Displacement Damage and Gas Production Data for ESS Structural Materials

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Content

- Background
- Data evaluation methodology (KIT)
- Displacement damage and gas production cross-section data
- Fe, Cr, Ni & others for n & p induced reactions up to 3 GeV
- Application to ESS windowless liquid metal target
- Conclusions
Background

- ESS target and structural materials subjected to intense neutron and proton irradiation
- Materials properties deteriorated due to displacement damages and gas generation
- Very few data available for materials and energy range relevant to ESS
- Evaluation effort at KIT for providing data of n & p induced reactions up to 3 GeV
- Focus on Fe, Cr & Ni
**Displacement damage cross-section**

\[ \sigma_d(E_p) = \sum_i \int_{E_d}^{T_i^{\text{max}}} \frac{d\sigma(E, Z, A, Z, A_i)}{dT_i} \cdot \eta(T) \cdot N_{\text{NRT}}(T, Z, A, Z, A_i) dT_i \]

\( d\sigma/dT \) : recoil energy distribution
\( E_d \) : effective threshold displacement energy

Defect production efficiency
\[ \eta(T) = \frac{N_D}{N_{\text{NRT}}} \]

\( N_D(T) \) : number of Frenkel pairs produced by PKA (MD, BCA, experiment)

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**MD = Molecular Dynamics**

**BCA = Binary Collision Approximation**

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NRT model


Number of defects produced by PKA

\[ N_{\text{NRT}}(T) = \frac{0.8}{2E_d} T_{\text{dam}} \]

\[ T_{\text{dam}}(T) = \frac{T}{1 + k \left( 3.4008 \varepsilon^{1/6} + 0.40244 \varepsilon^{3/4} + \varepsilon \right)} \]

Available experimental data and MD simulations show pronounced differences with NRT predictions

Typical \( \eta(T) \) values: 0.5 (Al), 0.3 (Fe), 0.3 (Cu)
Defect production calculation – KIT approach

Combined BCA-MD approach for the calculation of the number of stable displacements in atom lattices

Transition from BCA to MD at “critical” kinetic energy ($T_{\text{crit}}$)

- $T < T_{\text{crit}}$: MD
- $T > T_{\text{crit}}$: BCA

$T_{\text{crit}}$ typically between 30 – 60 keV

KIT codes IOTA and CASCADE

![Displacement production graph](attachment:image.png)

primary energy = 1 MeV
Example: $N_D/N_{\text{NRT}}$ for iron

![Graph showing defect production efficiency versus PKA energy (MeV)](image)

- **Fe+Fe**
- **MD: Voertler et al**
- **BCA, MD**

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Nucleon elastic scattering

- Optical potentials of Koning, Delaroche and Madland up to 400 MeV
- Relativistic approach above 400 MeV
Non-elastic scattering

Different models & codes

MCNPX: INC+PE+EQ
   INC: Bertini, ISABEL, CEM03, INCL4
   EQ: Dresner, ABLA

CASCADE (JINR, KIT): INC+EQ

DISCA-C (KIT): INC(+clusters)+EQ

TALYS: PE (exciton model) +EQ (H-F)

HMS ALICE: Hybrid model +EQ

GNASH: PE (exciton model) +EQ (H-F)

Evaluated displacement cross-section:

$$\sigma_{\text{displ}} = \sum_{m=1}^{M} W_m \sigma_{\text{displ},m}$$
Non-elastic scattering (cont’d)

Example: Displacement cross-sections (b) for non elastic interactions of 0.6 GeV neutrons and protons with $^{56}$Fe. Calculation of recoil spectra and displacement cross-sections using equally weighted models

