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DPA cross section library FermiDPA 1.0*

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Abstract

DPA cross section library FermiDPA 1.0 based on the industry standard NRT model calculations is described. The library contains DPA cross sections for neutrons in the energy range 10^{-5} eV 20 (150) MeV. Calculations used neutron-induced reaction cross sections from ENDFB-VII database of evaluated nuclear data. The NJOY99 nuclear data processing system's module HEATR was applied to calculate NRT model radiation damage cross sections. The FermiDPA 1.0 library is a database of 395 text files (for 395 known isotopes) with DPA cross sections. It is code-independent and can be implemented in any transport code.

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DPA cross section library FermiDPA 1.0 based on the industry standard NRT model calculations is described. The library contains DPA cross sections for neutrons in the energy range 10^{-5} eV – 20(150) MeV. Calculations used neutron-induced reaction cross sections from ENDFB-VII database of evaluated nuclear data. The NJOY99 nuclear data processing system's module HEATR was applied to calculate NRT model radiation damage cross sections. The FermiDPA 1.0 library is a database of 395 text files (for 395 known isotopes) with DPA cross sections. It is code-independent and can be implemented in any transport code.

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The code-independent atomic displacement (DPA) cross section library has been produced for low-energy neutrons. The new model encompasses the neutron energy range from 10^{-5} eV to 20-150 MeV using the ENDFB-VII [1] neutron cross section library database for 395 nuclides. The library was calculated using NRT [4] model as implemented in NJOY [2] code for all nuclides covered by ENDFB-VII ($N_{NRT} = \frac{0.8}{2 \cdot E_d} \cdot T_{dam}$, E_d – threshold energy, T_{dam} – damage energy) and in the energy range available in the library, from 10^{-5} eV to 150 MeV (or to 20 MeV for some isotopes). In calculations effective threshold energies from [3] were used, ranging from 12 eV (for Mg) to 90 eV (for W), and having the value of 40 eV for the most of the elements.

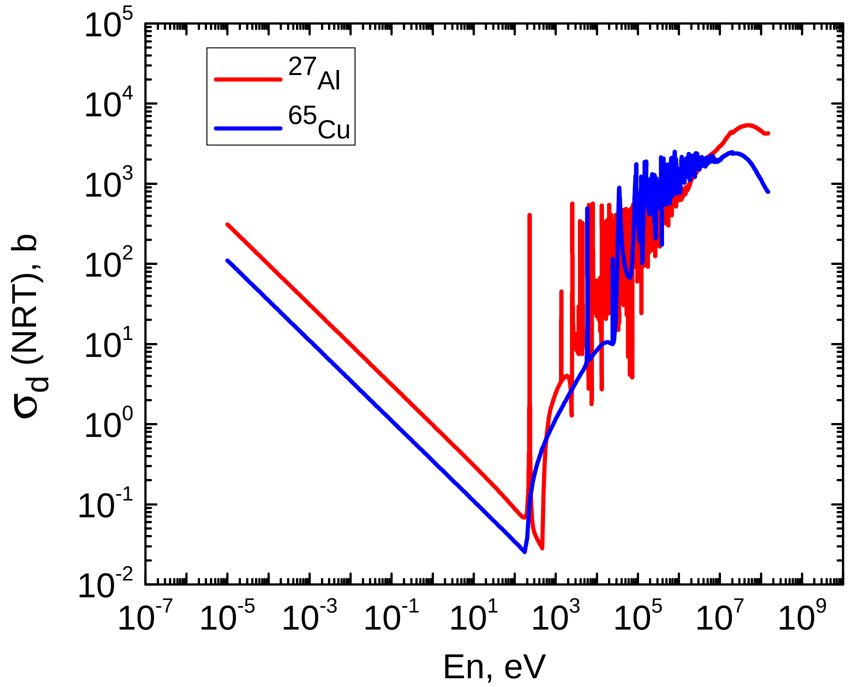

FIG. 1. NRT DPA cross sections from FermiDPA 1.0

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The FermiDPA 1.0 library is a set of 395 text files with the names containing the following fields : 1) the neutron identifier, 2) Z number of the element, 3) symbol of the element, and 4) mass number of the element. The first field is separated by a dash, while the other fields – by underscores, for example, $n - 013_A l_0 27.cs$ for Aluminum. The text in each file is organized in two columns, giving energy in eV, and cross-section in eV*barn, for instance :

```
1.000000E-05 1.014804E+05
1.062500E-05 9.845050E+04
```

