Karlsruhe Institute of Technology

DPA and gas production in intermediate and high energy particle interactions with accelerator components

A.Yu. Konobeev, U.Fischer

Karlsruhe Institute of Technology

Objectives

- Overview of recent developments in modeling of primary radiation damage relevant to dpa rate calculations
- Discussion of problems and perspectives of advanced radiation damage and gas production rate calculations at intermediate and high energies of primary particles

Radiation damage rate

$$K_d = \sum_p \int \sigma_d^{(p)}(E)\varphi^{(p)}(E)dE$$

Atomic displacement cross-section

$$\sigma_d^{(p)}(E_p) = \sum_r \int_{E_d}^{T_i^{max}} \frac{d\sigma^{(p)}(E_p, Z_T, A_T, Z_r, A_r)}{dT_r} N_D(T_r, Z_T, A_T, Z_r, A_r)dT_r$$

$N_D(T_r,Z_T,A_T,Z_i,A_r)dT_r$: number of stable defects produced

$d\sigma(E_p,Z_T,A_T, Z_r, A_r)/dT$: recoil energy distribution

Nuclear physics + solid state physics

Experimental data relevant to dpa calculations

Large data sets, compilations, measurements at high energies

Quantity	Projectile	Energy	Target	Reference
Displacement cross-section	p, d, ^{4}He, (electrons)	0.0005 to 20 MeV, (0.2 to 4 MeV)	Al, V, Fe, SS, Ni, Cu, Nb, Mo, Pd, Ag, Ta, W, Pt, Au	P. Jung, *J. Nucl. Mater. 117, 70 (1983)*
$\langle K_d \rangle$, $\langle \xi \rangle$	neutrons	reactor spectra	Mg, Al, K, Ti, V, Fe, SS, Co, Ni, Cu, Zn, Ga, Zr, Nb, Mo, Pd, Ag, Cd, Sn, Ta, W, Re, Pt, Au, Pb	C.H.M. Broeders et al, *J. Nucl. Mater. 328, 197 (2004)*

Quantity	Projectile	Energy	Target	Reference
Displacement cross-section	O, Ar, Kr, Xe, Pb, U	0.096 to 4.68 GeV	Fe (Ed = 25 eV)	A. Dunlop et al, *Nucl. Instr. Meth. B90, 330 (1994)*
Displacement cross-section	protons	1.1, 1.94 GeV	Cu, W	G.A. Greene et al, *AccApp ('03)*

R.S. Averback et al, *J. Nucl. Mater. 113, 211 (1983)*
S.J. Zinkle et al, *J. Nucl. Mater. 199, 173 (1993)*
K. Nordlund et al, *OECD (2013)*

Quantity: Defect production efficiency
Energy of ion: up to 50 keV
Target: Al, Fe, Ni, Cu

NRT: reference model

M.J.Norgett, M.T.Robinson, I.M.Torrens, *Nucl. Eng. Des.* 33, 50 (1975)

$$N_{NRT}(T) = \frac{0.8}{2E_d} T_{dam},$$

$$T_{dam}(T) = \frac{T}{1 + k(Z_{PKA}, A_{PKA}) g(Z_{PKA}, A_{PKA}, Z_T, A_T)}$$

Implemented in codes: Robinson formula

$$T_{dam}(T) = \frac{T}{1 + k(Z_{PKA}, A_{PKA}, Z_T, A_T) g(Z_{PKA}, A_{PKA}, Z_T, A_T)}$$

Internal limitations: monatomic materials, $E_{max} < 25\ Z_{PKA}^{4/3} A_{PKA}$ keV

Example. Fe+Fe: $E_{max} \approx 108$ MeV

Fe+Fe, E_{PKA}= 200 keV, E_d= 40 eV

NRT	NJOY code	MCNPX code	SRIM code
1100	1100	1100	1200

Al+Fe, E_{PKA}= 200 keV, E_d= 40 eV

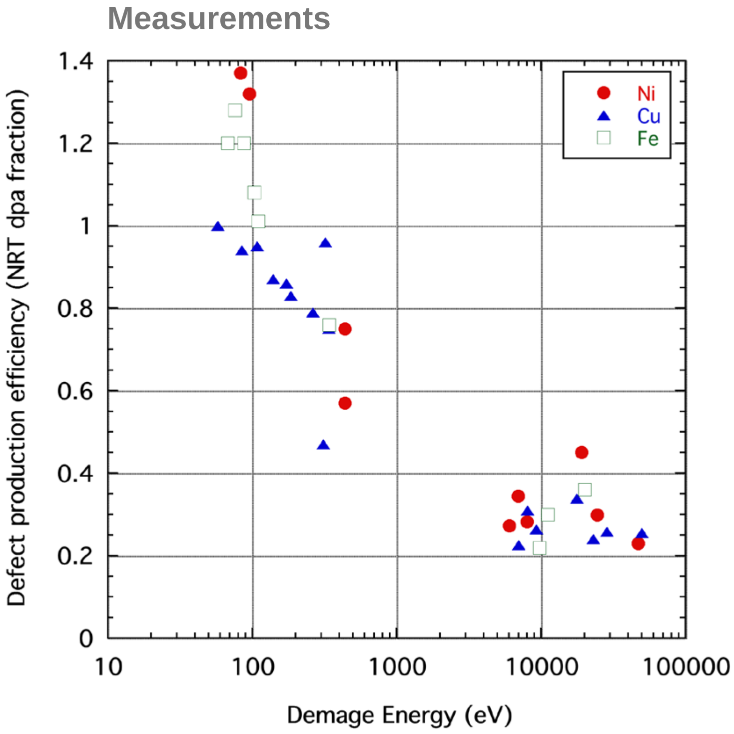
NRT	NJOY code	MCNPX code	SRIM code
900	690	760	920

Be+Fe, E_{PKA}= 200 keV, E_d= 40 eV

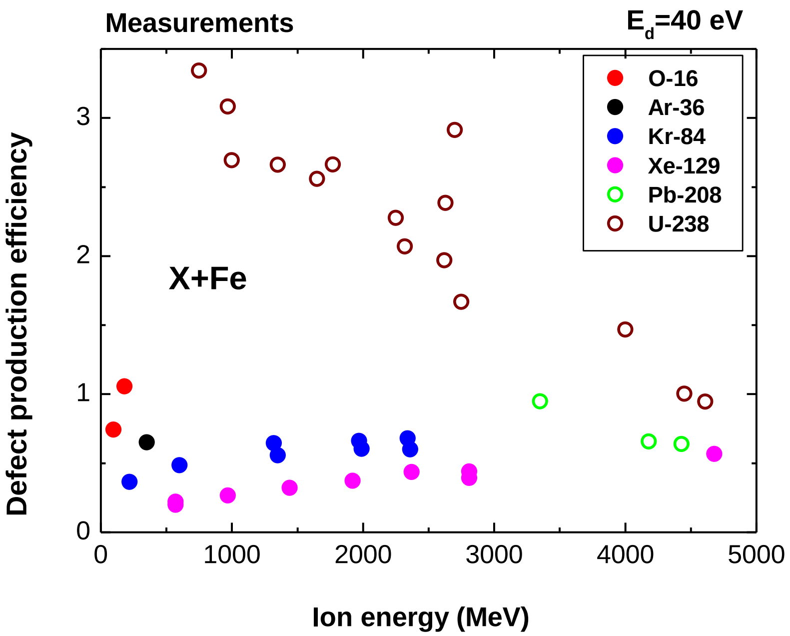
NRT	NJOY code	MCNPX code	SRIM code
530	170	220	240

Defect production efficiency

$$\xi(T) = \frac{N_D}{N_{NRT}}$$

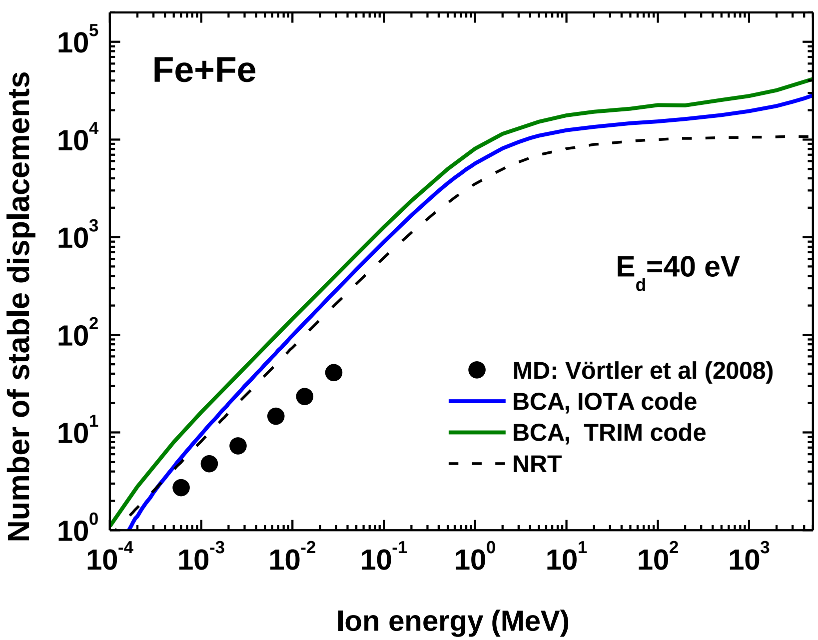


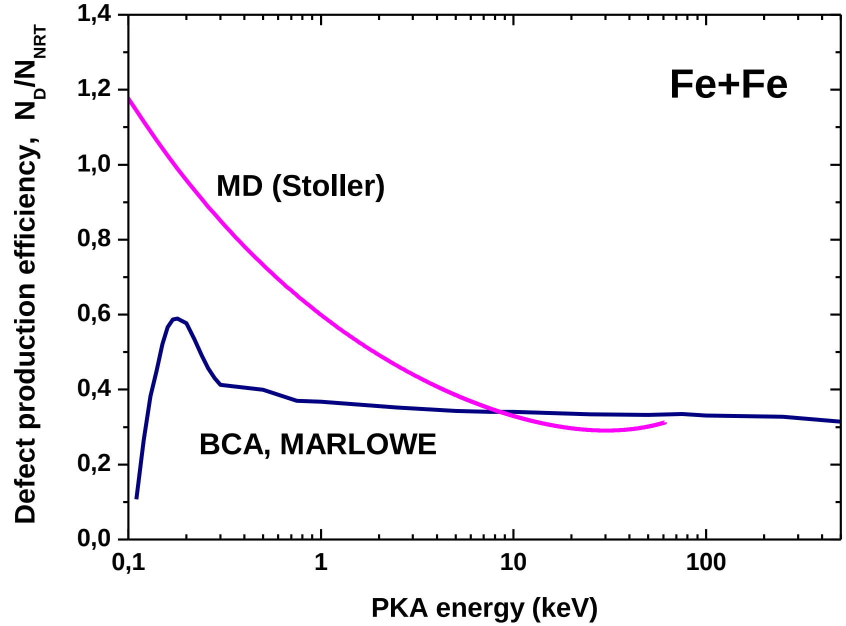
K.Nordlund et al, OECD (2013)