<table>
<thead>
<tr>
<th>Nuclear model</th>
<th>Neutrons</th>
<th>Protons</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bertini/Dresner</td>
<td>807</td>
<td>727</td>
</tr>
<tr>
<td>Bertini/ABLA</td>
<td>864</td>
<td>775</td>
</tr>
<tr>
<td>ISABEL/Dresner</td>
<td>815</td>
<td>732</td>
</tr>
<tr>
<td>ISABEL/ABLA</td>
<td>857</td>
<td>776</td>
</tr>
<tr>
<td>CEM03</td>
<td>781</td>
<td>712</td>
</tr>
<tr>
<td>INCL4/Dresner</td>
<td>956</td>
<td>849</td>
</tr>
<tr>
<td>INCL4/ABLA</td>
<td>1002</td>
<td>894</td>
</tr>
<tr>
<td>CASCADE</td>
<td>796</td>
<td>717</td>
</tr>
<tr>
<td>DISCA-C</td>
<td>870</td>
<td>786</td>
</tr>
<tr>
<td><strong>Average value</strong></td>
<td><strong>861 ± 75</strong></td>
<td><strong>774 ± 62</strong></td>
</tr>
</tbody>
</table>
Evaluated Fe displacement damage cross-sections up to 3 GeV

Neutron induced

Proton induced

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Evaluated Cr displacement damage cross-sections up to 3 GeV

Neutron induced

Proton induced

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Evaluated Ni displacement damage cross-sections up to 3 GeV

Neutron induced

Proton induced

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Gas production cross-sections

Proton-, deuteron-, triton, $^3$He-, $^4$He- production

Experimental data
EXFOR, JINR compilation (1972), and more

$(p,x)$ reactions
Fe, Ni: 24 measurements
Cr: K.Goebel et al, CERN (1964)

Data correction
Cutoff energy: Bertrand F.E., Peelle R.W. (1973)
Calculations

ALICE/ASH (KIT) : GDH(+non-equilibrium cluster emission) +EQ
TALYS (NRG): PE exciton model +EQ (H-F)
DISCA-C (KIT): INC(+clusters)+EQ
CASCADE (JINR, KIT): INC(+improved coalescence model) +EQ
MCNPX models: for illustration purposes only

Evaluation ...

... comes later
**MCNPX model calculations**

**Fe(p,p')x**

- Alard (75)
- Bertrand (73); Fe-nat (corr)
- Herbach (06) (corr)

**Proton energy (MeV)**

**Fe(p,t)x**

- Alard (75)
- Bertrand (73); Fe-nat (corr)
- Bogatin (76)
- Brun (82)
- Currie (56, 59)
- Fireman (62)
- Goebel (58, 61, 64)
- Herbach (06) (corr)

**Proton energy (MeV)**

**Fe(p, 3He)x**

- Alard (75)
- Ammon (08)
- Bieri (62)
- Goebel (64)

**Proton energy (MeV)**

**Fe(p, α)x**

- Alard (75)
- Ammon (08)
- Bieri (62)
- Goebel (64)

**Proton energy (MeV)**

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Examples of available evaluations and model calculations

**Fe(p,p')x**

- Alard (75)
- Bertrand (73): Fe-nat (corr)
- Herbach (96) (corr)

**Fe(p,α)x**

- Alard (75)
- Ammon (08)
- Bieri (62)
- Goebel (64)
- Green (88)
- Jung (91)
- Michel (95)
- Schaeffer (59)

Proton energy (MeV) vs. proton production cross-section (mb)

Proton energy (MeV) vs. α-particle production cross-section (mb)

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More model calculations ...

Fe(p,d)x

Proton energy (MeV)

deuteron production cross-section (mb)

Fe(p,t)x

triton production cross-section (mb)

Fe(p,3He)x

Proton energy (MeV)

3He production cross-section (mb)
**KIT evaluated cross-section data**

**I. Theoretical data**
- ALICE/ASH, CASCADE
- TALYS: up to several MeV

**II: Experimental data**

**III. Evaluated data = final data**
- BEKED code system (KIT)
- Uncertainties & co-variance information
- Generalised Least Square Method (GLSM) + Unified Monte Carlo (UMC) of D. L. Smith.