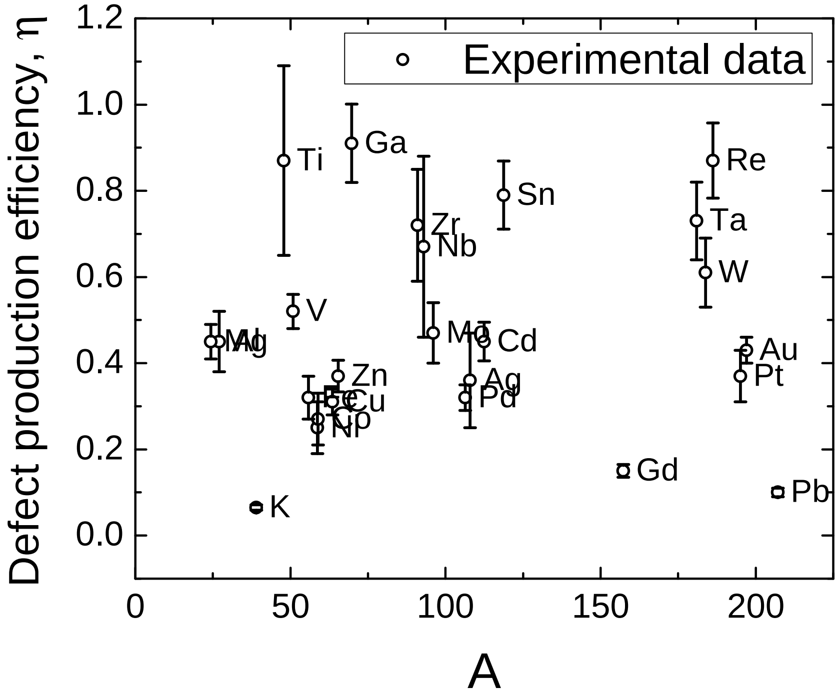

FIG. 2. Defect production efficiencies, η

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1.125000E-05 9.567670E+04

1.187500E-05 9.312487E+04

1.250000E-05 9.076685E+04

1.312500E-05 8.857937E+04

1.375000E-05 8.654279E+04

1.437500E-05 8.464052E+04

1.500000E-05 8.285843E+04

1.562500E-05 8.118434E+04

1.625000E-05 7.960778E+04

1.687500E-05 7.811966E+04

1.750000E-05 7.671200E+04

1.812500E-05 7.537778E+04

1.875000E-05 7.411084E+04

2.000000E-05 7.175751E+04

...

To obtain cross-sections in barns, one needs to apply the following transformation : $\frac{\sigma*0.8}{2*E_d}$, where E_d is taken, for example, from [3]. The Fermilab 1.0 library requires 93 Mb of disk space.

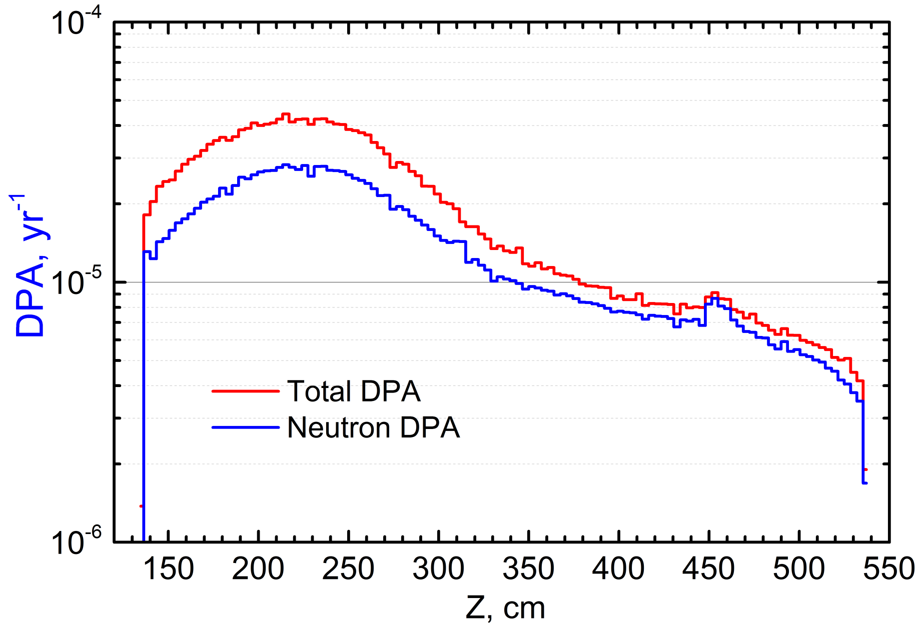

FIG. 3. Total and neutron-induced DPA

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In calculations, the effective threshold energies from [3] were used, ranging from 12 eV (for Mg) to 90 eV (for W), and having the value of 40 eV for the most of the elements. For each particle type, the DPA rate can be calculated using the equation :

