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Joint ICTP-IAEA Advanced Workshop on Multi-Scale Modelling for Characterization and Basic Understanding of Radiation Damage Mechanisms in Materials

12 - 23 April 2010

Modelling of cascade and sub-cascade formation in fission and fusion structural materials under fast neutron and ion irradiations

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A.I. Ryazanov, E.V.Semenov

Outline

- Introduction
- Theoretical Model
- Numerical Calculations of cascade and sub-cascade formation for different Fusion and Fission Neutron Facilities:

ITER, DEMO, IFMIF, HFIR.

- Conclusions

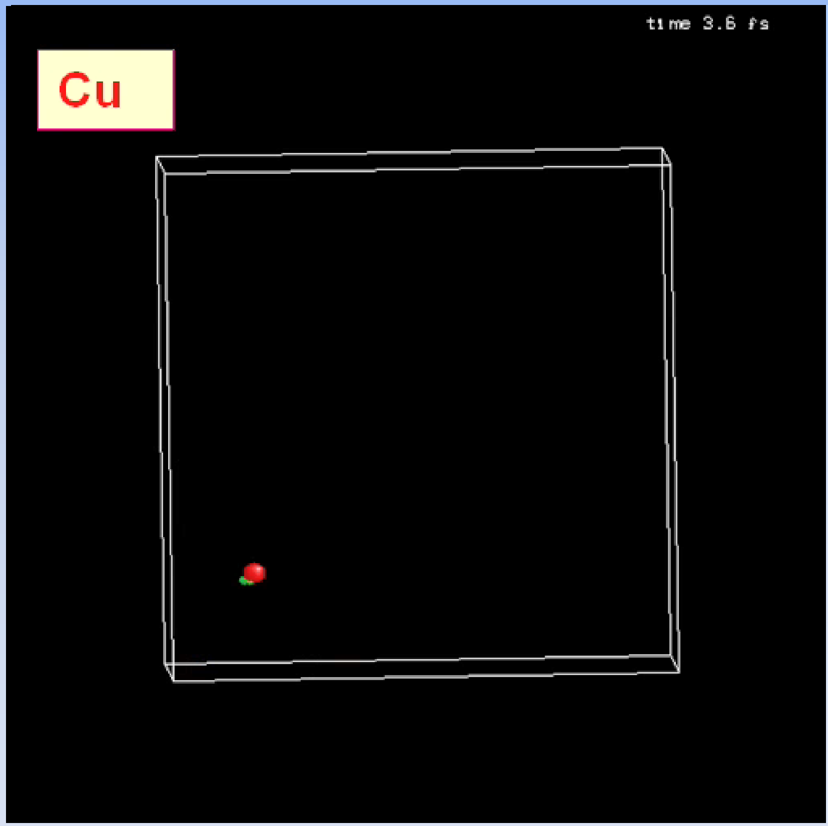
Introduction

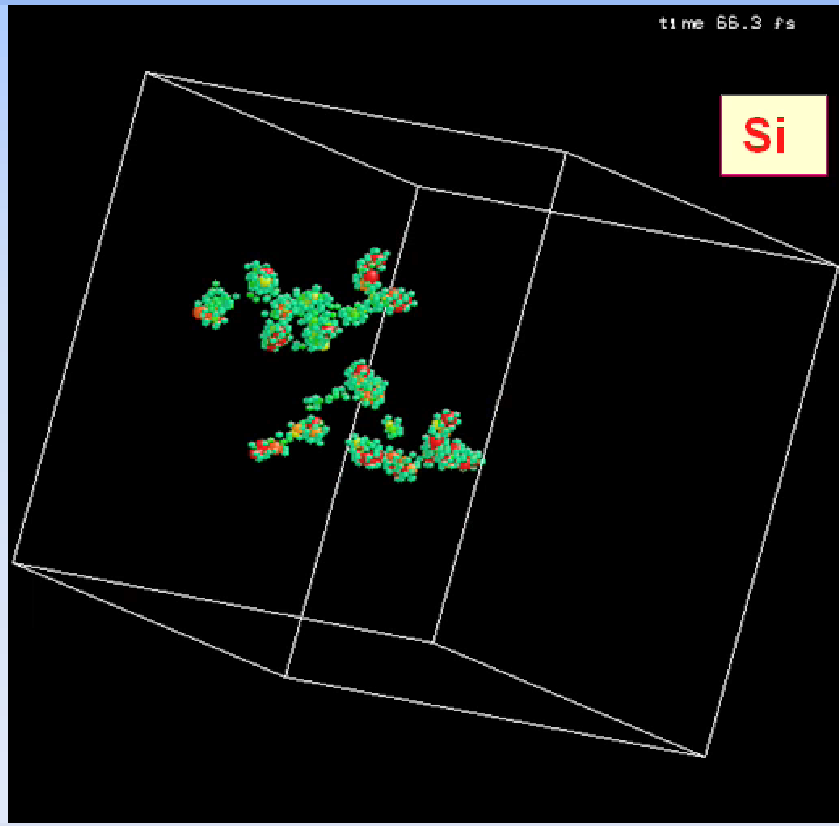
- Point defect clusters (dislocation loops, voids, bubbles) under fast neutron irradiation in fusion structural materials are formed into cascades and sub-cascades.

- 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 should be taking into account for calculations of PKA and recoil atom energy spectra.

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



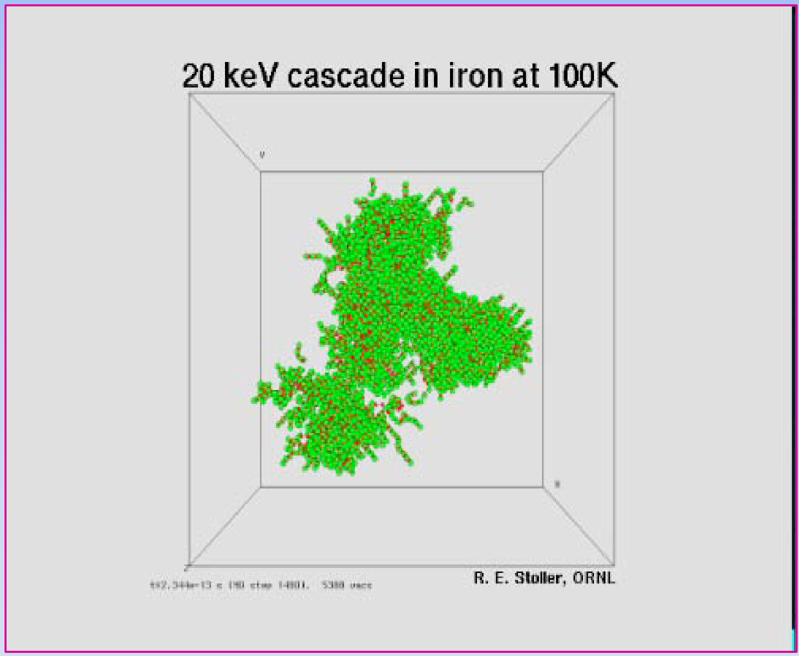


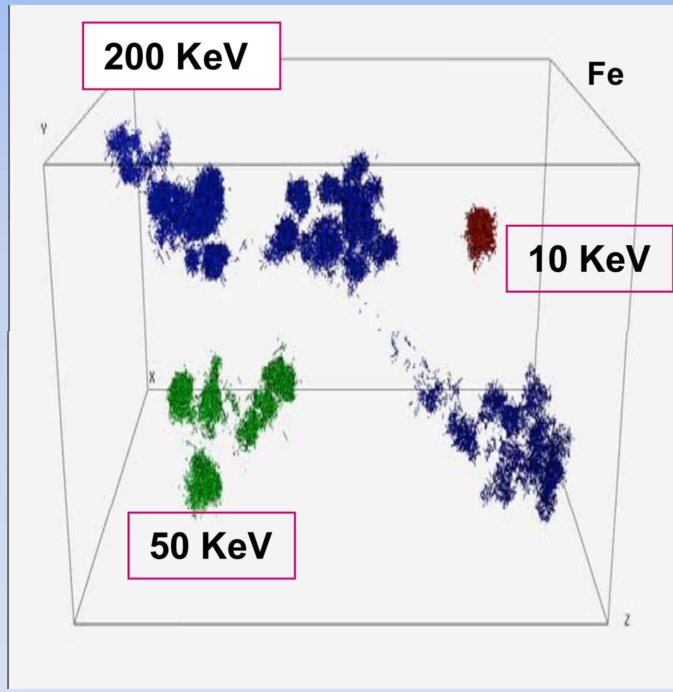
K. Nordlund (1998)

movie

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

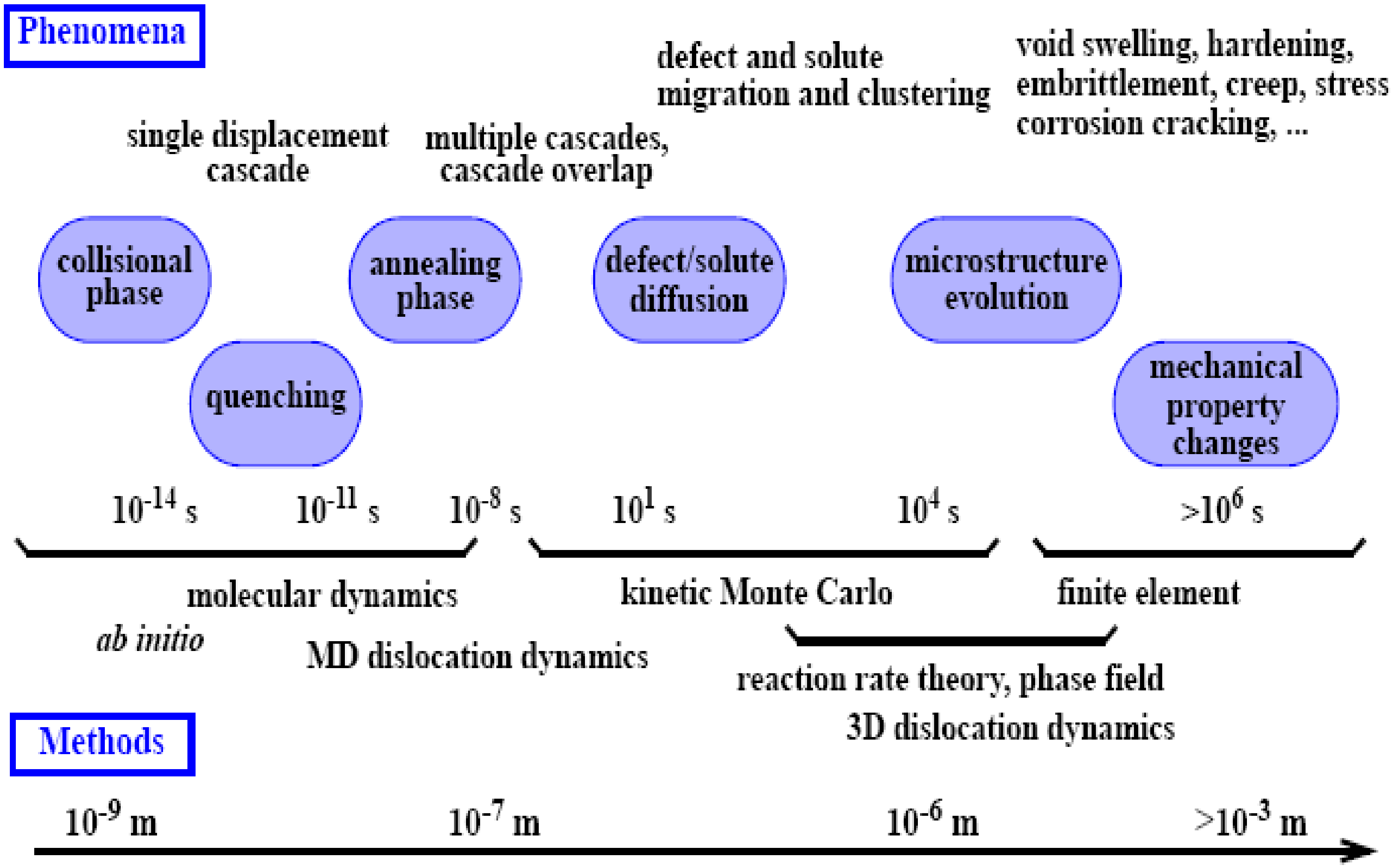
- Subcascade formation leads to asymptotic behavior at high energies
- Agrees with experimental data (TEM, etc.) (S. Zinkle, 2004)





R.E. Stoller, 2004

Schematic diagram: relevant phenomena and computational methods



R. Stoller

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 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

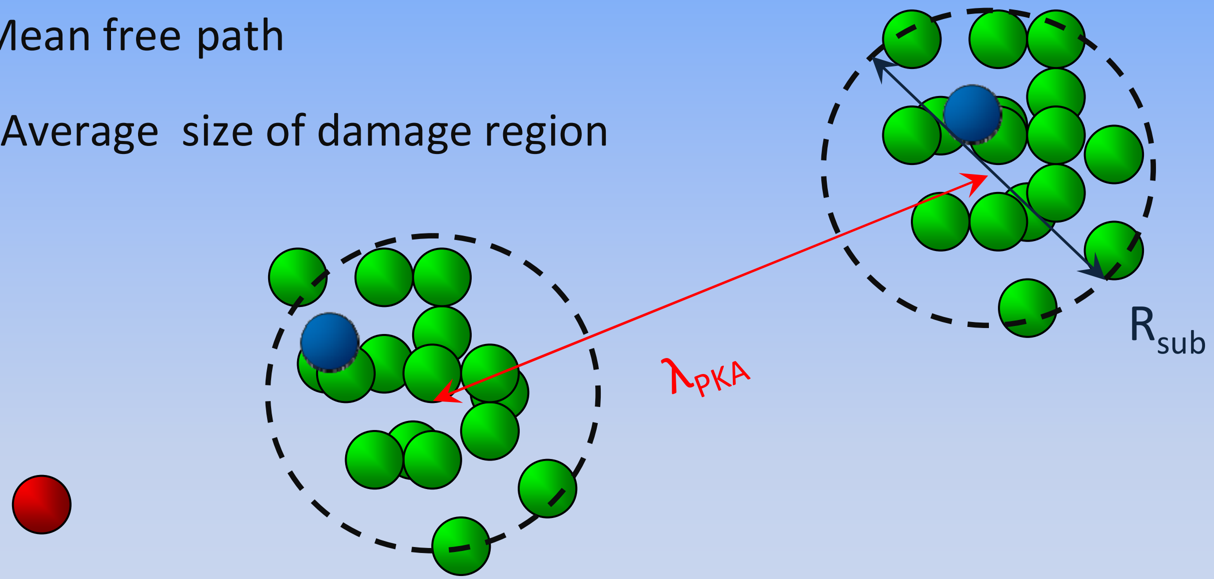
movie

PKA

SKA

λ_{PKA} Mean free path

R_{sub} Average size of damage region

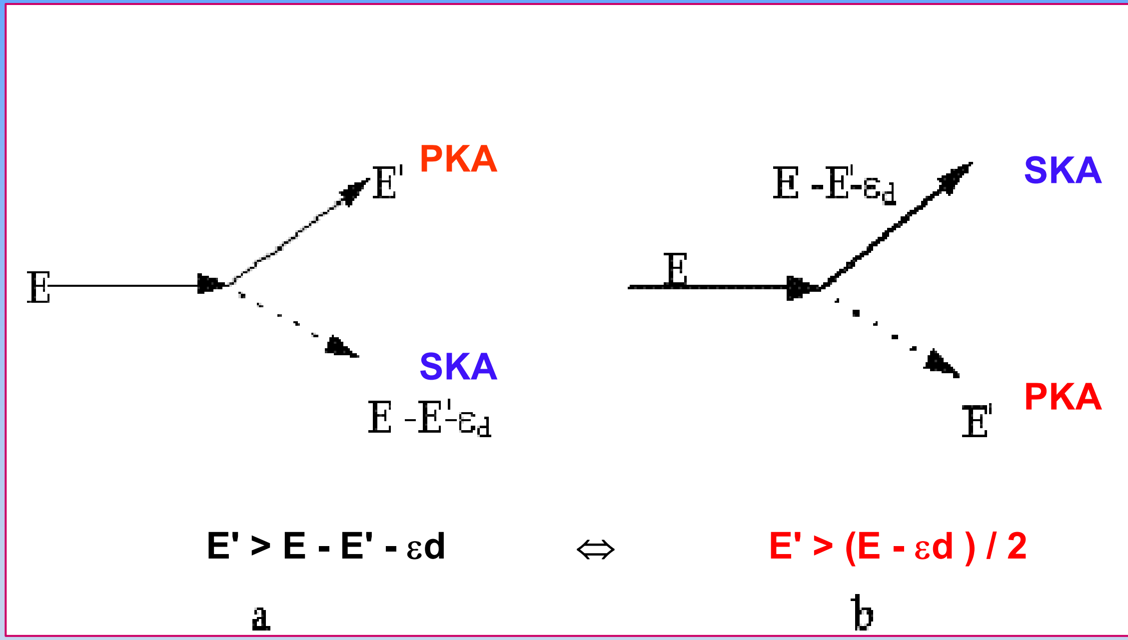


Sub-cascade formation criterion:

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

movie

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***

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

$\lambda_{PKA}(E)$ - 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

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

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

N_a is the density of target atoms,

$$\left(\frac{dT}{dx}\right)_{tot} = \left(\frac{dT}{dx}\right)_{n} + \left(\frac{dT}{dx}\right)_{e}$$

$$\left(\frac{dT}{dx}\right)_{n} = \frac{N_a \varepsilon}{T} \int_{0}^{T^2/\varepsilon^2} \left(\frac{\pi a^2}{2t^{1/2}}\right) \frac{\lambda t^{1/2-m}\,dt}{(1+(2\lambda t^{1-m})^q)^{1/q}}$$

