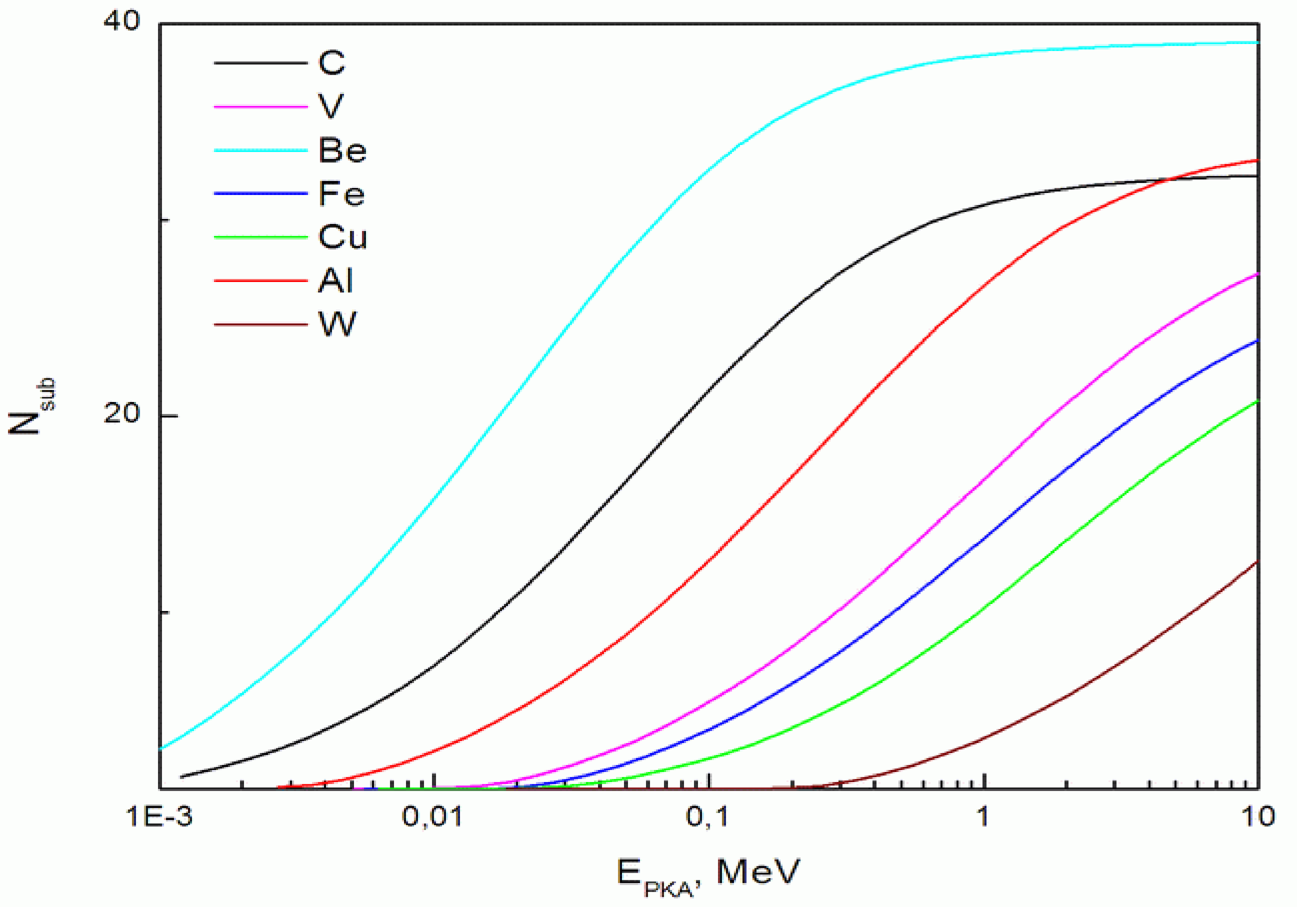
$\sigma_{el}(E_n, T)$ - Differential elastic cross section for scattering of fast neutron with energy ***En*** on atom with the energy transfer ***T*** to atom

$N_{sc}(T)$ - Number of sub-cascades produced by PKA with energy ***T***

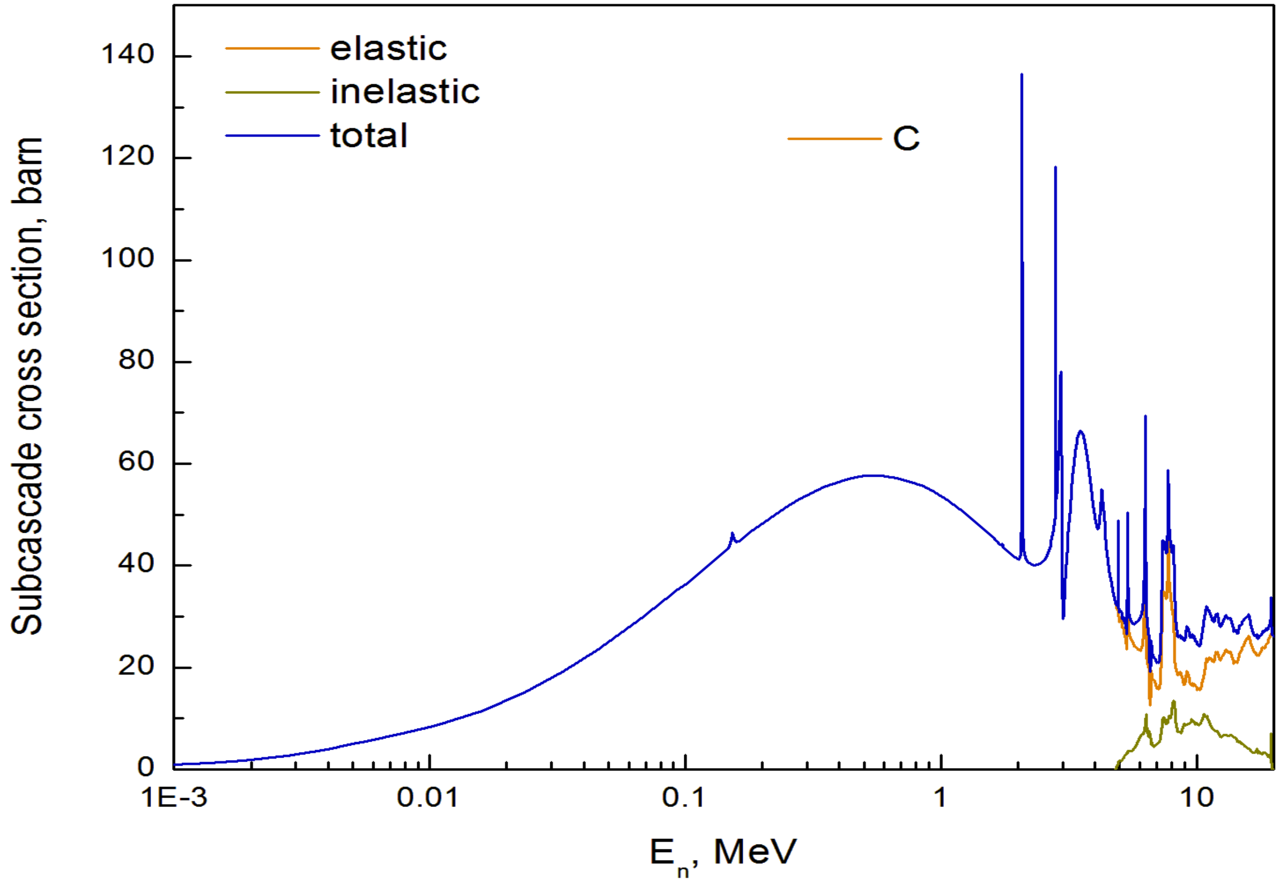
E_{sf} - Sub-cascade formation energy

$$E_{\max} = E_n \frac{4 m_n M_{PKA}}{(m_n + M_{PKA})^2}$$

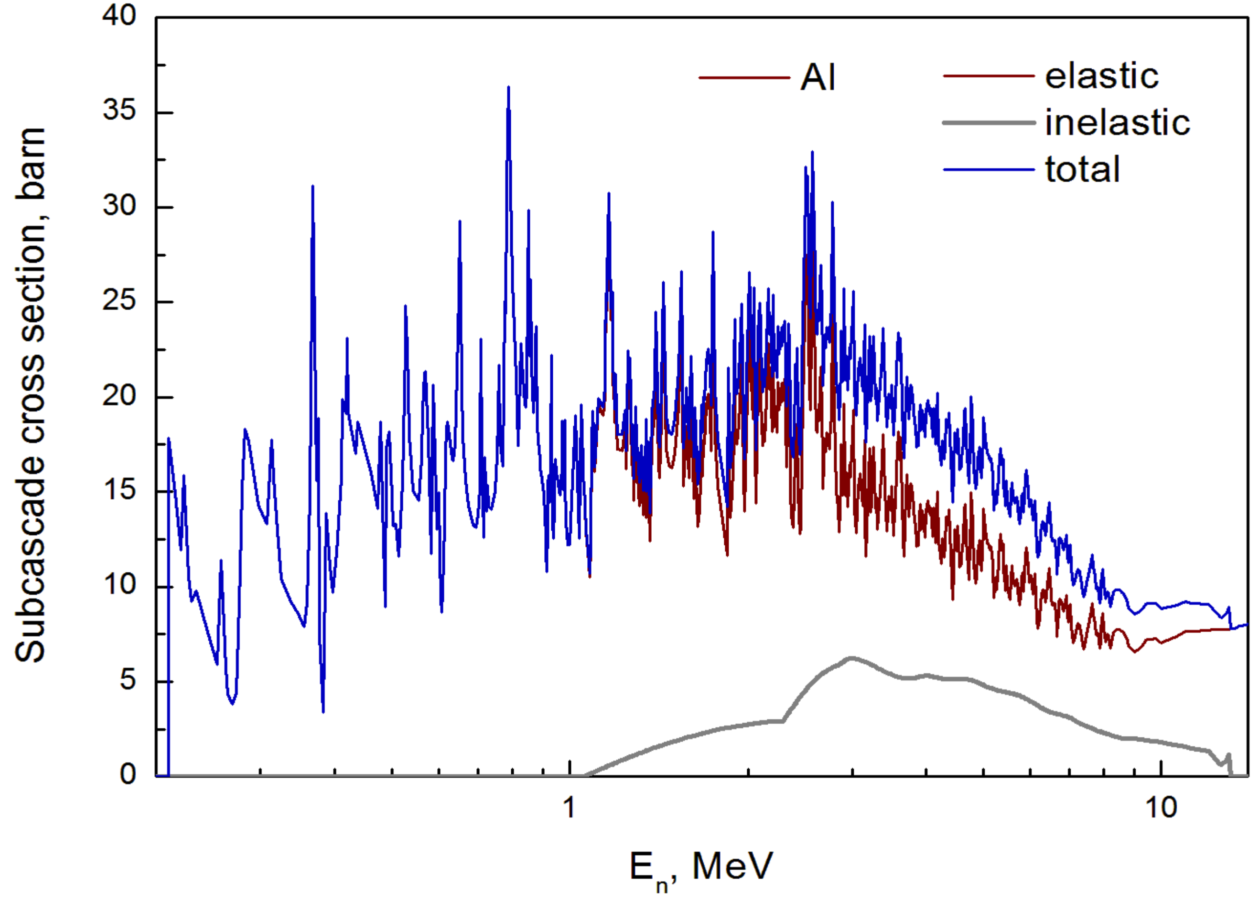
Number of Sub-cascades as a Function of PKA Energy



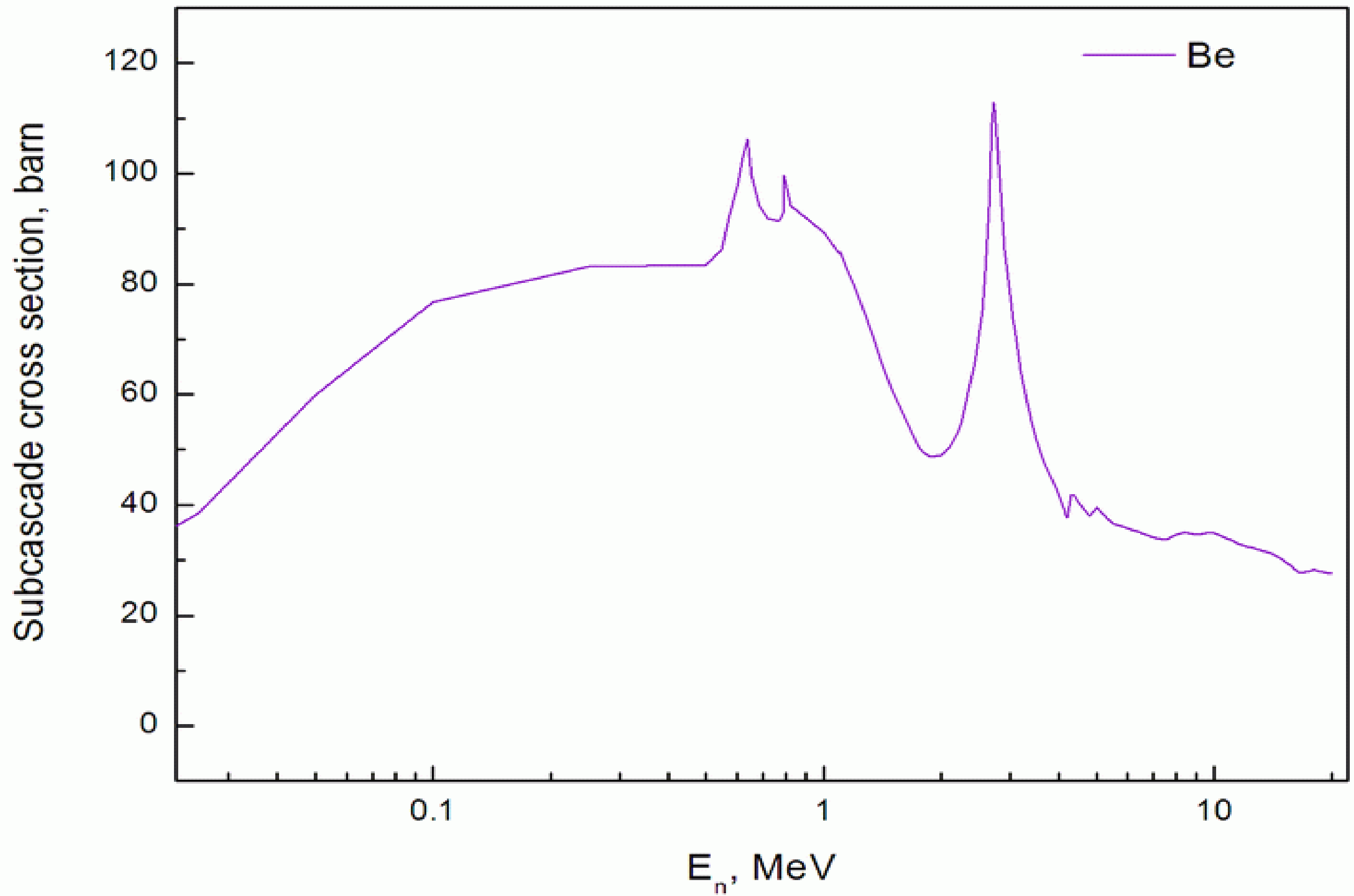
Cross Section of Sub-cascade Formation in C as a Function of Neutron Energy



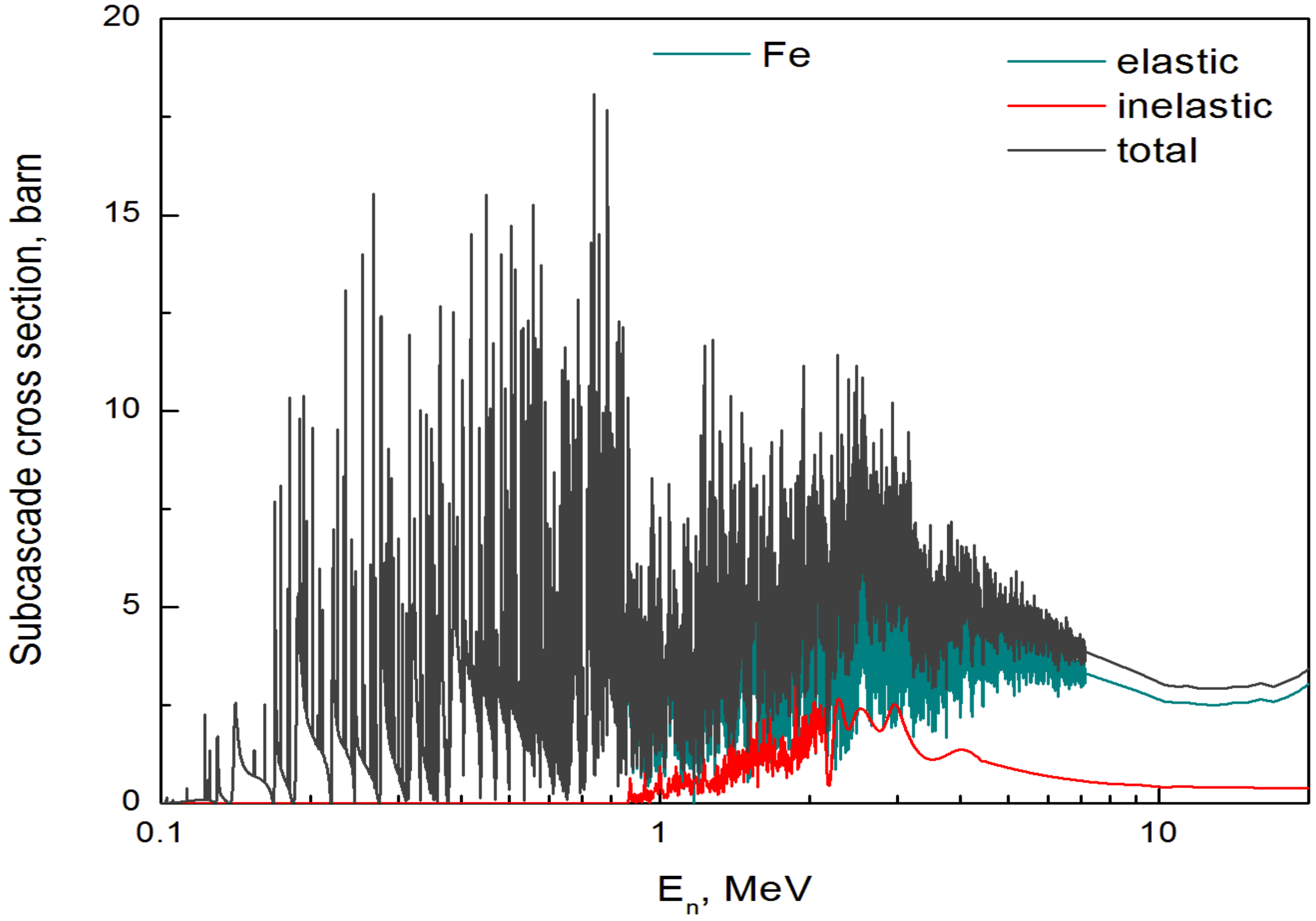
Cross Section of Sub-cascade Formation in Al as a Function of Neutron Energy



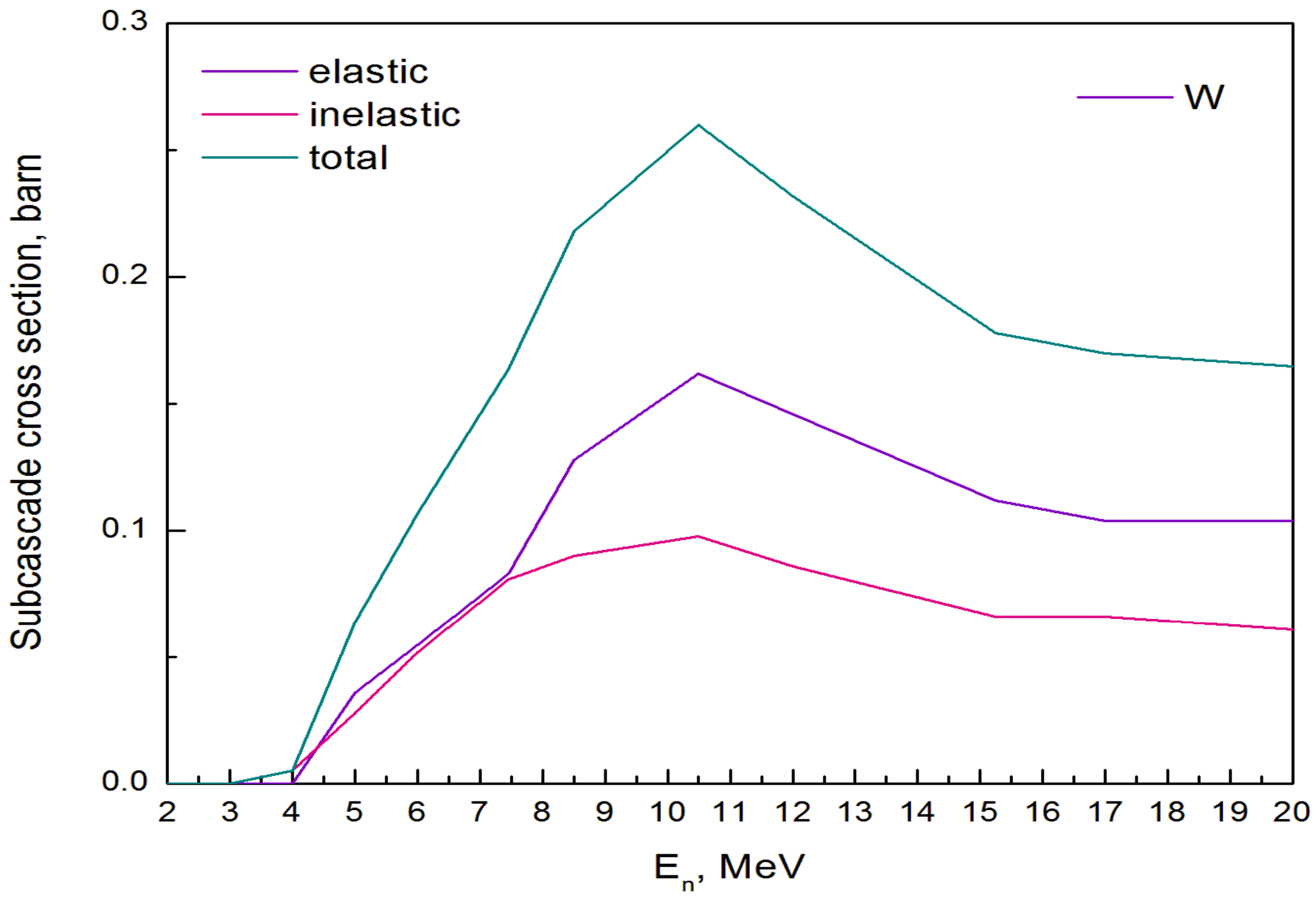
Cross Section of Sub-cascade Formation in Be as a Function of Neutron Energy