$$DPA = \int_0^{T_{max}} \sigma_d(T) \cdot \phi(T) dT, \tag{1}$$

where $DPA = N_d/N_0 \cdot t$ (DPA rate per proton), ϕ – particle flux, σ_d – defect production cross section, N_d – defects per unit volume, N_0 – atomic density, t – irradiation time. A practical calculation of DPA rate in MARS15 in a particular volume using `FermiDPA 1.0` cross sections can be reduced to the computation of the quantity :

$$DPA = \sum_N \frac{l_s \cdot \sigma_d}{V \cdot N}, \tag{2}$$

where l_s – step length of a neutron in the volume, N – number of Monte-Carlo events, V – volume.

In particuilar, the general equation for the defect production cross sections by neutrons has the form :

$$\sigma_d(E_n) = \sum_i \int_{E_d}^{T_i^{max}} \frac{d\sigma(E_n, Z_T, A_T, Z_i, A_i)}{dT_i} \cdot \nu(T_i, Z_T, A_T, Z_i, A_i) dT_i, \tag{3}$$

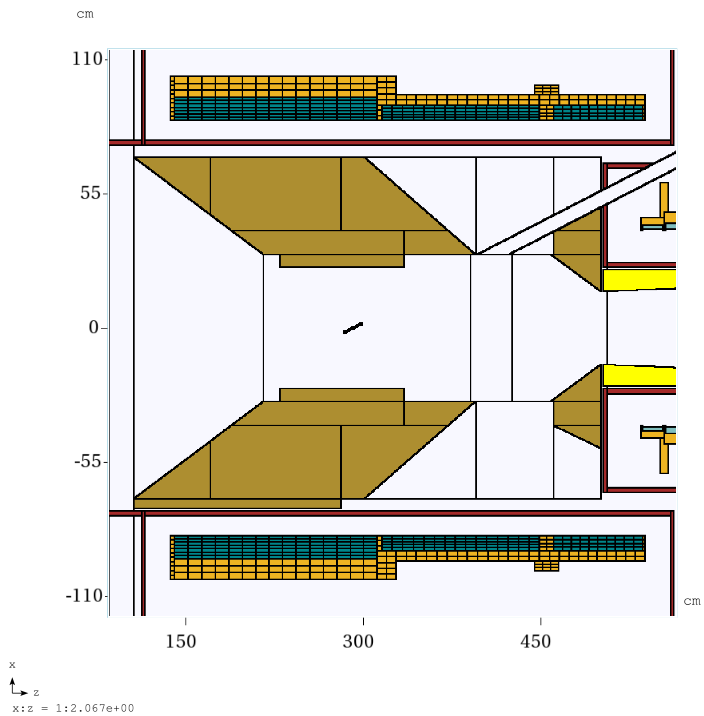

FIG. 4. Mu2e PS MARS15 model (reduced option)

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where E_n - neutron energy, $d\sigma/dT_i$ - the recoil atom formation cross section, A_i, Z_i, A_T, and Z_T - atomic and mass numbers of the recoil and target nuclei, $\nu(T_i)$ - number of defects produced by PKA with the kinetic energy T_i, E_d - displacement threshold energy, T_i^{max} - maximum PKA energy; the number of defects $\nu(T) = \eta \cdot 0.8/(2 \cdot E_d) \cdot T_{dam}(T)$, E_d – threshold energy, T_{dam} – damage energy equal to the energy transferred to the lattice with subtraction of the electronic stopping losses), η – defect production efficiency. The summation is performed over all the recoils.

For materials at low temperatures ($\leq$ 4.2 K), like the superconducting magnet coil material, the NRT DPA rates need to be corrected using experimental defect production efficiency η, which is the ratio of a number of single interstitial atom vacancy pairs (Frenkel pairs) produced in a material to the number of defects calculated using NRT model.

The values of η have been measured experimentally [3] for many important materials for a number of neutron spectra in the reactor energy range (below 14.5 MeV). Scaling the DPA rate obtained using NRT model to the experimental ones using η leads to a decrease of the resulting one by a factor of 2 – 3 (see Fig. 2) on average, because in the case of HRS "hot spot" on coils, which is near the spent beam exit close to the middle of the first coil (see Fig. 4), more than 99% of neutrons have energies below 14.5 MeV. For the HRS coils neutrons contribute to the total DPA about 70% (see Fig. 3). This explains significant (up to 40%) growth of DPA levels when the new DPA model was used instead of the old one.

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[4] M.J. Norgett *et al.*, Nuclear Engineering and Design, **33**, 50 (1975).