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TITLE: ADVANCED NUCLEAR DATA FOR RADIATION-DAMAGE CALCULATIONS

AUTHOR(S): Robert E. MacFarlane and D. Graham Foster, Jr., T-2

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ADVANCED NUCLEAR DATA FOR RADIATION DAMAGE CALCULATIONS

Robert E. MACFARLANE and D. Graham FOSTER, JR.

Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, U.S.A.

Accurate calculations of atomic displacement damage in materials exposed to neutrons require detailed spectra for primary recoil nuclei. Such data are not available from direct experimental measurements. Moreover, they cannot always be computed accurately starting from evaluated nuclear data libraries such as ENDF/B-V that were developed primarily for neutron transport applications, because these libraries lack detailed energy-and-angle distributions for outgoing charged particles. Fortunately, a new generation of nuclear model codes is now available that can be used to fill in the missing spectra. One example is the preequilibrium statistical-model code GNASH. For heating and damage applications, a supplementary code called RECOIL has been developed. RECOIL uses detailed reaction data from GNASH, together with angular distributions based on Kalbach-Mann systematics to compute the energy and angle distributions of recoil nuclei. The energy-angle distributions for recoil nuclei and outgoing particles are written out in the new ENDF/B "File 6" format. The result is a complete set of nuclear data that can be used to calculate displacement-energy production, heat production, gas production, transmutation, and activation. Sample results for iron are given and compared to the results of conventional damage models such as those used in NJOY.

1. INTRODUCTION

One important component of radiation damage in fusion reactor materials is the large cluster of displaced atoms produced by the recoil nucleus from a neutron-induced reaction. The number of atoms displaced depends on the energy of the recoil nucleus and the partition of this energy between atomic motion and electronic excitations. For metals, the displacement damage is often assumed to be proportional to a "damage-energy production cross section," obtained by folding the energy spectrum of the primary recoil nucleus together with a partition function derived from electron screening theory. Therefore, the nuclear part of the problem is reduced to obtaining accurate recoil spectra.

In some cases, it is quite easy to calculate the required recoil spectra.[1] For elastic scattering, they can be computed by conservation of momentum using angular distributions available from the Evaluated Nuclear Data Files (ENDF/B).[2] Recoils from discrete-level inelastic scattering can also be computed accurately in this way because the photon momentum can be neglected. Finally, recoils from the radiative capture reaction (n,γ) can be calculated. In this case, the photon momentum cannot be neglected below 25-100 keV, but reasonable approximations[1] are available for this range. These methods allow for accurate calculations of damage-energy production from thermal energies to the thresholds of the more complex reactions. These thresholds vary from a few MeV for light metals to a few hundred keV for heavy metals.

Fusion devices, however, have many neutrons in the 1 to 14-MeV range. It is important to include the so-called "continuum" scattering reaction, other absorption reactions such as (n,p) and (n,α), and (n,2n) reactions. Even higher neutron energies will be common in d-Li sources such as the Fusion Materials Irradiation Test Facility (FMIT). This will require more attention to three-particle reactions like (n,n'α). At these high energies, the current generation of damage and heating codes rapidly loses accuracy, because the required spectra are not available in compilations such as ENDF/B-V, which were primarily intended for neutron-transport applications.

Fortunately, it is now becoming possible to compute the spectra of particles emitted from these high-energy reactions with reasonable accuracy using modern preequilibirum statistical-model codes such as GNASH.[3] A description of the methods used in GNASH is given in Section 2. These spectra can be combined with angular distributions based on Kalbach-Mann systematics[4] (see Section 3) to obtain distributions in energy and angle for the recoil nucleus. This step is performed by the RECOIL code described in Section 4. Instead of the traditional damage cross section, RECOIL tabulates all the particle and recoil distributions directly using the new ENDF/B File 6 format (see Section 5). These tabulated spectra can then be used in a subsequent code to compute damage in metals, or the same recoil data can be used with a different partition function to compute damage for non-metallic materials such as ceramics. Some results and comparisons for iron are given in Section 6.