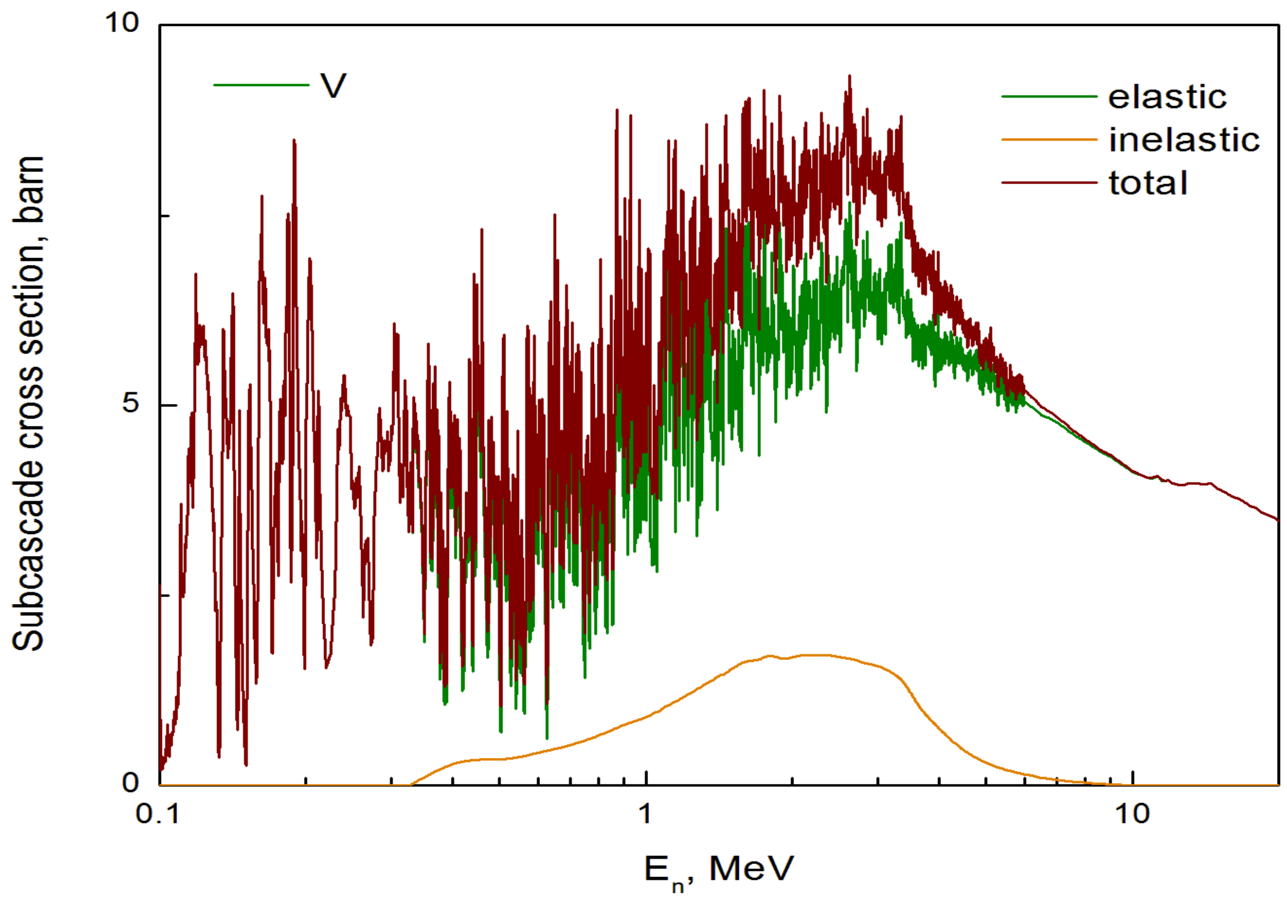
Cross Section of Sub-cascade Formation in Fe as a Function of Neutron Energy



Cross Section of Sub-cascade Formation in W as a Function of Neutron Energy



Cross Section of Sub-cascade Formation in V as a Function of Neutron Energy



Calculations of Sub-cascade Generation Rates in different Materials under Neutron Irradiation

$$G_{sf}(E_n) = \int_{E_{sf}}^{E_n} \Phi(E_n^{/}) \Sigma_{sf}(E_n^{/}) dE_n^{/}$$

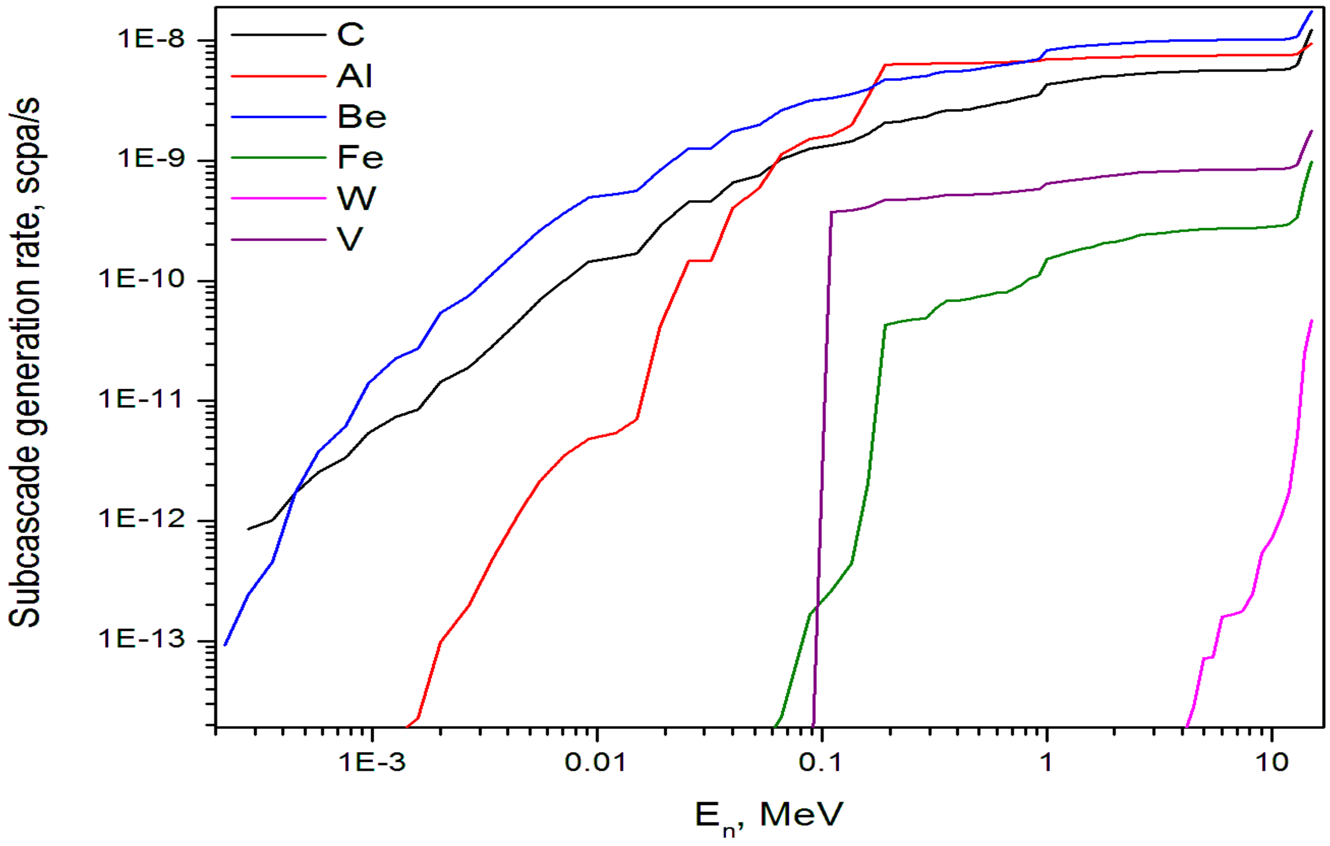
$G_{sf}(E_n)$ - Generation rate of sub-cascade formation as a function of neutron energy ***En***

$\Sigma_{sf}(E_n^{/})$ - Cross section of sub-cascade formation as a function of neutron energy ***En***

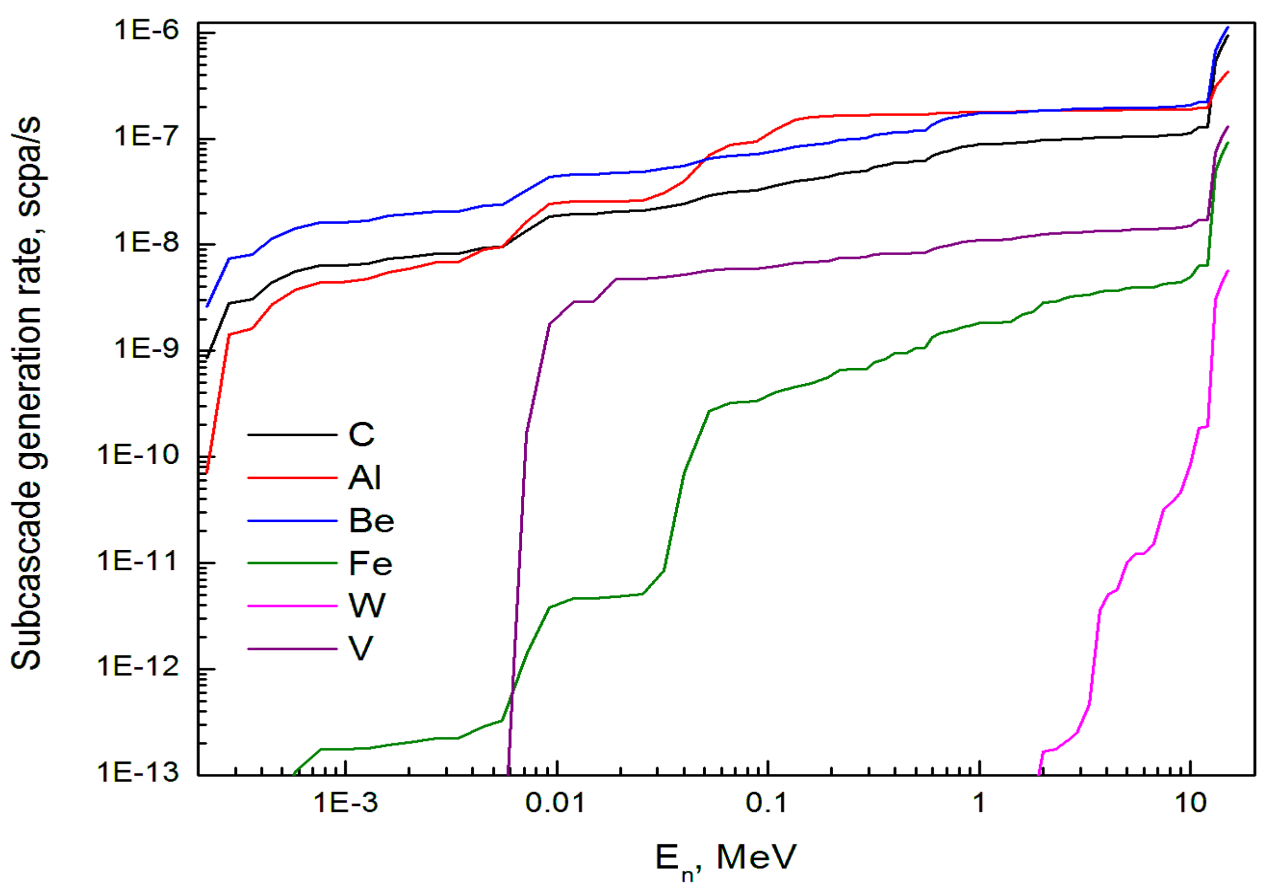
$\Phi(E_n^{/})$ - Energy flux of fast neutrons in differential fusion facilities

E_{sf} - Sub-cascade formation energy

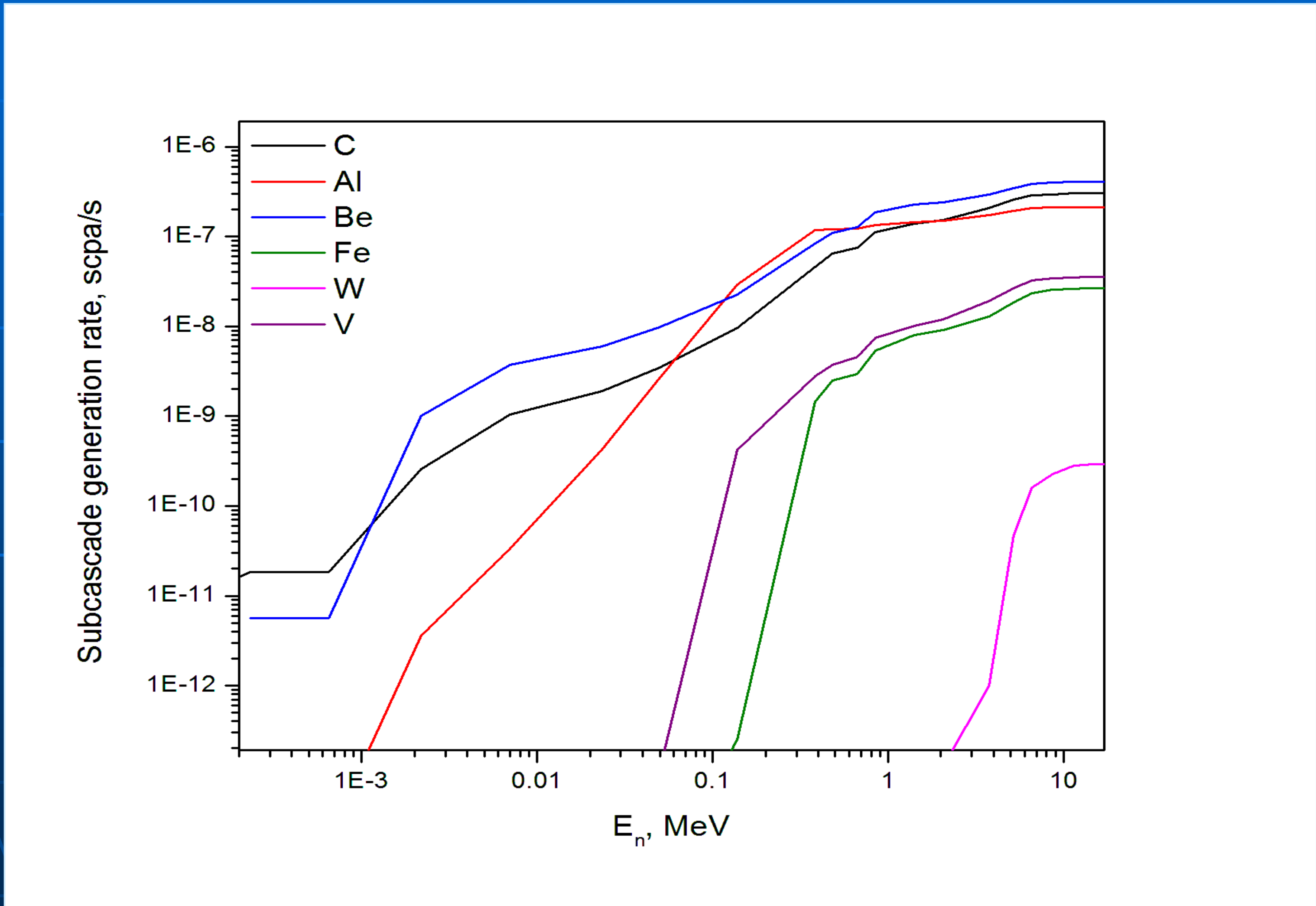
Sub-cascade Generation Rate in different Materials under Neutron Irradiation in DEMO



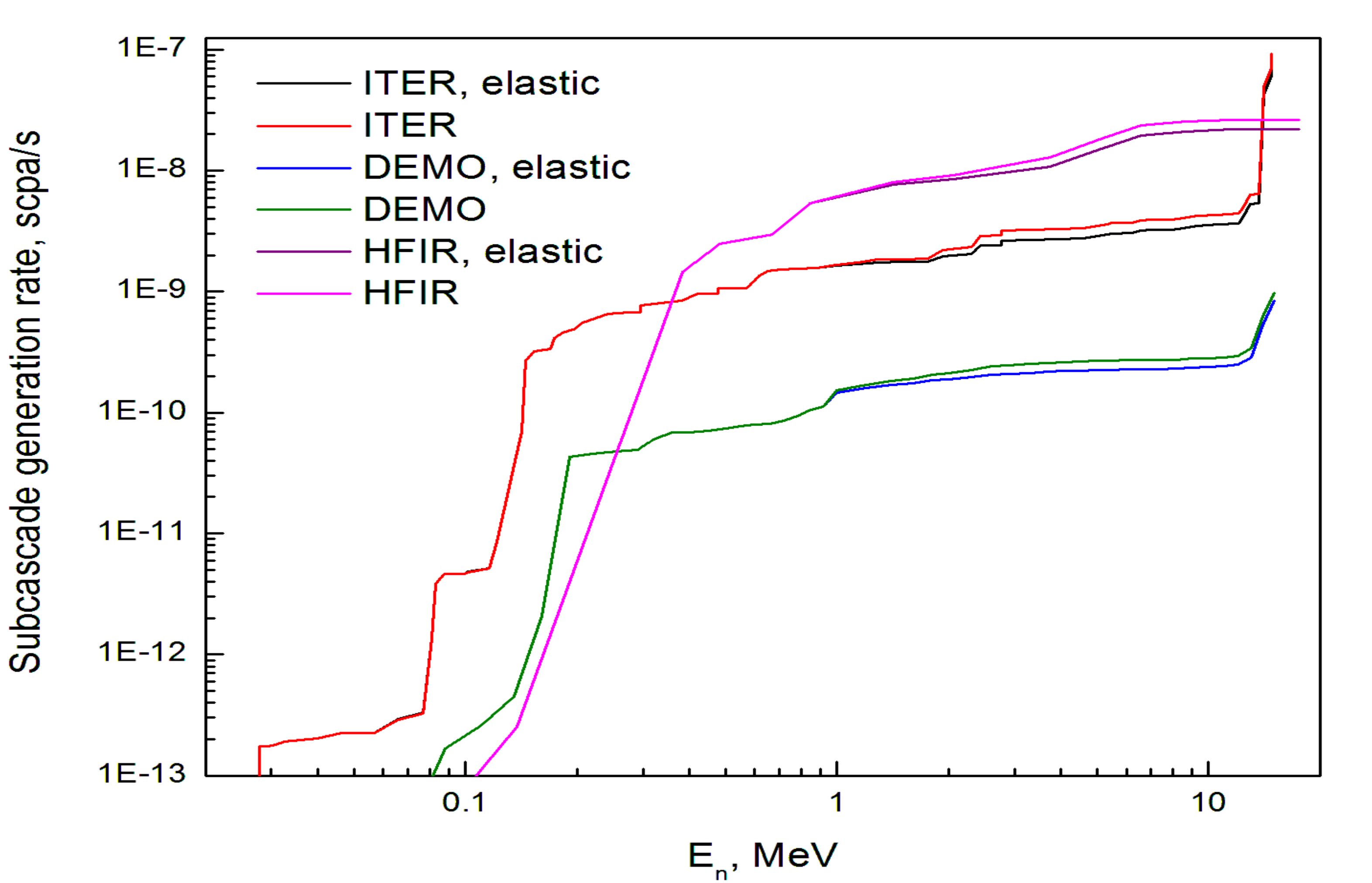
Sub-cascade Generation Rate in different Materials under Neutron Irradiation in ITER