A.Dunlop et al, (1994)

BCA model: fast, but not always reliable





R.E.Stoller et al, *Nucl. Instr. Meth. Phys Res.* B310, 75 (2013)
"On the use of SRIM for computing radiation damage exposure"

MD: most realistic simulation

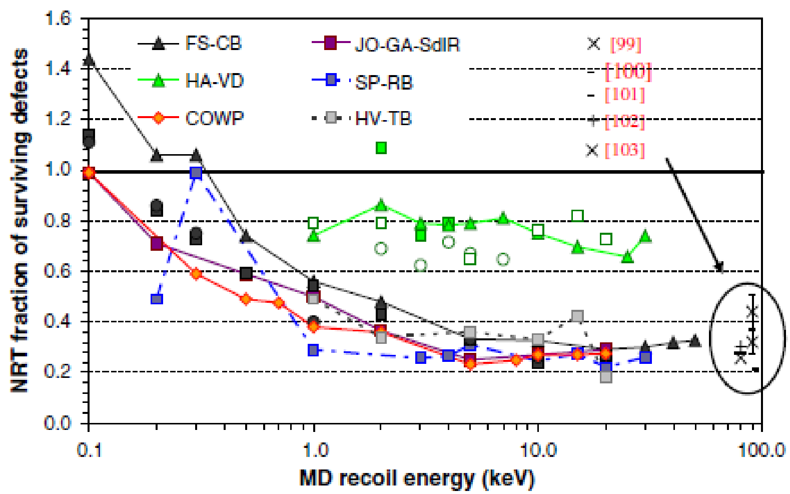
Electronic stopping: treated implicitly

- friction forces
- $E_{MD} \approx T_{dam}$ or $T_{PKA} \approx E_{MD} + E_{el}$

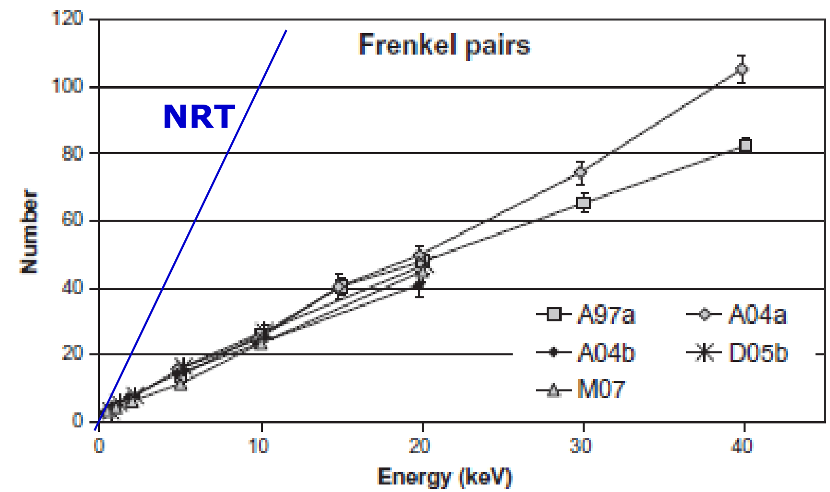
Brief discussion: C.P. Race at al, (2010); K.Nordlund, OECD (2013)

Interatomic potential

Fe+Fe



L. Malerba (2006)



L. Malerba et al (2010)

MD studies relevant to dpa rate calculations

Metals: Al, Ti, V, Fe, Ni, Cu, Zr, Mo, W, Pt, Au

Alloys: Fe-Cr, Fe-Cr-C, Ni_3Al, Ni-Fe, Cu-Au, U-Mo

Semiconductors: Si, Ge, GaN

Carbides: SiC, Fe_3C, WC

Oxides: MgO, UO_2

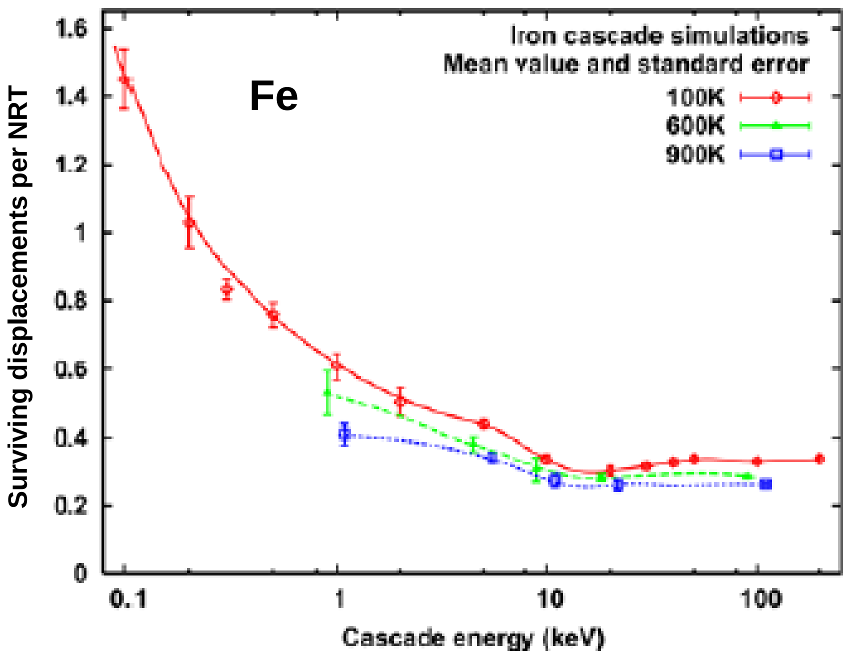
Spinel: $MgAl_2O_4$, $MgGa_2O_4$, $MgIn_2O_4$

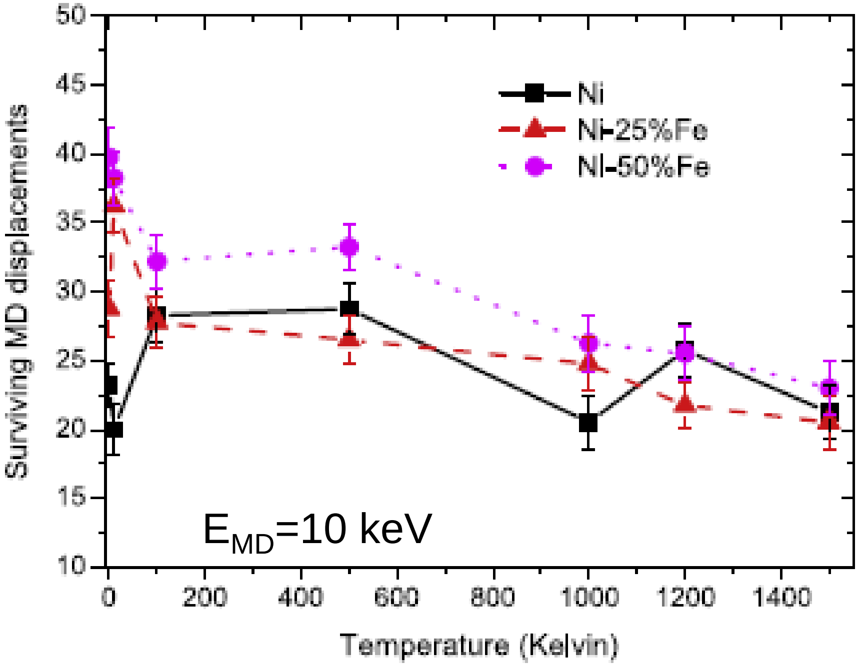
Zirconolite: $CaZrTi_2O_7$

Energy (E_{MD}): up to several tens of keV, Fe - 200 keV (Stoller)

Temperature: 0 – 1500 K

Temperature: definite, but modest influence on N_D value





R.E.Stoller, IAEA (2013)

C.Wang et al, NIMB 321, 49 (2014)

"Cascade energy", "E_{PKA}" in MD articles = $E_{MD} \approx T_{dam}$ (not PKA kinetic energy)

Recently proposed alternative to NRT formula

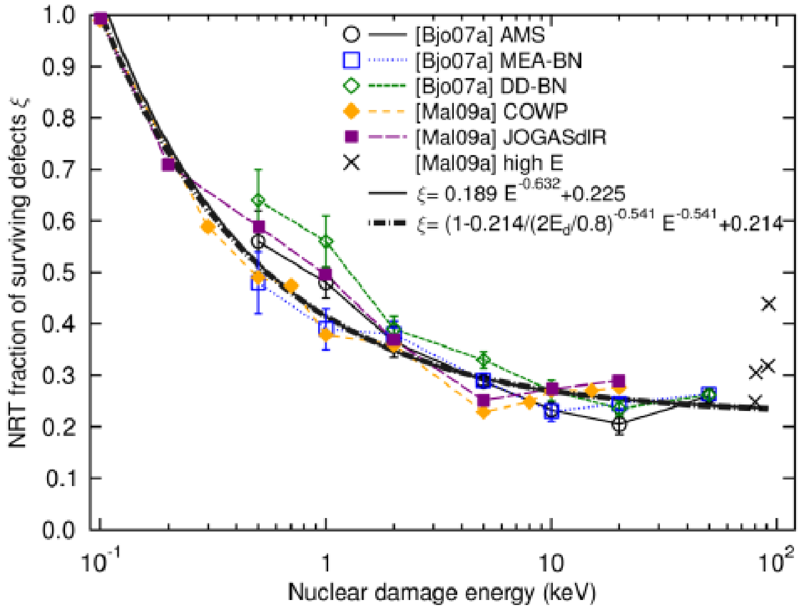
Generalizing the MD results

K.Nordlund, IAEA (2012)