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KIT evaluated data - examples

Fe(p,p')x

Proton production cross-section (mb)

Proton energy (MeV)

Alard (75)

Bertrand (73): Fe-nat (corr)

Herbach (06) (corr)

Fe(p,d)x

Proton energy (MeV)

Alard (75)

Bertrand (73): Fe-56 (corr)

Herbach (06) (corr)

Wu (79): Ni-58 (corr)

Ni-58 (corr)

KIT evaluated data - examples

Proton production cross-section (mb)

Proton energy (MeV)

Wu (79): Ni-58 (corr)

Lefort (61)

Mekhedov (67)

Schaeffer (58)

Fe(p,t)x

Triton production cross-section (mb)

Proton energy (MeV)

Alard (75)

Bertrand (73): Fe-56 (corr)

Herbach (06) (corr)

Wu (79): Ni-58 (corr)

Goebel (58, 61, 64)

Fireman (55, 57)
KIT evaluated data – examples (cont’d)

Fe(p, $^3$He)x

Fe(p, $\alpha$)x

Fe(n, $\alpha$)x

Proton energy (MeV)

Neutron energy (MeV)

$\alpha$-particle production cross-section (mb)

$\alpha$-particle production cross-section (mb)

LANSCE (05)
Paulsen (81)
Wattecamps (83)

evaluated data

Alard (75)
Ammon (88)
Bieri (62)
Goebel (64)
Green (88)
Jung (91)
Michel (95)
Schaeffer (59)

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KIT evaluated data files

- Neutron & proton data up to 3 GeV
- Fe, Cr, Ni + Al, Zr, Cu, W
- Data files in standard ENDF-6 format
- Gas production cross-sections for p-, d-, t-, \(^3\)He, \(^4\)He (MT=203-207)
- Displacement cross-sections for BCA-MD (MT=900) and NRT (MT=901)
- Data files can be processed into ACE format for direct use with MCNPX(*)

(*) p data require patch or secondary input

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Windowless Liquid Metal Target Design for ESS

Proton beams impinge liquid metal at 15° inclination angle
No direct interaction of proton beam and solid structures
Radiation damage to structure walls due to neutron irradiation

See A. Class et al, Windowless liquid metal target concept for ESS, this workshop

SS-316 structure walls
Neutronics calculations

- MCNPX, Version 2.7a, using CEM cascade model
- Source: Proton beam $E_p = 2500$ MeV with Gaussian profile incident at $15\degree$ on PbBi free surface target
- Geometry model: PbBi enclosed in SS-316 steel frame
- Calculations of n-, p-flux, heating, dpa, gas production distributions using mesh tallies
- Use of evaluated dpa & gas production cross-section data for dpa and gas production rates in SS-316
- Typically 10 million source particle histories tracked with fractional standard deviation (FSD) around 1 %. 

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Neutronics results for target side wall (SS-316)

Neutron flux density [cm$^{-2}$s$^{-1}$]

- Max. $3 \times 10^{14}$ cm$^{-2}$s$^{-1}$

H production [appm/fpy]

- Max. 760 appm/fpy

Displacement damage [dpa/fpy]

- Max. 9 dpa$_{NRT}$/fpy

He production [appm/fpy]

- Max. 160 appm/fpy

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Neutronics results for bottom wall (SS-316)

Neutron flux density [cm$^{-2}$s$^{-1}$]  

\[
\text{max. } 9.3 \cdot 10^{14} \text{ cm}^{-2}\text{s}^{-1}
\]

H production [appm/fpy]  

\[
\text{max. } 4600 \text{ appm/fpy}
\]

Displacement damage [dpa/fpy]  

\[
\text{max. } 28 \text{ dpa}_{NRT}/\text{fpy}
\]

He production [appm/fpy]  

\[
\text{max. } 780 \text{ appm/fpy}
\]
Neutronics results for upper wall (SS-316)

Neutron flux density [cm\(^{-2}\)s\(^{-1}\)]

- max. \(1.2 \cdot 10^{15}\) cm\(^{-2}\)s\(^{-1}\)

H production [appm/fpy]

- max. 10000 appm/fpy

Displacement damage [dpa/fpy]

- max. 43 dpa\(_\text{NRT}/\text{fpy}\)

He production [appm/fpy]

- max. 1700 appm/fpy
Conclusions

- Evaluations performed for displacement and gas production data using advanced KIT approach
- Data for Fe, Cr, Ni (+Al, Zr, Cu, W), n - and p induced reactions up to 3 GeV
- ENDF data files available upon request
- Application analyses for ESS windowless liquid metal target
- Data can be used with MCNP/MCNPX
  ... and other codes