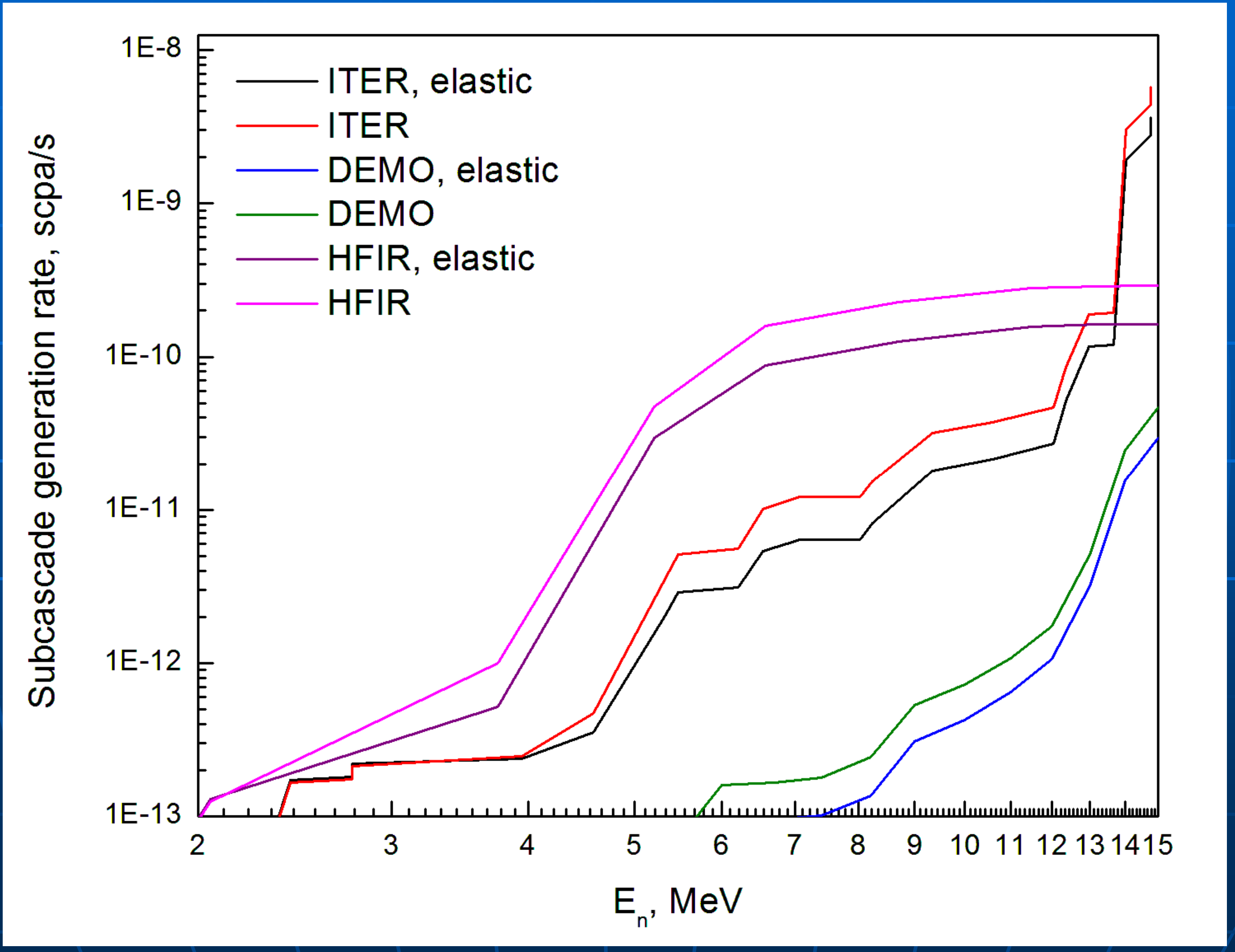
Sub-cascade Generation Rate in different Materials under Neutron Irradiation in HFIR



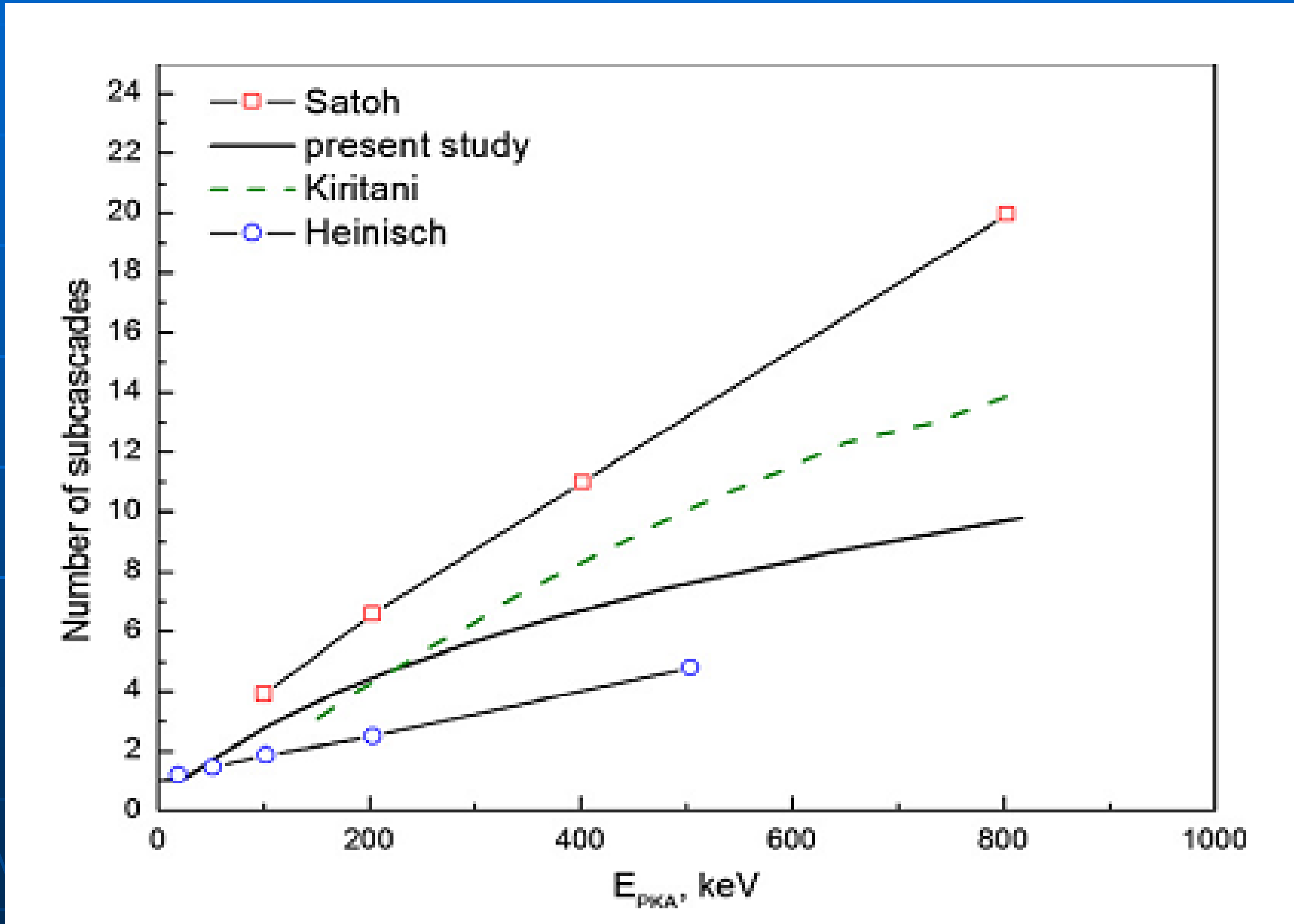
Subcascade Generation Rate for Fe in different Fusion and Fission Facilities



Sub-cascade Generation Rate for W in different Fusion and Fission Facilities

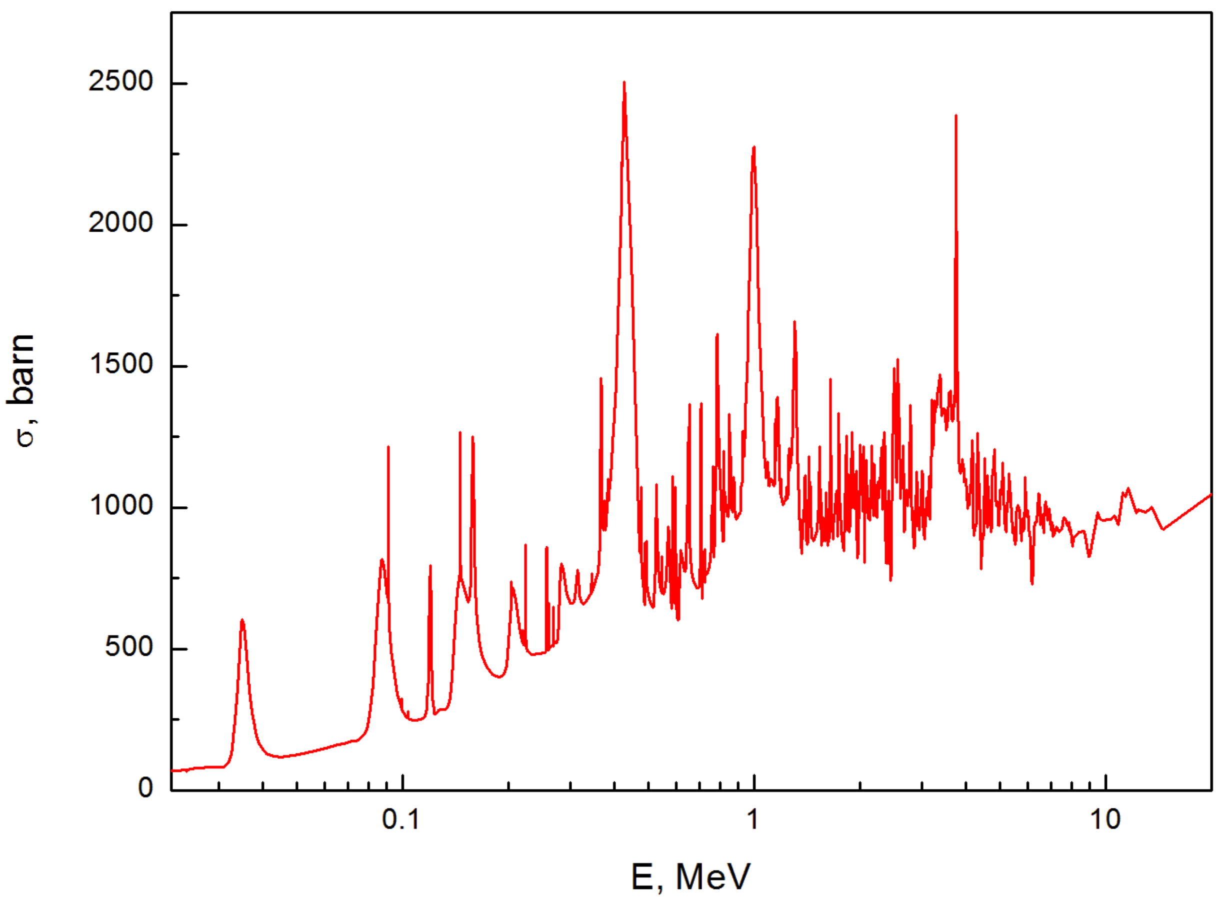


Comparison of the theoretical results from previous studies for number of sub-cascades in Cu with the experimental data

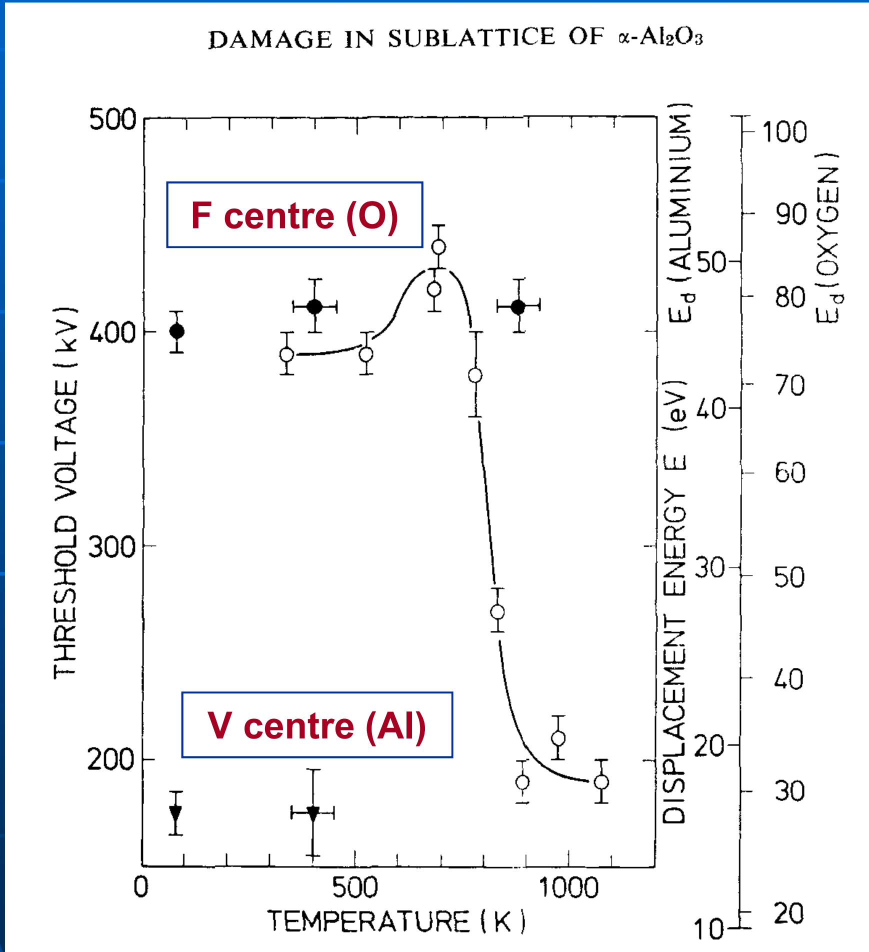


Calculations of primary radiation point defects in diatomic materials (Al_2O_3)

Cross section of primary point defect production in Al_2O_3 under neutron irradiation



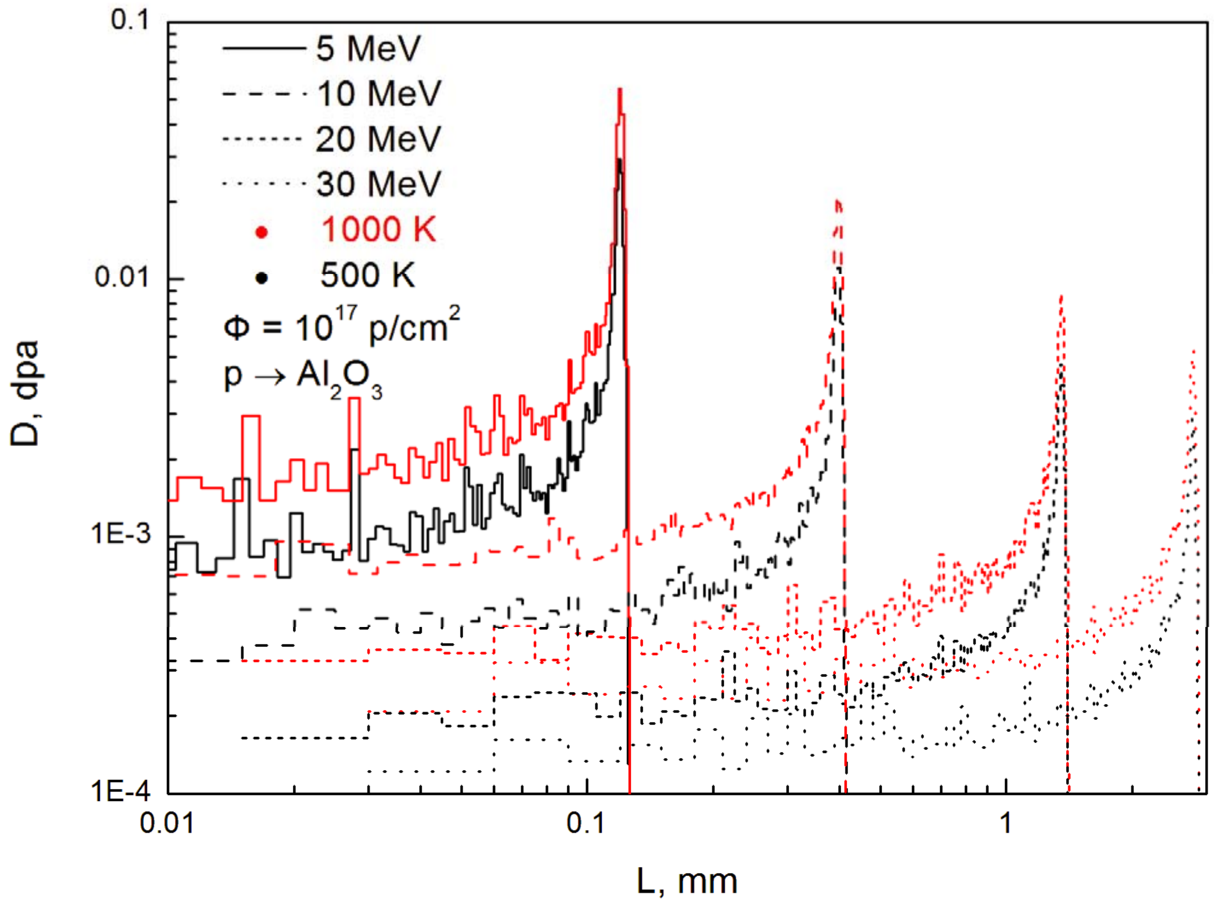
Temperature dependence of threshold energies for point defect production for Al and O atoms into Al_2O_3



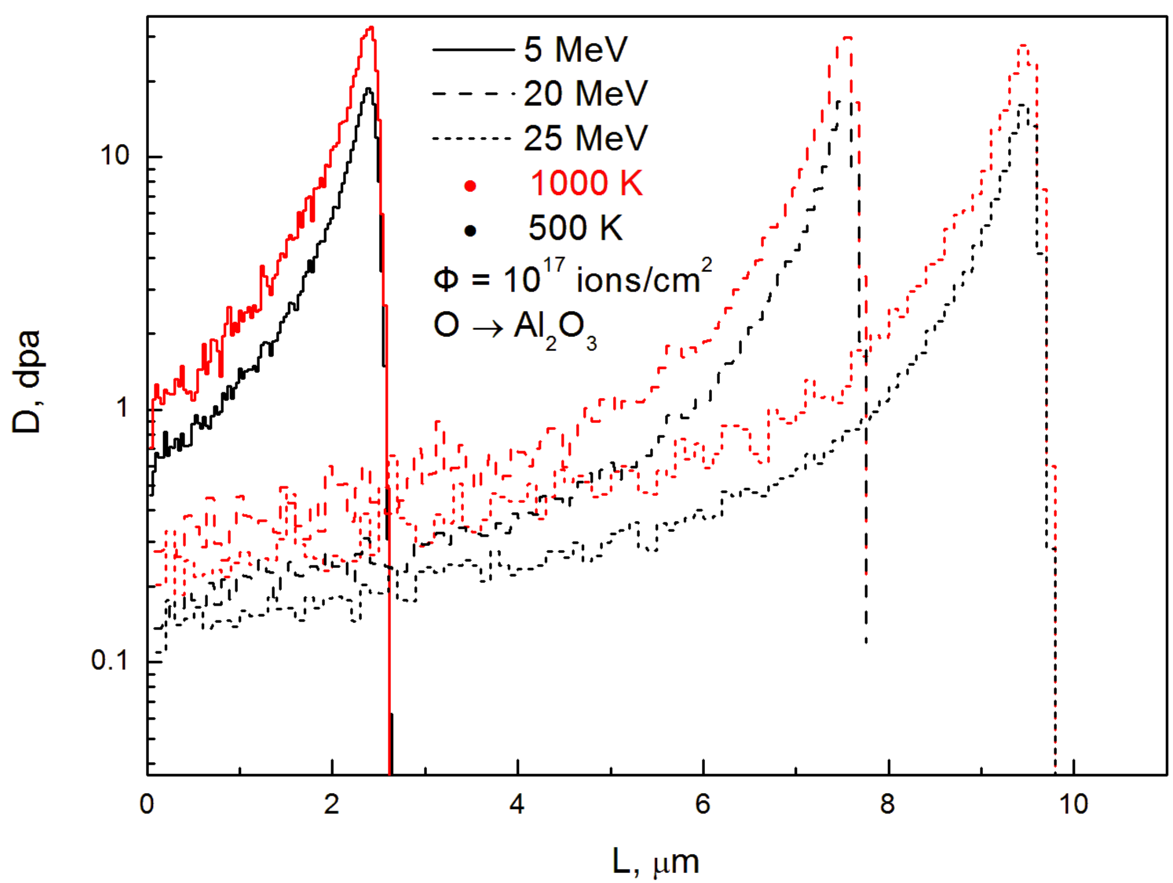
G.P.Pells et al.

Rad.Effect., 74 (1983) 181.