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

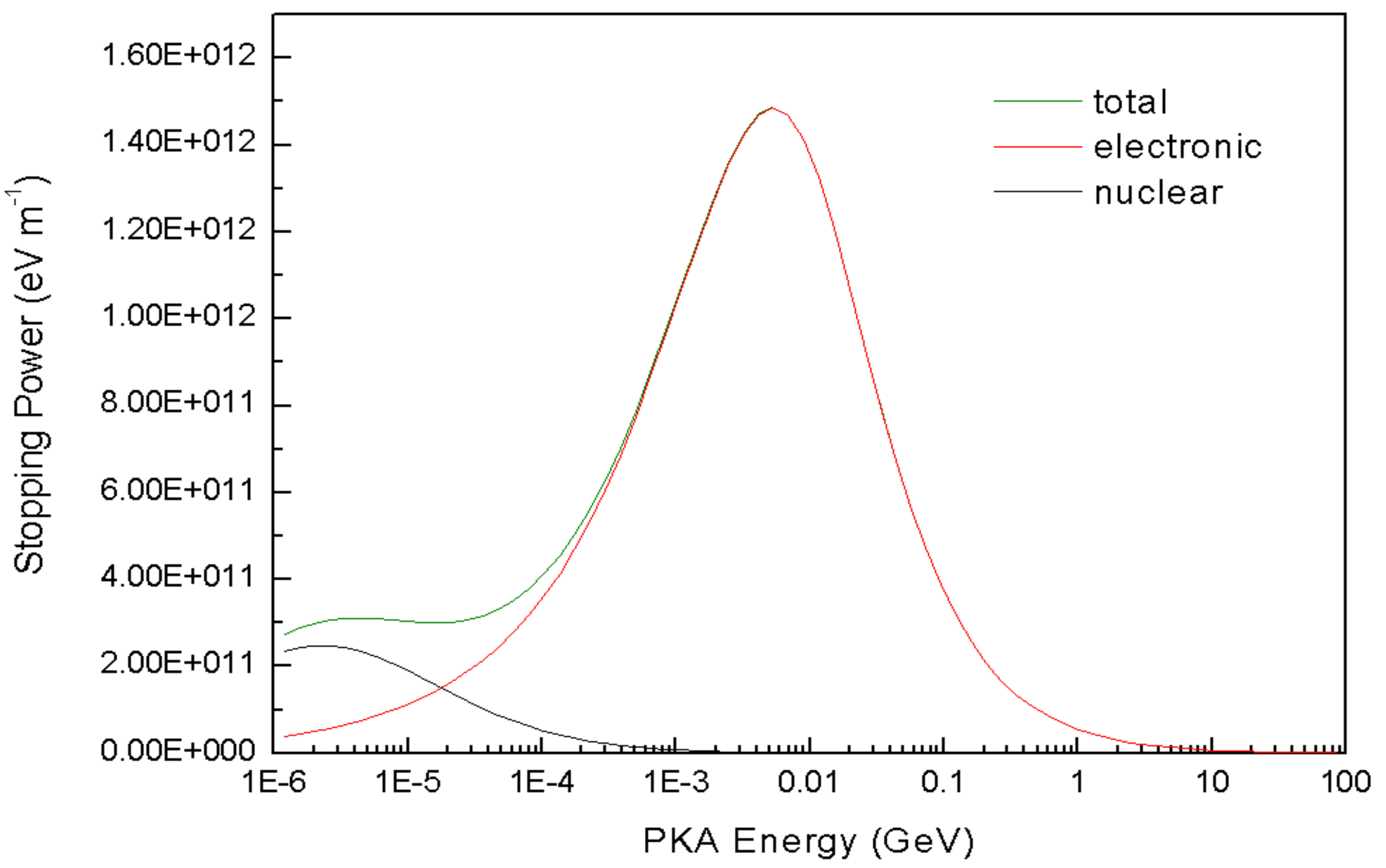
$$S_L(T) = k_L T^{1/2}$$

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

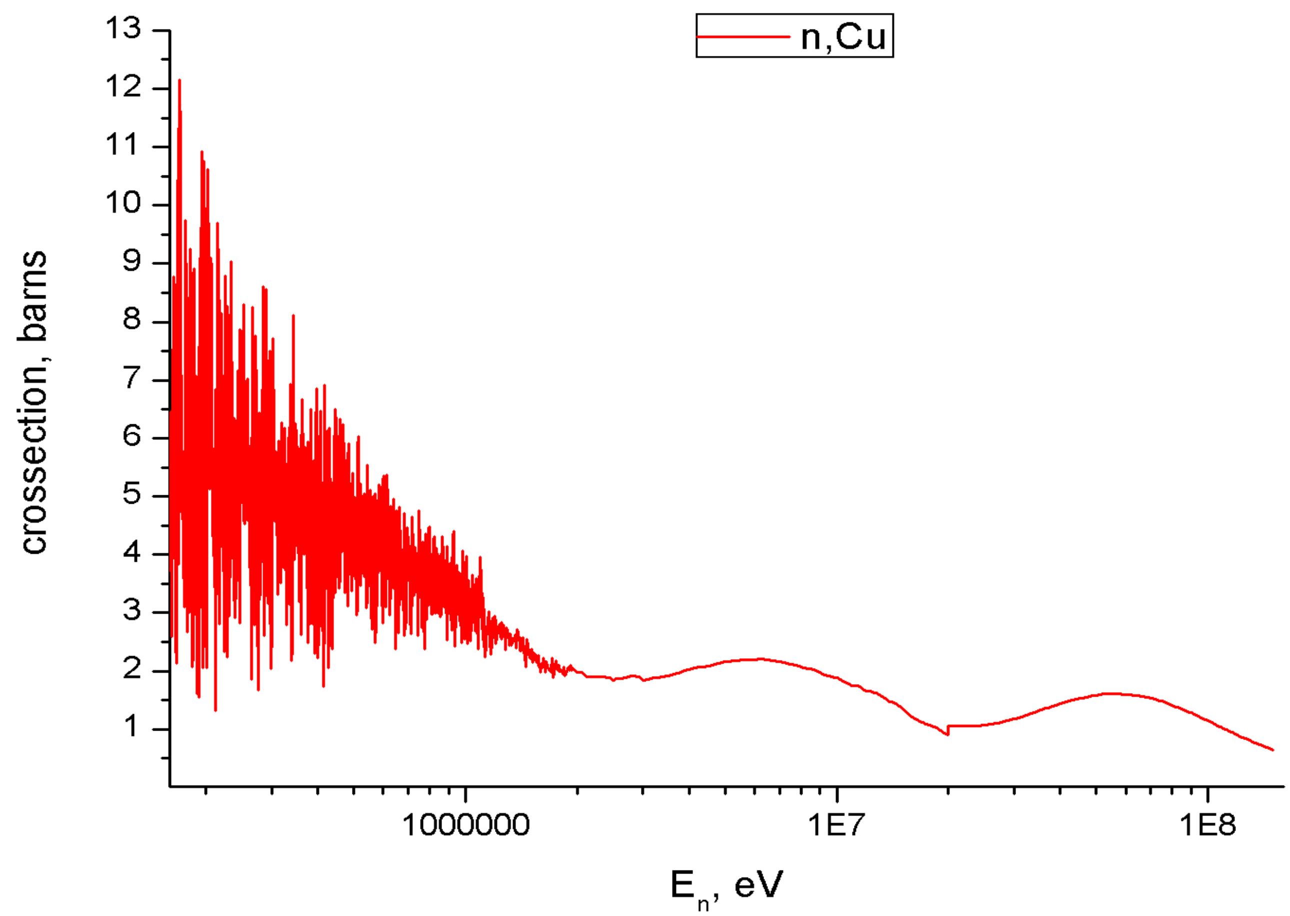
$$S_{BB}(T) = \frac{8\pi Z^2 e^4}{I \varepsilon_b} \ln\left(\varepsilon_b + 1 + \frac{5}{\varepsilon_b}\right)$$

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

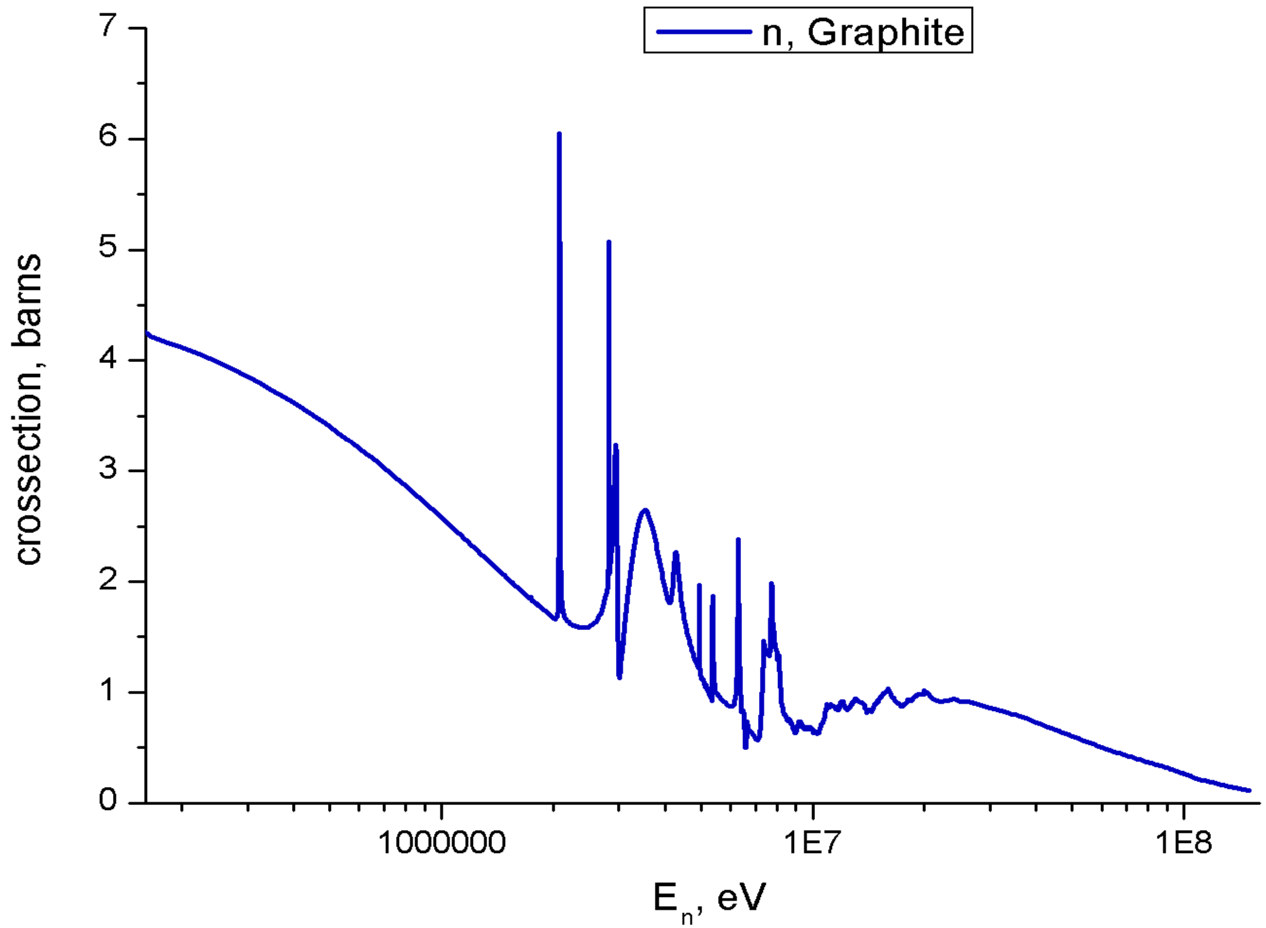
Total Energy Loss for Moving Atoms in Graphite



Cross section of elastic interaction of fast neutrons with Cu Atoms (from ENDF-B IV)



Cross section of elastic interaction of fast neutrons with C Atoms (from ENDF-B IV)



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

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

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

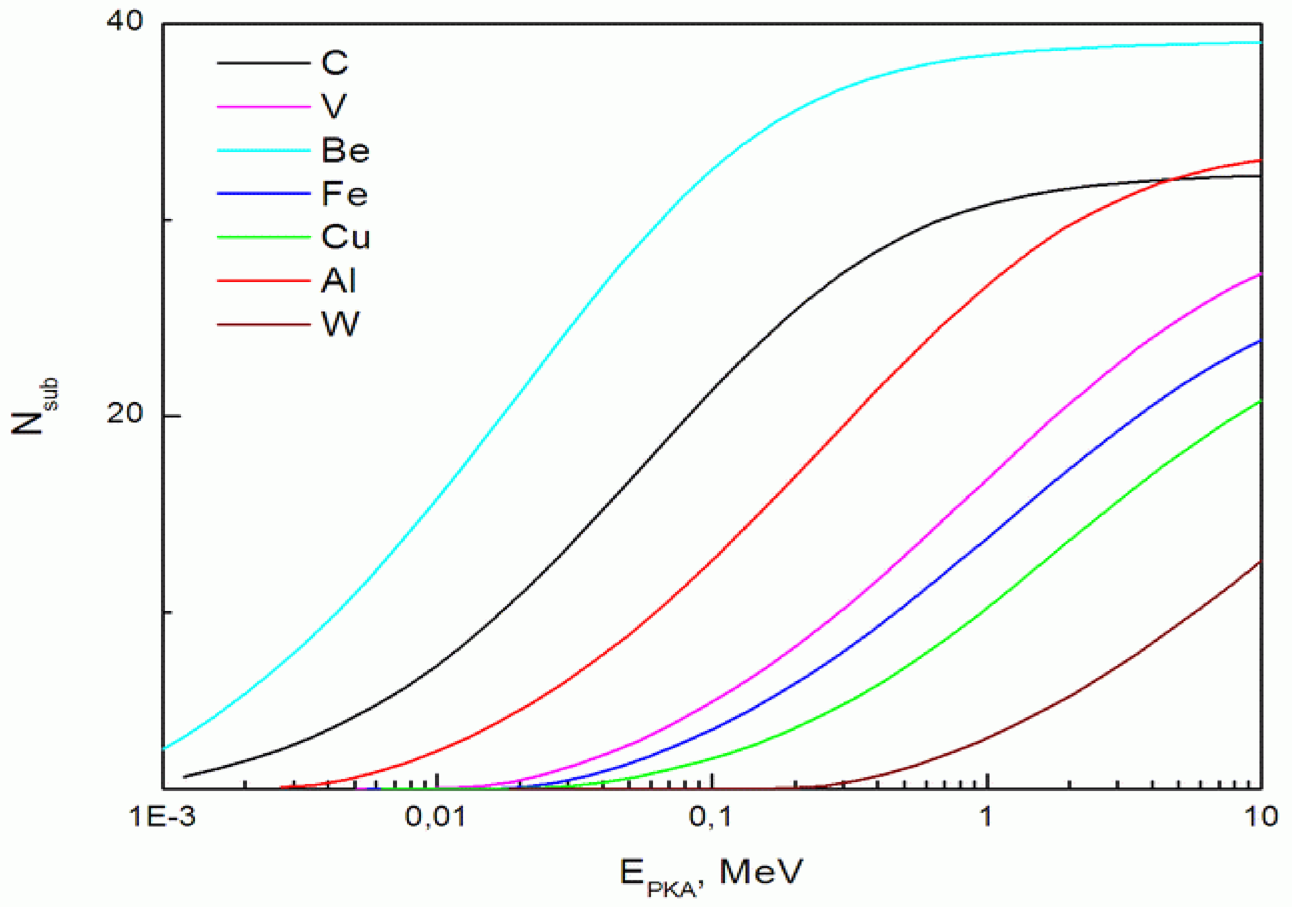
$\sigma_{el}(E_n, T)$ - Differential elastic cross section for scattering of fast neutron with energy *En* on atom with the energy transfer *T* to atom

