

Comparison of NRT-dpa cross sections calculated by NJOY-2012.50 with ASTM standard for ^{nat}Fe

The NJOY code is widely used to calculate displacement cross section dpa.

The procedure usually consists of:

- (i) computing of the Damage Energy T_d (MT = 444) by NJOY from the evaluated cross section files.
- (ii) calculation of the dpa- cross section as:

$$\sigma_{dpa} = 0.8 T_d / (2 E_d), \text{ where } E_d \text{ average displacement energy (40 eV for Iron)} \quad (1)$$

Figs. 1 and 2 below compare the dpa cross sections for natural Fe:

- from **Standard ASTM E693-12** (Table 1 in [1]), where it was calculated by NJOY-97 from ENDF/B-VII.1-5 using the NRT convention [2] for conversion of damage energy into dpa:

$N_d(T_d) = \begin{cases} 0 & T_d < E_d \\ 1 & E_d \leq T_d < 2 E_d / \beta \\ \frac{\beta T_d}{2 E_d} & 2 E_d / \beta \leq T_d < \infty \end{cases}$	$\beta = 0.8$ <p>(for Fe: $2E_d/\beta = 100$ eV)</p>
	(2)

- calculated by default version of NJOY-2012.50 from ENDF/B-VII.1 files with this [input](#) - “NJOY2012(default)”

The reason for **50% discrepancies** in vicinity of 1 keV: calculation of dpa cross section using formula (1) and T_d from NJOY neglects the NRT definition (2) for Fe recoils energies between 40 and 100 eV (corresponding elastic neutron energies 0.58 and 1.45 keV).

To overcome this and follow typical procedure (1), T_d should be modified in function $df(e,zr,ar,zl,al)$ of the HEATR module as:

```

real (kr) :: el, rel, denom, fl, ep, dam, Exxx ! ***: to define Exxx
.....
else
ep=e*rel
dam=e/(1+fl*(c3*ep**sixth+c4*ep**threeq+ep))
! ***: re-definition of Damage Energy < 2Ed/betta to get NRT-dpa from it
Exxx=2*break/0.8
if(e.lt.break) dam=0
if(break.le.e.and.e.lt.Exxx) dam=Exxx
! ***: end of modification
df=dam
endif
    
```

After such modification of NJOY (i.e., exactly the same NRT convention for counting of the displaced atoms above E_d will be used) the [NJOY2012\(NRT\)/ENDF/B-VII.1](#) and **ASTM standard** agree much better (the difference left – probably come from the different versions of evaluated files, codes, ...).

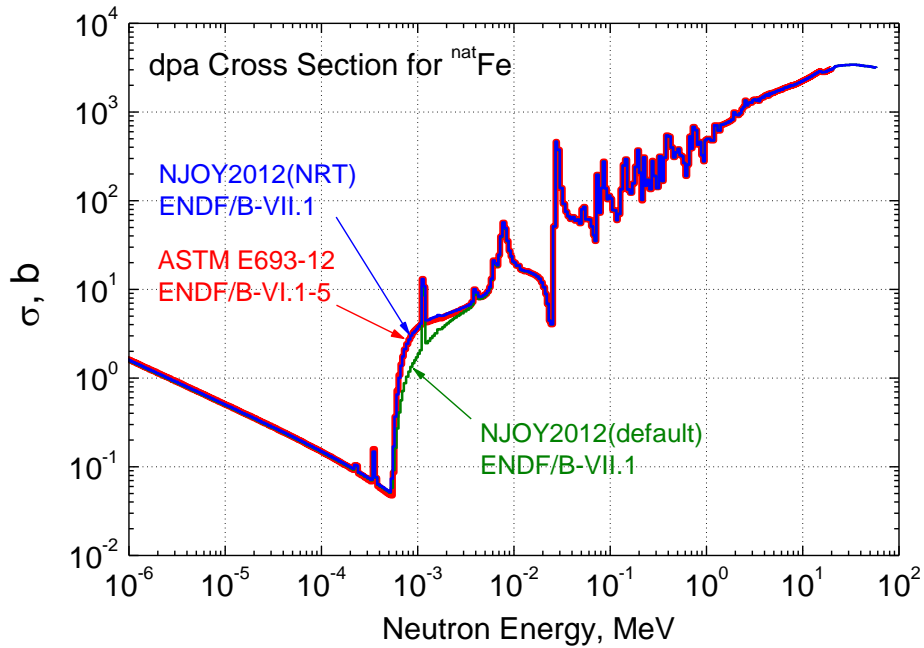


Fig. 1. NRT dpa cross section for ^{nat}Fe: **ASTM E693 standard** and calculated by **default** and **modified (NRT)** versions of NJOY-2012.50 from the ENDF/B-VII.1 files.

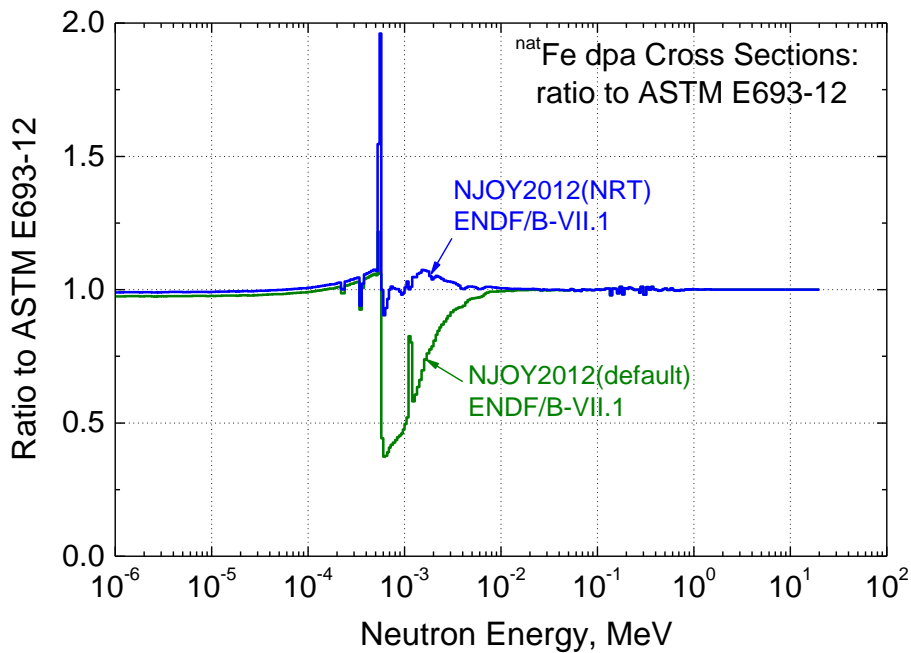


Fig. 2. Ratio of NRT dpa cross sections for ^{nat}Fe to ASTM E693 standard: calculated by **default** and **modified(NRT)** versions of NJOY-2012.50 from the ENDF/B-VII.1 files.

References

1. ASTM E693-12: "Standard Practice for Characterizing Neutron Exposures in Iron and Low Alloy Steels in Terms of Displacements Per Atom (DPA)", <http://www.astm.org/Standards/E693.htm>
2. M. J. Norgett, T. Robinson and I. Torrens, A proposed method of calculating displacement dose rates, Nucl. Eng. Des. 33 (1975) 50