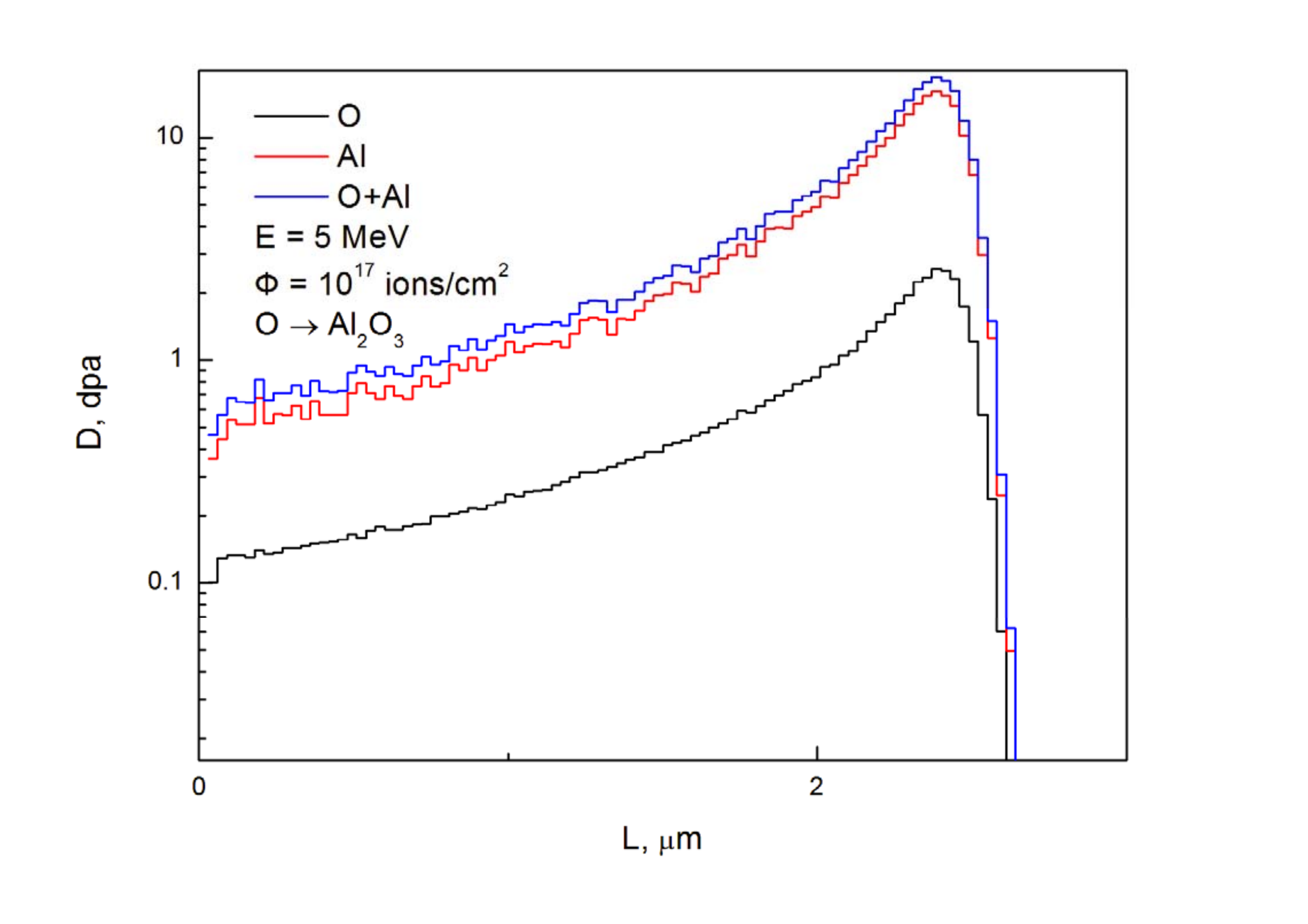
Distribution of point defect production under proton irradiation into Al_2O_3 at two temperatures: T_1=500 K and T_2=1000 K



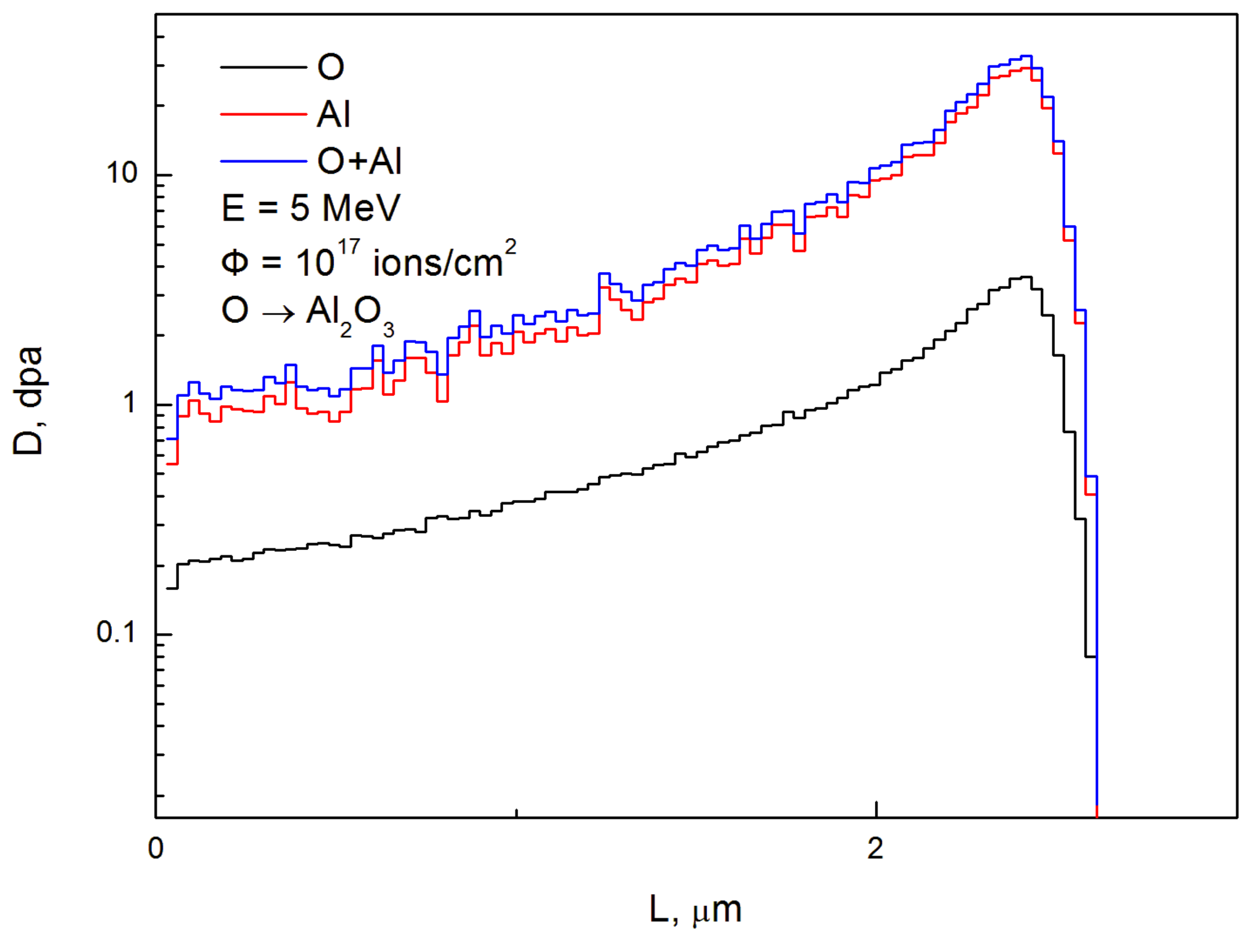
Distribution of point defect production under oxygen ion irradiation into Al_2O_3 at two temperatures: T_1=500 K and T_2=1000 K



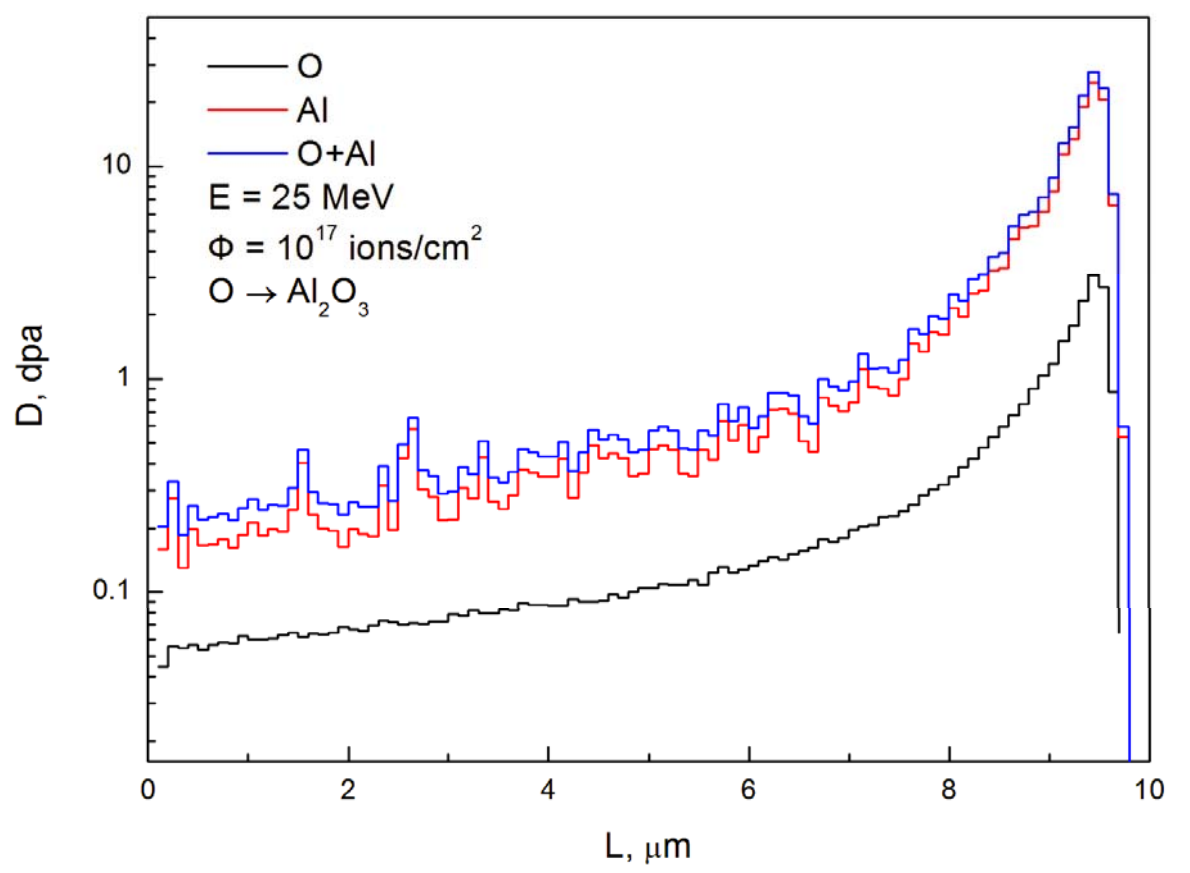
Distribution profiles of point defects due to displacements of O and Al atoms into Al_2O_3 under 5 MeV oxygen ion irradiation at T = 500 K



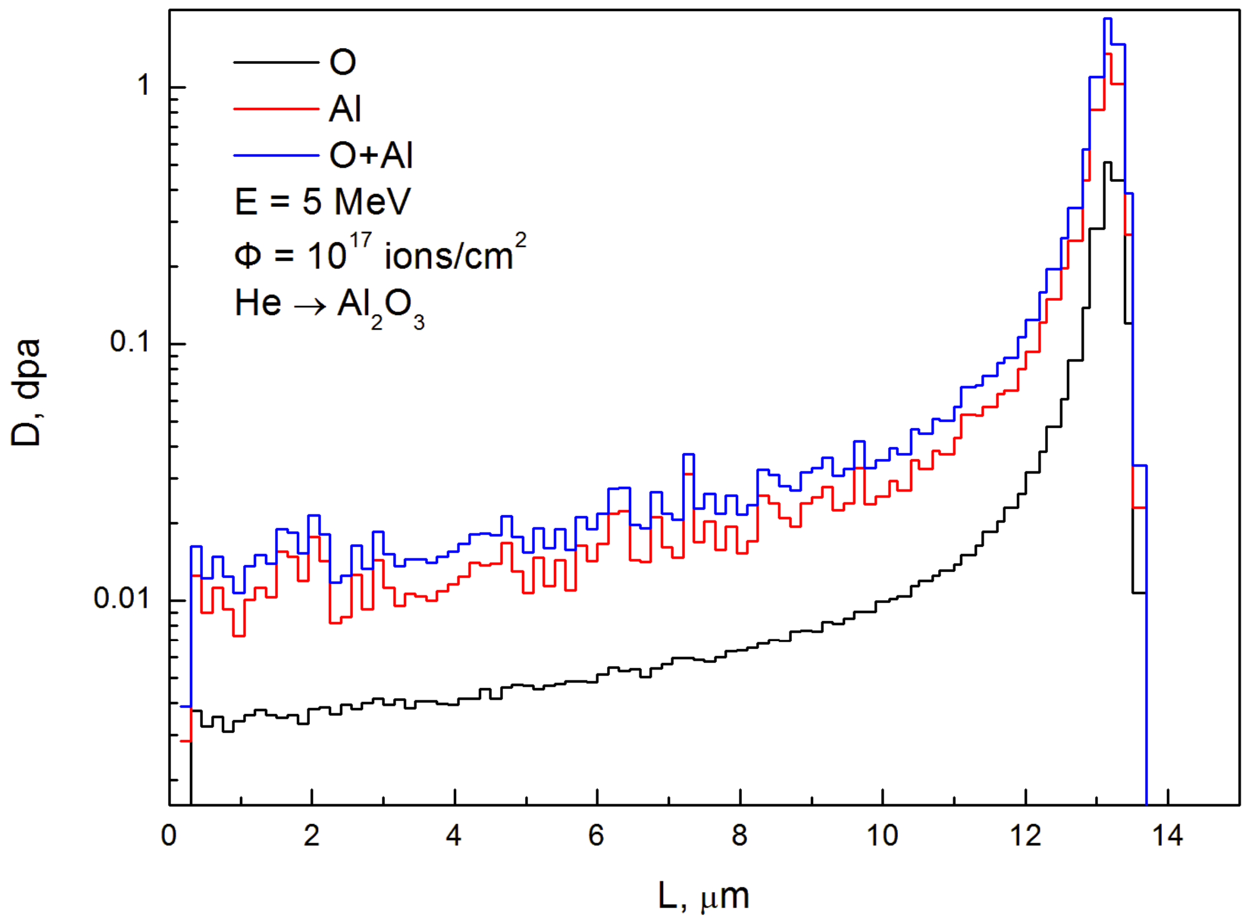
Distribution profiles of point defects due to displacements of O and Al atoms into Al_2O_3 under 5 MeV oxygen ion irradiation at T = 1000 K



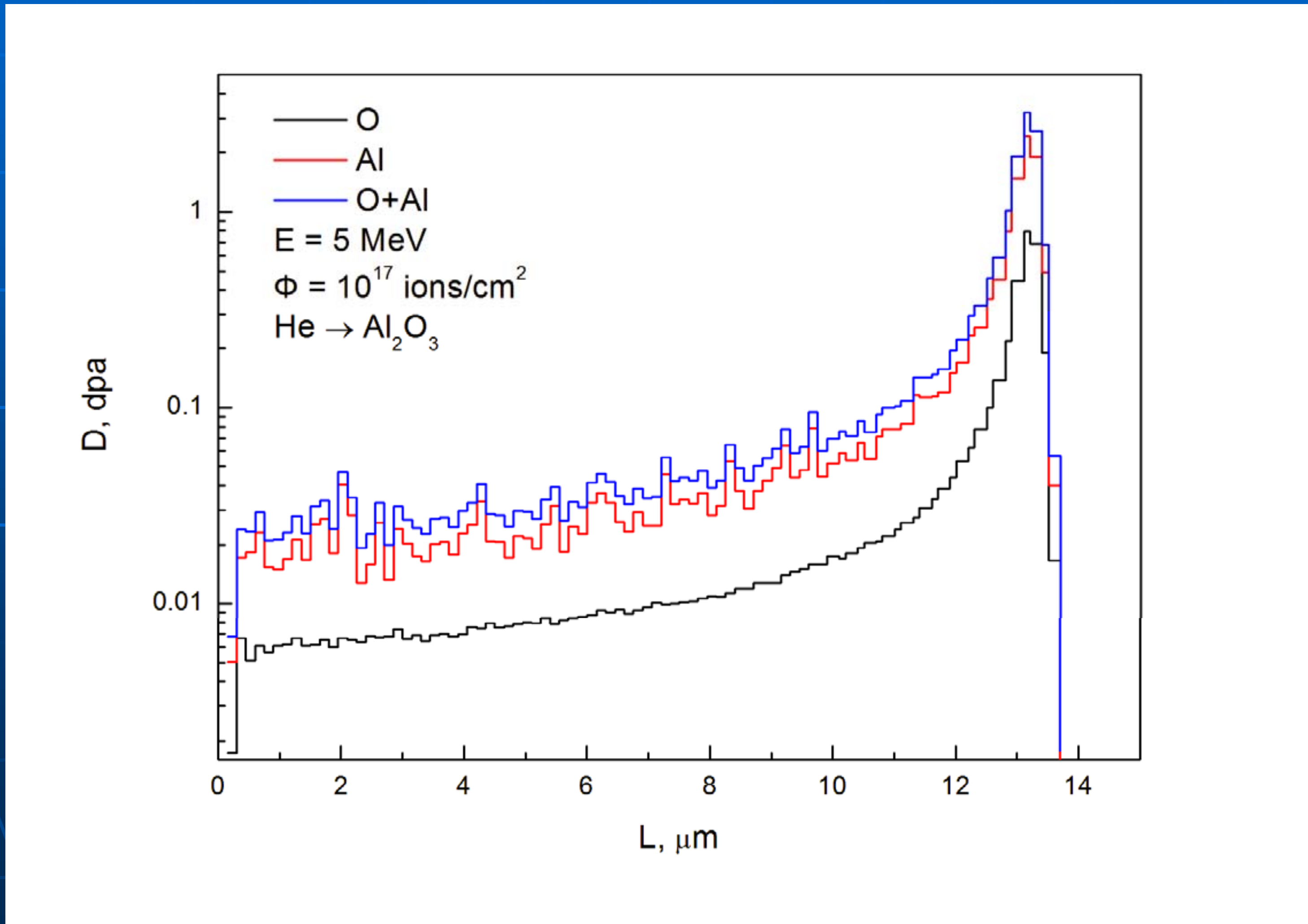
Distribution profiles of point defects due to displacements of O and Al atoms into Al_2O_3 under 25 MeV oxygen ion irradiation at T = 1000 K



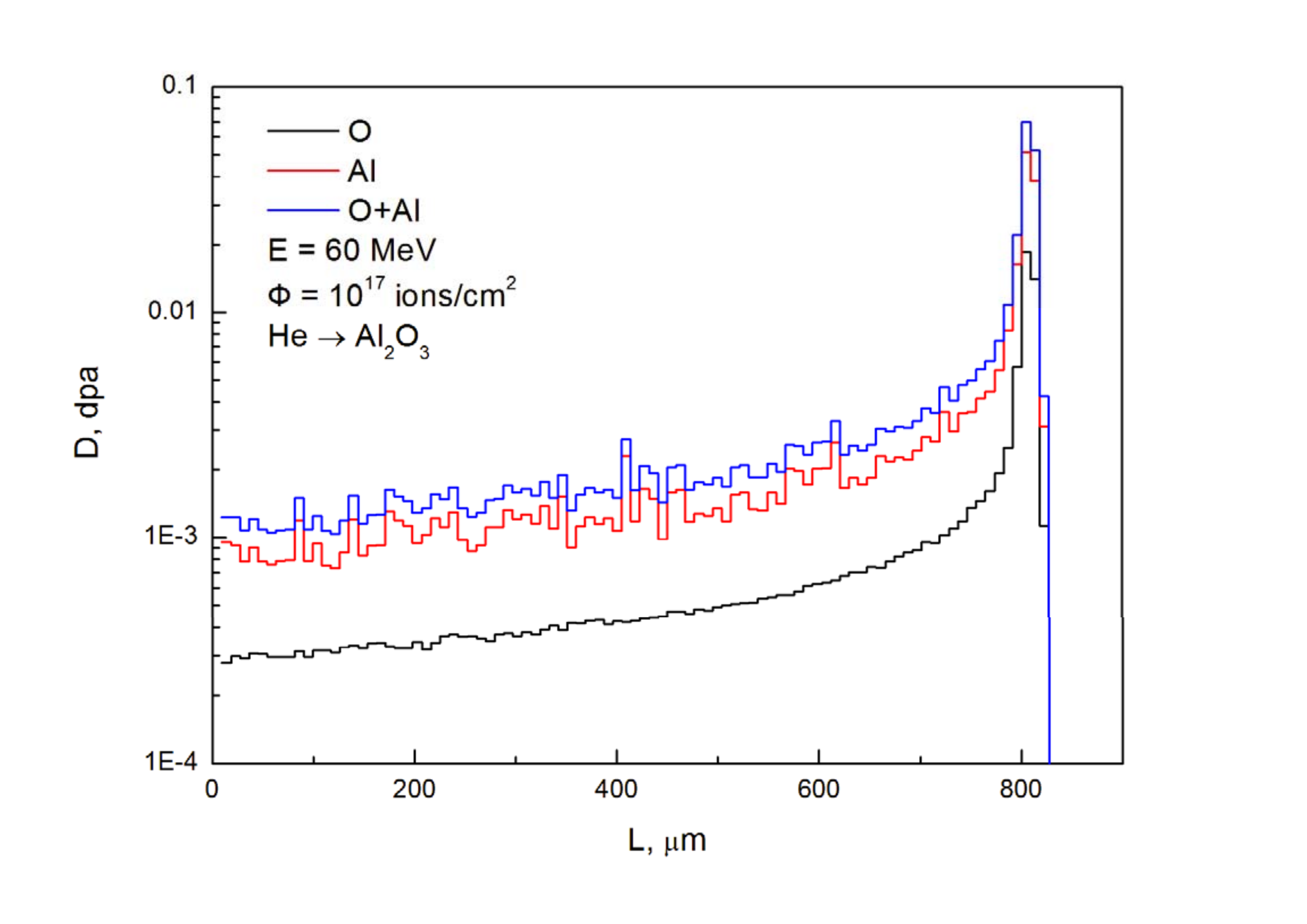
Distribution profiles of point defects due to displacements of O and Al atoms into Al_2O_3 under 5 MeV helium ion irradiation at T=500 K