"Athermal recombination corrected displacement damage (arc-dpa):"

$$\xi(E) = \frac{1-c}{(2E_d/0.8)^b} E^b + c$$

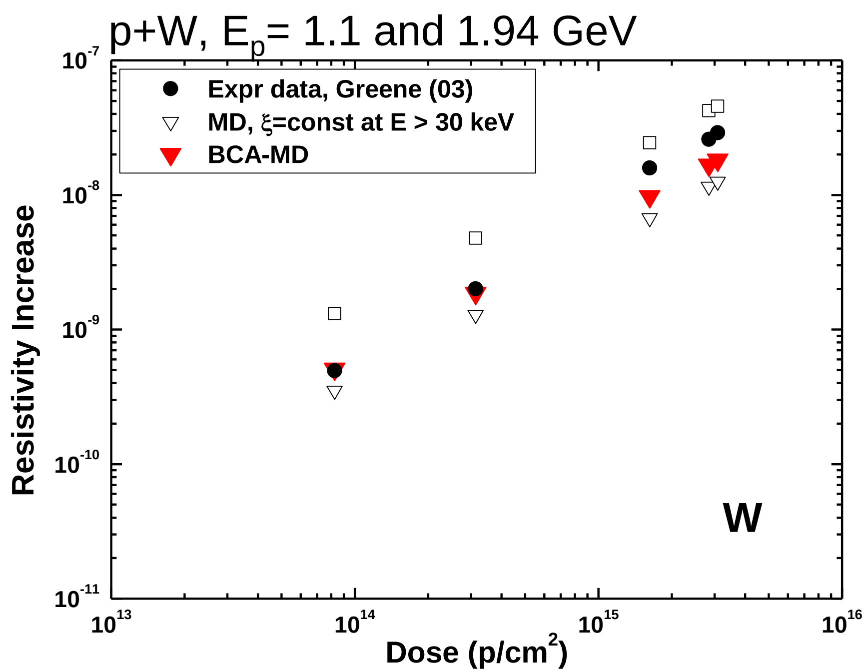
c and *b*: parameters

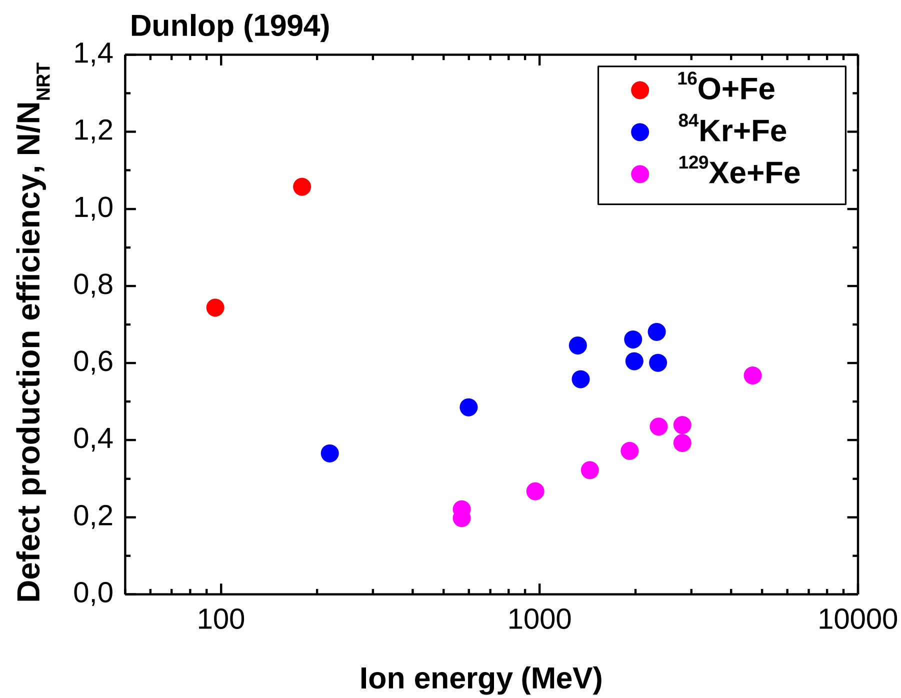


Extrapolation of MD results to higher energies

Simple solution: “constant efficiency” approximations

ξ = const at energies above 30-50 keV





Combined BCA–MD simulations

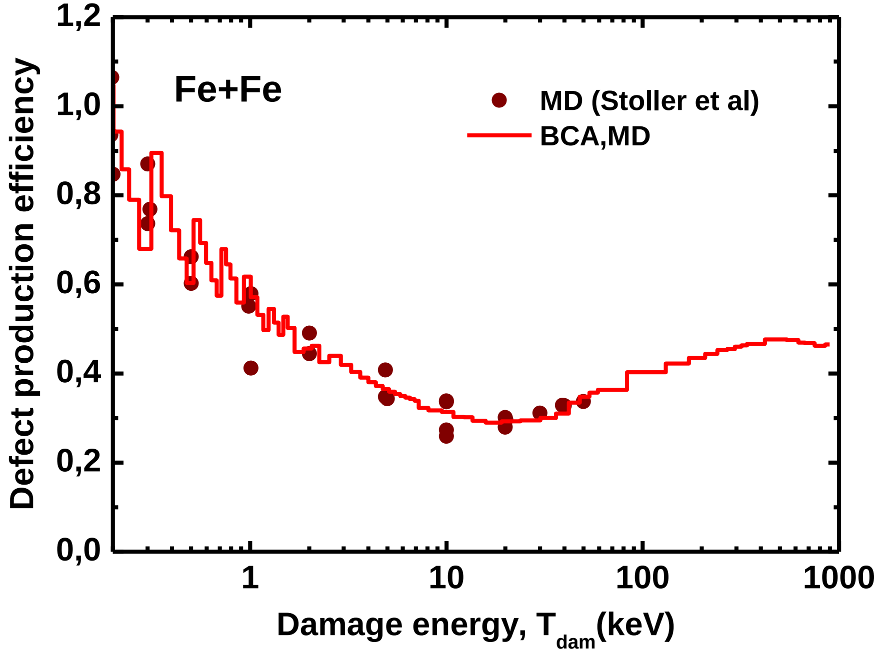
Karlsruhe Institute of Technology

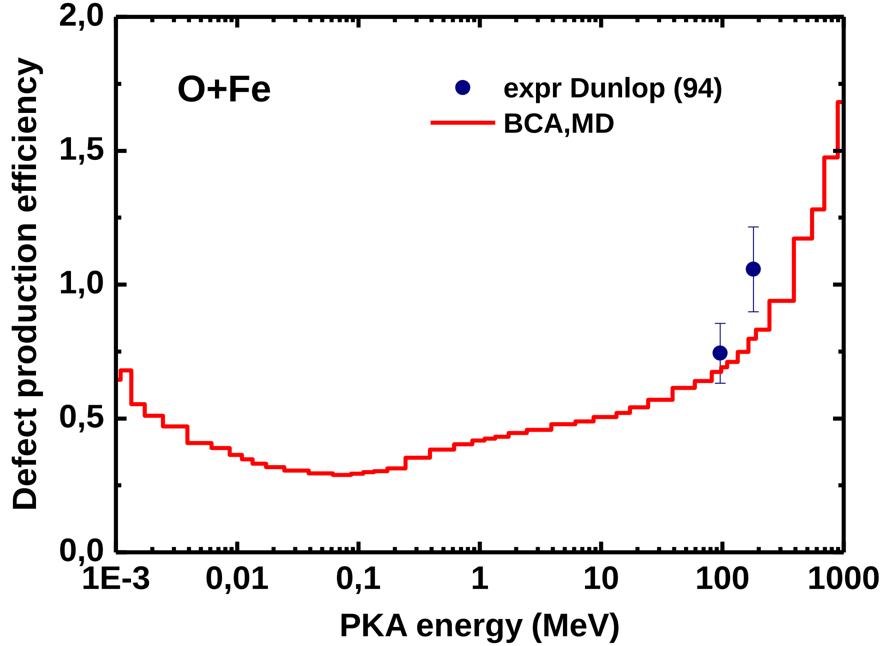
Moving ion: transition from BCA to MD at the certain "critical" kinetic energy ($T_{crit} \approx 30 - 60$ keV)

$T < T_{crit}$: MD (results)

$T > T_{crit}$: BCA

BCA-MD: IOTA code (KIT)





Kinetic Monte Carlo simulations

MD: up to nanoseconds

KMC: up to 10^4 s

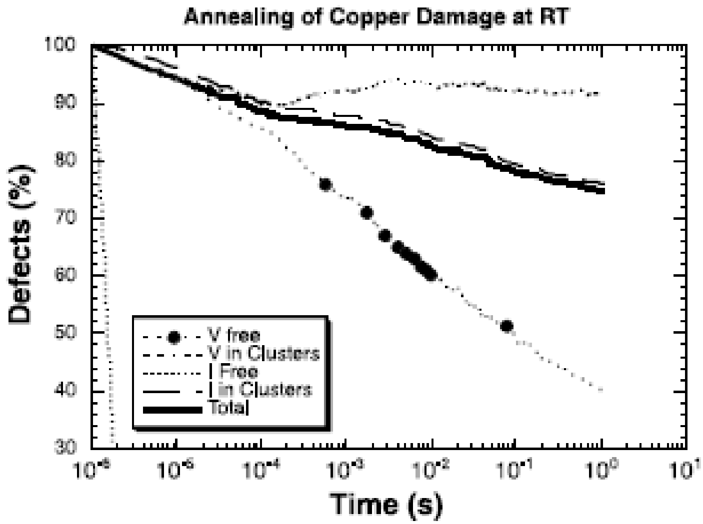
"Objects": Individual defects, clusters, impurities etc

Object KMC (OKMC) and event KMC (EKMC)

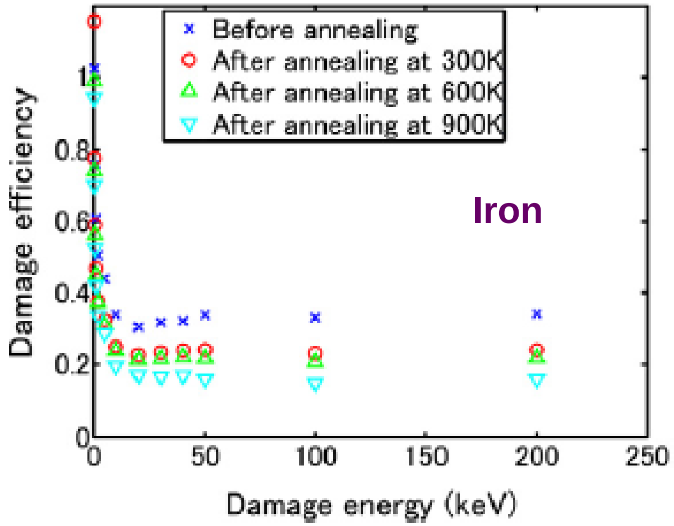
OKMC:

- atomic KMC (AKMC): explicit modeling
- "OKMC": no detailed treatment

C.S. Becquart, B.D.Wirth (2012)

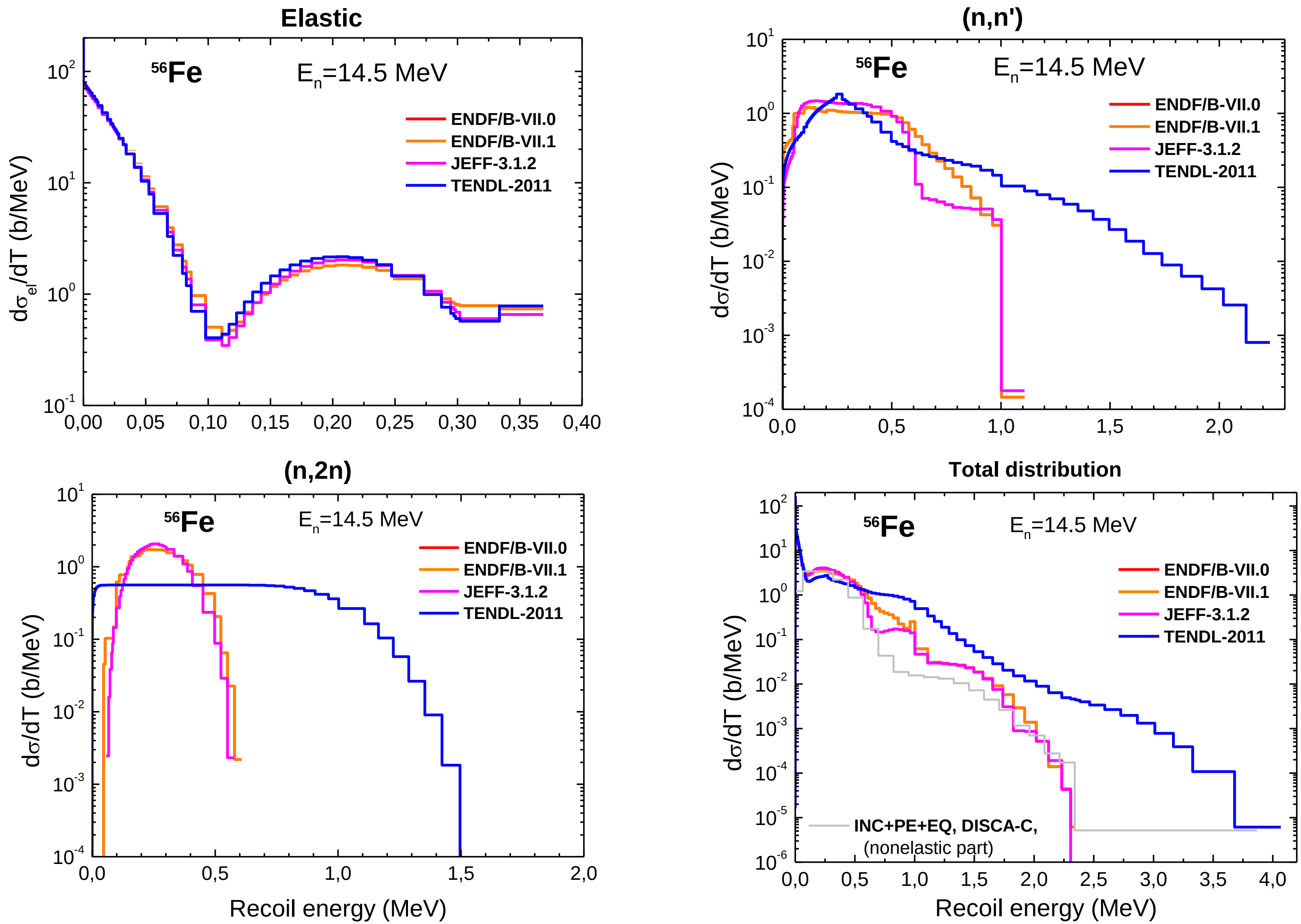


M.J.Caturla et al, (2001)

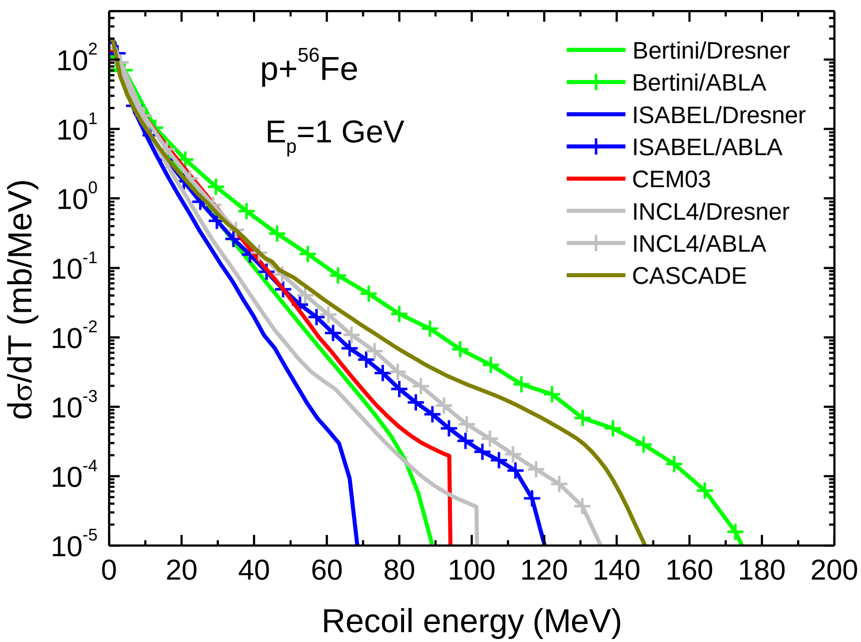


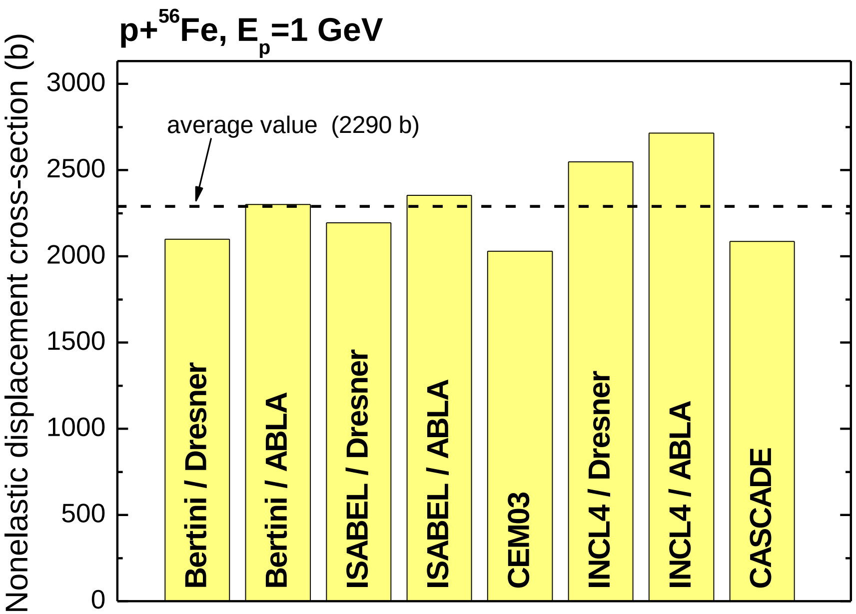
T.Suzudo et al, (2012)

Recoil energy distributions



Example of calculated recoil energy distribution





Evaluated displacement cross-section

$$\sigma_d(E) = \sum_{i=1}^{M} w_m \sigma_{d,m}(E) \left(\sum_{m=1}^{M} w_m \right)^{-1}$$

Improved dpa rate calculations using particle transport codes

1. Complete simulation
   - Nuclear interactions
   - Particle transport
   - Heavy ion transport: BCA+MD(+KMC)

Questionable

- Computer power
- Uncertainty of results (global IAP (?))
- No advantage over less time consuming methods (in most cases)

2. "Almost complete" simulation

- Nuclear interactions
- Particle transport
- Heavy ion transport:

  BCA + MD (results) + KMC (corrections)

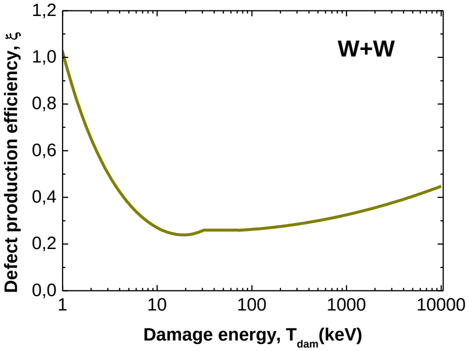
BCA: SRIM/TRIM, IOTA(KIT) etc.