2. THE GNASH CODE

The GNASH claculation begins with the compound system formed by the interaction of a neutron having a specified laboratory energy with a particular target nucleus. A set of residual nuclei is then defined that can be reached from the initial compound system by various sequences of particle emission. Each nucleus is characterized by a particular separation energy, a set of discrete levels, and a set of continuum energy bins.

For every bin of each compound system, GNASH computes the probability of particle or photon emission. At high enough incident energy, particle emissions from the first compound system are affected by preequilibirum processes that are calculated using the Master Equation model of Kalbach.[5] As will be seen later, the "preequilibrium ratio" versus energy for each particle is useful for determining its angular distribution. Particle emission probabilities are determined from transmission coefficients based on optical model parameters. For materials like iron, these optical model parameters can be adjusted[6,7] to give good agreement with measured cross sections. The good agreement obtained gives confidence in the results for unmeasured isotopes or energy ranges.

Gamma emission is important due to its effect (through competition) on particle emission, as well as for its direct effects. Continuum emission is computed using transmission coefficients based on the Brink-Axel giant dipole resonance model.[8] For iron, the coefficients were normalized to give good fits to capture cross sections.[6,7] Detailed transition probabilities can be input for discrete photon emission.

GNASH represents continuum excitation energy regions through use of a level density model. For iron, the model of Gilbert and Cameron[9] with the parameters of Cook[10] was employed. Additionally, adjustments were made at lower excitation energies to match available discrete level information.

During a calculation, GNASH prepares a printer output file containing run parameters, a preequilibrium summary, discrete-level data, cross sections, and various accumulated spectra for particles and photons. Additionally, it provides detailed transition probabilities in the form of "population increments" on an auxilliary binary output file. As discussed in Section 4, these population increments can be used to derive particle spectra by reaction.

3. KALBACH-MANN SYSTEMATICS

By studying existing measurements of secondary-particle spectra for incident particle energies between 20 and 60 MeV, Kalbach and Mann[4] have derived a simple technique for predicting such distributions with reasonable accuracy. The form of their result adopted for ENDF/B-VI is

$$f(\mu,E\to E') = \sum_{\ell} \frac{2\ell+1}{2} f_\ell(E\to E')P_\ell(\mu) \quad , \qquad (1)$$

where

$$f_\ell = \begin{cases} a_\ell & \text{if } \ell = 2,4,6,\ldots, \\ ra_\ell/(1+r) & \text{if } \ell = 1,3,5,\ldots, \end{cases} \qquad (2)$$

$$a_\ell = \frac{2f_0}{1+\exp[A_\ell(B_\ell-E')]} \quad , \qquad (3)$$

$$A_\ell = 0.036 + 0.0039[\ell(\ell+1)]\text{MeV}^{-1} \quad , \qquad (4)$$

and

$$B_\ell = 92.0 - 90.0 \frac{1}{\sqrt{\ell(\ell+1)}} \text{ MeV} . \qquad (5)$$

In Eq. (2), r is the "preequilibrium ratio" that is obtained from GNASH. Note that f_0 is the total emission probability for a particular E and E'. These coefficients are for the center of mass of the initial colliding system.

The Kalbach-Mann representation implies that energetic emitted particles (which usually have $r \sim 1$) will have forward-peaked distributions. On the other hand, low-energy particles or particles from states with a high compound-nucleus fraction ($r \sim 0$) will be emitted with nearly isotropic distributions.

4. THE RECOIL CODE

RECOIL begins by reading and re-organizing the information available from a completed GNASH run. Preequilibrium ratios and photon level data are read from the printer output file. Global parameters, energy level schemes, and population increment data are read from the auxiliary binary output file. While this information is being gathered, the RECOIL code can optionally exclude neutron compound elastic scattering, neutron discrete-inelastic scattering, and/or discrete-level particle production steps from the reaction data. These reactions and the "shape elastic" term can normally be computed more accurately using optical model codes.