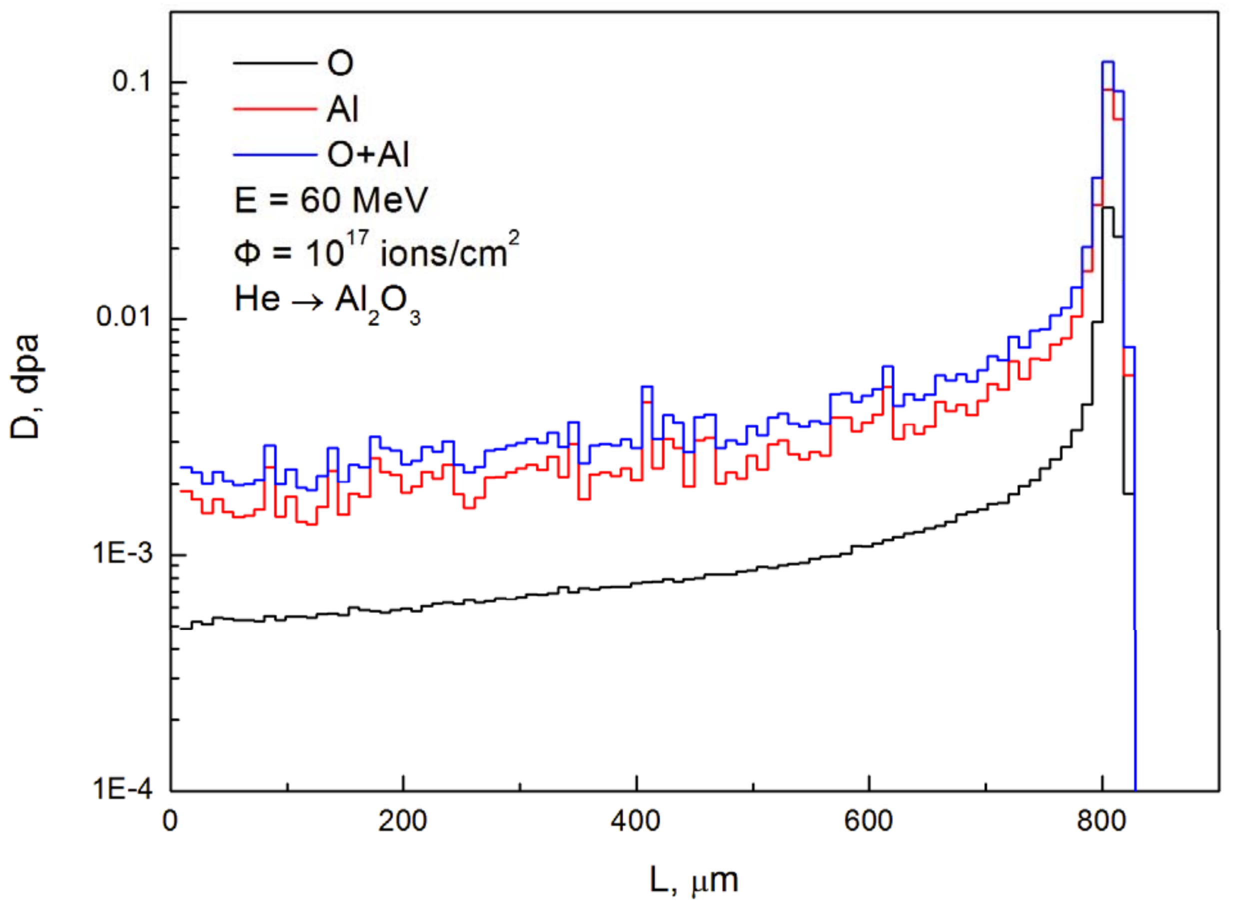
Distribution profiles of point defects due to displacements of O and Al atoms into Al_2O_3 under 5 MeV helium ion irradiation at T=1000 K



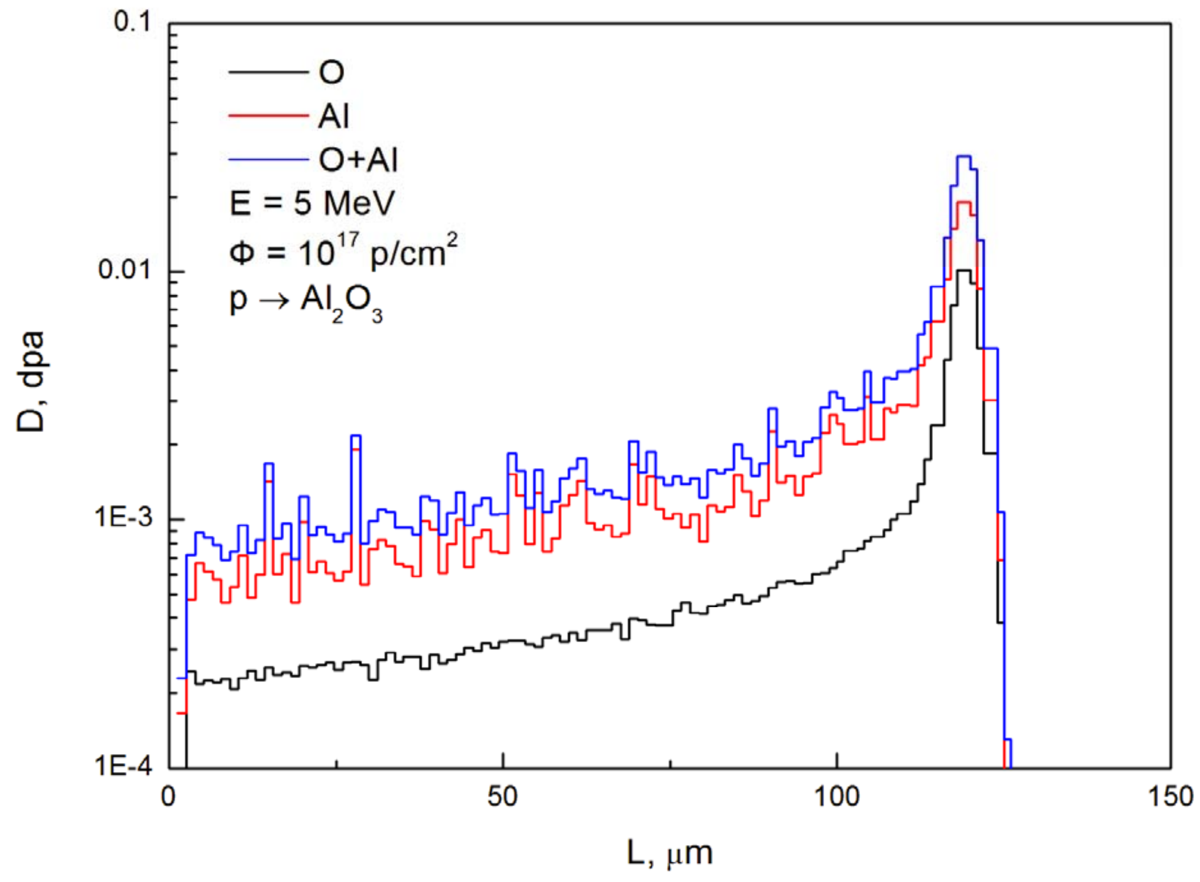
Distribution profiles of point defects due to displacements of O and Al atoms into Al_2O_3 under 60 MeV helium ion irradiation at T=500 K



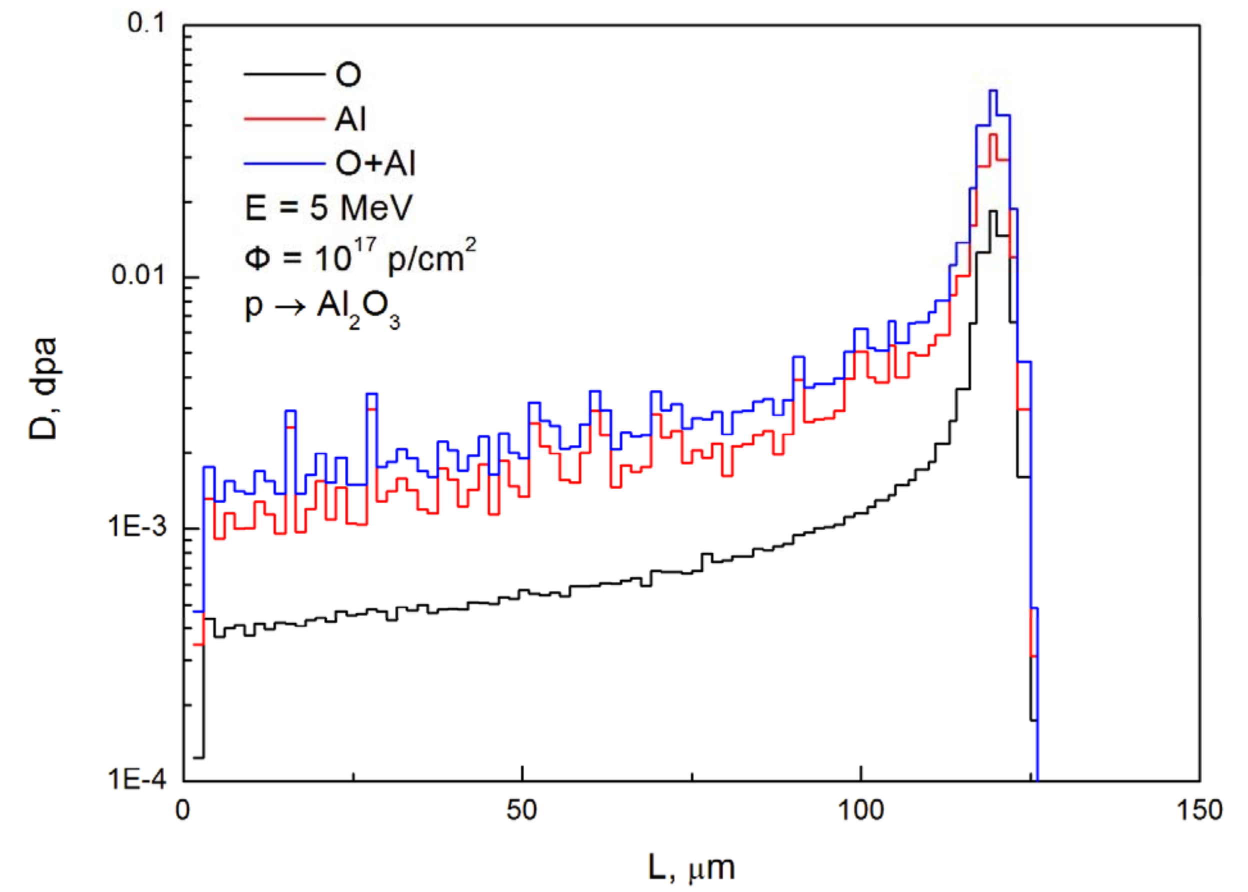
Distribution profiles of point defects due to displacements of O and Al atoms into Al_2O_3 under 60 MeV helium ion irradiation at T=1000 K



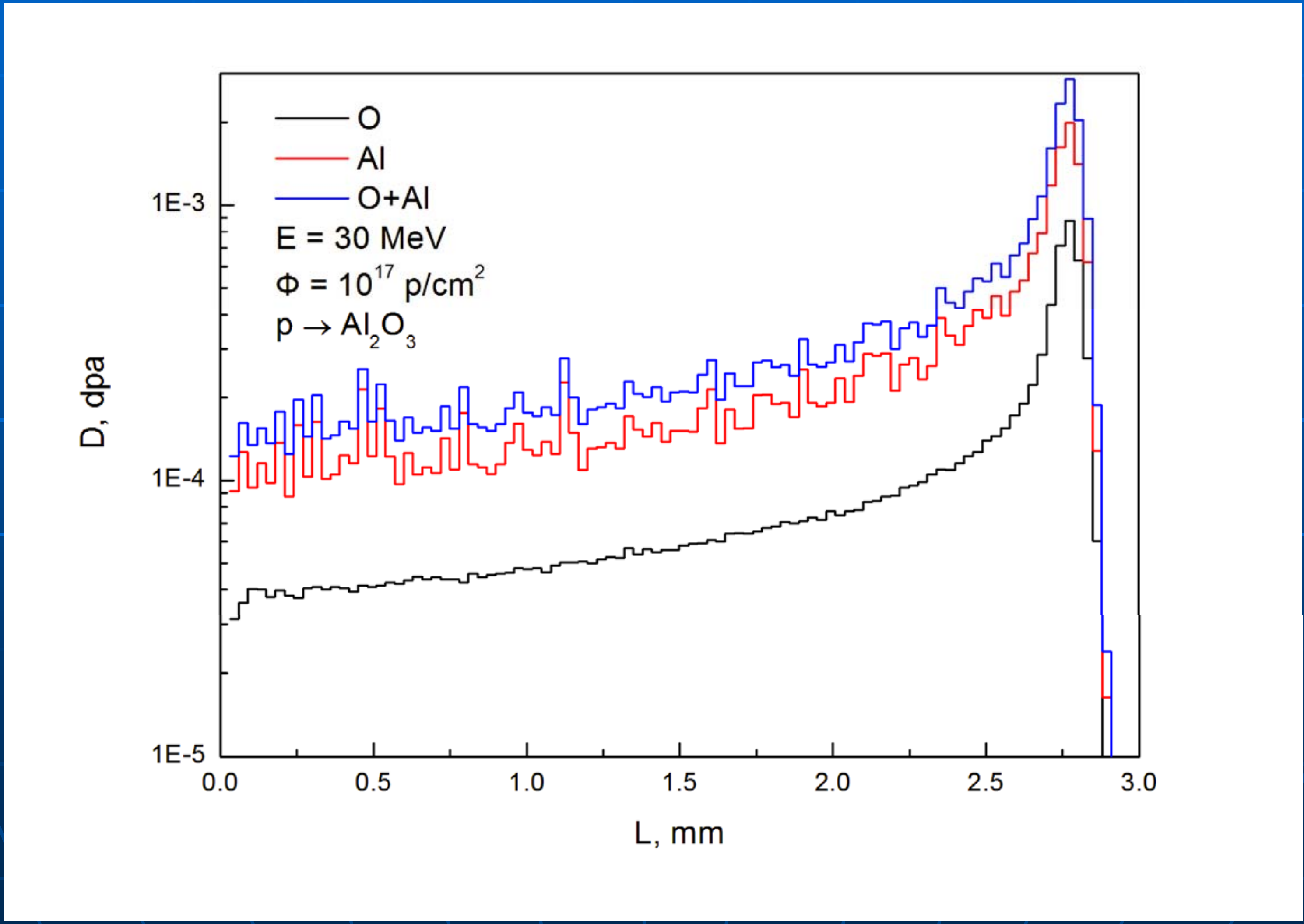
Distribution profiles of point defects due to displacements of O and Al atoms into Al_2O_3 under 5 MeV proton irradiation at T=500 K



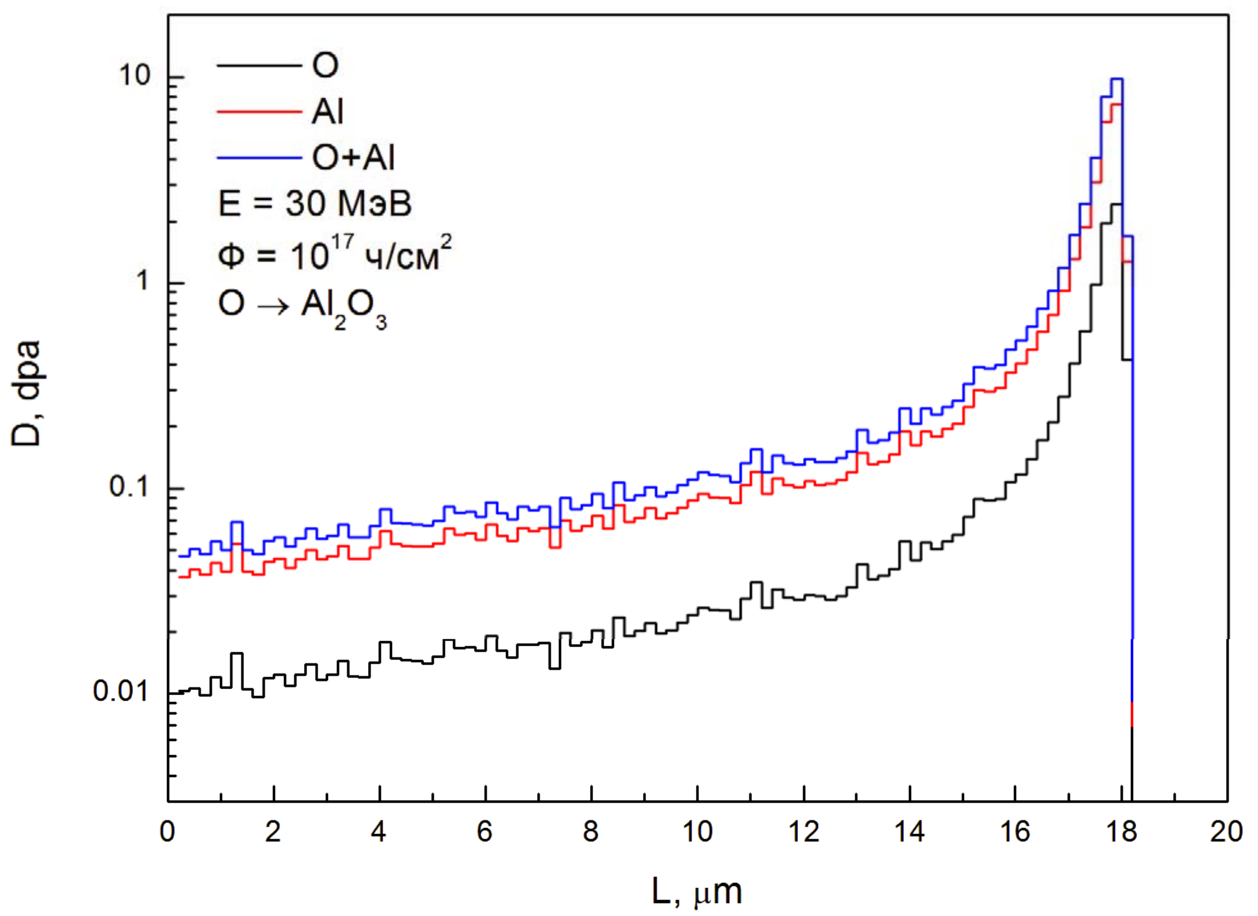
Distribution profiles of point defects due to displacements of O and Al atoms into Al_2O_3 under 5 MeV proton irradiation at T=1000 K



Distribution profiles of point defects due to displacements of O and Al atoms into Al_2O_3 under 30 MeV proton irradiation at T=500 K



Distribution profiles of point defects due to displacements of O and Al atoms into Al_2O_3 under 30 MeV proton irradiation at T=1000 K



Damage calculations in Al2O3 using Boltzmann Transport Equation: comparing neutron and ion irradiation

1. Yu.D.Lizunov, A.I Ryazanov et al., Rad.Effects, v.60 (1982) 95,

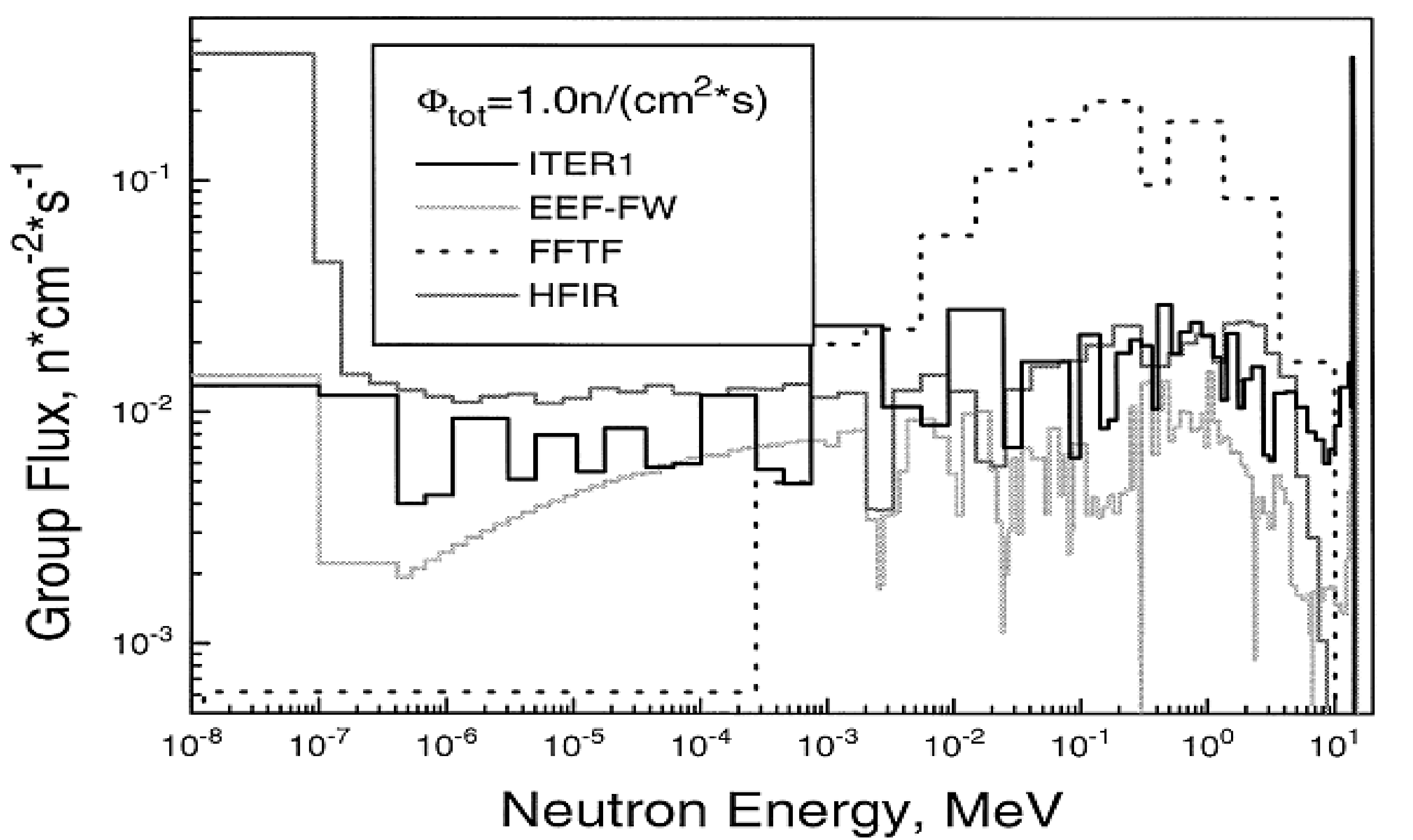
2. Yu.D.Lizunov, A.I Ryazanov et al., Rad.Effects, v.107 (1989) 185,

3. Yu.D.Lizunov, A.I Ryazanov et al., Preprint IAE-52-98/11,1991, Moscow,

4. Yu.D.Lizunov, A.I Ryazanov et al., J.Nucl.Mat.,250 (1997) 236.

5. Yu.D.Lizunov, A.I Ryazanov et al., J.Nucl.Mat.,253 (1998) 104.

Neutron group spectra for fusion environments EEF, ITER and for fission reactors HFIR, FFTF .