MD, KMC: modeling precedes

Compromise

Neutron and proton low energy data (ENDF/B, JEFF, JENDL etc)

3. Modeling using pre-calculated ξ(T) dependence



ξ(T): parameterized or pointwise

Implemented: MARS15, FLUKA, PHITS

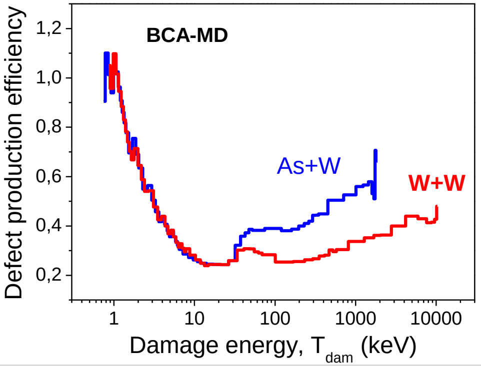
Simulation: BCA-MD

Correction: measured <ξ> values, *JNM 328, 197 (2004)*

Important

- Evaluated data at low energies (ENDF/B, JEFF, JENDL etc): processing dpa- cross-sections with ξ(T)

- ξ(T) dependence for various PKA



4. Modeling using pre-evaluated σ_d cross-sections

The most flexible way to keep

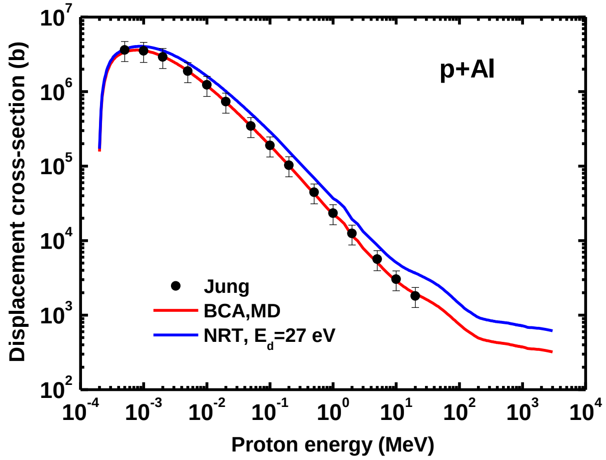
- justified theoretical information
- experimental data

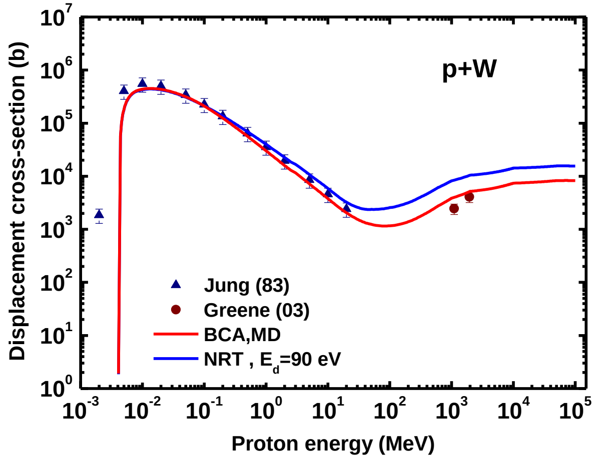
DXS data file (KIT, 2011-2014) (IAEA)

Projectile: neutron, proton

Energy: 10^{-5} eV to 3 GeV

Target: Al, Ti, V, Cr, Fe, Ni, Cu, Zr, W





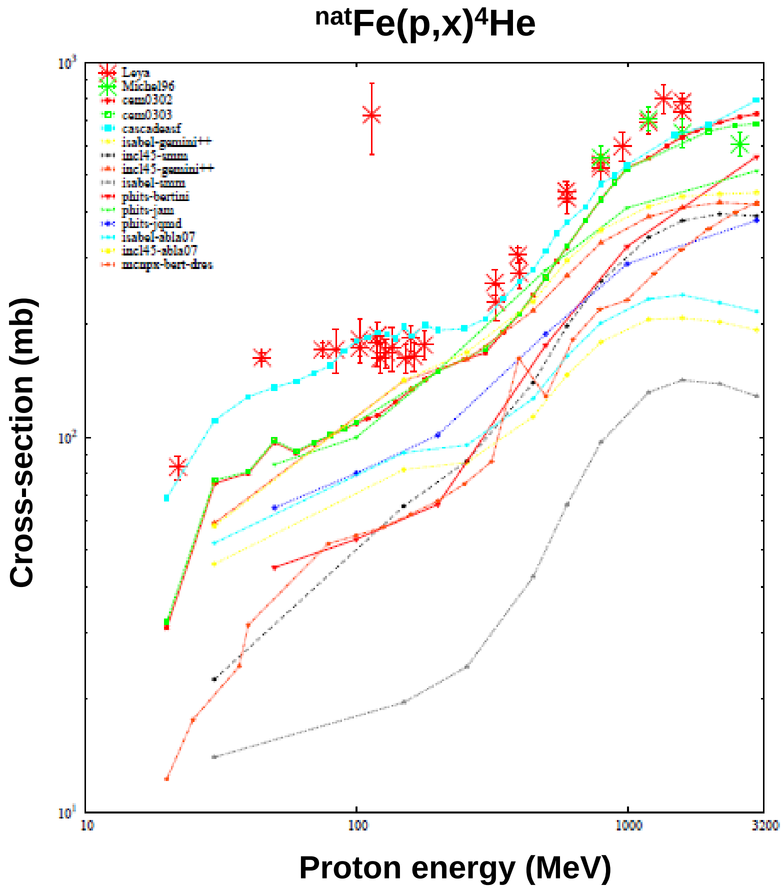
Gas production rate calculations

proton, deuteron, triton, ^{3}He, α-particle

Non-equilibrium emission

Phenomenological models:

- pick-up
- knock-on
- coalescence



IAEA Benchmark of Spallation Models, 2008

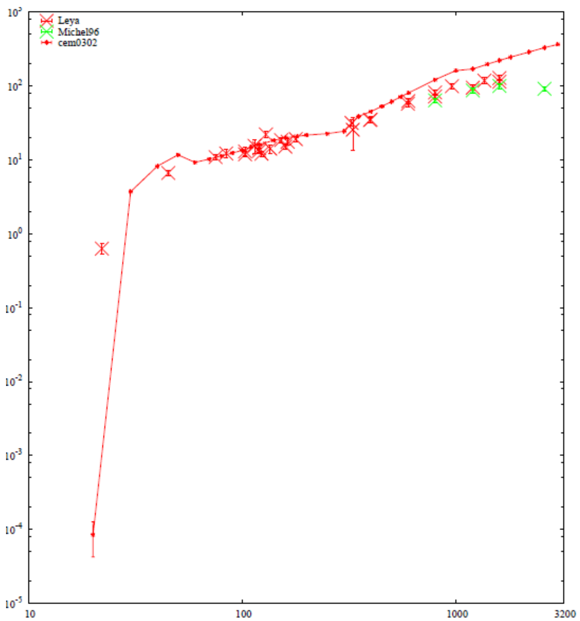
Energy of primary nucleons > 200 MeV

Success of coalescence model

CEM03

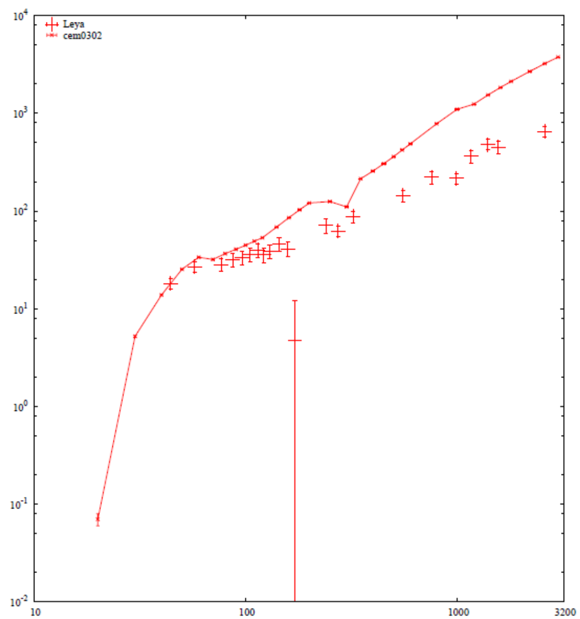
Cross-section (mb)

$^{nat}Fe(p,x)^3He$



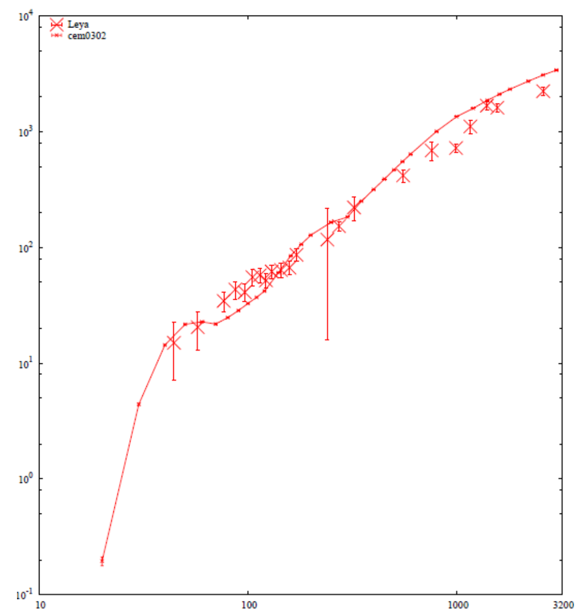
Proton energy (MeV)

$^{nat}Pb(p,x)^3He(cum)$



Proton energy (MeV)