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

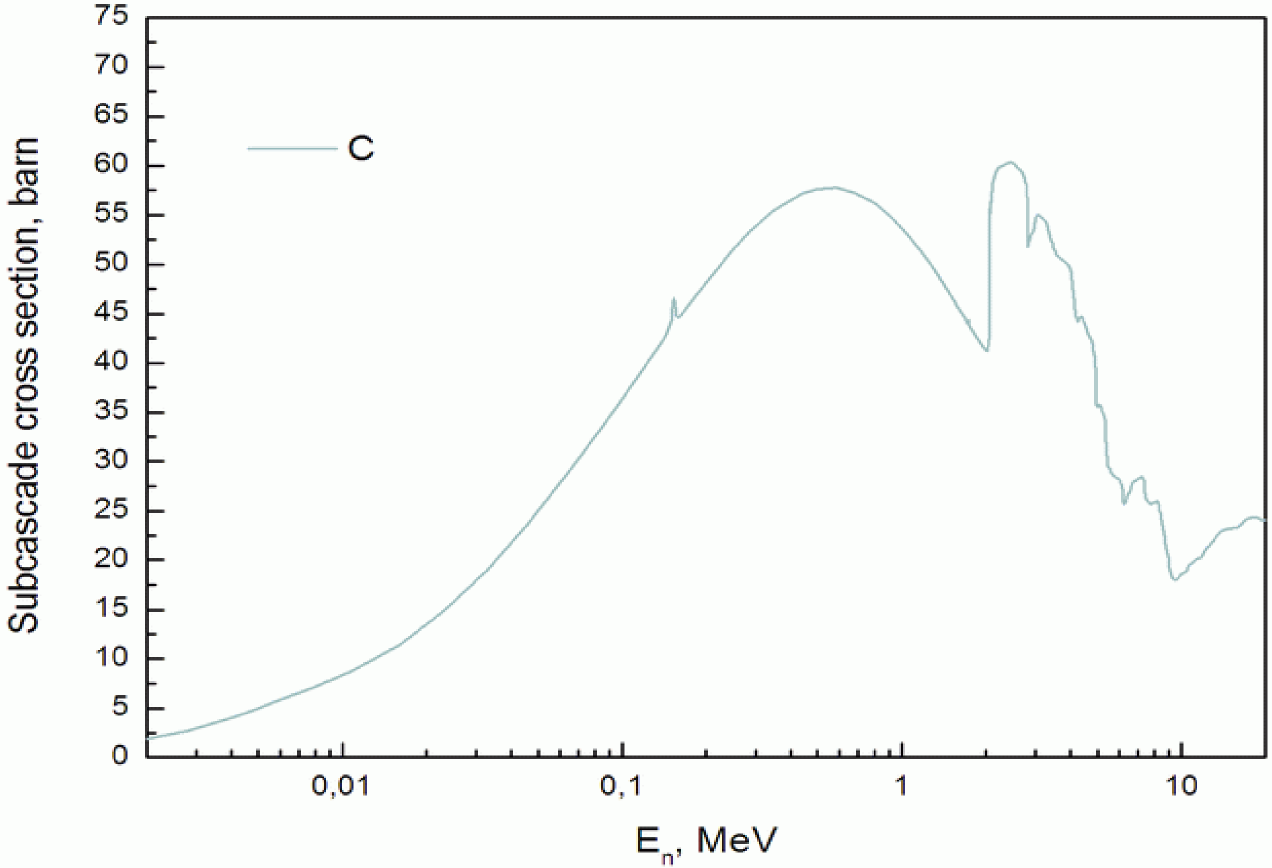
E_{sf} - Sub-cascade formation energy

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

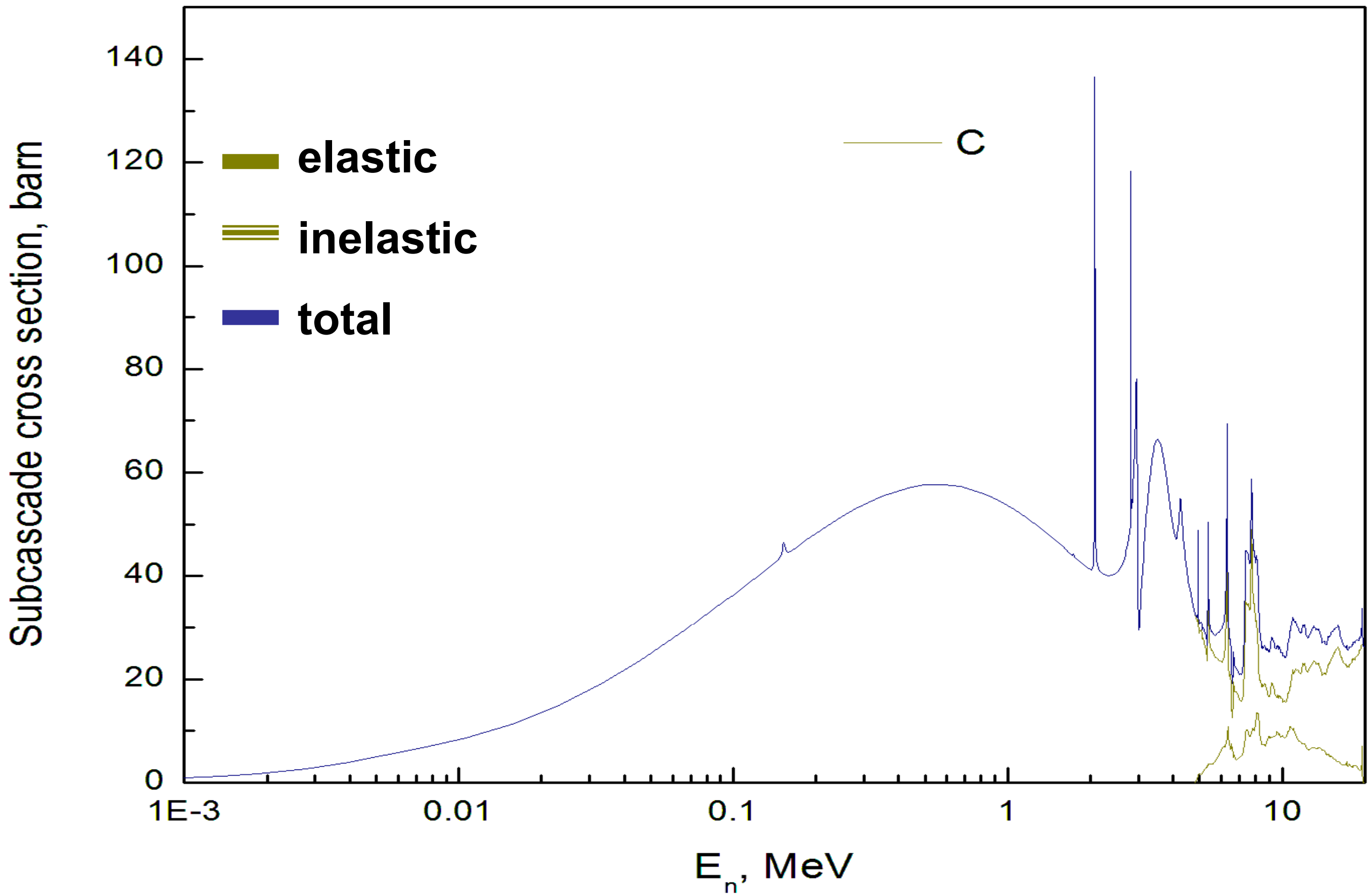
Number of Sub-cascades as a Function of PKA Energy



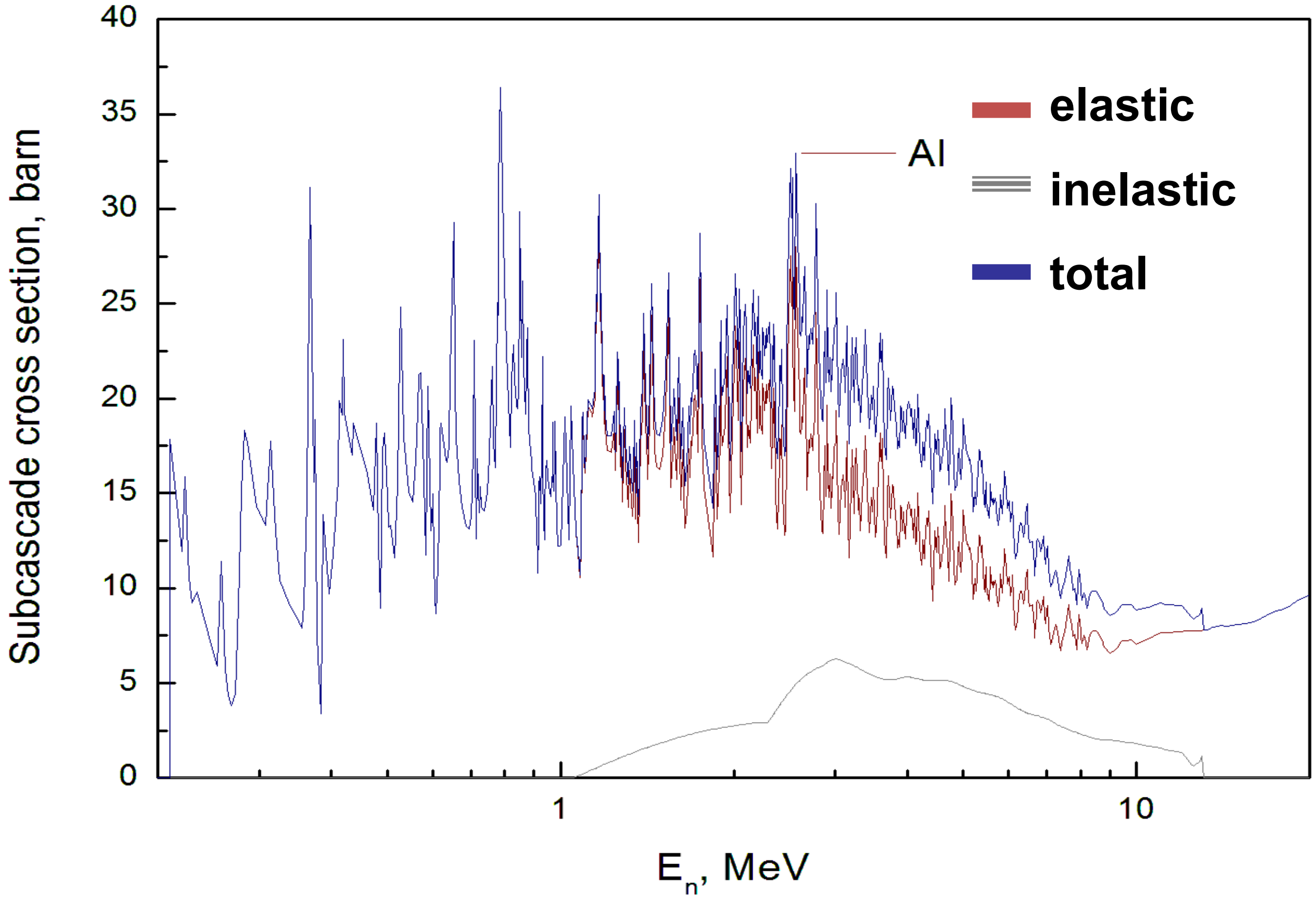
Cross Section of Sub-cascade Formation in C as a Function of Neutron Energy



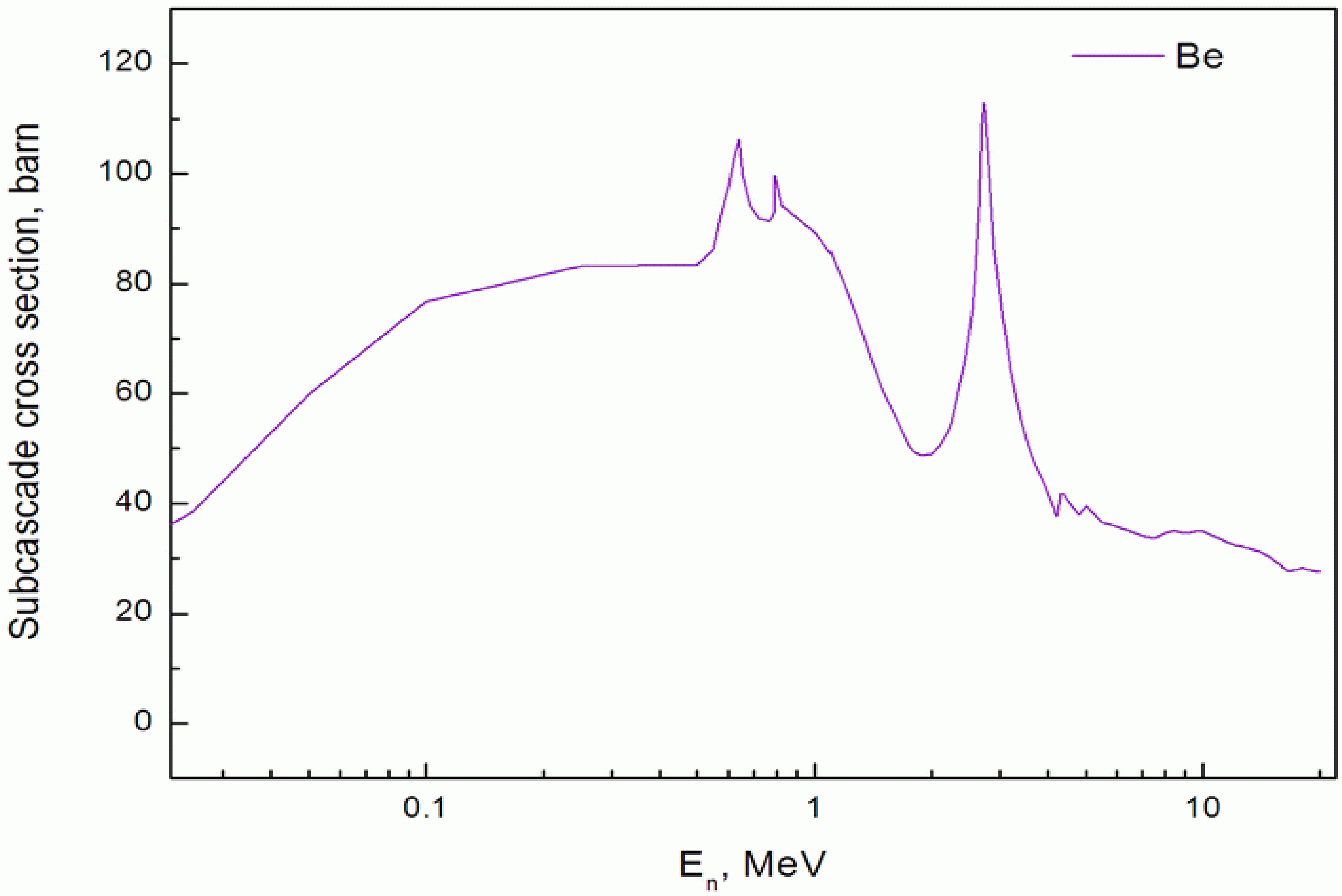
Cross Section of Sub-cascade Formation in C as a Function of Neutron Energy



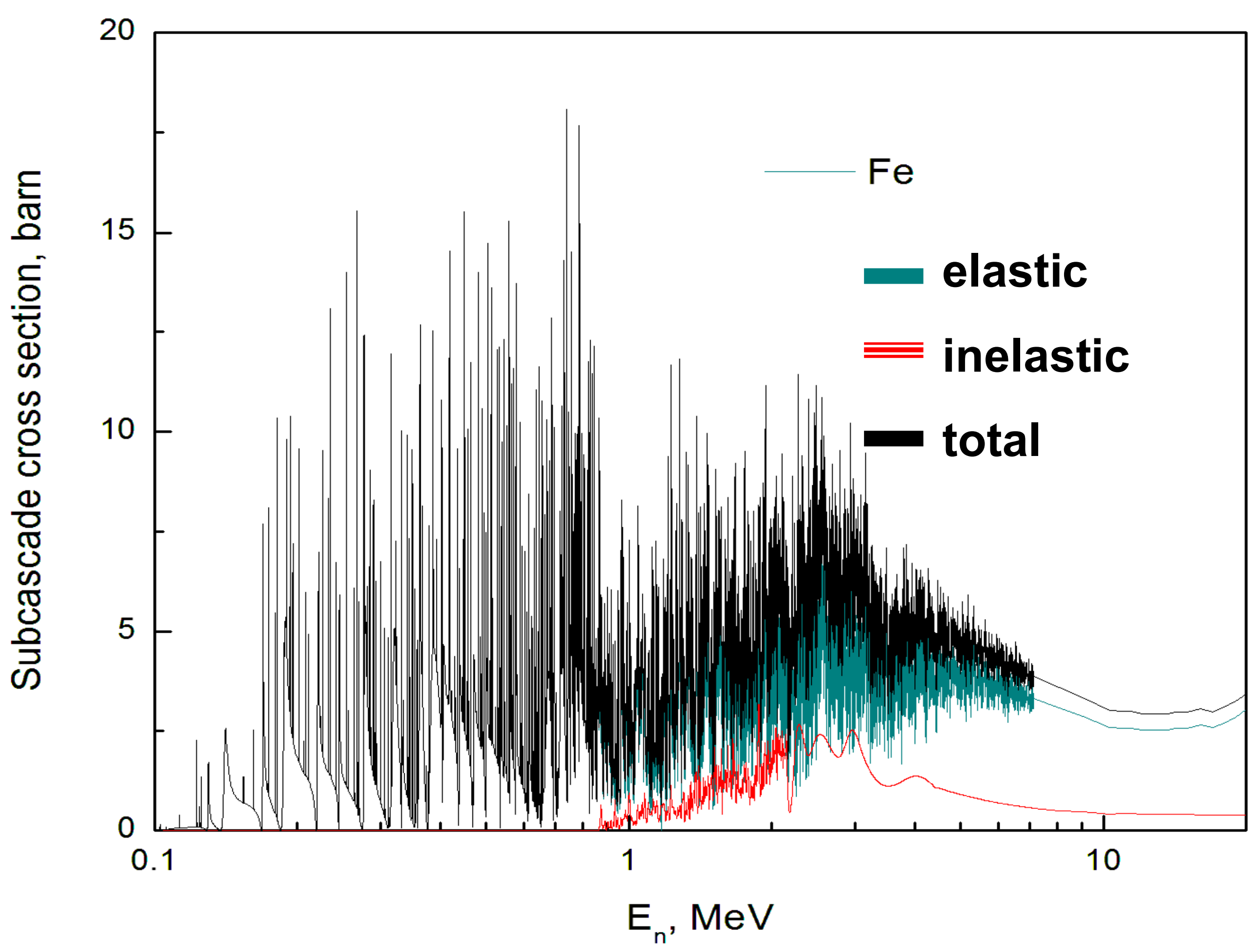
Cross Section of Sub-cascade Formation in Al as a Function of Neutron Energy