Boltzmann transport equations for slowing down ions and knocked-on atoms in one-dimensional plane geometry.

$$(\Omega * e_x)\frac{d\Phi_\kappa(x,\Omega,E)}{dx} - \frac{d}{dE}\left[S_k(E)\Phi_\kappa(x,\Omega,E)\right] = I_k + q_k(x,\Omega,E)$$

$\Phi_\kappa(x,\Omega,E)$ is the scalar flux for the *k*-th sort of moving atoms that can be either knocked-on atoms or slowing down ions.

$S_k(E)$ is the electronic stopping power for k-th sort of moving atoms, $q_k(x,\Omega,E)$ is the source of the -type of moving atoms.

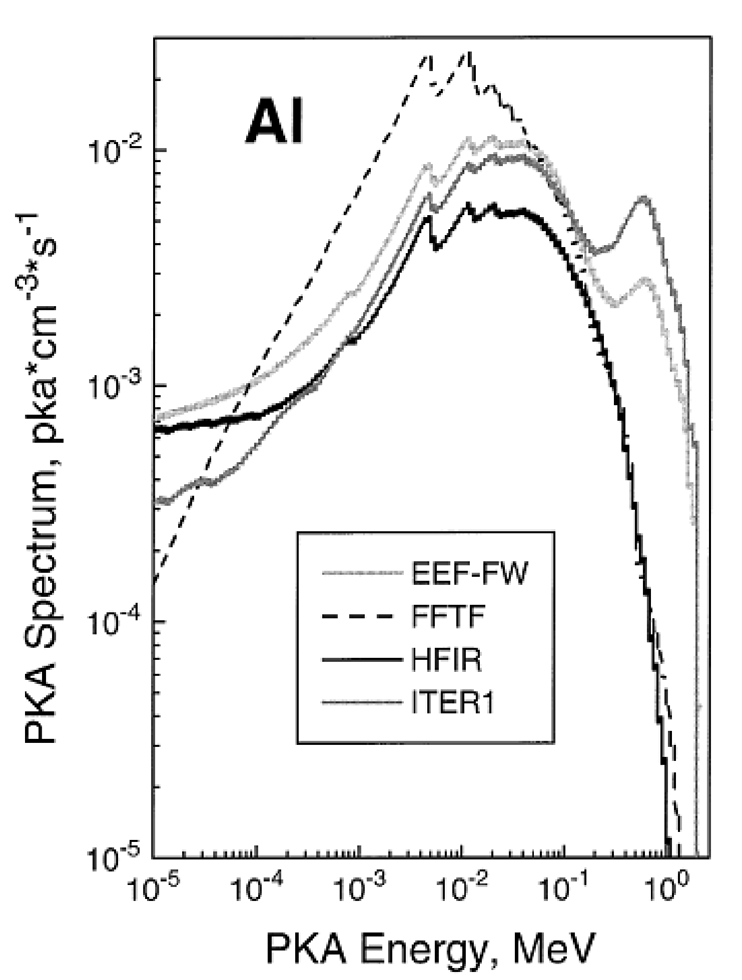
I_k stands for the collision integral of the *k*-th sort of moving particles:

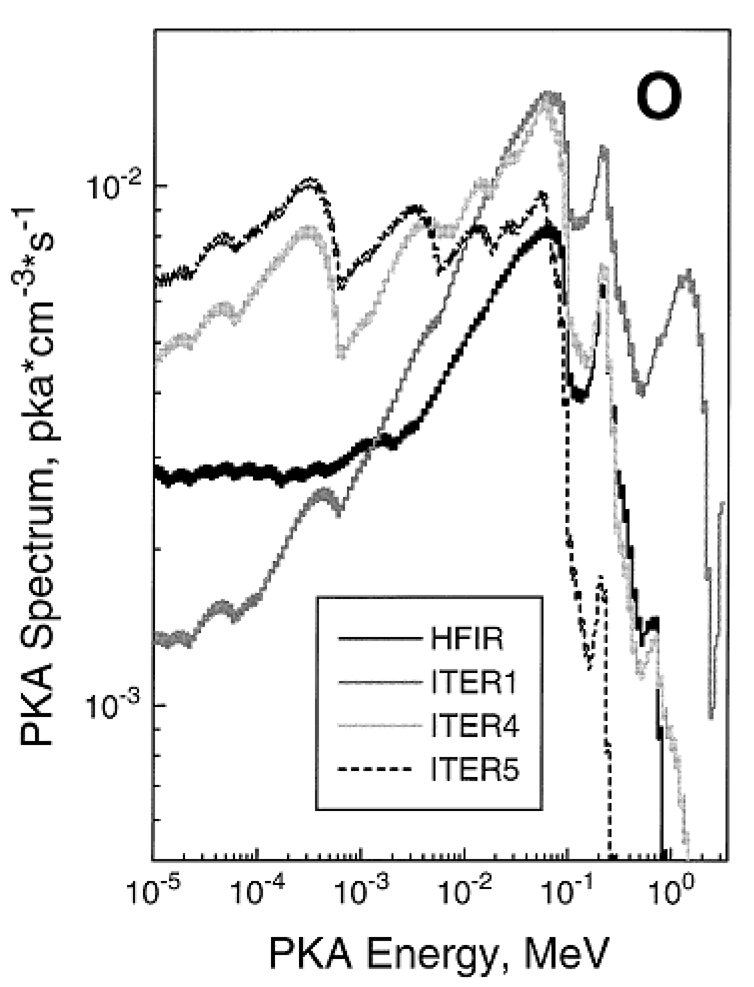
$$I_k =_i N_i \int d\sigma_{ki}(E',\Omega' \to E,\Omega;\Omega'')\Phi_\kappa(x,\Omega',E')dE'd\Omega'$$
$$-_i N_i \Phi_\kappa(x,\Omega,E)\int d\sigma_{ki}(E,\Omega \to E',\Omega';\Omega'')dE'd\Omega'$$
$$+N_{ki}\int d\sigma_{ik}(E',\Omega' \to E'-E,\Omega'';\Omega)\Phi_i(x,\Omega',E')dE'd\Omega'$$

N_i is the atomic concentration of the i-th sort of atoms.

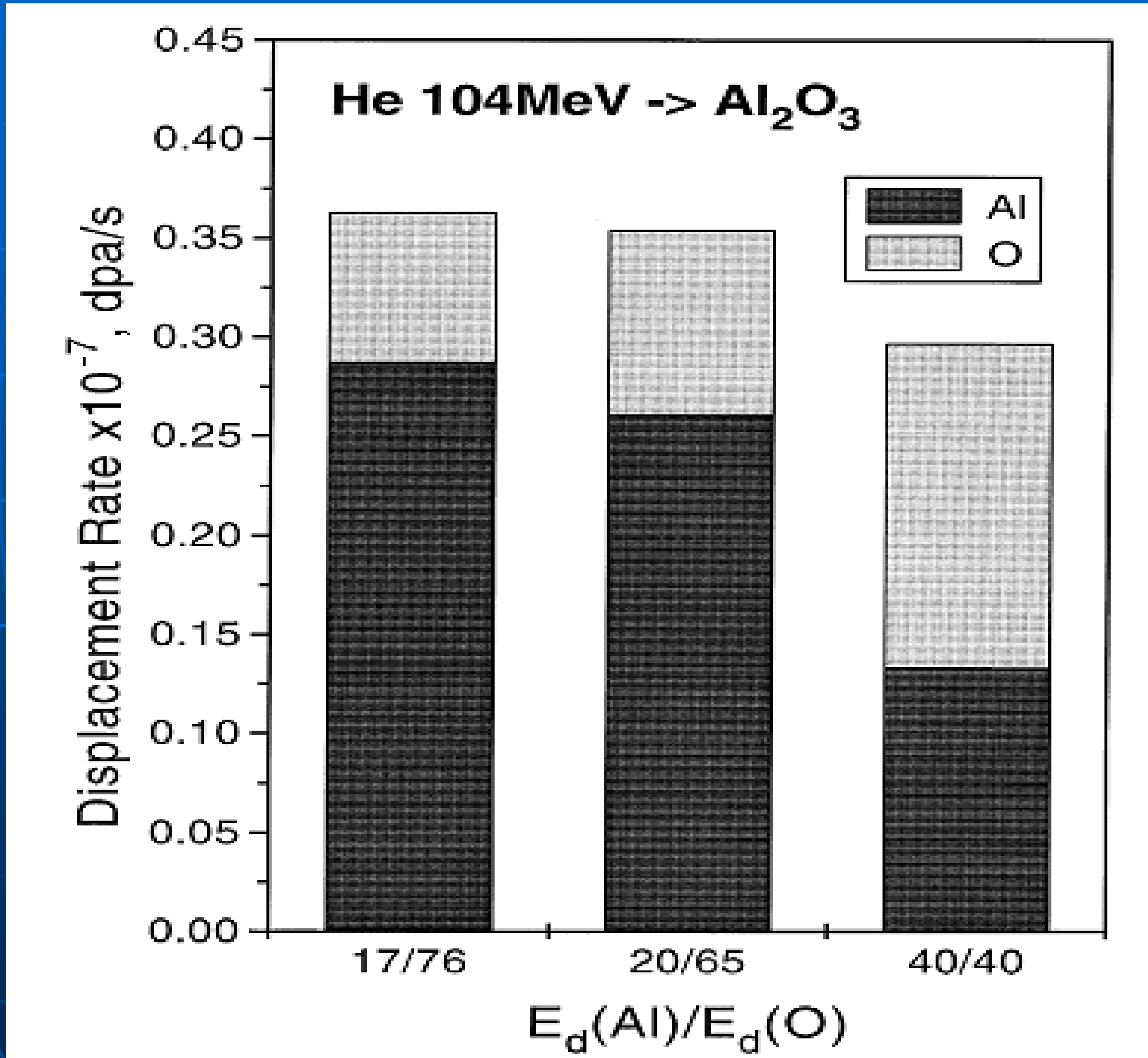
$d\sigma_{ki}(E,\Omega \to E',\Omega';\Omega'')$ is differential cross-section of collisions between *k*-th type of atoms with energy *E* moving in Ω direction and *i*-th type of atoms in the target.

Primary recoil aluminum and oxygen spectra for several neutron environments. All neutron fluxes are normalized to the total flux of 10E18 n/(m2s)

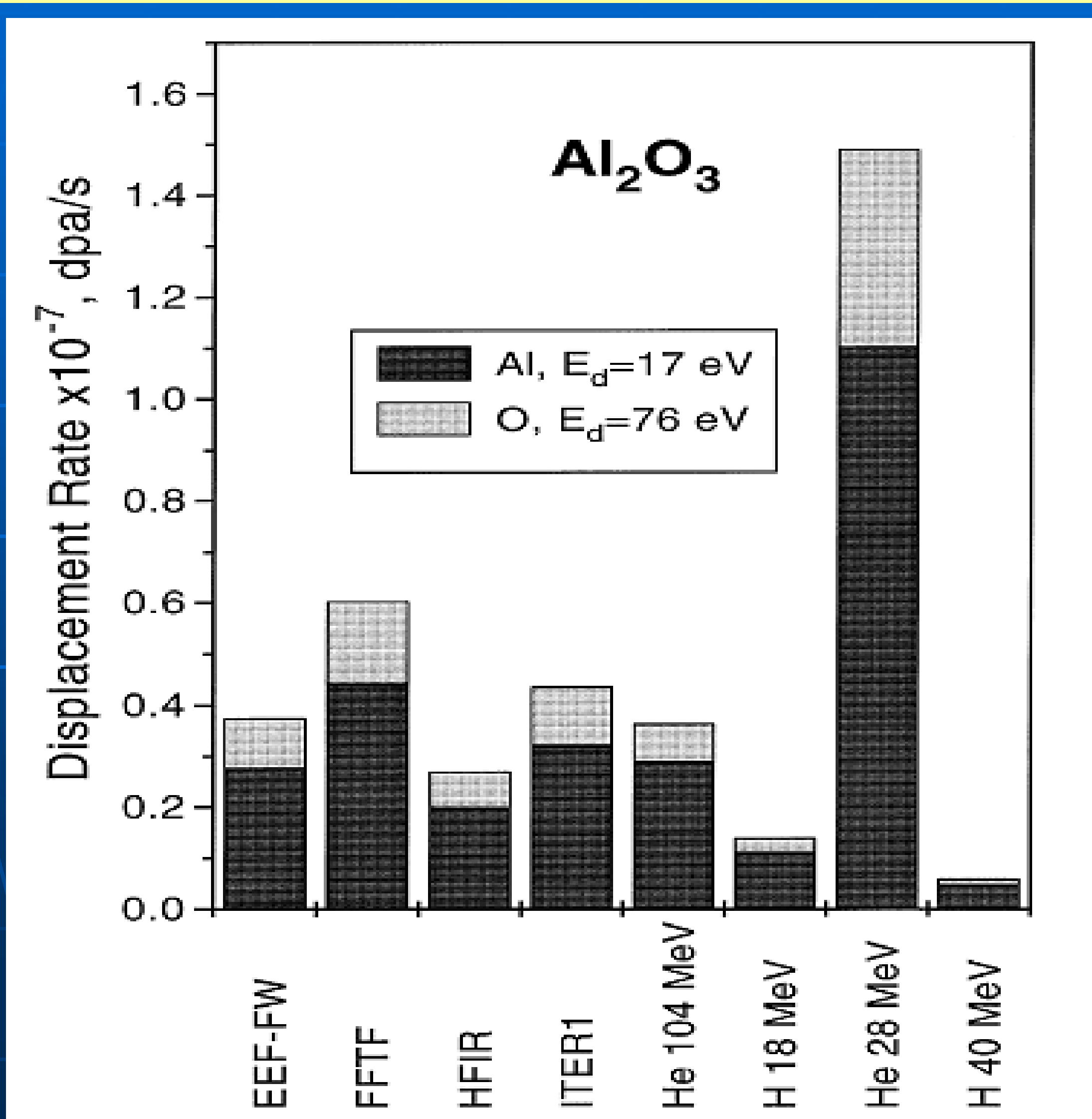




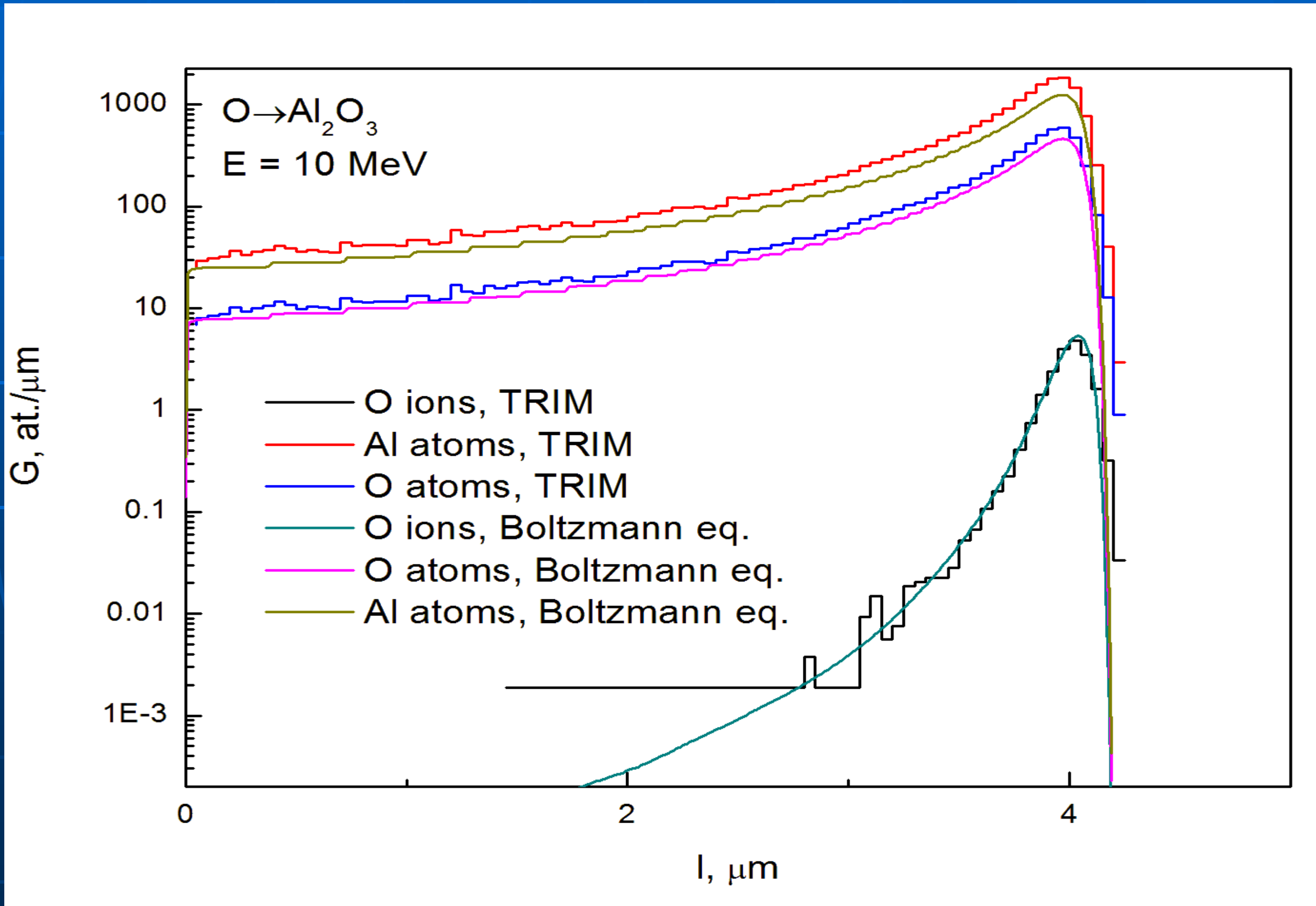
Radiation damage rates in the different sublattices of Al_2O_3 bombarded by 104 MeV He (+2q) ions



Displacement damage rates in alumina for several neutron and ion sources. All neutron fluxes are normalized to the total flux 10E18 (n/m2s) and the light ions to a beam current of 10E-2 A/m2

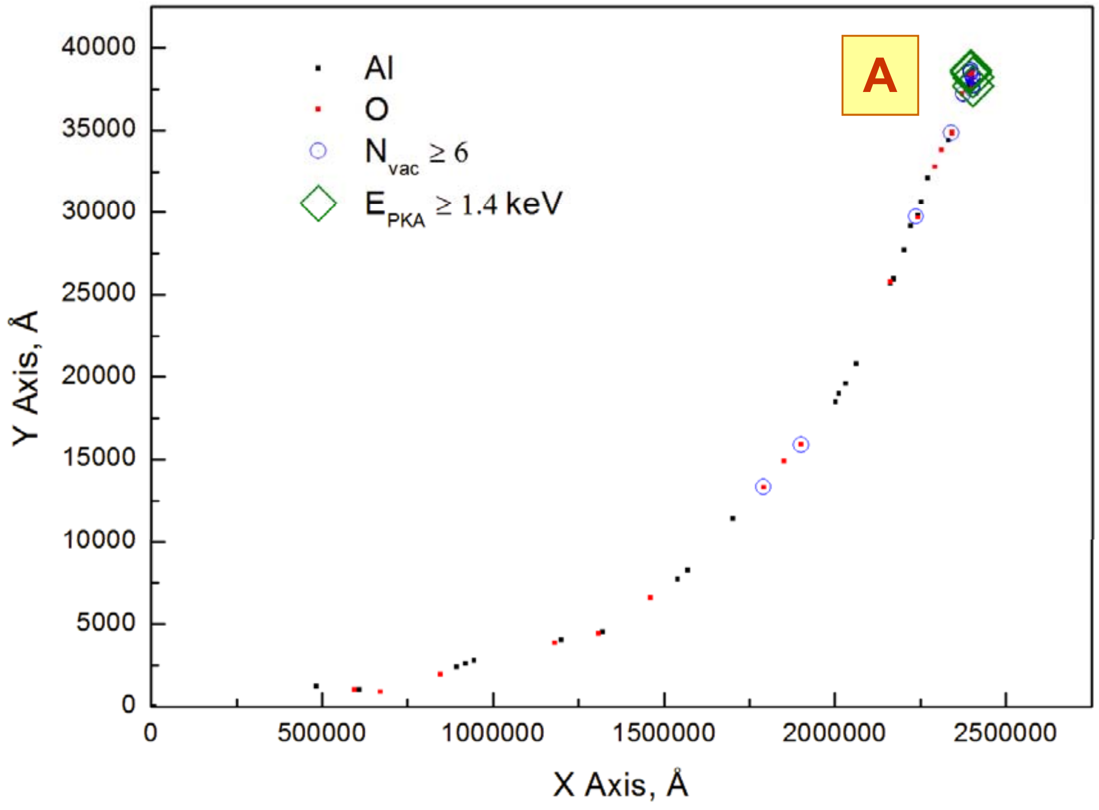


Calculations of damage profiles for displaced oxygen and aluminum atoms per ion using TRIM and Boltzmann Equation