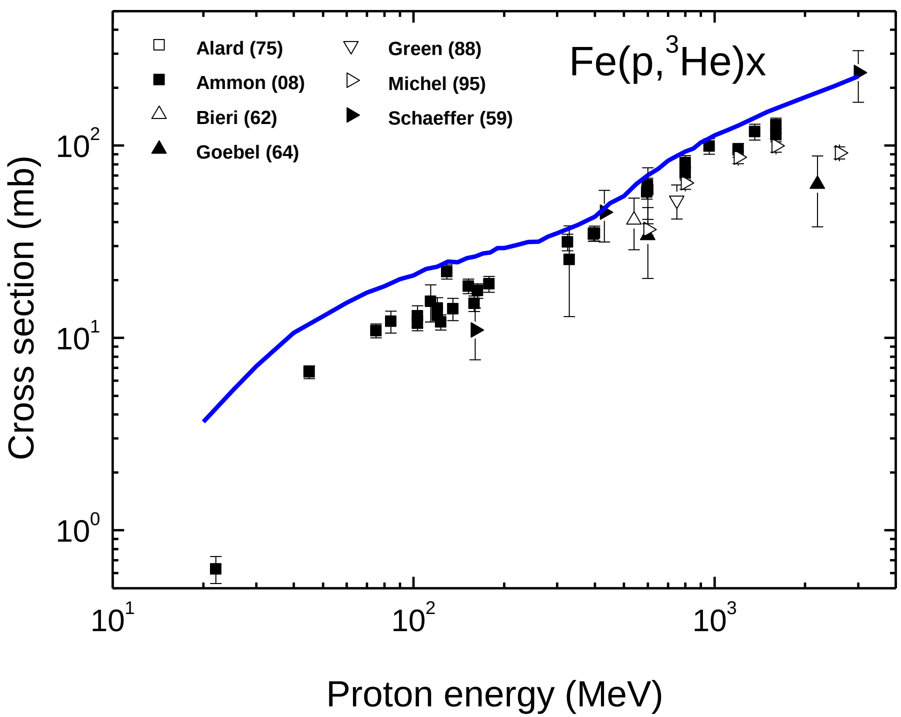
$^{nat}Pb(p,x)^4He$

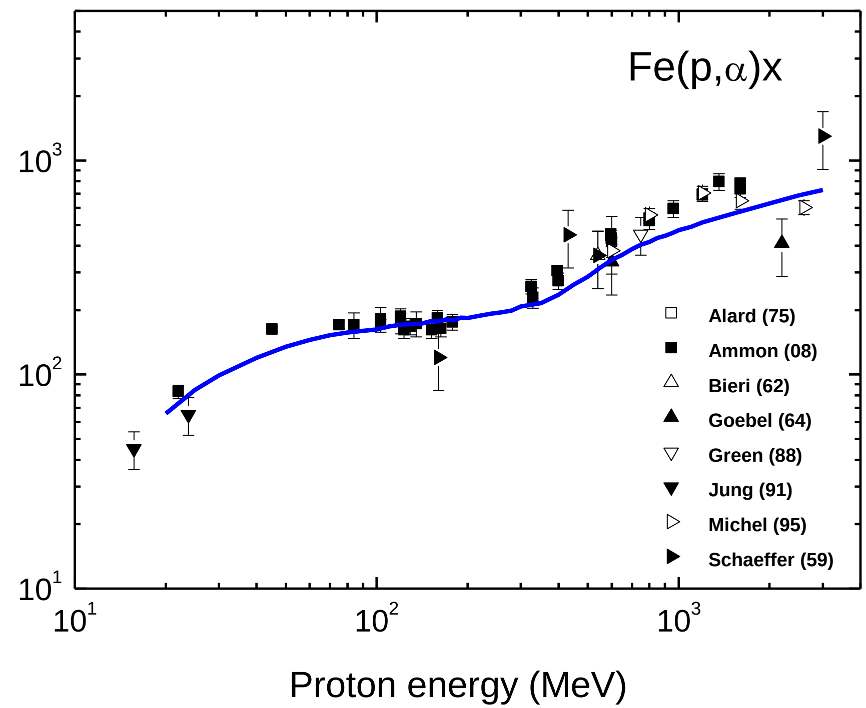


Proton energy (MeV)

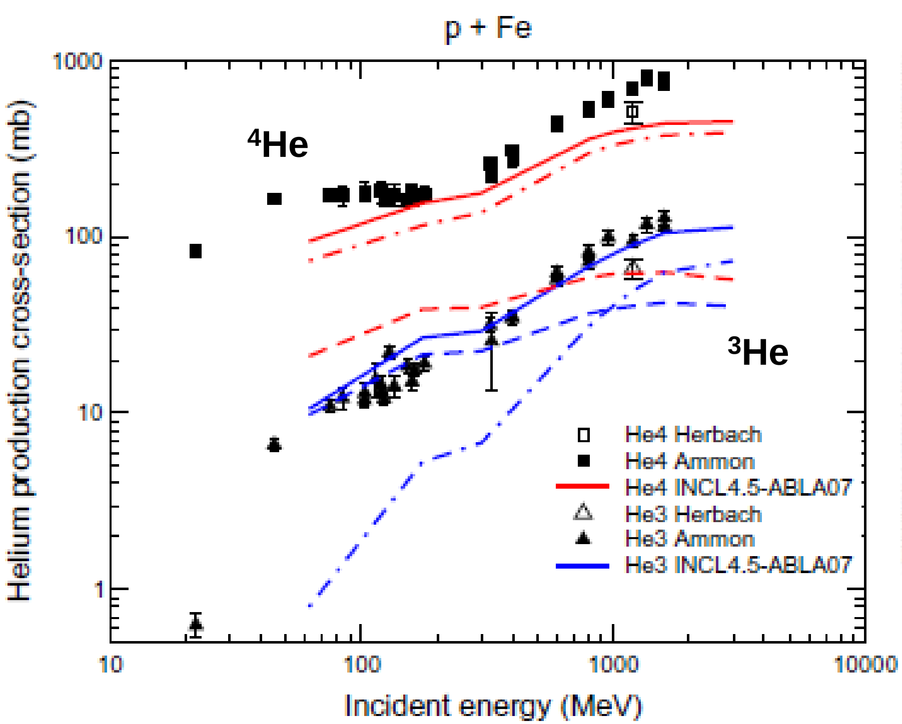
https://www-nds.iaea.org/spallations/spal_cal.html

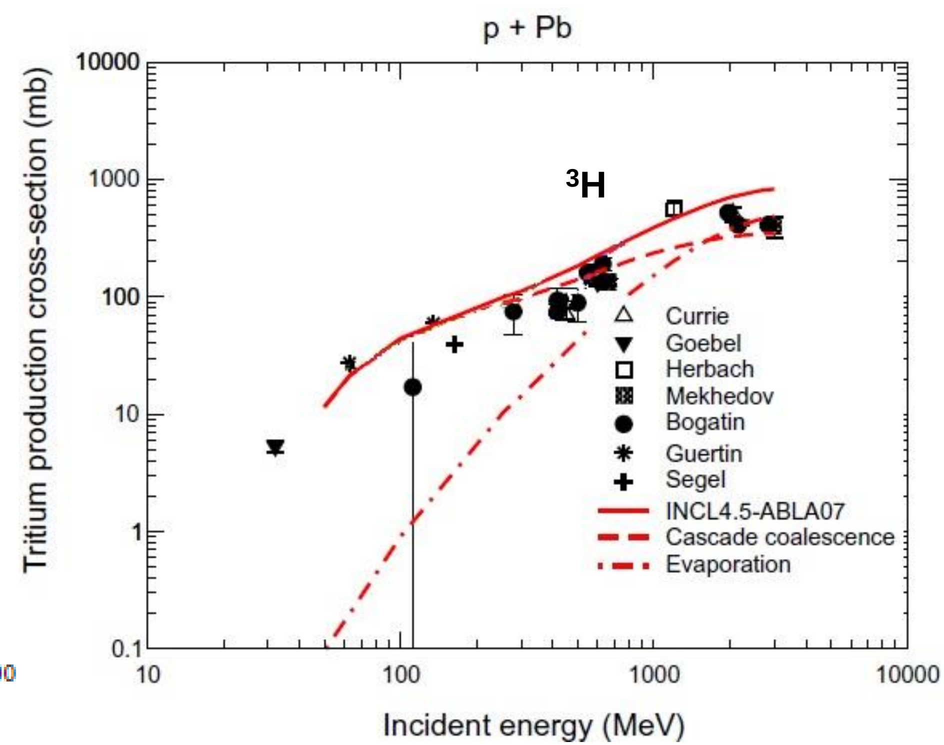
CASCADE-2012





INCL4



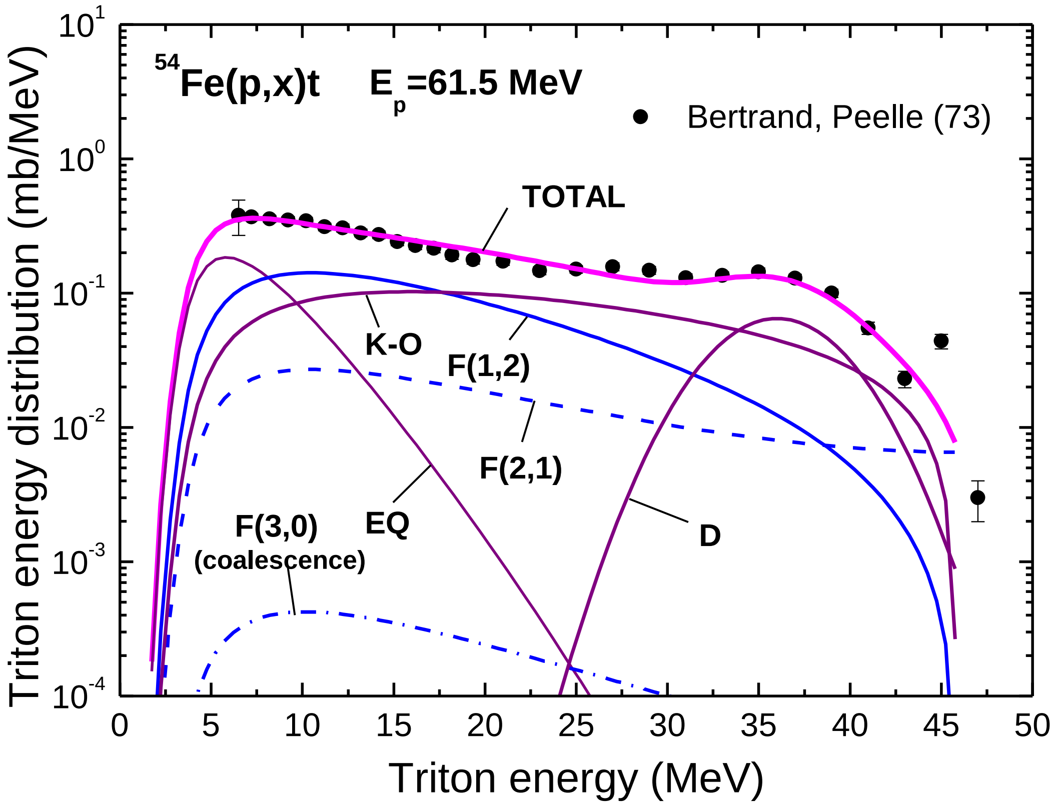


S.Leray et al,. NIMB 268, 581 (2010)

Energy of primary nucleons < 200 MeV

Combined approach

$$\frac{d\sigma}{d\varepsilon} = \frac{d\sigma^{P-U,C}}{d\varepsilon} + \frac{d\sigma^{K-O}}{d\varepsilon} + \frac{d\sigma^{D}}{d\varepsilon}$$



ALICE/ASH

JEFF, May 2011

Improved gas rate calculations using particle transport codes

1. Calculations + pre-evaluated (calculated) data

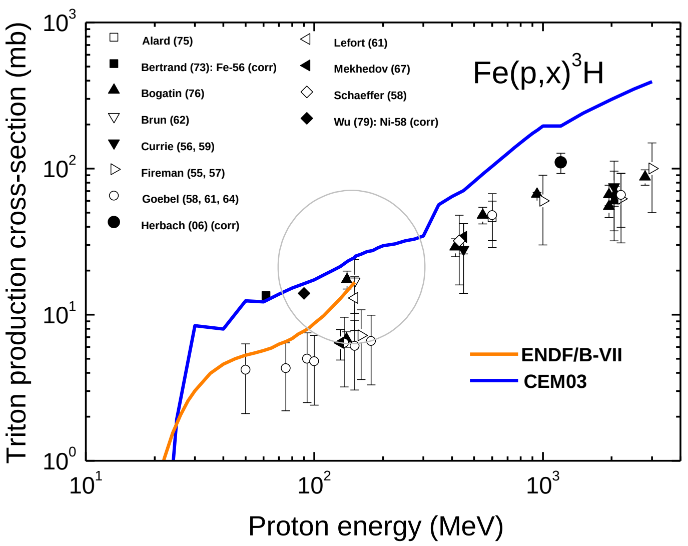
<u>Energy of incident nucleons < 150-200 MeV</u>