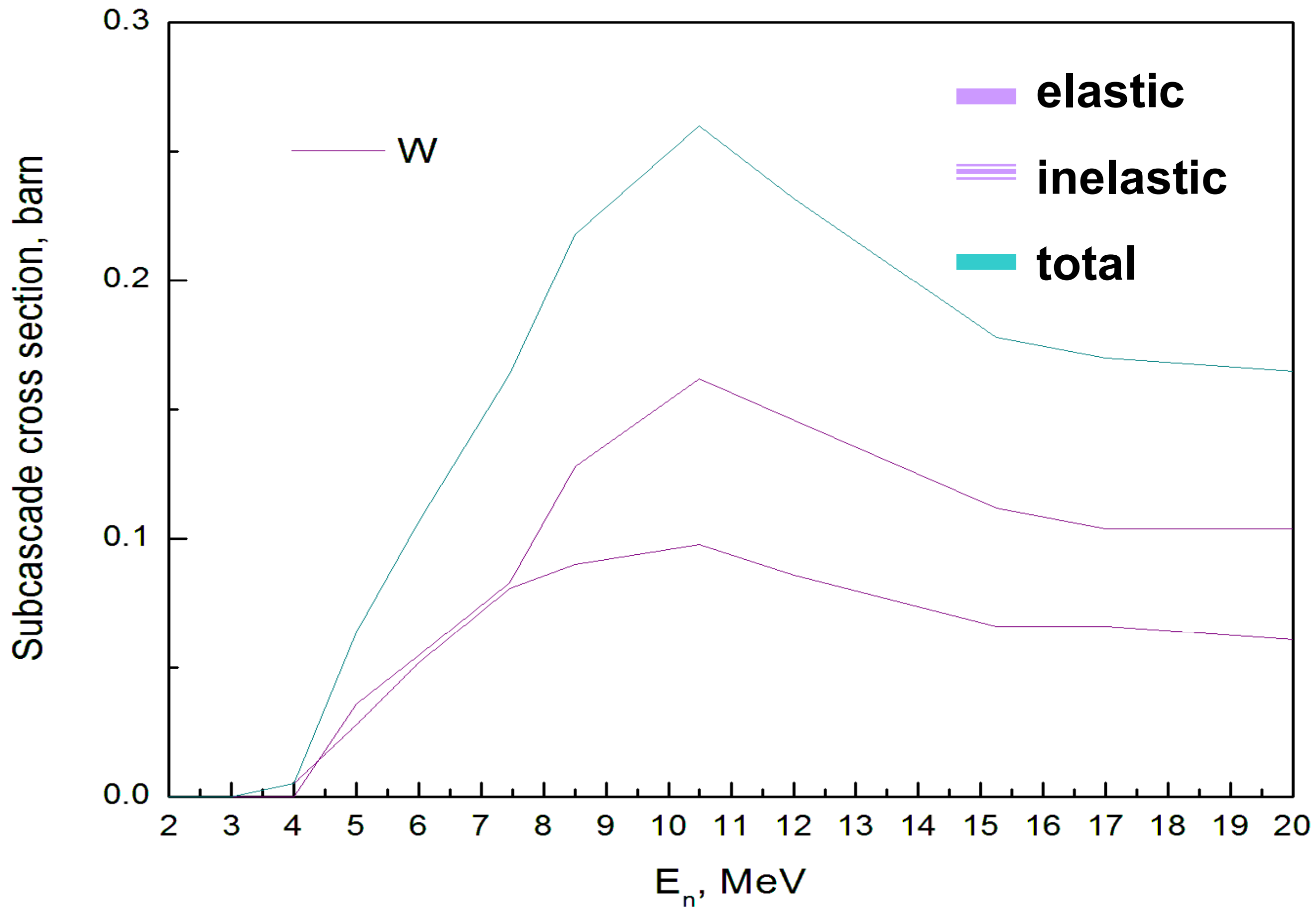
Cross Section of Sub-cascade Formation in Be as a Function of Neutron Energy



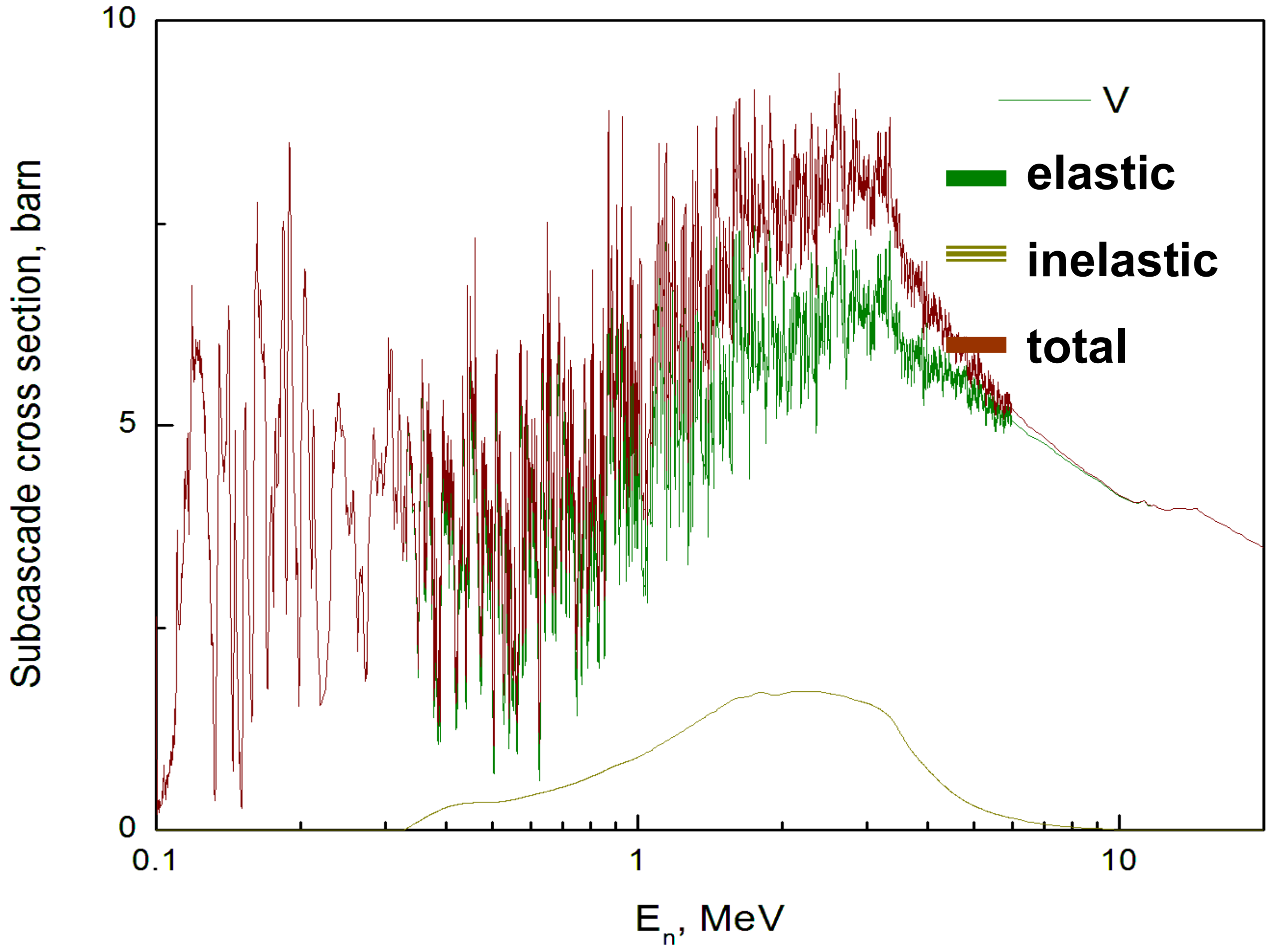
Cross Section of Sub-cascade Formation in Fe as a Function of Neutron Energy



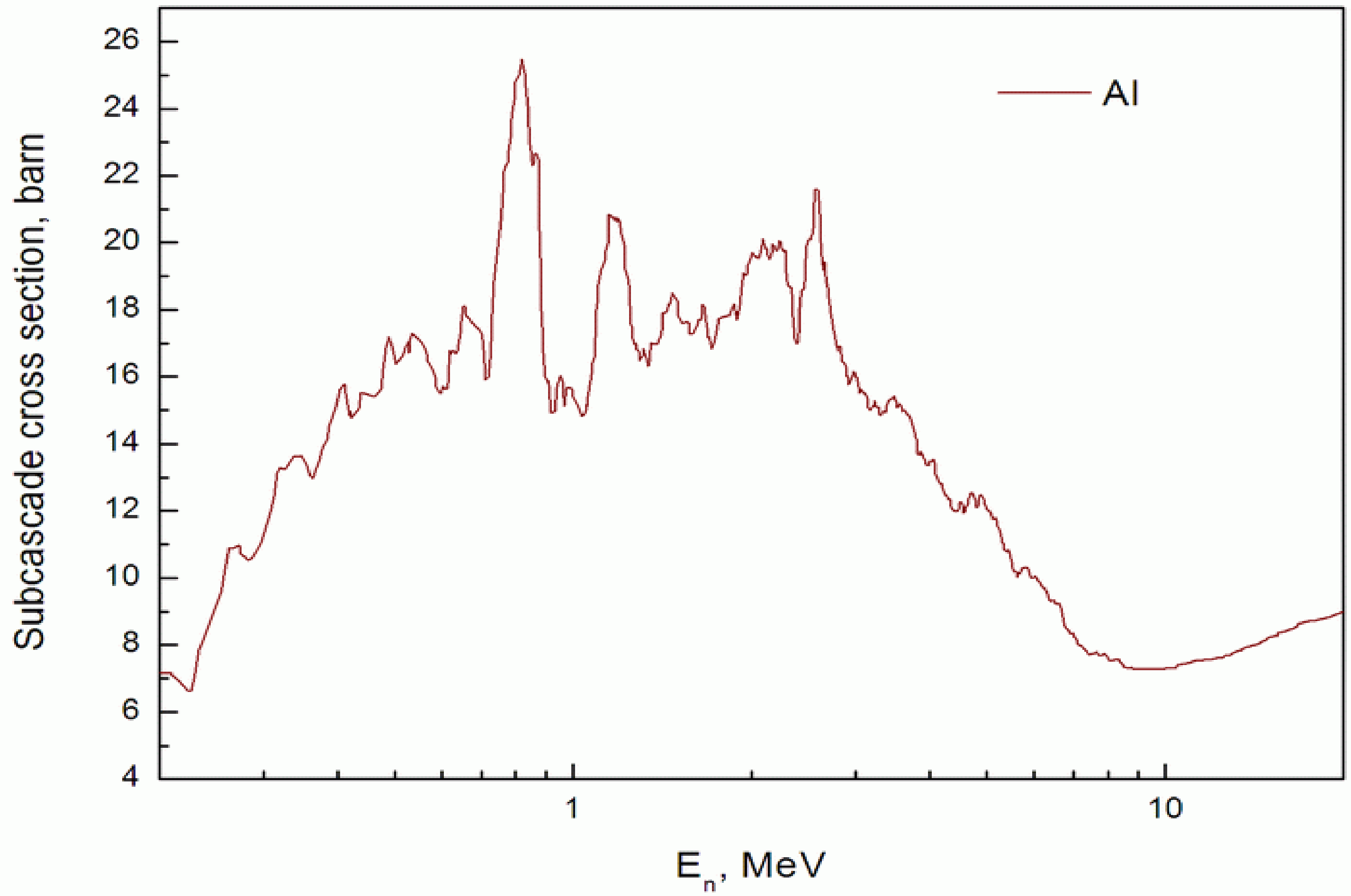
Cross Section of Sub-cascade Formation in W as a Function of Neutron Energy



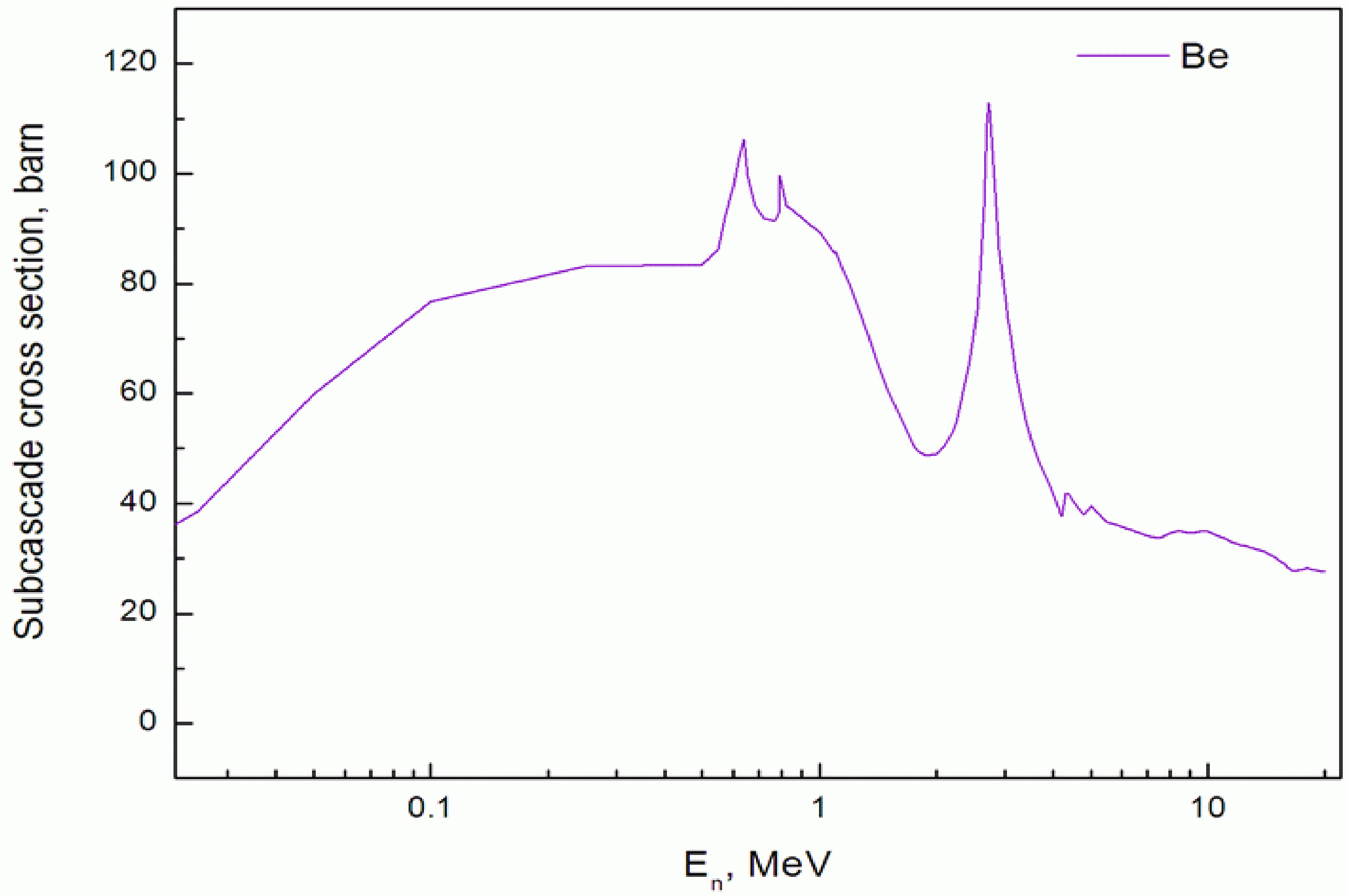
Cross Section of Sub-cascade Formation in V as a Function of Neutron Energy



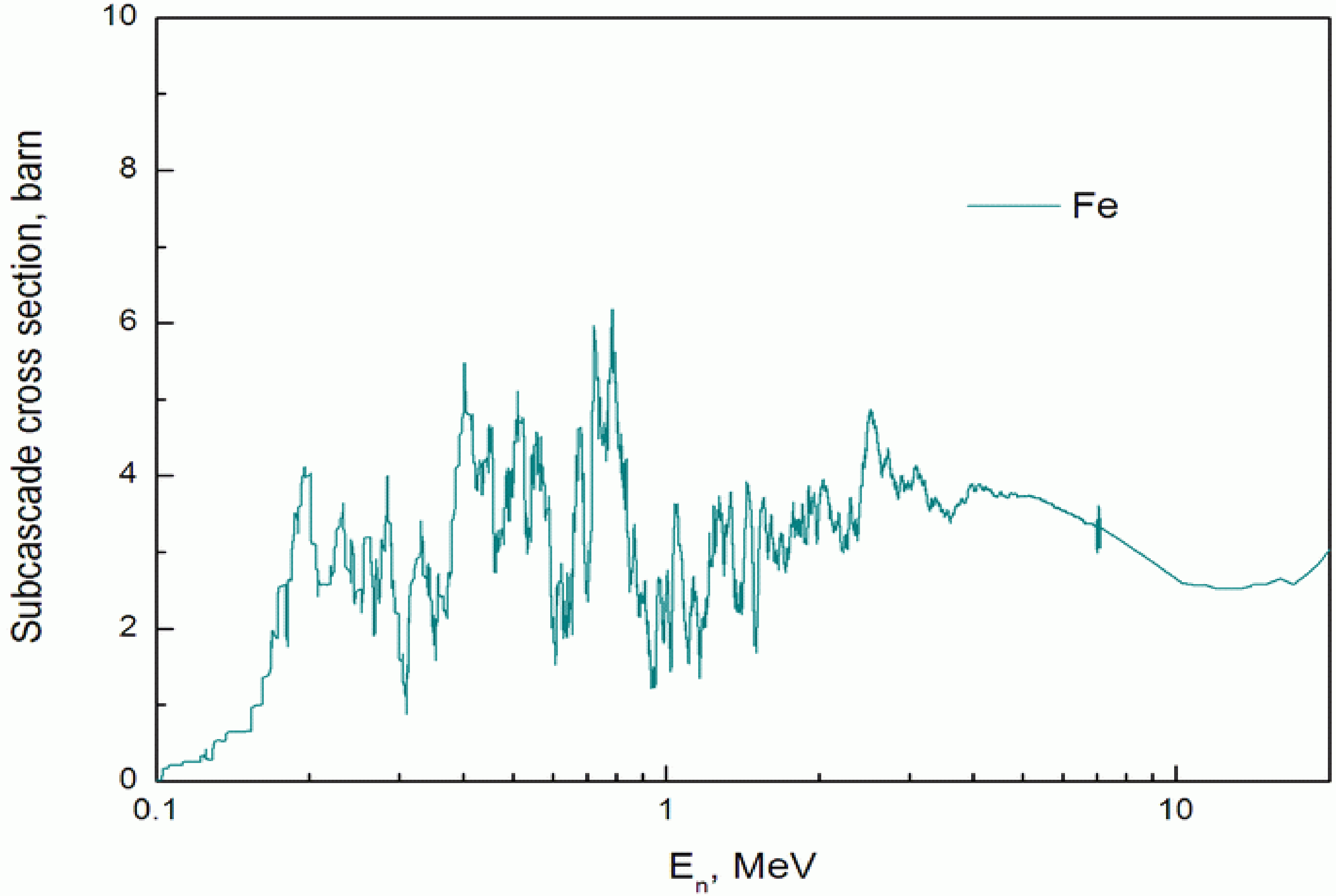
Cross Section of Sub-cascade Formation in Al as a Function of Neutron Energy



