

NJOY/BERSILLON-01 - 11 June 1993

Remark about the damage calculation in NJOY

by

**O. Bersillon
CEA BRC**

CEA

COMMISSARIAT A L'ENERGIE ATOMIQUE

DIRECTION DES APPLICATIONS MILITAIRES
CENTRE D'ETUDES DE BRUYERES-LE-CHATEL
SERVICE DE PHYSIQUE ET TECHNIQUES NUCLEAIRES
Section Recherches Fondamentales et Prospectives

O. Bersillon
☎ 69.26.54.14

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Monsieur Enrico SARTORI ↩

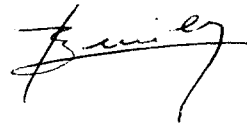
Nuclear Data Bank
OECD Nuclear Energy Agency
Le Seine St-Germain
12 boulevard des Iles
92130 ISSY-LES-MOULINEAUX

Cher Enrico,

Je te fais parvenir quelques remarques sur ce qui semble être une petite erreur dans le programme NJOY 91.38 au niveau du calcul du dommage. Pourrais-tu transmettre le document ci-joint à Bob MacFarlane pour lui demander son avis ?

Merci d'avance.

O. BERSILLON



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NJOY / BERSILLON - 01

Remark about the damage calculation in NJOY

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Olivier BERSILLON, June 1993

I tried to calculate the damage for ^{28}Si with NJOY 91.38. As a result it appears a large discontinuity in the damage around 5 keV . This discontinuity is entirely related to the elastic scattering contribution.

Looking in the code, it appears that the elastic scattering damage is calculated only for $E > \text{ENX}$ (line heatr.1200) where ENX is defined by

```
ENX = 6.25 / AFACT      (heatr.1163)
and AFACT = AWP/((AWR+1)**2 (heatr.1149)
```

which, for ^{28}Si , gives $\text{ENX} \simeq 5.26\text{ keV}$.

This "threshold energy" ENX seems to be related to the fact that the damage is non-zero only if the kinetic energy of the recoiling nucleus is greater than 25 eV .

But I have some doubt about the validity of the definition of ENX , which, to my opinion, should read

```
ENX = 6.25 / AFACT / AWR
(see my calculations below).
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Using this modification I get a nice shoulder for the low energy damage (above 188 eV instead of a discontinuity around 5.26 keV).

I would be glad to have your comments about this point.

Calculation of ENX

Using usual indices for a nuclear reaction (1 = incoming particle, 2 = target nucleus, 3 = outgoing particle, 4 = residual nucleus), the CM kinetic energy of the residual nucleus is given by

$$\bar{E}_4 = \frac{m_3}{M} \left(\frac{m_2}{M} (E_1 + Q) \right),$$

where E_1 is the lab kinetic energy of the incoming particle and $M = m_1 + m_2 = m_3 + m_4$.

In the lab system, we get

$$E_4 = \frac{m_3}{M} \left(\frac{m_2}{M} (E_1 + Q) \right) (1 + 2\gamma_4\mu_4 + \gamma_4^2),$$

where μ_4 is the cosine of the CM scattering angle and, for elastic scattering, $Q = 0$ and $\gamma_4 = 1$, so that, with $\mu_4 = -\mu_3$

$$E_4 = \frac{m_3 m_2}{M^2} 2E_1(1 - \mu_3).$$

For a given lab incident energy E_1 , the maximum value of μ_3 is given by

$$\mu_{3max} = 1 - \frac{M^2}{m_2 m_3} \frac{E_{4min}}{2E_1},$$

where $E_{4min} = 25 \text{ eV}$ in NJOY. In order to get a cosine greater than -1 , we must have

$$E_1 > \frac{M^2}{m_2 m_3} \frac{E_{4min}}{4},$$

which, coming back to the NJOY notations, reads

$$E_1 > \frac{(AWR + 1)^2}{AWR * AWP} \frac{25.0}{4}.$$

So, it seems that in NJOY the quantity AWR is missing in the denominator.