ENDF/B, JENDL, JEFF

TENDL

Neutron data: 2630 nuclides, Z=1 - 110

Proton data : 2629 nuclides, Z= 1 - 109



Transition to model calculations around 150 MeV

smoothed curves: “hybrid” LAHET approach, $\min[E_1/E_2, 1.0]$

Energy of incident nucleons above 150 MeV

Promising: INC + PE + HF

HF: at least at low excitation energies

WE: improved level density (GSM), optical model for σ_{inv}

CEM95+STAPRE Yavshits et al, Nucl. Const. 2000

CASCADEX (CASCADE+TALYS) Stankovskiy et al, NIMA, 2008

CASCADE/ASF Broeders et al, NIMA, 2005

CASCADE+TALYS KIT, 2011

MC + deterministic models

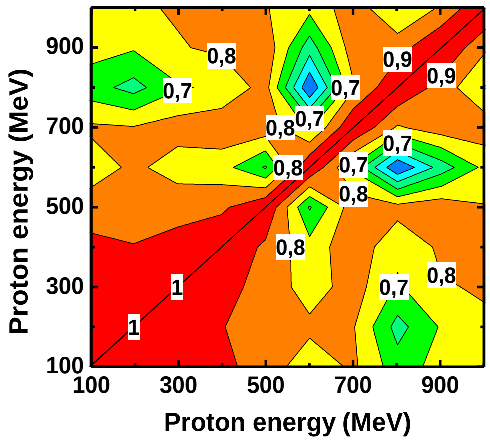
2. Use of evaluated data, σ(E)

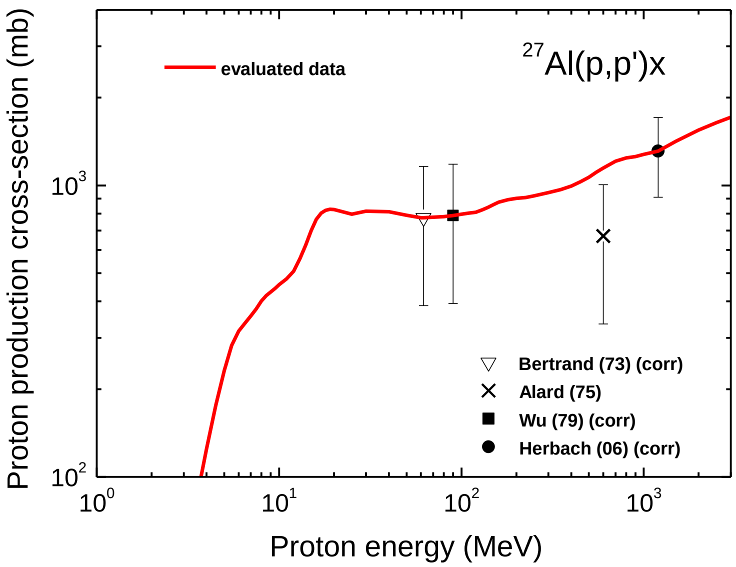
DXS data file (KIT, 2011-2014) (IAEA)

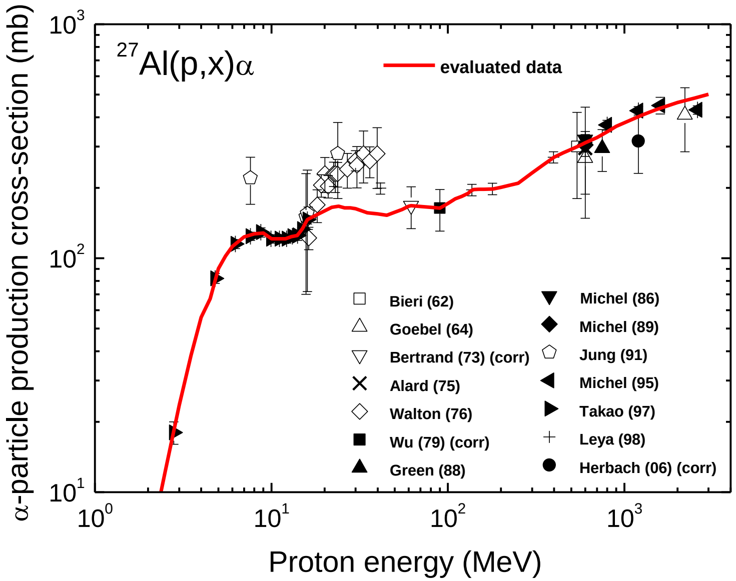
Projectile: neutron, proton

Energy: 10^{-5} eV to 3 GeV

Target: Al, Ti, Cr, Fe, Ni, W







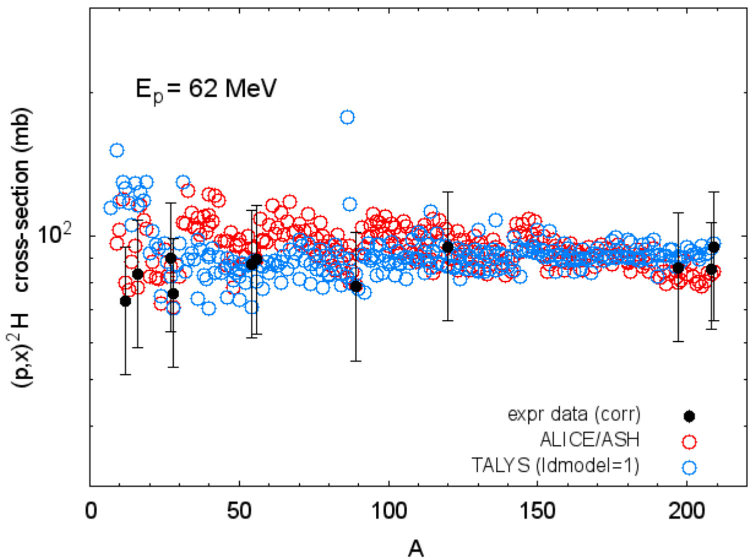
3. Use of evaluated data, σ(A)

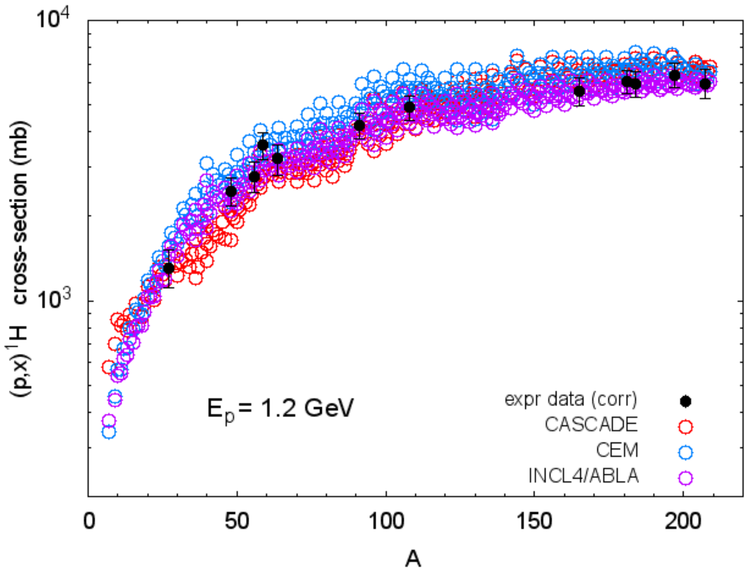
Evaluated σ(A) are not „systematics" data

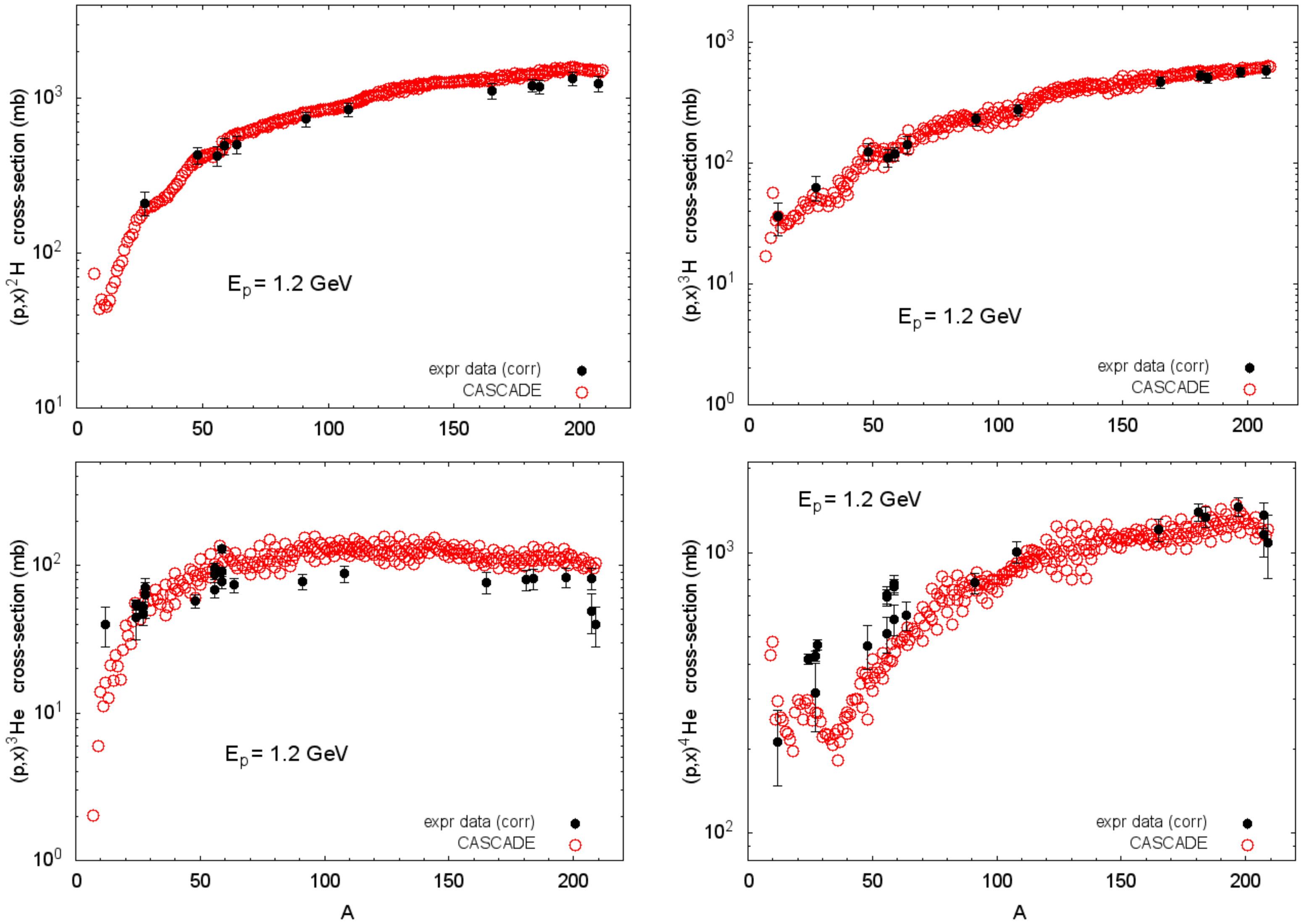
Choice of incident proton energies: a number of measurements