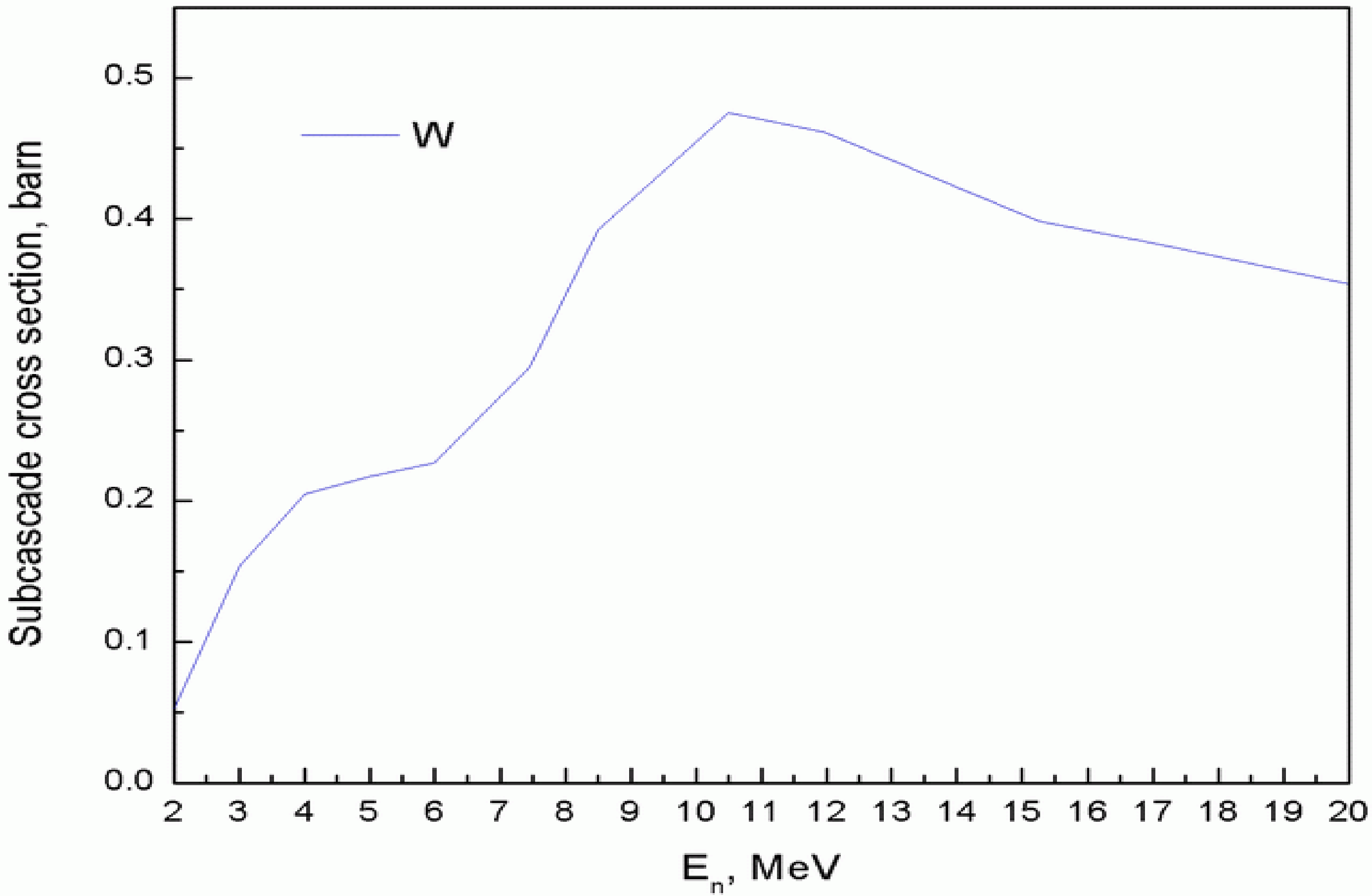
Cross Section of Sub-cascade Formation in Be as a Function of Neutron Energy



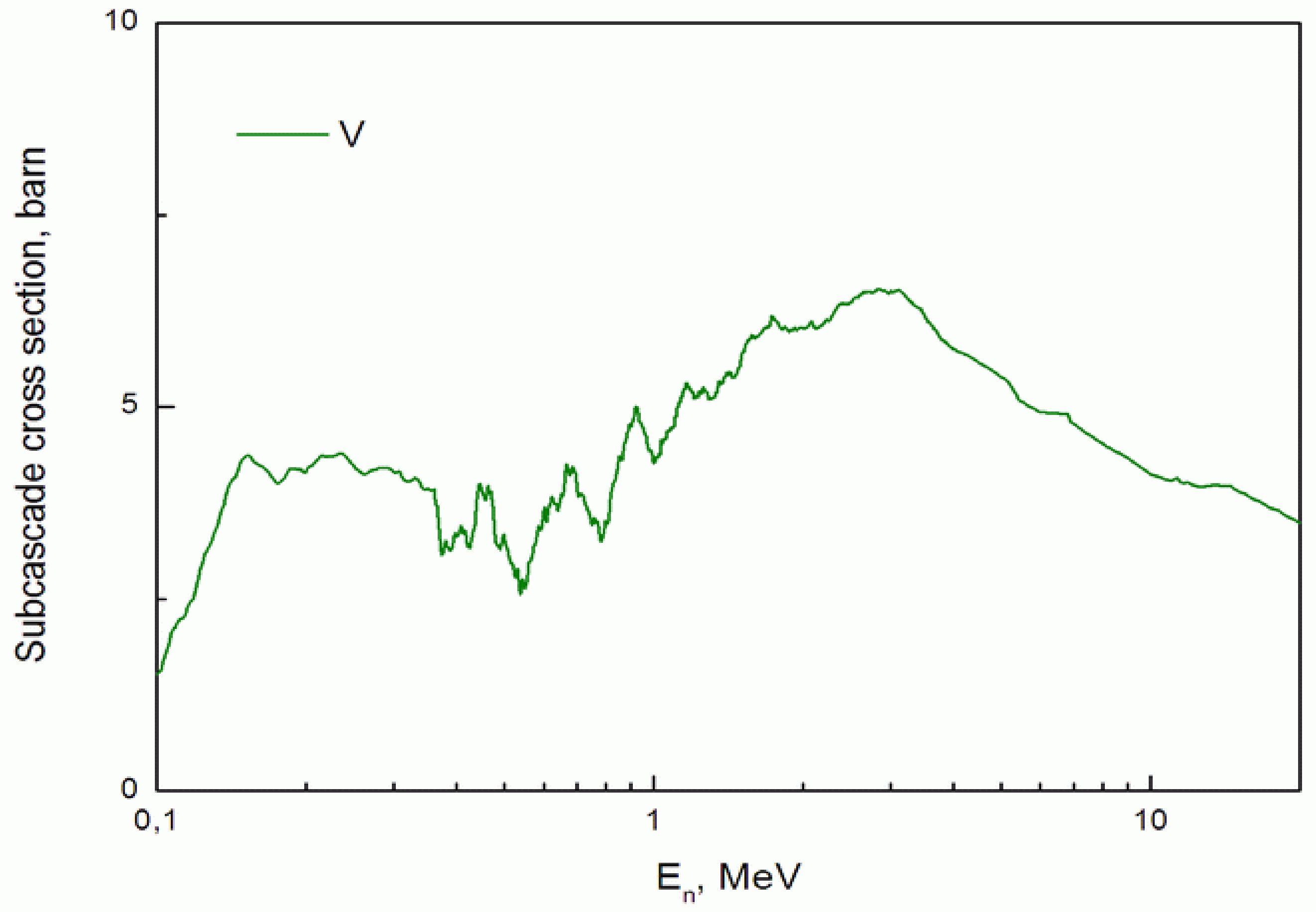
Cross Section of Sub-cascade Formation in Fe as a Function of Neutron Energy



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

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

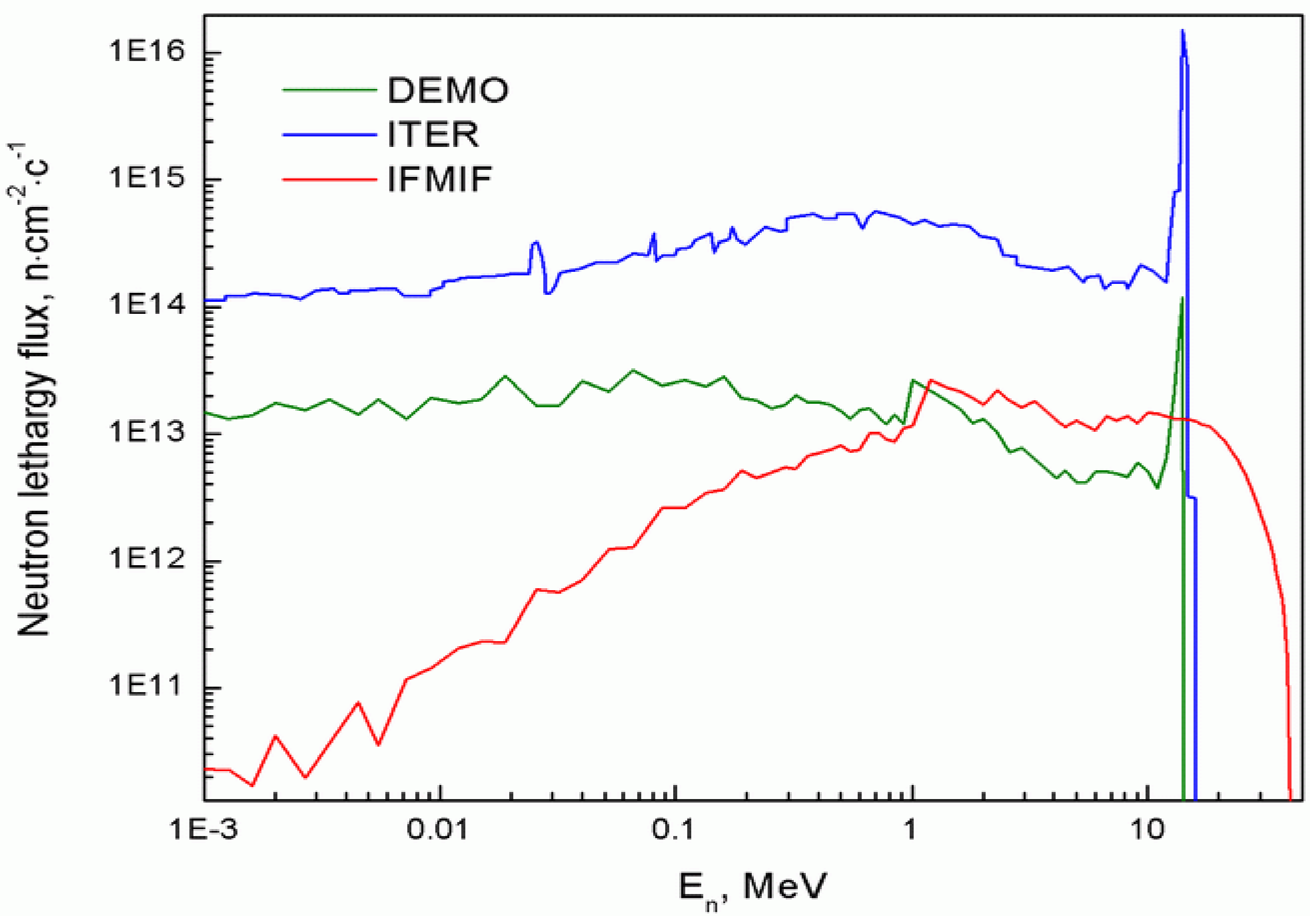
$G_{sf}(E_n)$ **- Generation rate of sub-cascade formation as a function of neutron energy *En***

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

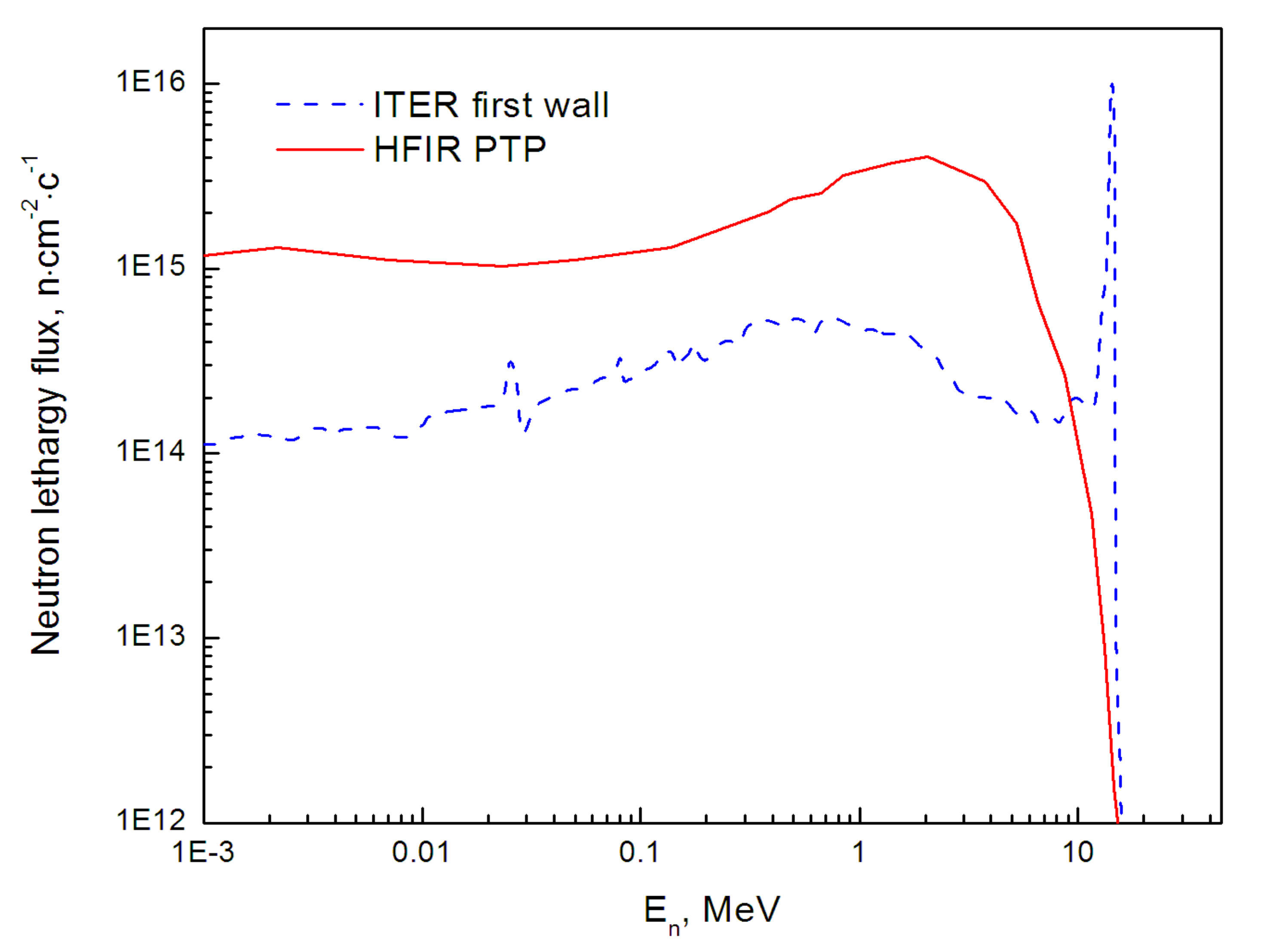
$\Phi(E_n^{/})$ **- Energy flux of fast neutrons in differential fusion facilities**

