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Remark about the damage calculation in NJOY

by

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Monsieur Enrico SARTORI

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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

Remark about the damage calculation in NJOY

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 > 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 $ENX \simeq 5.26\,keV$.

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).

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

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

where E_1 is the lab kinetic energy of the incoming particule 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 $E_{4min} = 25\,eV$ 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.