JEFF-DOC-1223: NRT and MD models formalism

Norgett, Robinson & Torrens (NRT) model assesses initial no. of knock-on atoms:

Available Energy for lattice damage : $$E_a(E) = \sum_i \int_{E_d}^{T} \frac{d\sigma(E,T_i)}{dT_i} P(T_i)\ dT_i$$

where $P(T_i)$ - the portion of initial recoil energy T_i transferred to lattice atom

Displacement XS: $$\sigma = \frac{0.8}{2E_d} E_a$$

where E_d – energy needed to eject atom from lattice (= 40 eV for Fe)

Molecular Dynamics (MD) assesses survived defects after cascade cooling:

Point defects (Frenkel pairs), N_{FP}: $$\eta_{FP}(T) = \frac{N_{FP}}{N_{NRT}}$$

Interstitial Clusters, N_{IC}: $$\eta_{IC}(T) = \frac{N_{IC}}{N_{NRT}}$$

NJOY modification to incorporate defect surviving fraction from MD/BCA

Module HEATR calculates:

$$(MT = 444) = E_a(E) = \sum_i \int_{E_d}^{T} \frac{d\sigma(E, T_i)}{dT_i} P(T_i)\ dT_i \qquad \sigma = \frac{0.8}{2E_d} E_a$$

where $P(T_i)$ – partition function = the portion of recoil energy T_i transferred to lattice atom

function df(e,zr,ar,zl,al):

```
c   ********************************************************************  heatr.1707
c   damage function using the lindhard partition of                       heatr.1708
c   energy between atomic and electronic motion                           heatr.1709
c   call with e=0 for each reaction to precompute the constants           heatr.1710
c   ********************************************************************  heatr.1711
```

This function returns damage energy for every recoils having energy $e = T$

To account for MD results this df-function has to be multiplied by surviving fraction η :

either *function of e = T:* $df = df * \eta(T)$

or function of $df = E_{md}$: $df = df * \eta(df)$