Modeling of sub-cascade formation in diatomic materials

Modeling of subcascade formation in Al_2O_3 under 30 MeV He ion irradiation

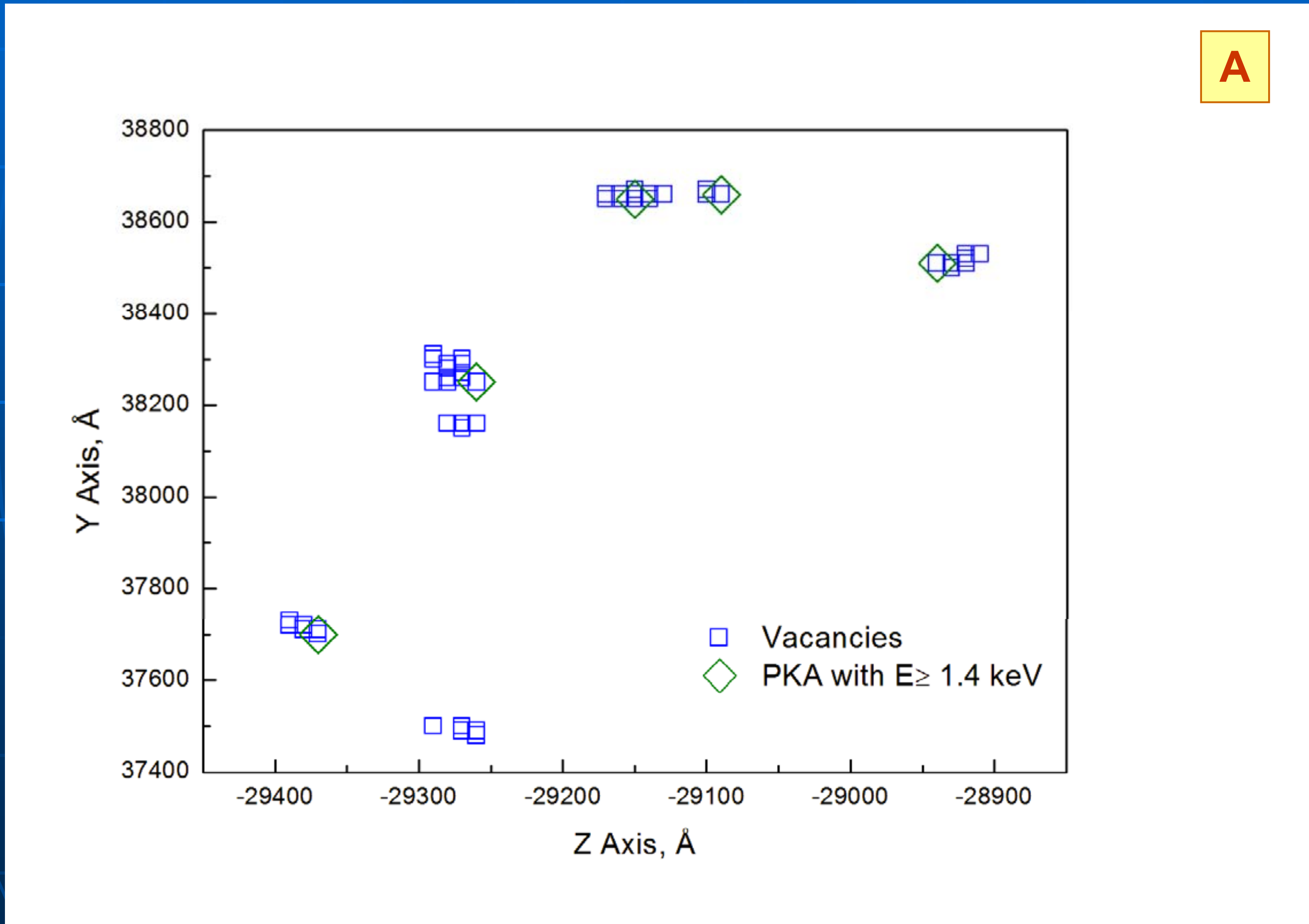


SRIM-2010

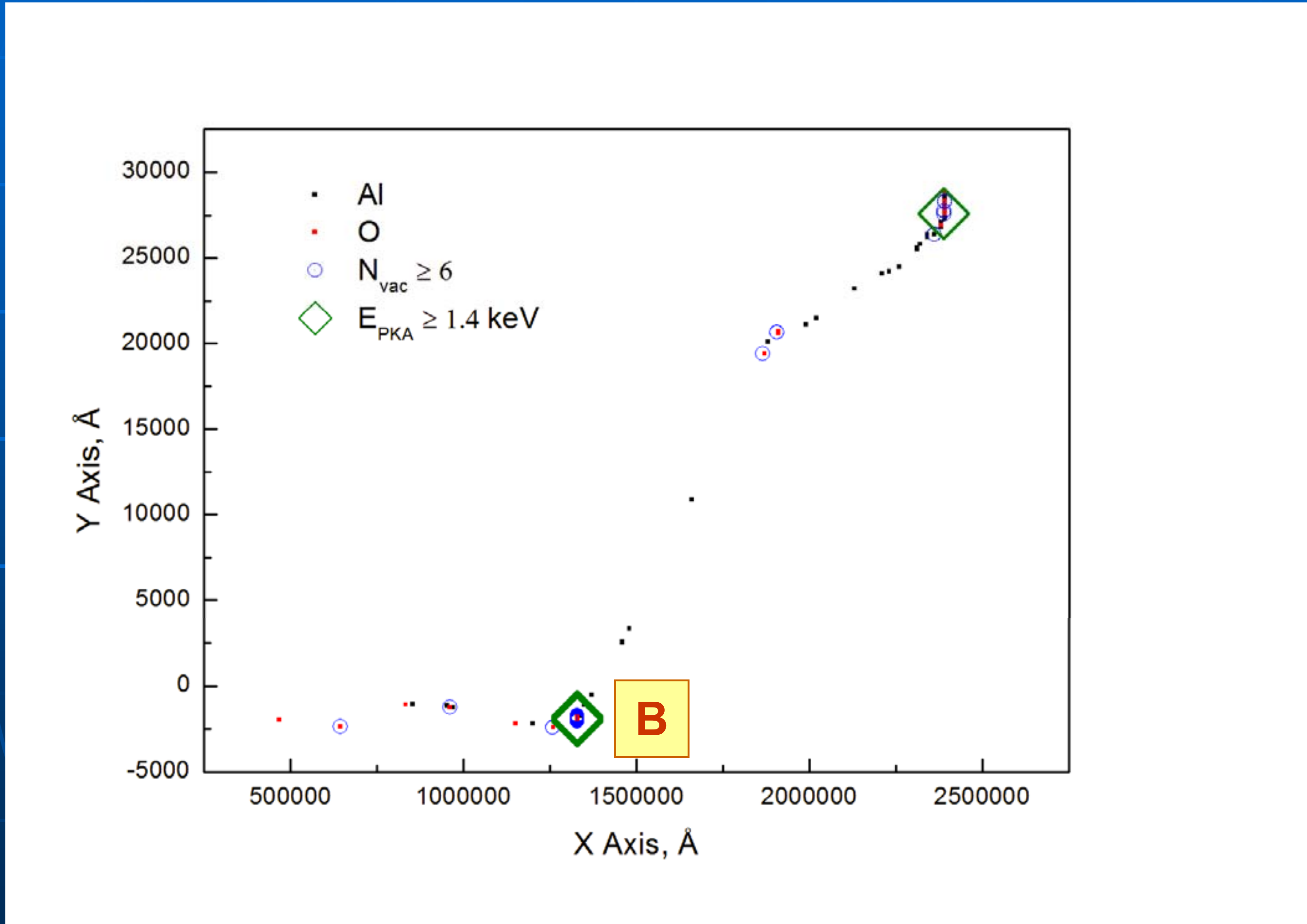
E_{PKA} (Al) >1.4 KeV

E_{PKA} (O) >0.4 KeV

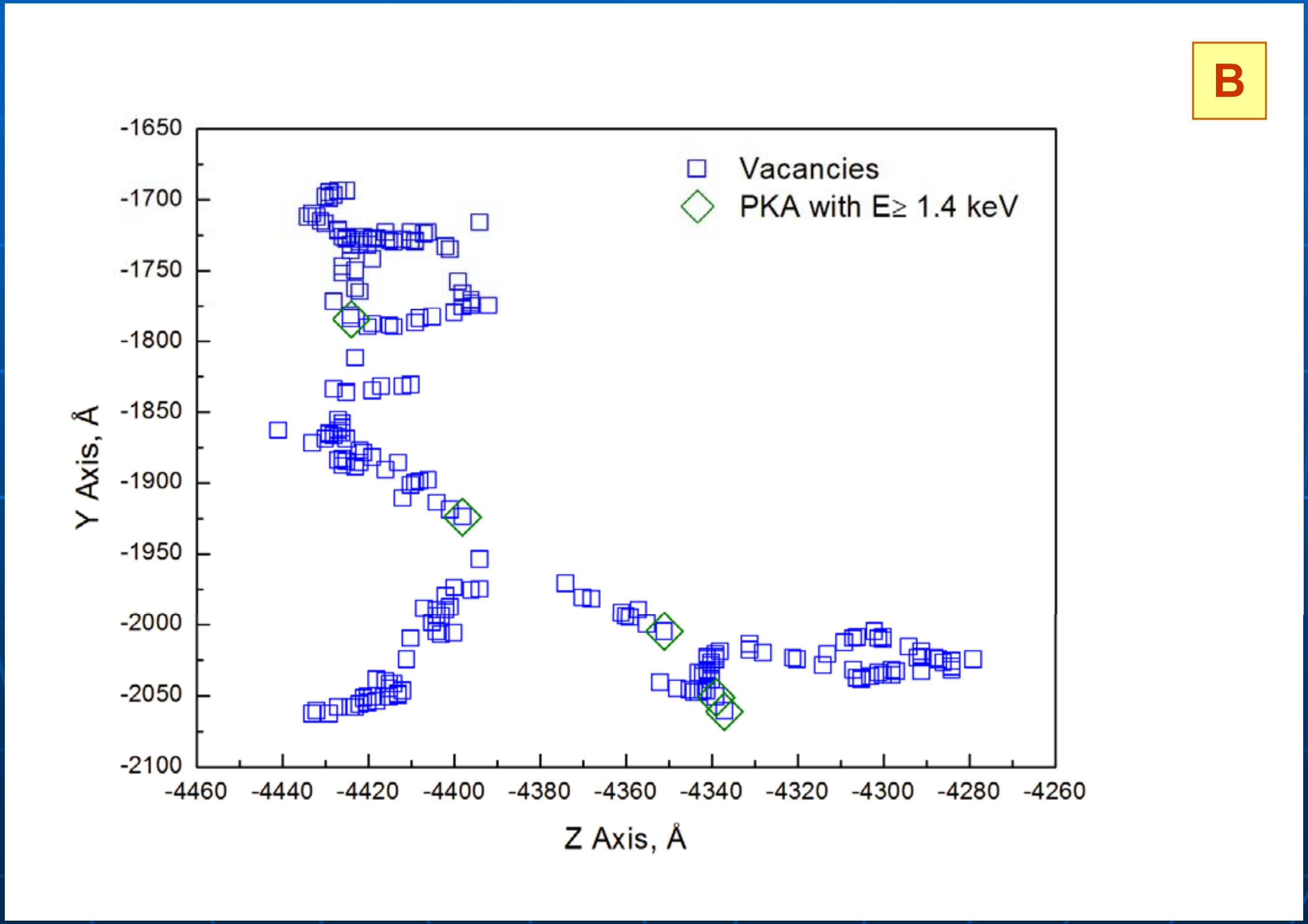
Modeling of subcascade formation in Al_2O_3 near the end of penetration depth of 30 MeV He ion (A area)



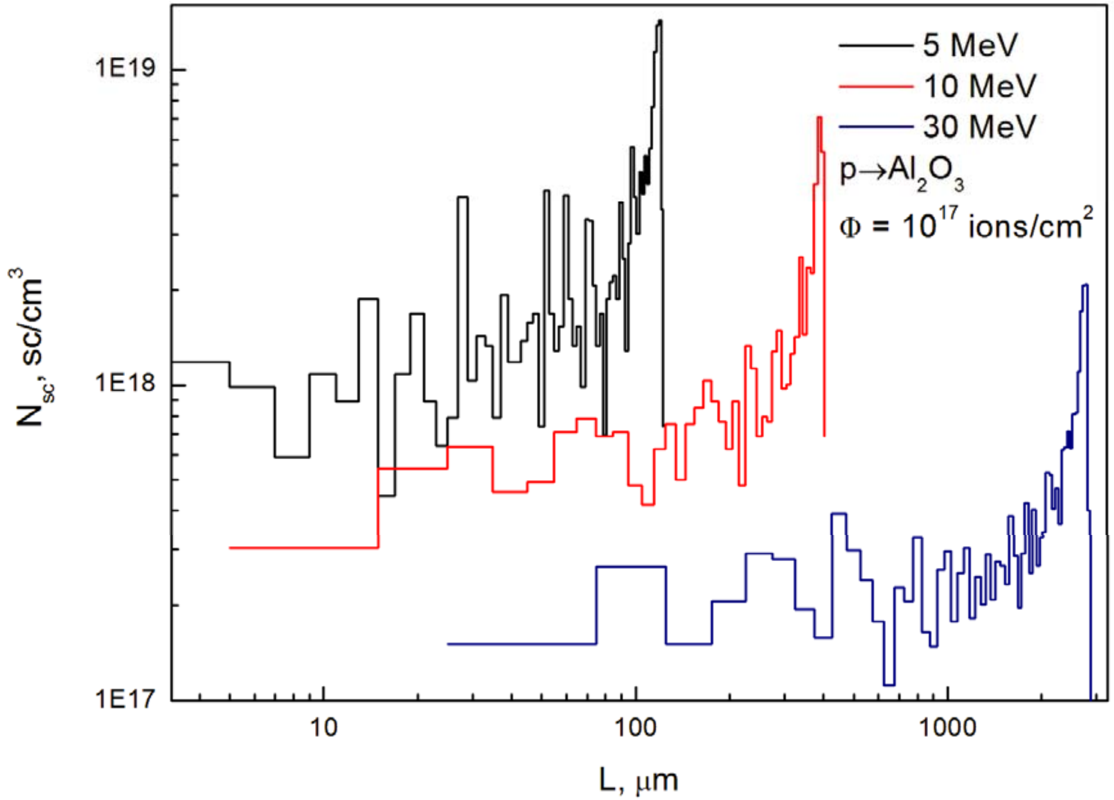
Modeling of subcascade formation in Al_2O_3 under 30 MeV He ion irradiation



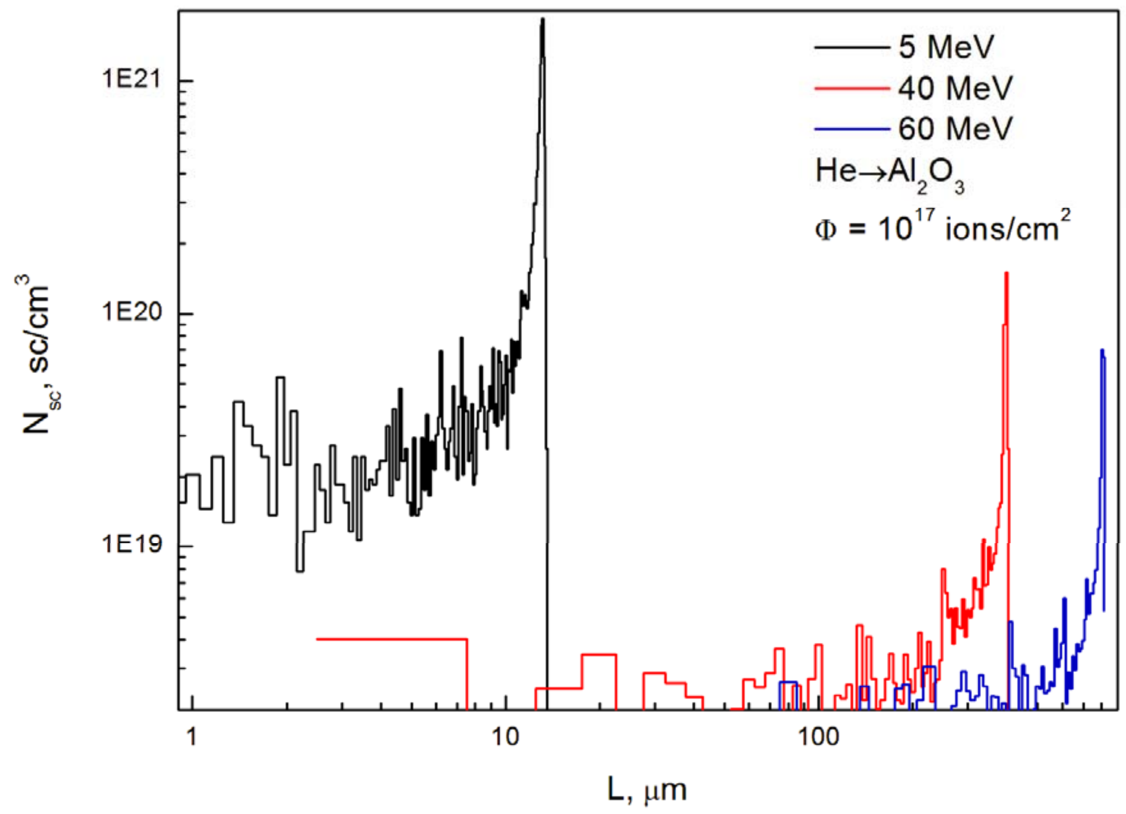
Modeling of sub-cascade formation in Al_2O_3 near the middle of penetration depth of 30 MeV He ion (B area)



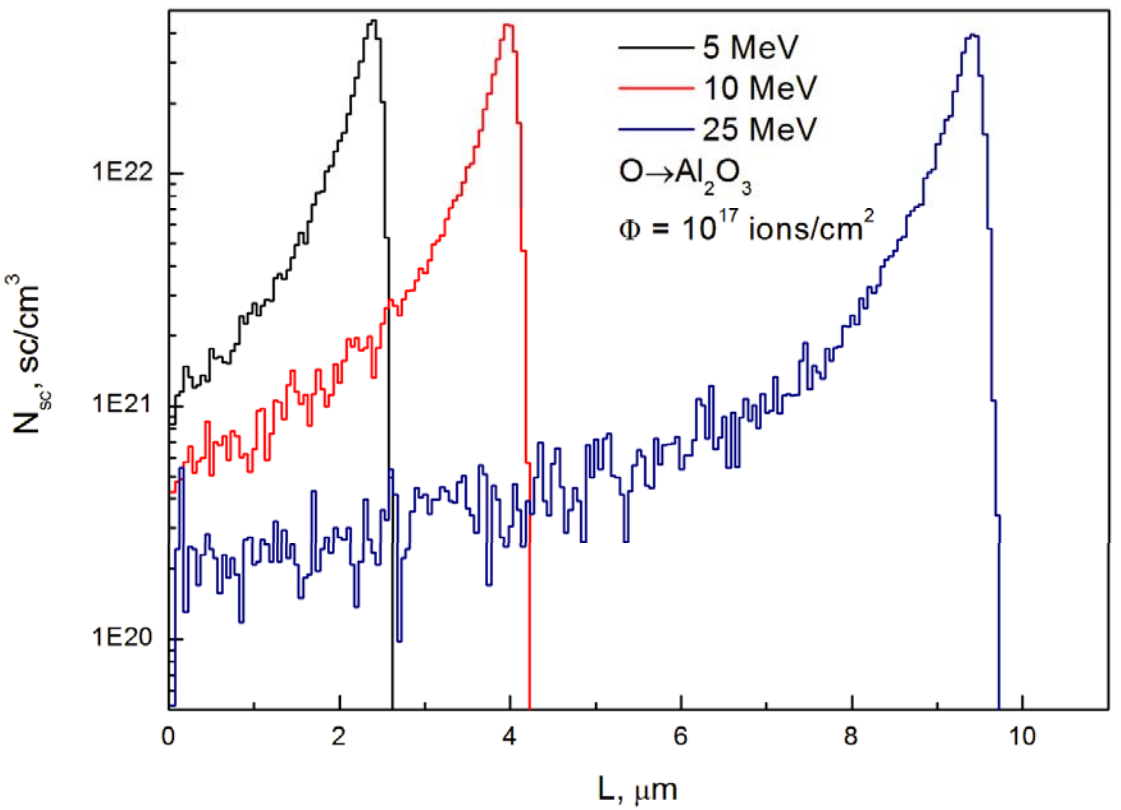
Distribution of sub-cascade density along penetration depth of protons with the different energies