E_{sf} **- Sub-cascade formation energy**

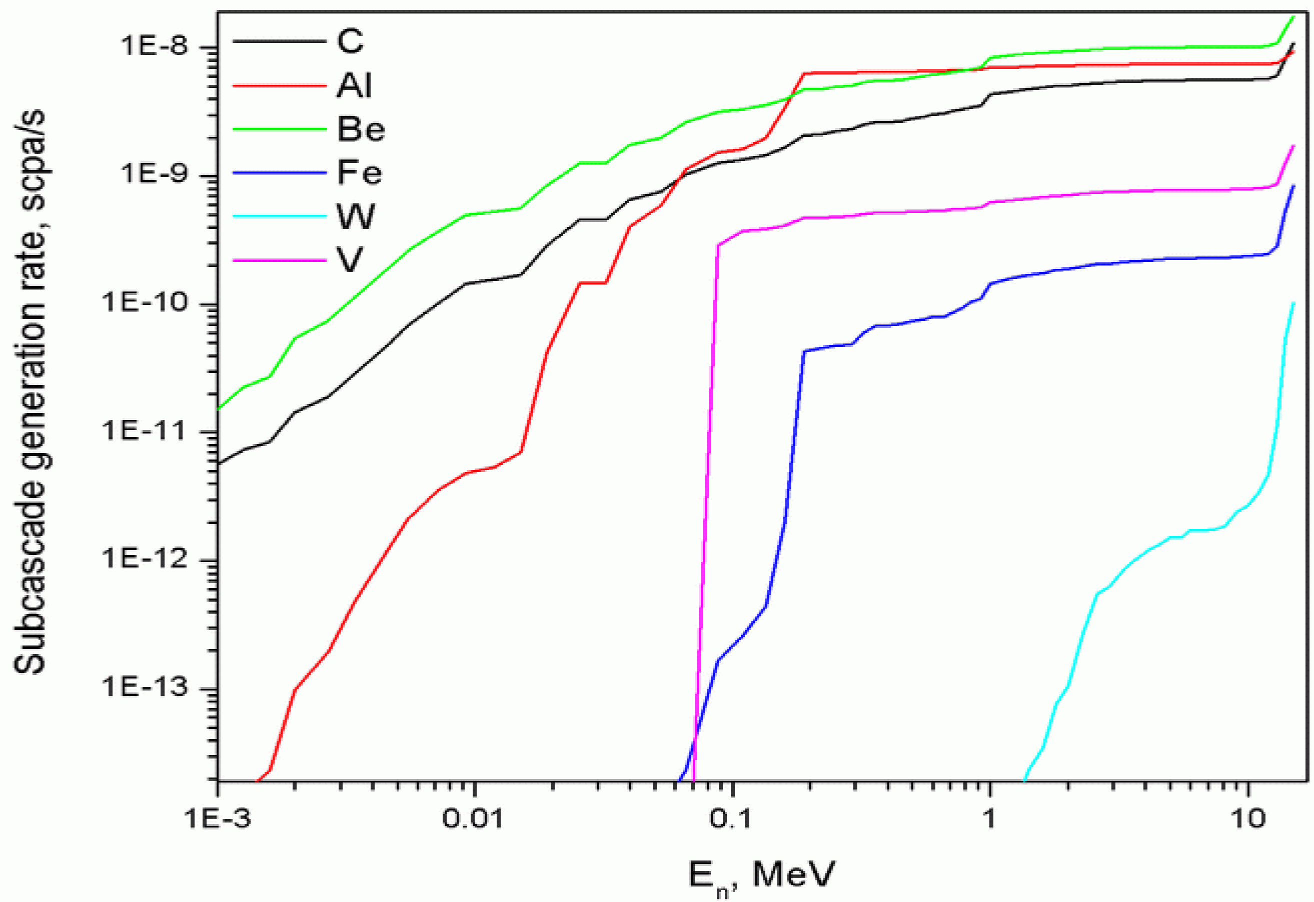
Neutron Energy Fluxes for different Fast Neutron Facilities



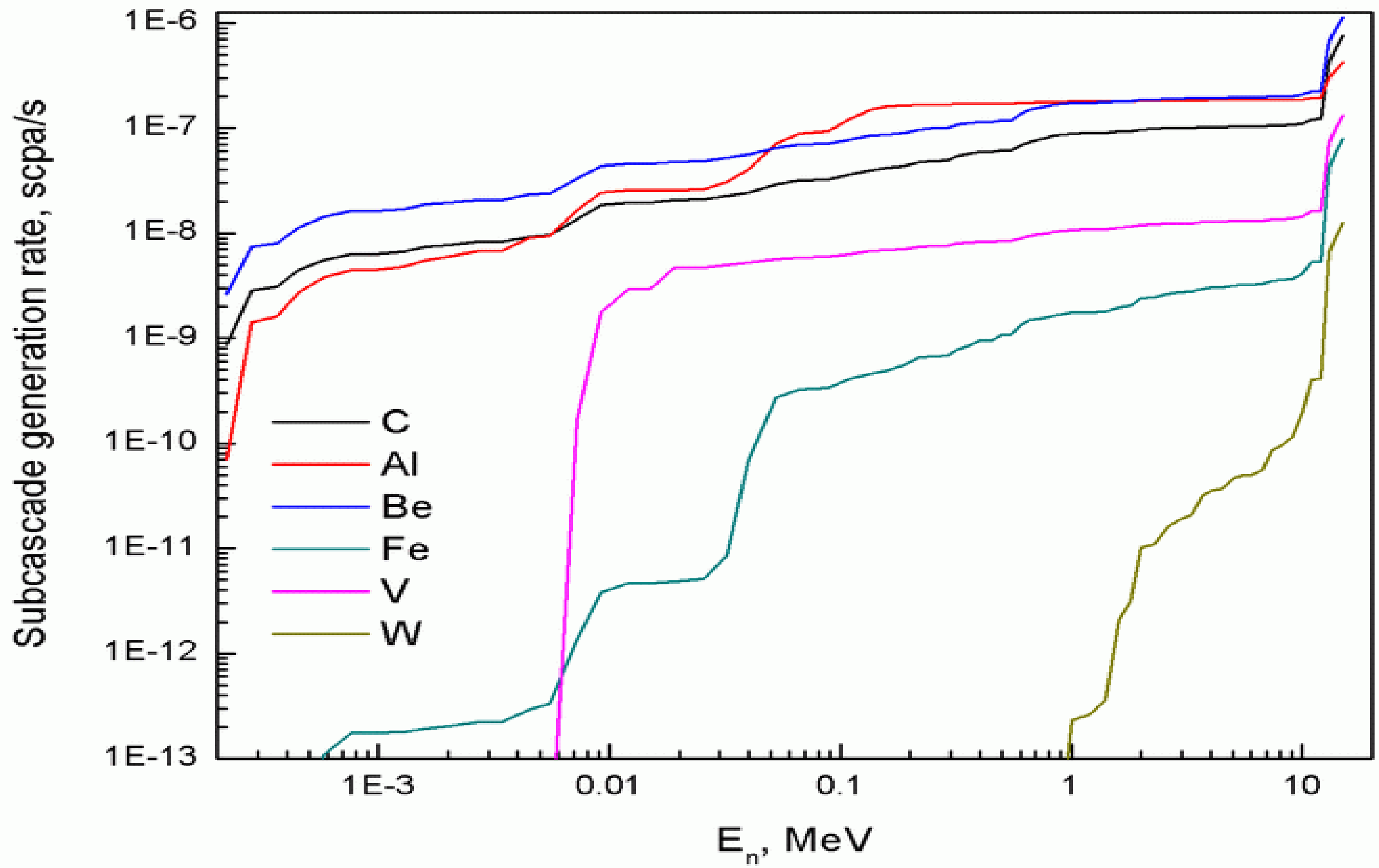
Neutron Energy Fluxes for different Fast Neutron Facilities (HRIR, ITER)



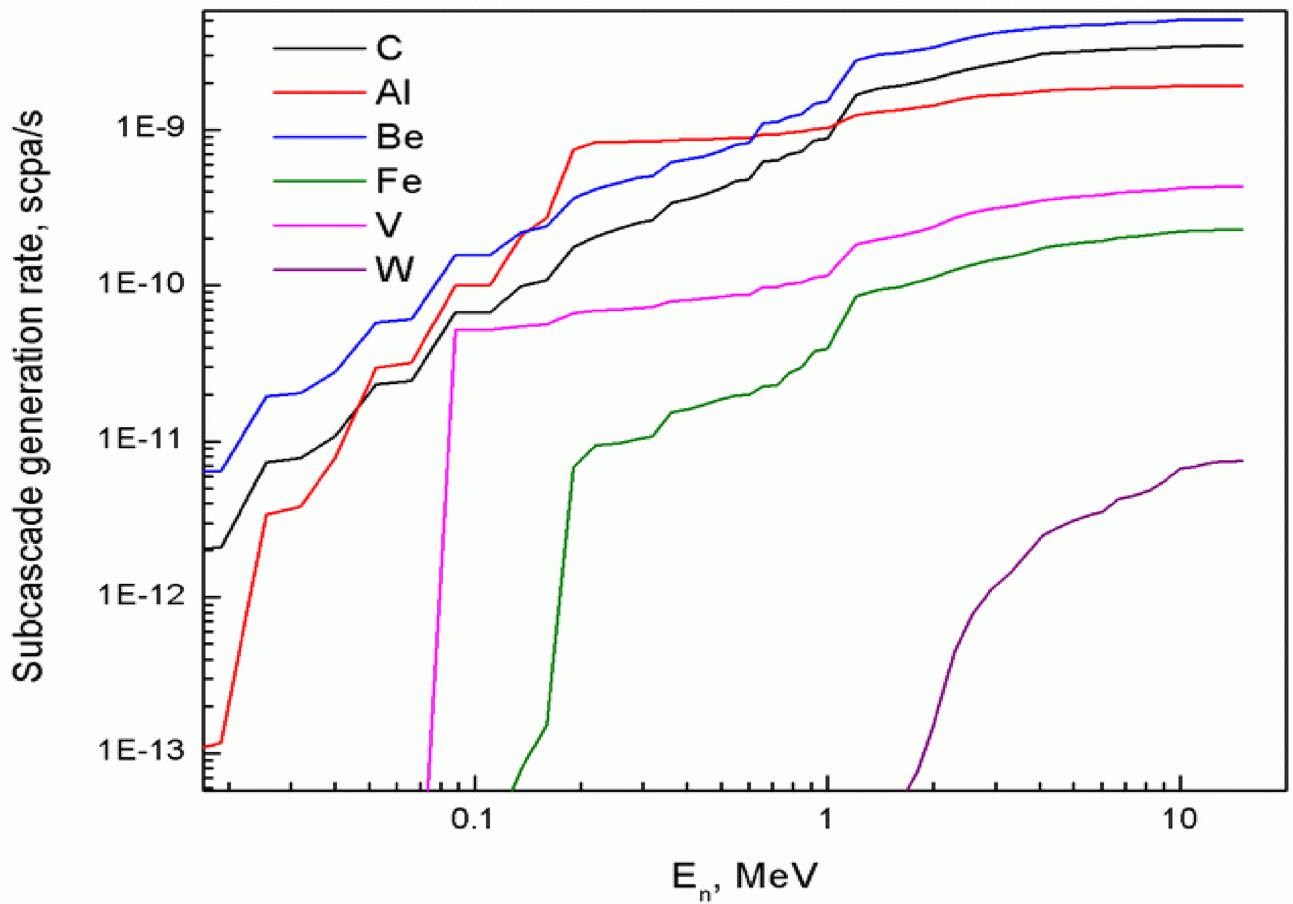
Sub-cascade Generation Rate in different Materials under Neutron Irradiation in DEMO



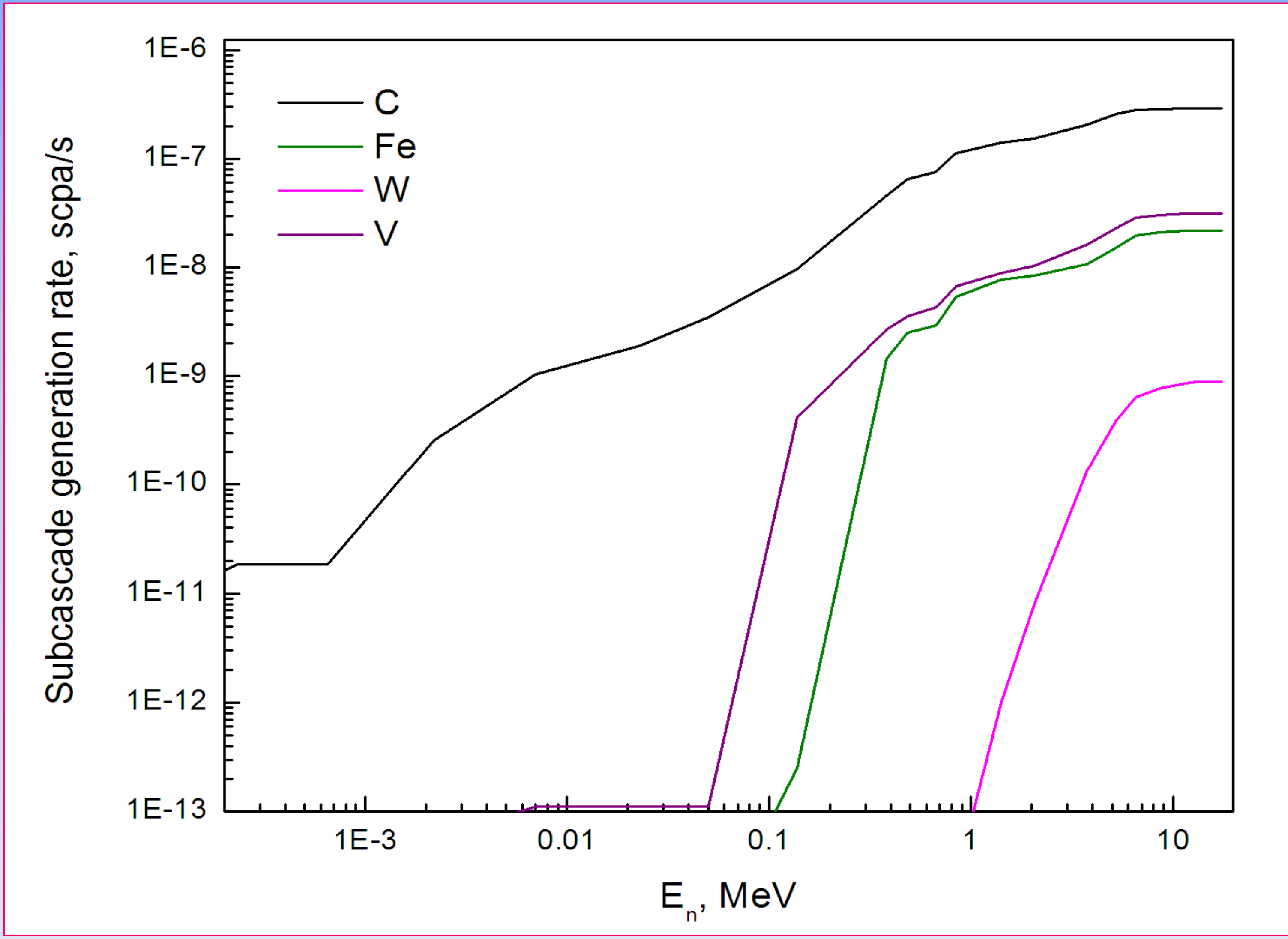
Sub-cascade Generation Rate in different Materials under Neutron Irradiation in ITER



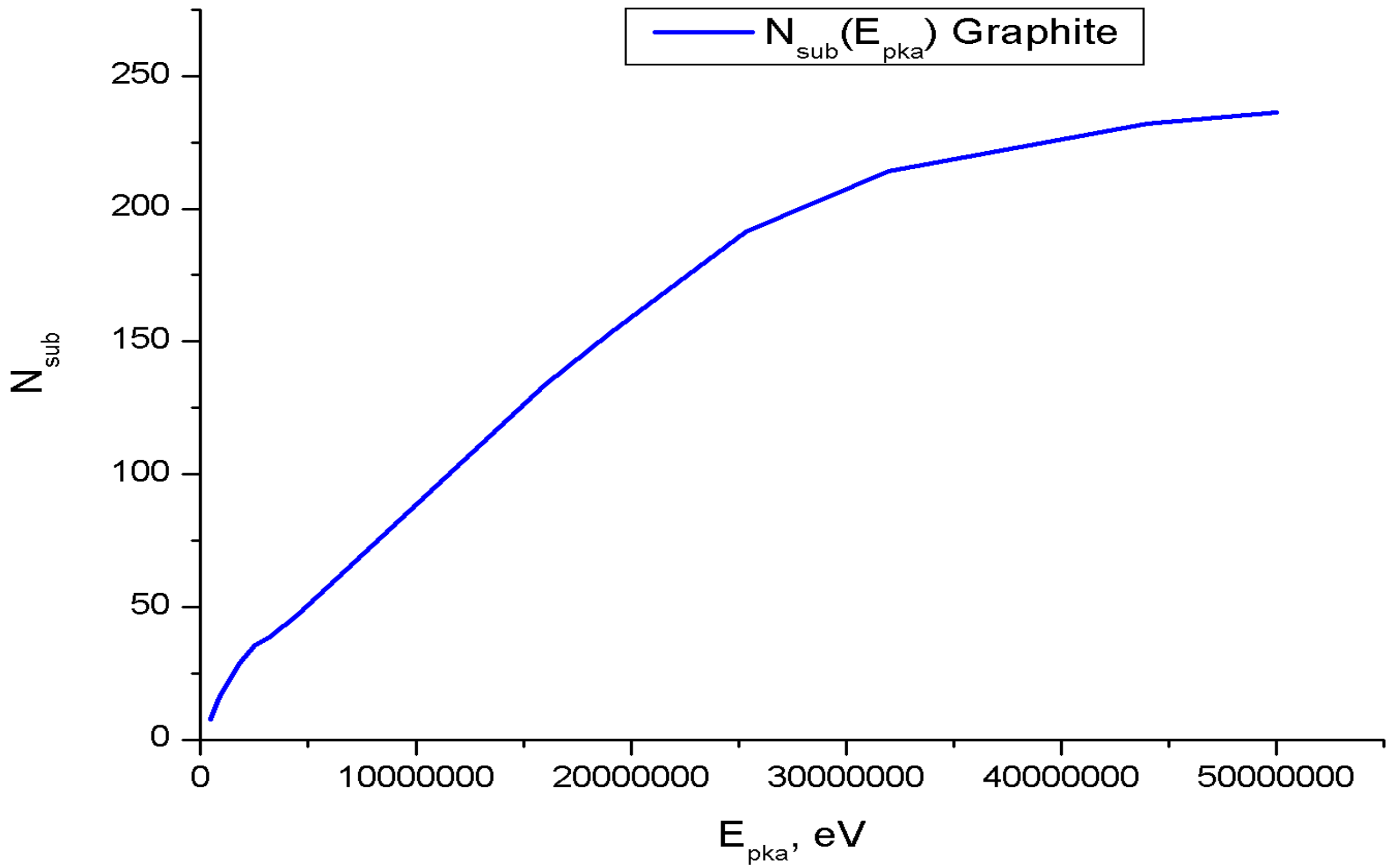
Sub-cascade Generation Rate in different Materials under Neutron Irradiation in IFMIF