Next, this reaction data is used to produce all possible "reaction stars." Each "star" consists of a series of steps characterized by a particular emitted particle of a particular energy. The probability of observing a particular star is just the product of the probabilities for each step as obtained from GNASH. Once a star has been formed, it is easy to determine that it belongs to a particular reaction, say (n,n'p). RECOIL ignores the order of the steps, and (n,n'p) will actually be the sum of (n,n'p) and (n,pn). Thus a "reaction" in this sense is characterized by a particular recoil nucleus.

The center-of-mass (CM) momentum of this recoil nucleus is simply the negative of the vector sum of the momenta of all emitted particles. For two-particle final states, the calculation is easy and reliable. The CM energy of the recoil is scaled from the energy of the emitted particle using the appropriate mass ratio and accumulated into the appropriate bin of the recoil spectrum. The angular distribution for the recoil nucleus is just the complement of the distribution of the emitted particle as given by Kalbach-Mann systematics.

For complex reactions, a more approximate method is used. The full angular range for each emitted particle is sampled systematically (not randomly), using a Kalbach-Mann or uniform distribution. This divides each "star" into a large number of "substars" each with its own probability. The energy and emission angle of the recoil nucleus of each substar are then computed and used to increment the energy-angle distribution for that particular recoil nucleus.

When all stars have been processed, the result is a set of reaction cross sections and coupled energy-angle distributions for each emitted particle and each recoil nucleus.

5. THE ENDF/B FILE 6 FORMAT

As mentioned in the Introduction, it is desirable to save these distributions in full detail for later use. For just this kind of application, a new ENDF/B format was recently adoped for use in ENDF/B-VI. This format is called "FILE 6, PRODUCT ENERGY-ANGLE DISTRIBUTIONS" and is a completely new form of the previously unused File 6.

For the purposes of this file, any reaction is defined by giving the production cross section for <u>each</u> reaction product as a product of a reaction cross section, a product yield or multiplicity, and a normalized distribution for the product in energy and angle. As usual, the cross section is given in File 3; the other two factors are given in File 6. Correlations and sequences are ignored; that is, the distributions given are those which would be seen by an observer outside of a "black box" looking at one particle at a time. The process being described may be a combination of several different reactions, and the product distribution may be described using several different representations.

For the GNASH results as processed by RECOIL, the most appropriate representation is "Tabulated Continuum Energy-Angle Distribution" (LAW=5) with Legendre coefficients (IANG=1) in the CM system (LCT=2). For each incident energy E, a set of secondary energies E' is defined. For each secondary-energy bin, an emission probability $f_0(E \to E')$ and its Legendre coefficients $f_\ell(E \to E')$ are given.

Other possible representations include discrete laws and a direct tabulation of the precompound ratio for the Kalbach-Mann representation.

Because the new File 6 gives explicit yields for each particle and residual nucleus, it can be used easily to generate gas production and activation cross sections. Thus, all the information needed for heating, damage, gas production, activation, neutron transport, and particle transport is provided by File 3 and File 6 in a uniform and consistent way.

6. RESULTS

Existing GNASH calculations for iron[6,7] have been processed into File 6 format using RECOIL and an auxiliary code called MAKE6. At the same time, heat production and damage-energy production were computed from the calculated spectra. Sample results for the nonelastic damage and total heating are given in Table I, together with corresponding results from previous methods.[1] For this example, the differences in damage production are modest with the RECOIL results at 14 MeV lying about 7% lower than

TABLE I

Comparison of Damage-Energy Production and Heat Production for ^{56}Fe Computed by RECOIL with Results for ENDF/B-V Natural Iron Computed by Conventional Methods (Ref. 1).