Selected: 62, 90, 150, 600, 800, and 1200 MeV

Example of calculations







$(p,x)^2H$ cross-section (mb)
$E_p = 1.2$ GeV
expr data (corr)
CASCADE
$(p,x)^3H$ cross-section (mb)
$E_p = 1.2$ GeV
expr data (corr)
CASCADE
$(p,x)^3He$ cross-section (mb)
$E_p = 1.2$ GeV
expr data (corr)
CASCADE
A
$(p,x)^4He$ cross-section (mb)
$E_p = 1.2$ GeV
expr data (corr)
CASCADE
A

Evaluated data

Proton, deuteron, triton, ^{3}He, ^{4}He –production cross-sections

278 targets from ^{7}Li to ^{209}Bi

Incident proton energies: 62, 90, 150, 600, 800, 1200 MeV

Measurements

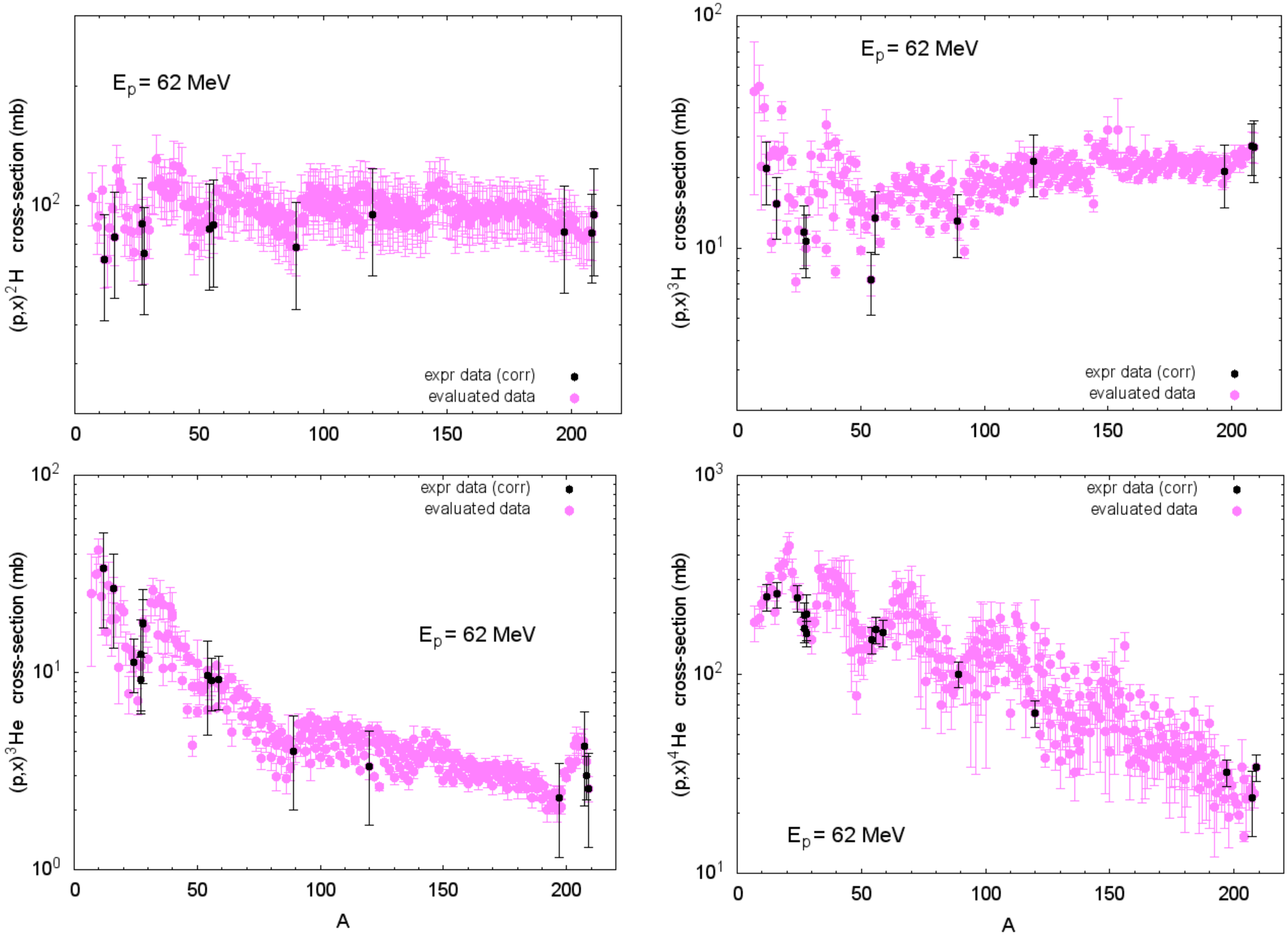
available data, corrected data

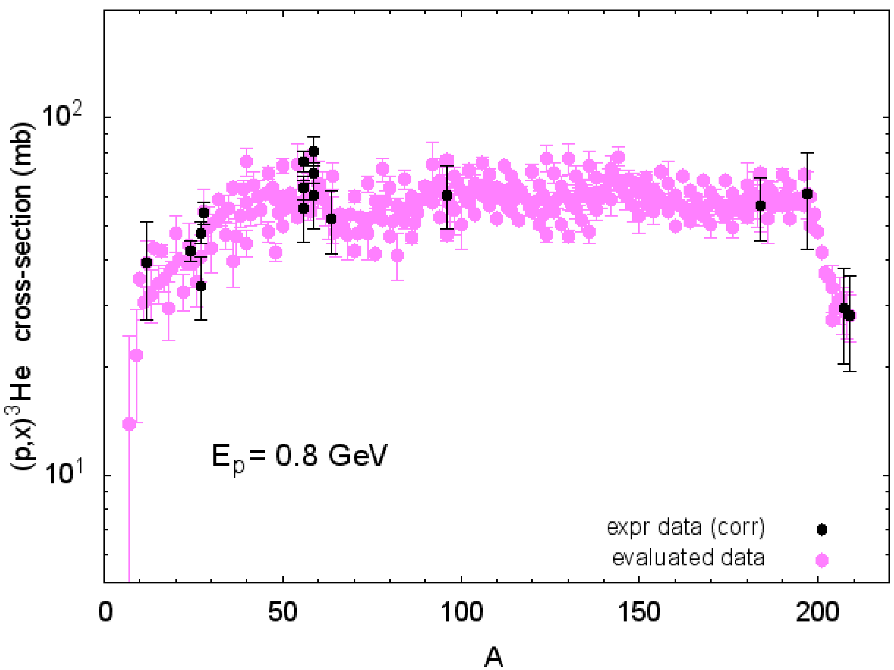
Calculations

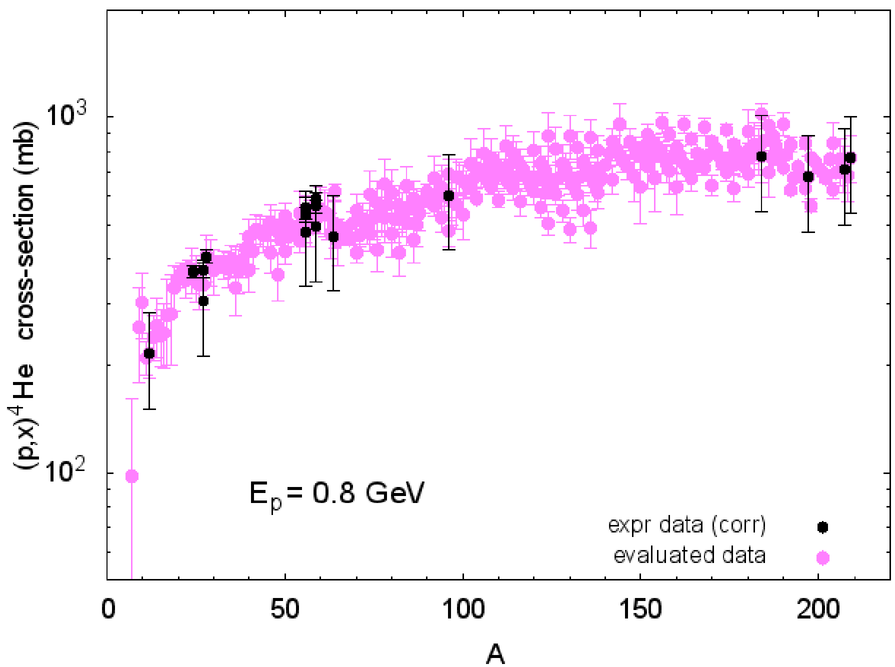
ALICE/ASH, TALYS (*ldmodel*=1,2,3)

CASCADE, CEM03, INCL4/ABLA

Examples of evaluated data




10^2
10^1
$(p,x)^3He$ cross-section (mb)
E_p = 0.8 GeV
expr data (corr)
evaluated data
0
50
100
150
200
A


10^3
10^2
$(p,x)^4He$ cross-section (mb)
E_p = 0.8 GeV
expr data (corr)
evaluated data
0
50
100
150
200
A

Conclusion

The use of modern approaches for calculation of the number of stable defects in irradiated materials improves markedly the reliability of calculated dpa rates

Advanced calculations assumes the direct simulation of radiation damage or the application of atomic displacement cross-sections obtained using BCA-MD modeling and available experimental data

Nuclear models implemented in popular computer codes predict gas production cross-section with varying degrees of success depending on the energy of projectiles

The use of cross-sections evaluated using nuclear model calculations and measured data is one of the most reliable and flexible approach for advanced calculation of gas production rate