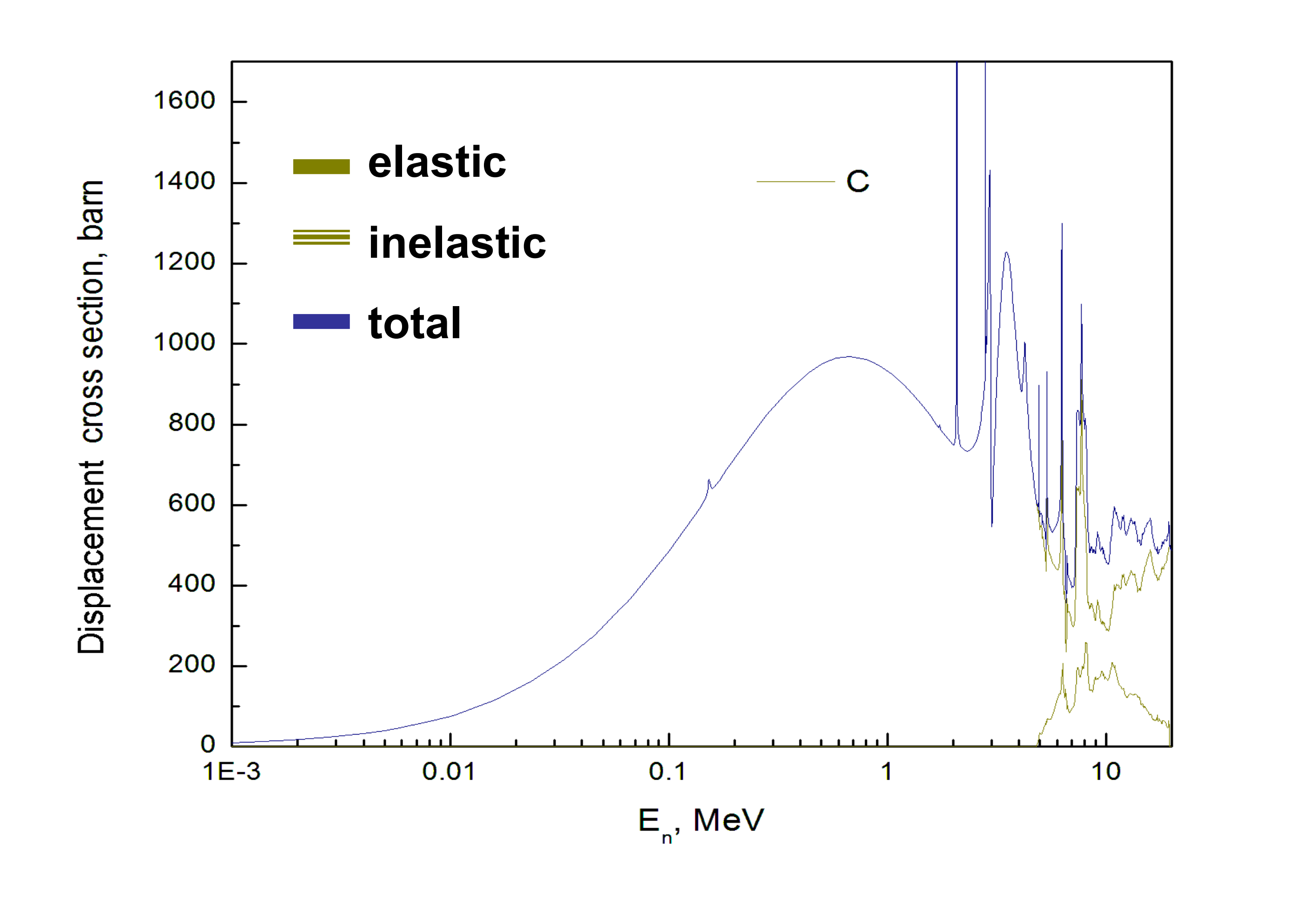
Sub-cascade Generation Rate in different Materials under Neutron Irradiation in HFIR



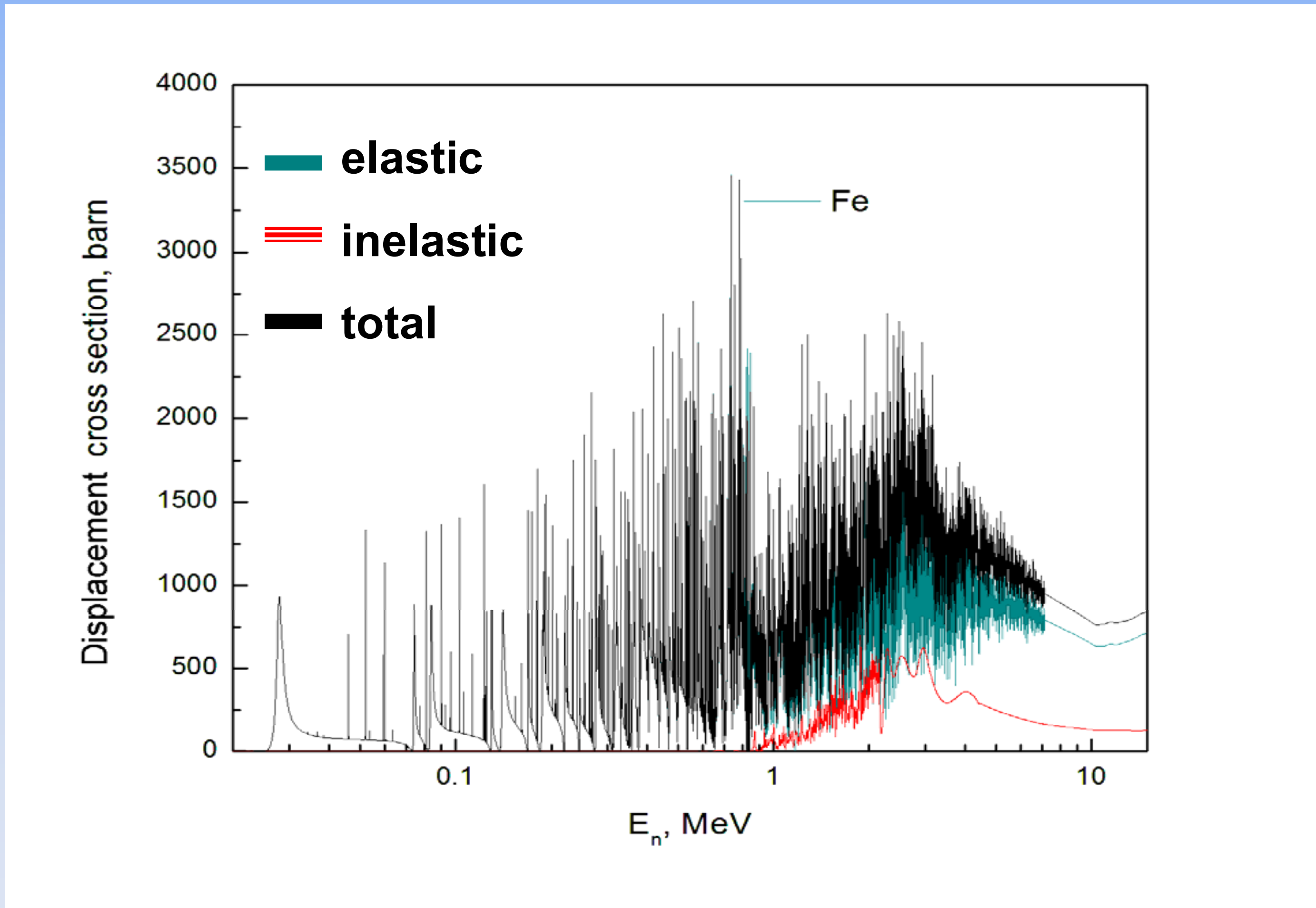
Number of Sub-cascades in C as a Function of PKA Energy



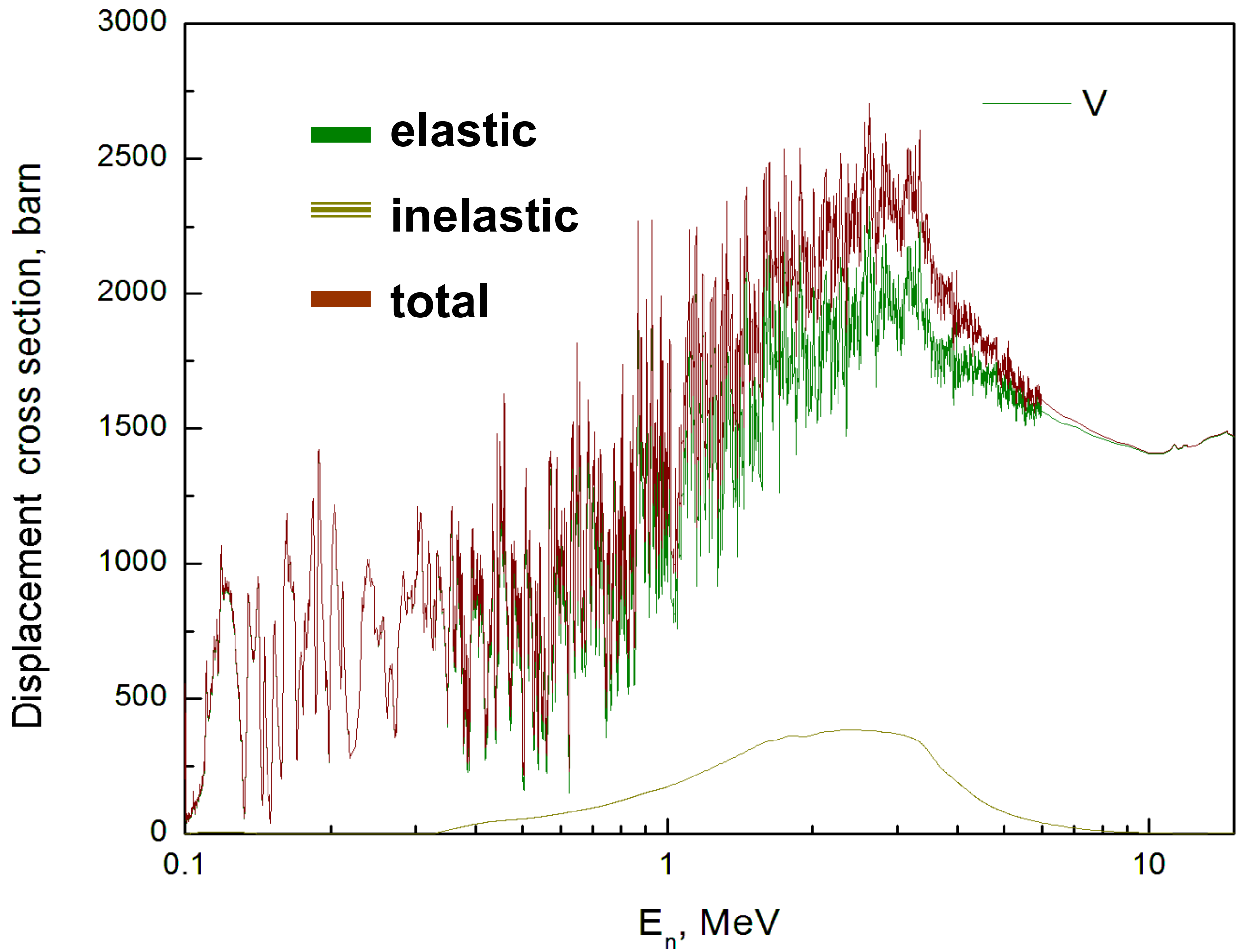
Cross Section of Point Defect Formation in C as a Function of Neutron Energy



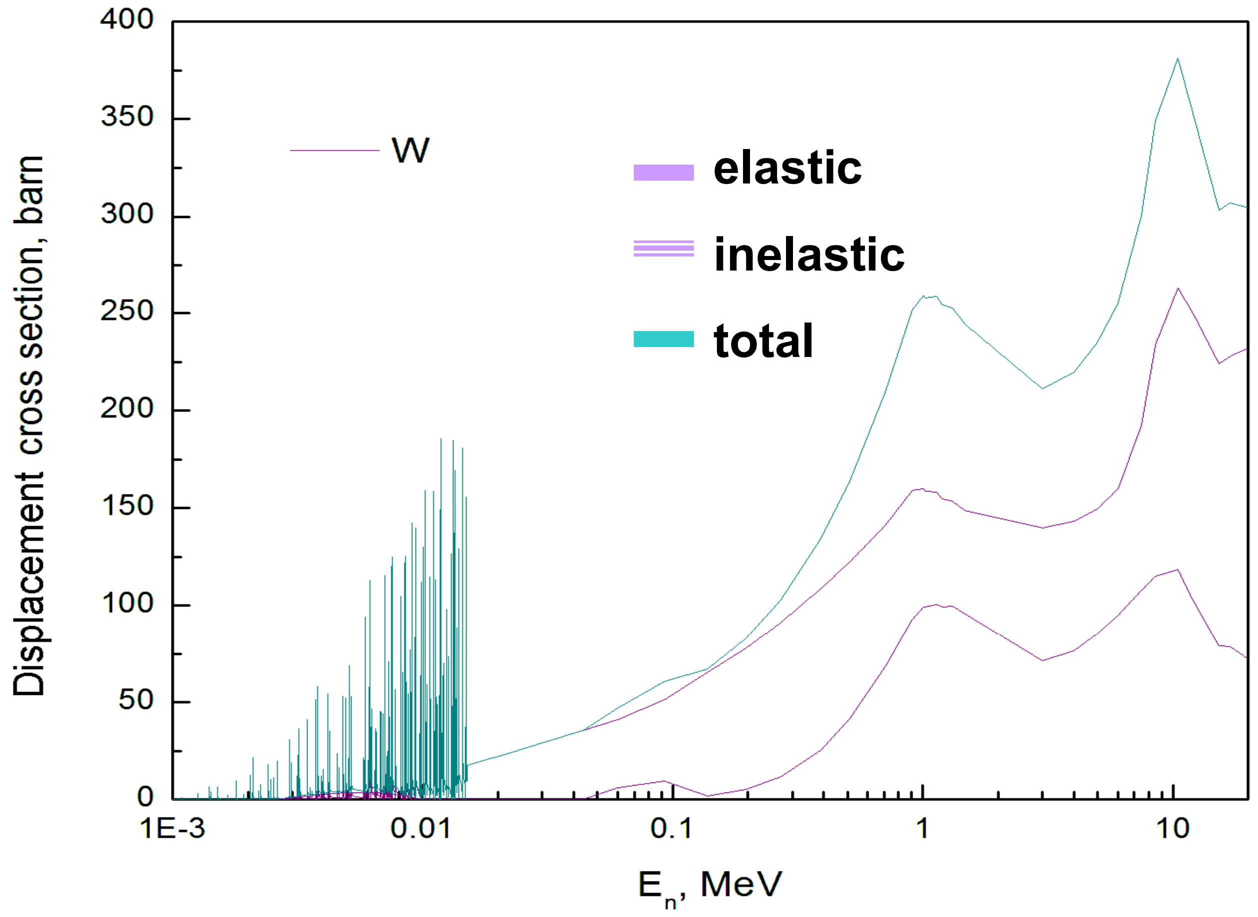
Cross Section of Point Defect Formation in Fe as a Function of Neutron Energy



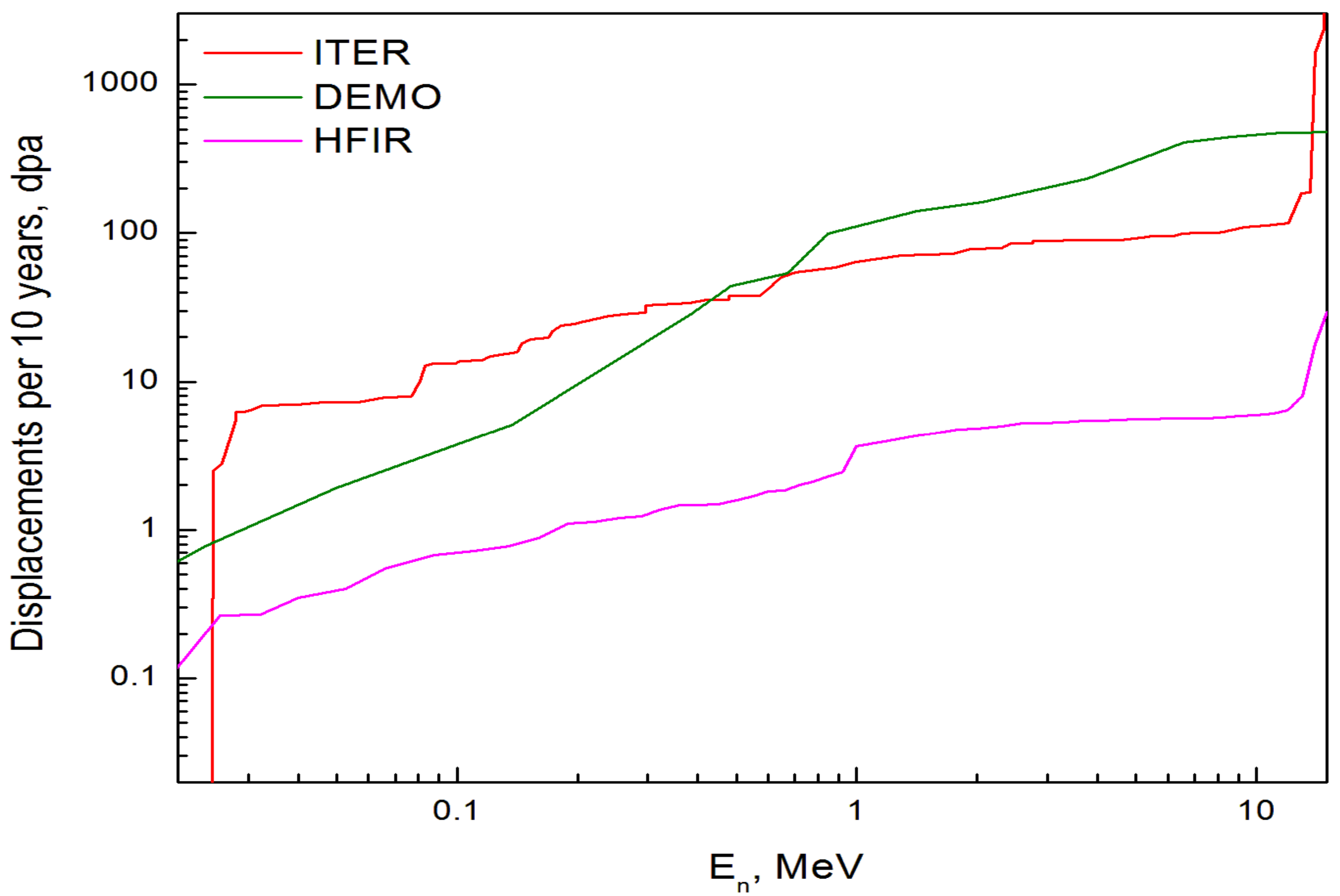
Cross Section of Point Defect Formation in V as a Function of Neutron Energy