Energy (MeV)	RECOIL Damage[a] (keV·b)	ENDF/B-V Damage[a] (keV·b)	RECOIL Heat (MeV·b)	ENDF/B-V Heat (MeV·b)
10	174.5	192.4	0.972	-0.095
11	183.8	207.1	1.104	0.026
12	193.2	219.4	1.237	0.390
13	204.0	225.6	1.421	-[illegible]863
14	215.8	231.9	1.622	-1.096
15	228.6	238.7	1.836	-2.451
16	241.9	252.1	2.083	-3.047
17	254.2	246.8	2.337	-0.310
18	265.9	262.3	2.614	1.482
19	275.7	261.0	2.871	2.006
20	283.7	259.5	3.106	2.602

[a] Nonelastic part only

results at 14 MeV lying about 7% lower than ENDF/B-V values. Improvement in the heating numbers is more dramatic. The difficulties in computing kerma from ENDF/B-V are well known;[11] for iron, the problems include neutron-photon energy-balance errors and the difficulty in working with a natural-element file.

Figure 1 compares two important parts of the calculated damage-energy production to the previous results. The RECOIL results have been adjusted to use the ENDF/B-V cross sections. Thus, the differences seen in the figure represent real spectral differences. In the case of (n,2n), there are differences in the neutron spectra coming from GNASH, but some of the difference comes from the two-step emission process modeled in RECOIL.

Finally, Fig. 2 shows two typical recoil spectra as computed by these methods. Note the effects of discrete levels which show up in the inelastic recoil spectrum at high energies.

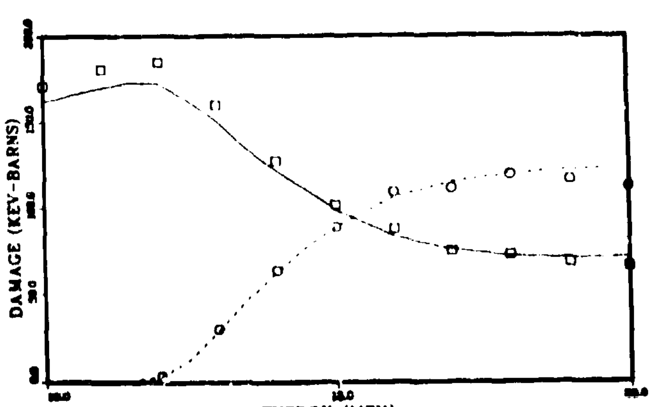

FIGURE 1
Calculated damage-energy production for ^{56}Fe inelastic (solid) and (n,2n) (dashed) compared with results for ENDF/B-V natural iron using conventional methods.[1] Calculations were renormalized to the ENDF/B cross sections in order to highlight the recoil spectrum differences.

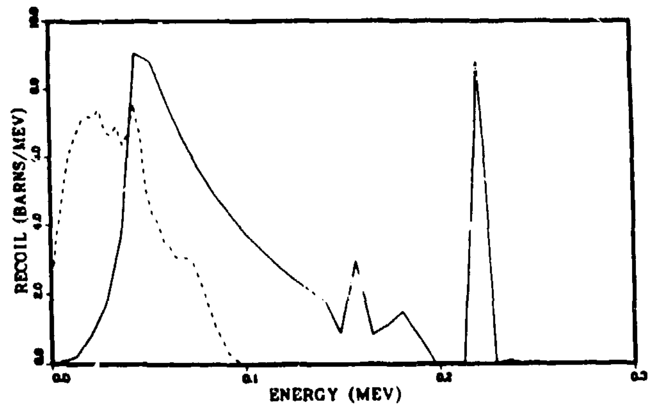

FIGURE 2
Typical recoil spectra for ^{56}Fe at 14 MeV. Solid curve is inelastic and dashed curve is (n,2n).

7. CONCLUSIONS

The RECOIL code and the new ENDF/B File 6 provide a convenient way to make nuclear model calculations available for applications. Preliminary results for energies up to 20 MeV show modest improvements in damage-energy calculations and dramatic improvements in kerma factors. In addition, these methods provide a way to obtain reliable nuclear parameters in the range 20-50 MeV, which will be important for future studies of damage in fusion reactor materials.

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