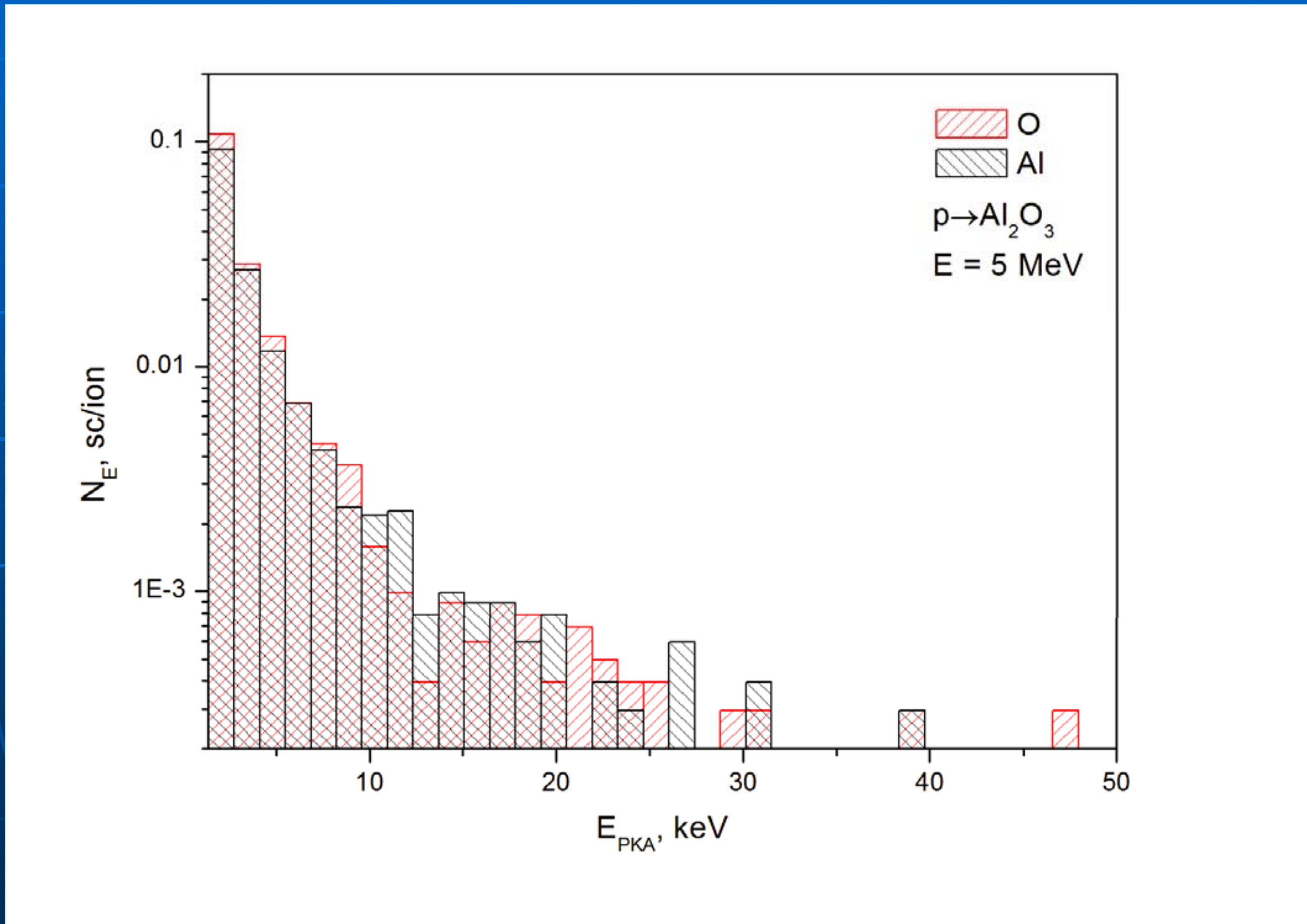
Distribution of sub-cascade density along penetration depth of He ions with the different energies



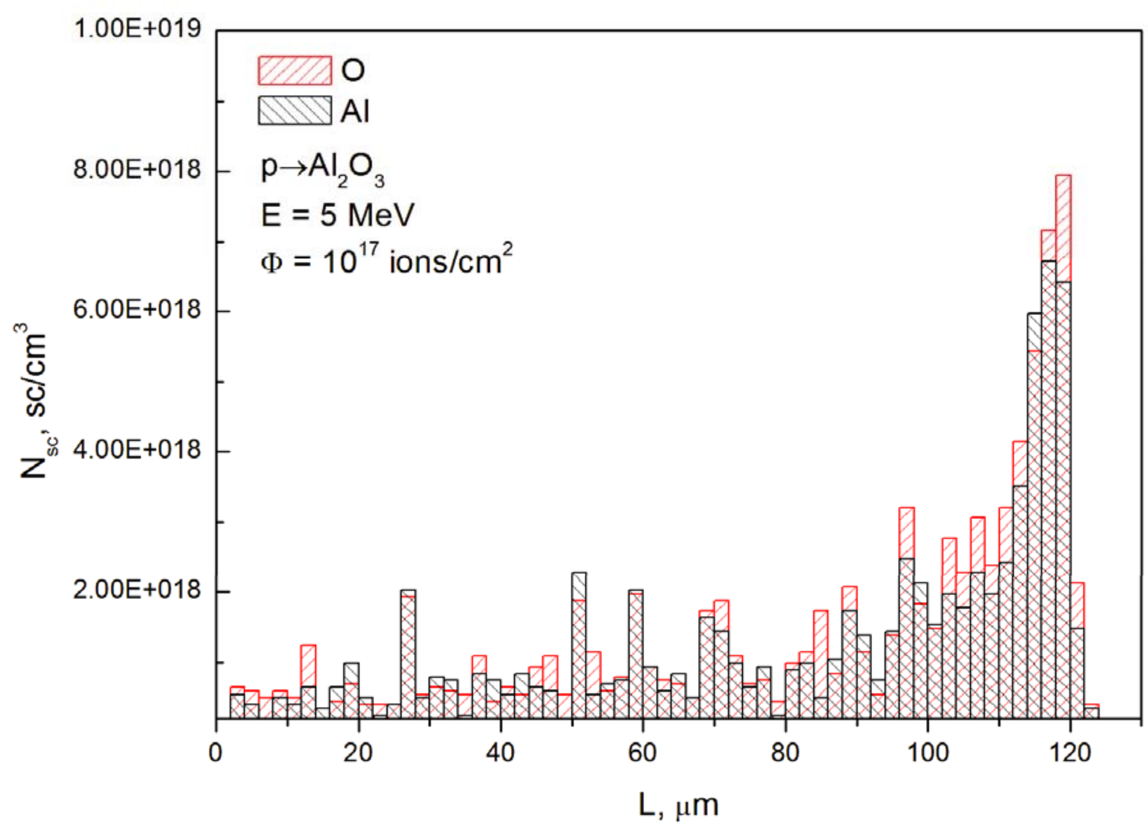
Distribution of sub-cascade density along penetration depth of oxygen ions with the different energies



Calculations of sub-cascade distribution in Al_2O_3 as a function of PKA energy under 5 MeV proton irradiation



Distribution profile of sub-cascade density along penetration depth of 5 MeV protons



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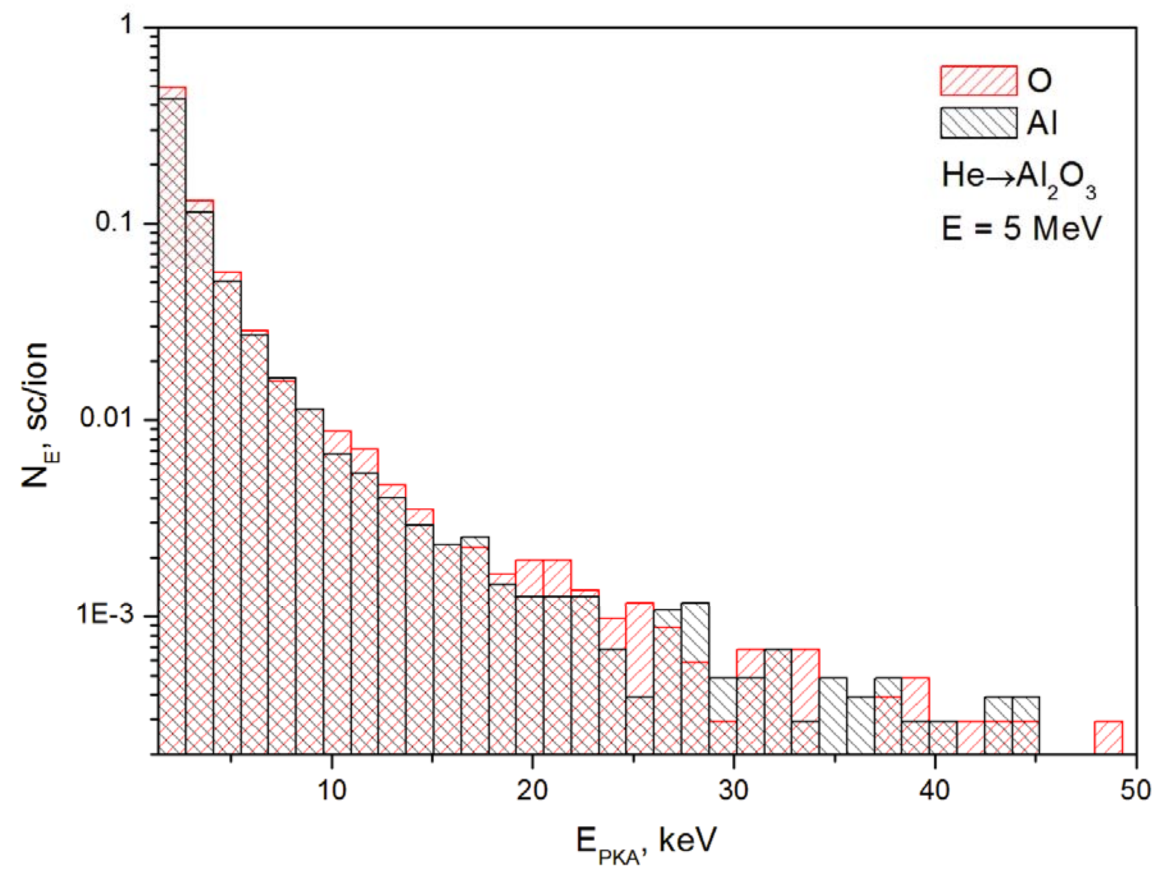
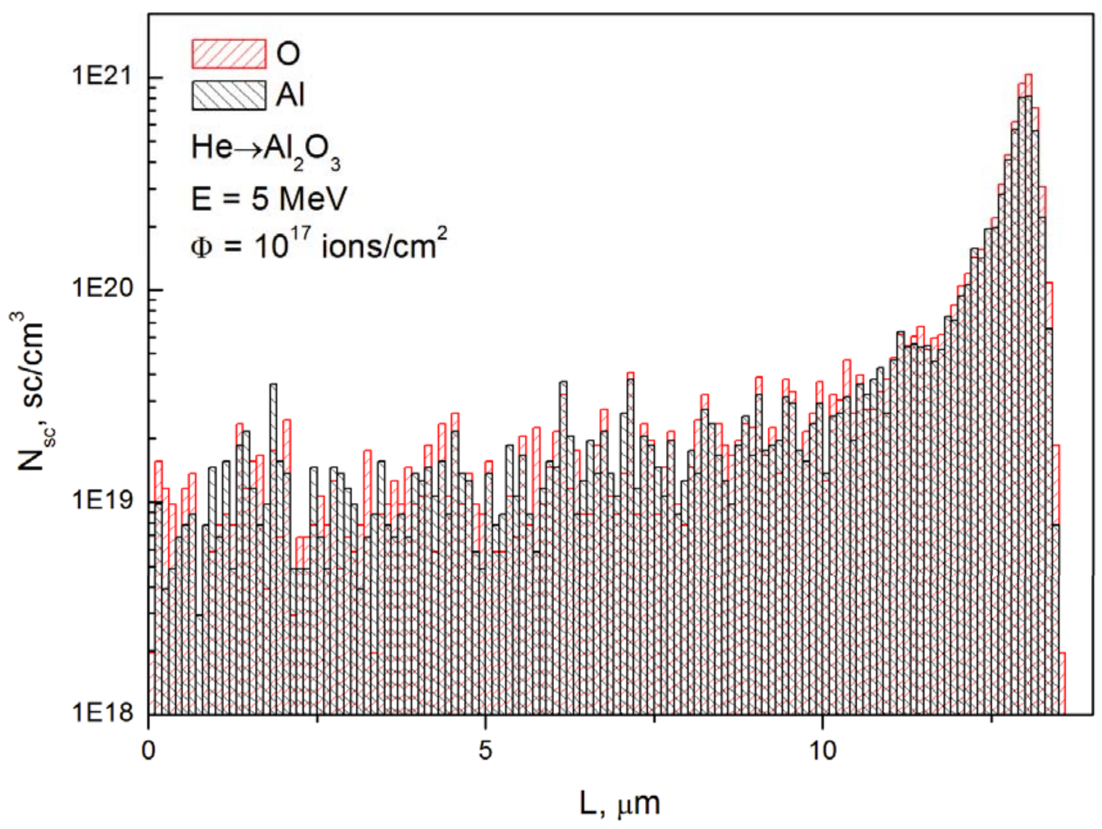
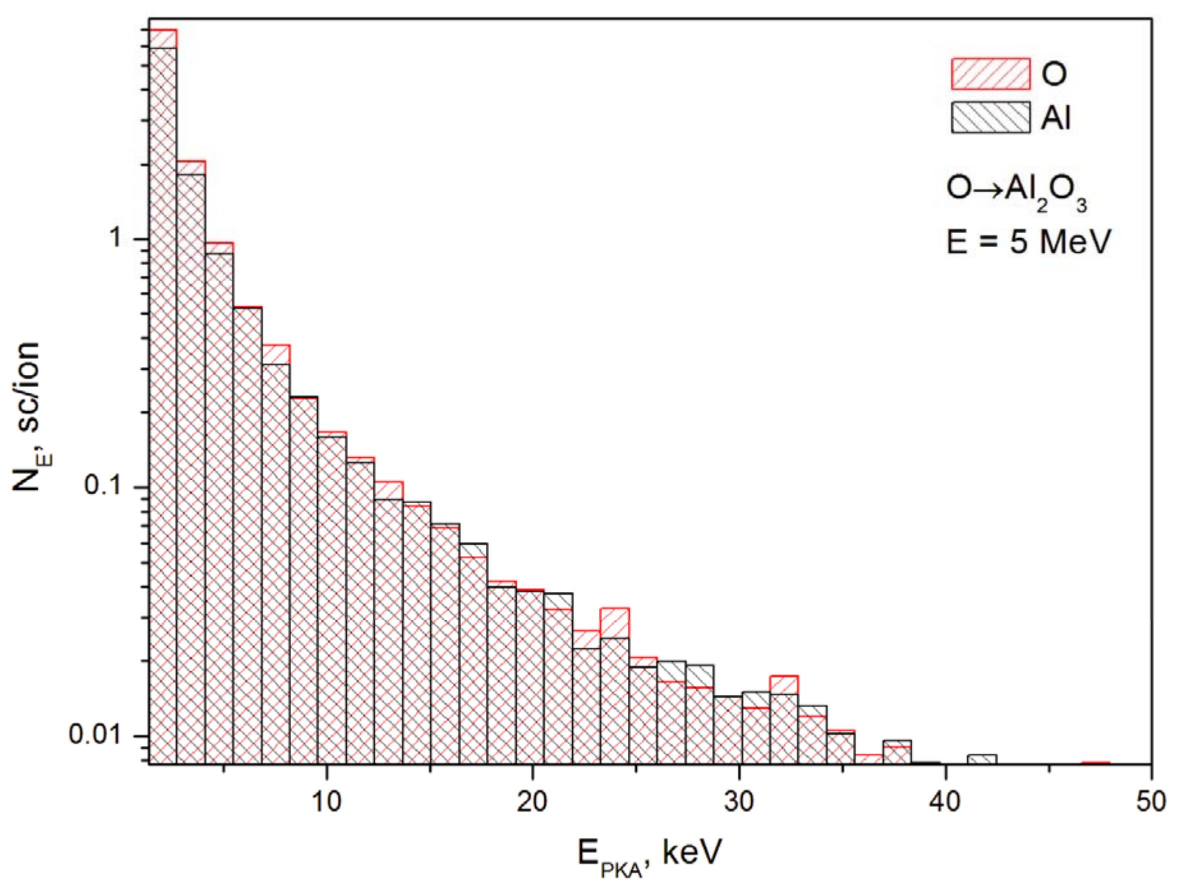
Calculations of sub-cascade distribution in Al_2O_3 as a function of PKA energy under 5 MeV He ion irradiation



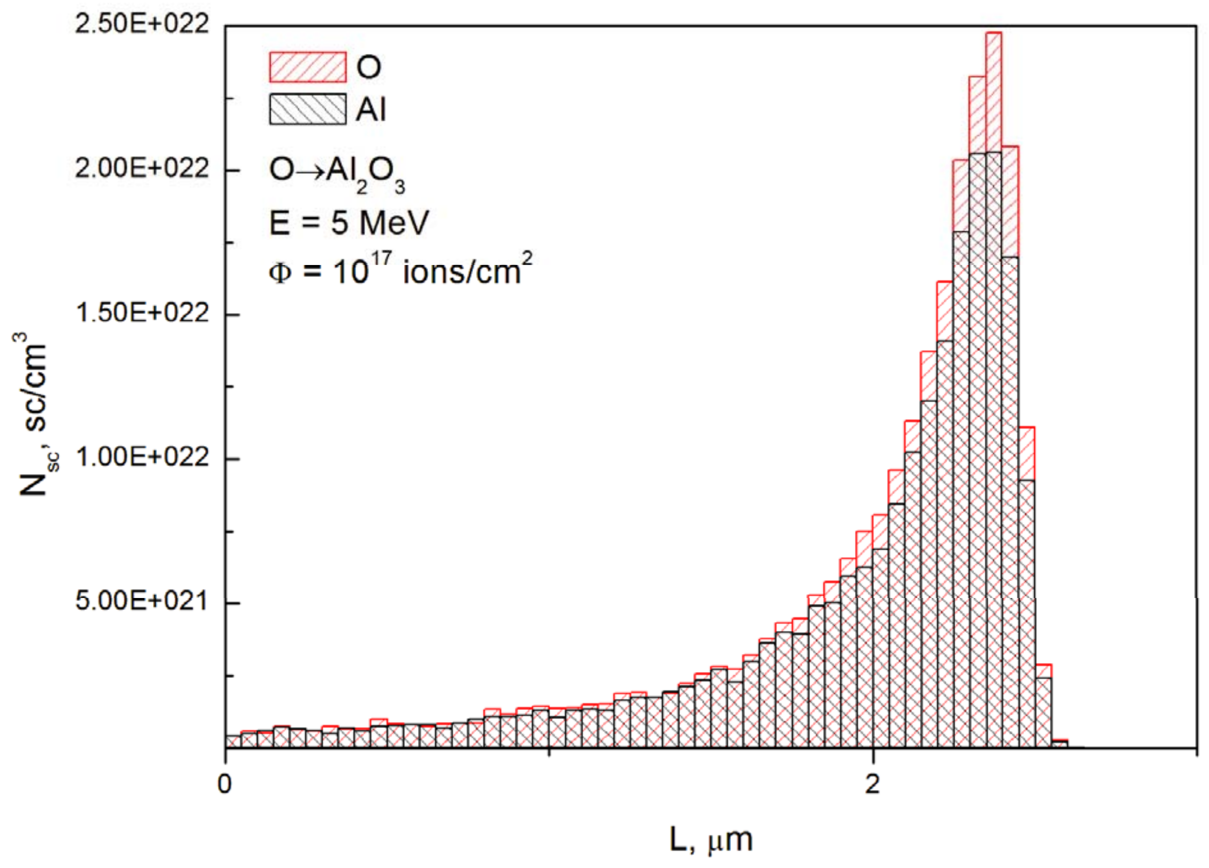
Distribution profile of sub-cascade density along penetration depth of 5 MeV He ions



Calculations of sub-cascade distribution in Al_2O_3 as a function of PKA energy under 5 MeV O ion irradiation



Distribution profile of sub-cascade density along penetration depth of 5 MeV oxygen ions



Summary

- Theoretical models and computer tools were developed for the investigations of radiation damage formation: cascades and sub-cascades in the fission and fusion structural materials: C, V, Be, Fe, Al, W taking into account elastic and inelastic collisions of fast neutrons with atoms in these materials .

- Numerical calculations have been made to determine generation rates of point defects, cascades and sub-cascades under neutron irradiation in ITER, DEMO and HFIR for different materials: C, V, Be, Fe, Al, W.

- It was shown, that the more strong effect of inelastic collisions of fast neutrons with atoms on the values of generation rates of point radiation defects and subcascade formations is realized in heavy materials (W, Fe and V).

- Developed theoretical models for diatomic material (Al2O3) allow to calculate radiation damage formation (point defects, cascades and sub-cascade formation) for fast neutron and ion irradiations.