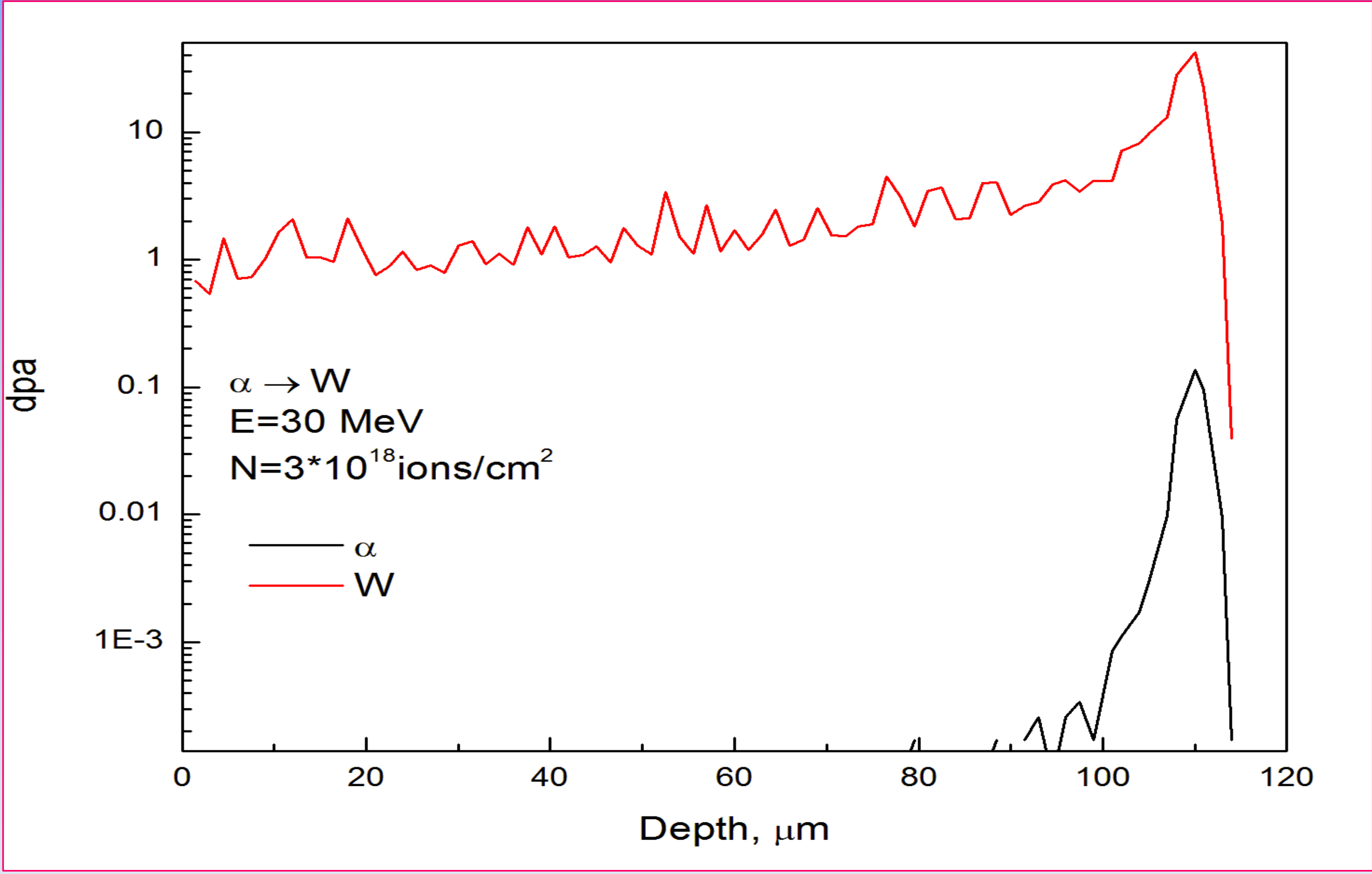
Cross Section of Point Defect Formation in W as a Function of Neutron Energy



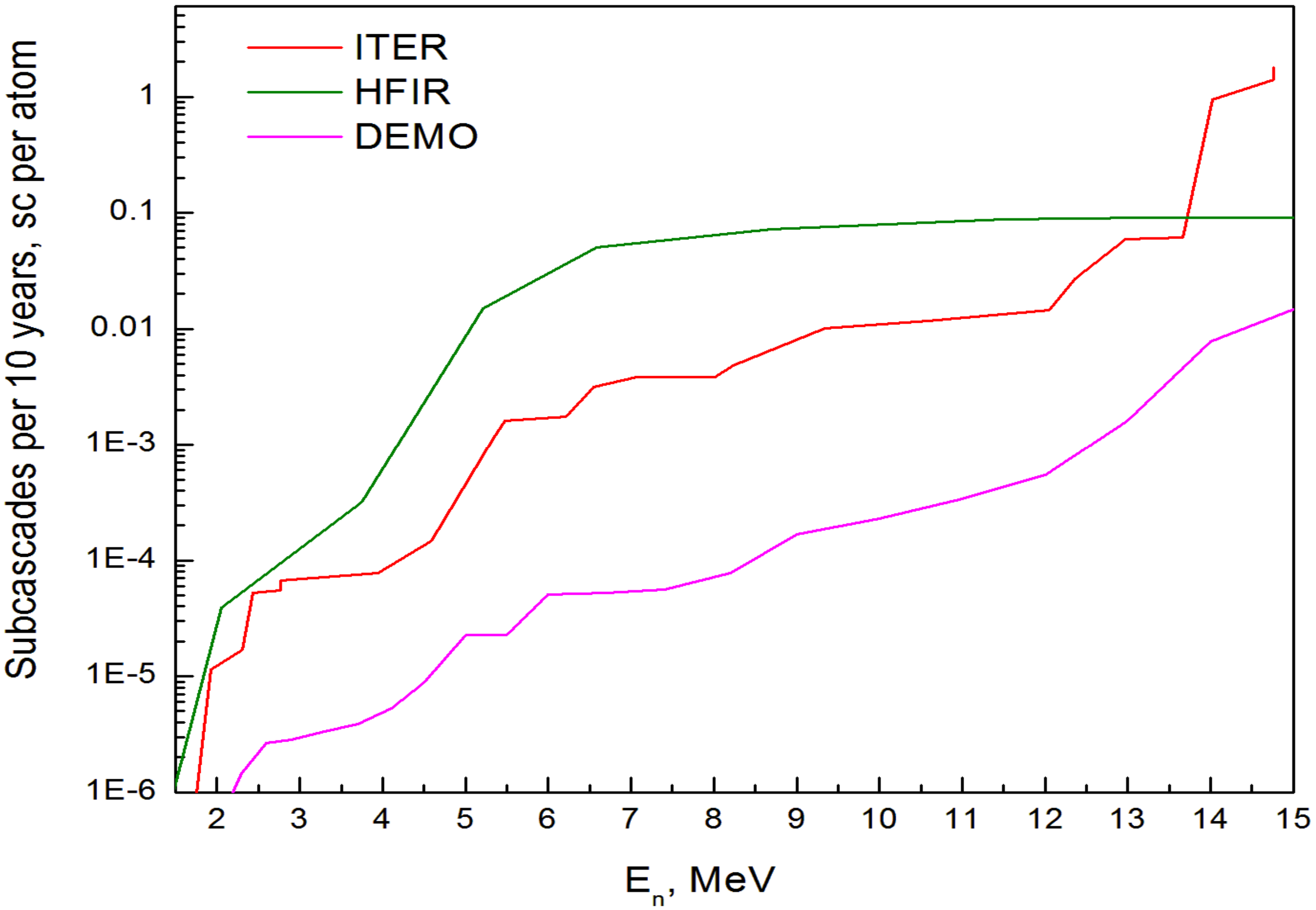
Accumulation of dpa level in W in different types of reactors: ITER,DEMO,HFIR during 10 years



Accumulation of dpa level in W under α-particle irradiation with the energy 30 MeV



Accumulation of subcascades in W in different types of reactors: ITER,DEMO,HFIR during 10 years

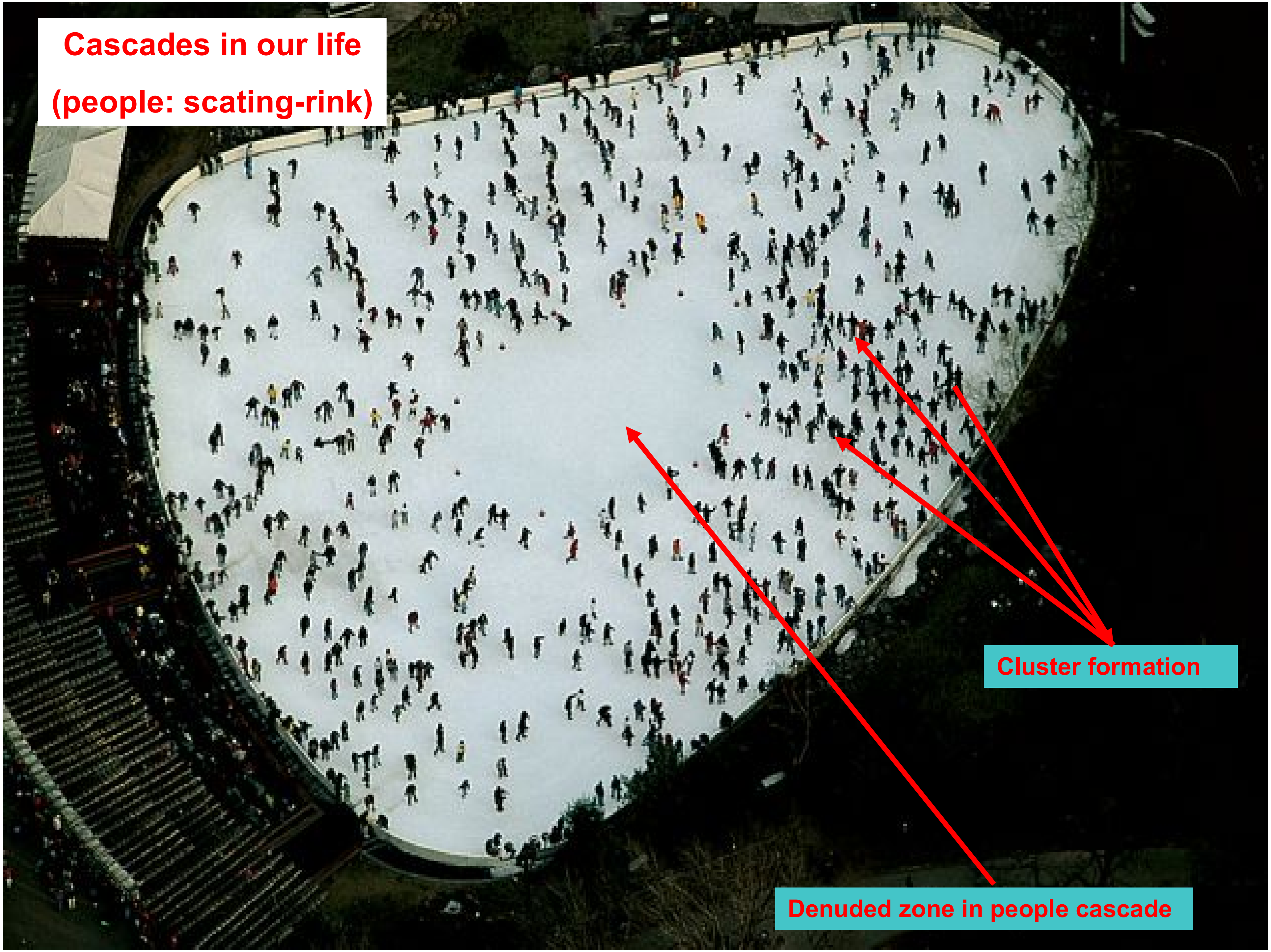


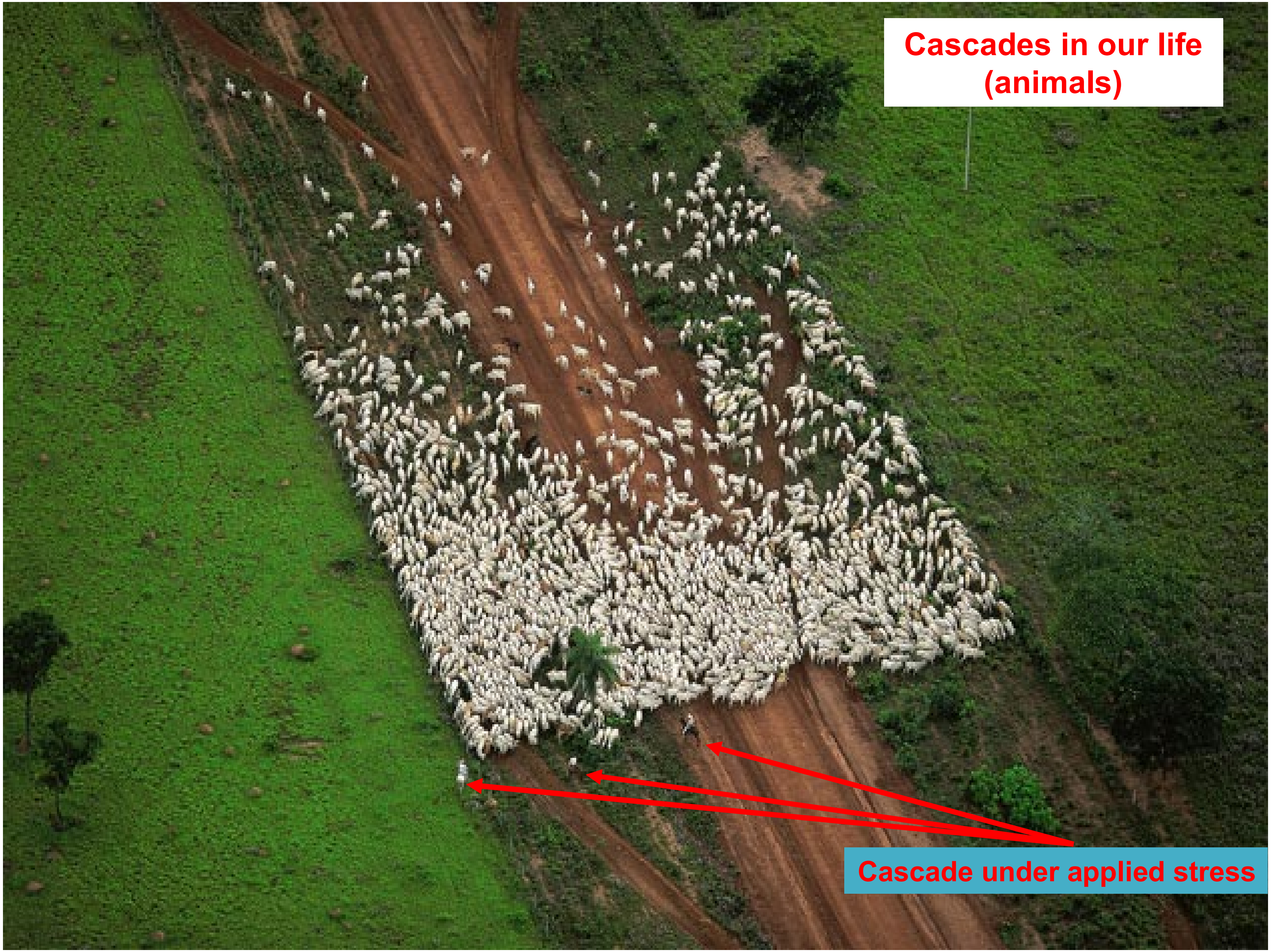
Summary

- Theoretical models and computer tools were developed for the investigations of radiation damage formation: cascades and sub-cascades in the fusion structural materials: C, V, Be, Fe, Al, W.

- Developed models allow to calculate the cascade and sub-cascade formation in fission and fusion structural materials taking into account electronic excitation, energy loss, elastic and inelastic collisions of fast neutrons with atoms of these materials using ENDF-B IV code.

- Numerical calculations have been made to determine generation rates of cascades and sub-cascades under fast ion irradiation for carbon and tungsten materials.


Cascades in our life
(people: scating-rink)
Cluster formation
Denuded zone in people cascade


Cascades in our life
(animals)
Cascade under applied stress

Thank you for your attention!