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Title: NJOY/HEATR: What It Calculates Now, What Should It Calculate?

Author(s): Kahler, Albert C. III

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NJOY/HEATR: What It Calculates Now, What Should It Calculate?

A. C. (Skip) Kahler
Theoretical Division
Los Alamos National Laboratory

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from nuclear reaction to point defects"

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Abstract

We review some basic aspects of the Evaluated Nuclear Data File (ENDF) format and summarize some of the processing options currently available in NJOY's HEATR module.

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Presentation Outline

- **Opening Remarks/Introduction**
- **Details of an ENDF File**
- **What NJOY/HEATR Calculates**
- **Conclusions**

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NJOY/HEATR … what it calculates now

- NJOY is an ENDF (Evaluated Nuclear Data File) Processing code.
  - What is ENDF?
    - A data file containing tabulated nuclear cross section data
      - Cross Section vs. Energy by reaction;
      - Angular distributions of outgoing reaction products;
      - Secondary Energy Distribution (outgoing particle energy distributions as a function of incident particle energy.
    - ENDF was initially developed in the mid-1960s
      - Has evolved through 7 primary "generations" over 40+ years;
      - The primary emphasis for much of this time has been to define what are believed to be increasingly accurate nuclear data;

        i.e. … best estimate of the mean value
      - Inclusion of uncertainties and covariances for these data is still an immature and evolving field.

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NJOY/HEATR … what it calculates now

- As a product of the 1960s, the ENDF format is rooted in an old technology
  - Data are given in a fixed record length (80 characters/line)
    - Specific record formats are defined containing integers and real numbers in fixed (i11 or 1pe11.0) format;
    - 6 values per record plus a fixed set of 4 control integers (matn, mf, mt, ns);
      - matn (I4) = material number (a unique number per nuclide within a given ENDF generation);
      - mf (I2) = a file number where a pre-defined type of data are defined;
        e.g. MF=3 = list of [σ(e), e]; MF=5 = secondary energy dists
      - mt (I3) = a specific reaction;
        e.g. MT=2 = elastic scattering; MT=16 = (n,2n); MT=102 = (n,γ)
      - ns (I5) = sequence number … allows you to sort your deck into proper order after having dropped the cards!

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NJOY/HEATR … what it calculates now

- The current ENDF format is known as ENDF-6
  - Used to define ENDF/B-VI.x and ENDF/B-VII.x data files.
- The latest version of the ENDF format manual is available from the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL)
  - http://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf
- CSEWG = Cross Section Evaluation Working Group
  - An advisory organization that coordinates evaluation work leading to new evaluated data files;
    - Also is responsible for maintaining and updating the ENDF format.
  - A new, "Generalized Nuclear Data" format is under development.
    - See the December, 2012 issue of Nuclear Data Sheets for details

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NJOY/HEATR … what it calculates now

- The opening slide says "NJOY is an ENDF Processing Code"
  - So … what does it "process"? We start with an ENDF-formatted file, what do we end up with?
  - Primary use is to develop application libraries for continuous energy transport calculations with LANL's MCNP code;
    - i.e., NJOY creates "ACE" files for MCNP use;
      - Cross sections, angular distributions, secondary energy distributions;
      - Derived quantities, such as KERMA (Kinetic Energy Release in Materials) and Radiation Damage.
  - Can also create multi-group files;
  - Can produce plots of cross sections & distributions;
  - Can produce plots of uncertainties and covariance matrices;
    - MF3 = cross sections; MF33 = cross section covariances

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NJOY/HEATR … what it calculates now

- KERMA – a "derived" quantity within the ENDF system
  - Has an assigned "MT" number in the ENDF format so that KERMA by reaction type is defined
    - MT for KERMA of reaction MT_R is defined to be $(300+MT_R)$
      - MT values from 301 to 450 are reserved for "energy release"
    - "derived" means these data are NOT part of an original ENDF-formatted file
      - Represents the results of a calculation within NJOY (or any other processing code), but is not a fundamental component of an evaluated file.

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NJOY/HEATR … what it calculates now

Heating, therefore, is often described by KERMA[28] (Kinetic Energy Release in Materials) coefficients $k_{ij}(E)$ defined such that the heating rate in a mixture is given by

$$H(E) = \sum_i \sum_j \rho_i k_{ij}(E)\phi(E) , \quad (160)$$

where ρ_i is the number density of material i, $k_{ij}(E)$ is the KERMA coefficient for material i and reaction j at incident energy E, and $\phi(E)$ is the neutron or photon scalar flux at E. KERMA is used just like a microscopic reaction cross section except that its units are energy × cross section (eV-barns for HEATR). When multiplied by a flux and number density, the result would give heating in eV/s.

The "direct method" for computing the KERMA coefficient is

$$k_{ij}(E) = \sum_\ell \overline{E}_{ij\ell}(E)\sigma_{ij}(E) , \quad (161)$$

where the sum is carried out over all charged products of the reaction including the recoil nucleus, and $\overline{E}_{ij\ell}$ is the total kinetic energy carried away by the ℓ^{th} species of secondary particle. These kinds of data are now becoming available for some materials with the advent of ENDF/B-VI and ENDF/B-VII, but earlier ENDF/B versions did not include the detailed spectral information needed to evaluate Eq. 161.

For this reason, NJOY computes KERMA factors for many materials by the "energy-balance method"[40]. The energy allocated to neutrons and photons is simply subtracted from the available energy to obtain the energy carried away by charged particles:

$$k_{ij}(E) = \left(E + Q_{ij} - \overline{E}_{ijn} - \overline{E}_{ij\gamma}\right)\sigma_{ij}(E) , \quad (162)$$

where Q_{ij} is the mass-difference Q value for material i and reaction j, $\overline{E}_n$ is the total energy of secondary neutrons including multiplicity, and $\overline{E}_\gamma$ is the energy of secondary photons including photon yields.

Use eq. 161 when possible, but usually can't with pre-ENDF/B-VI.x files due to incomplete spectra (particularly for the heavy recoil product).

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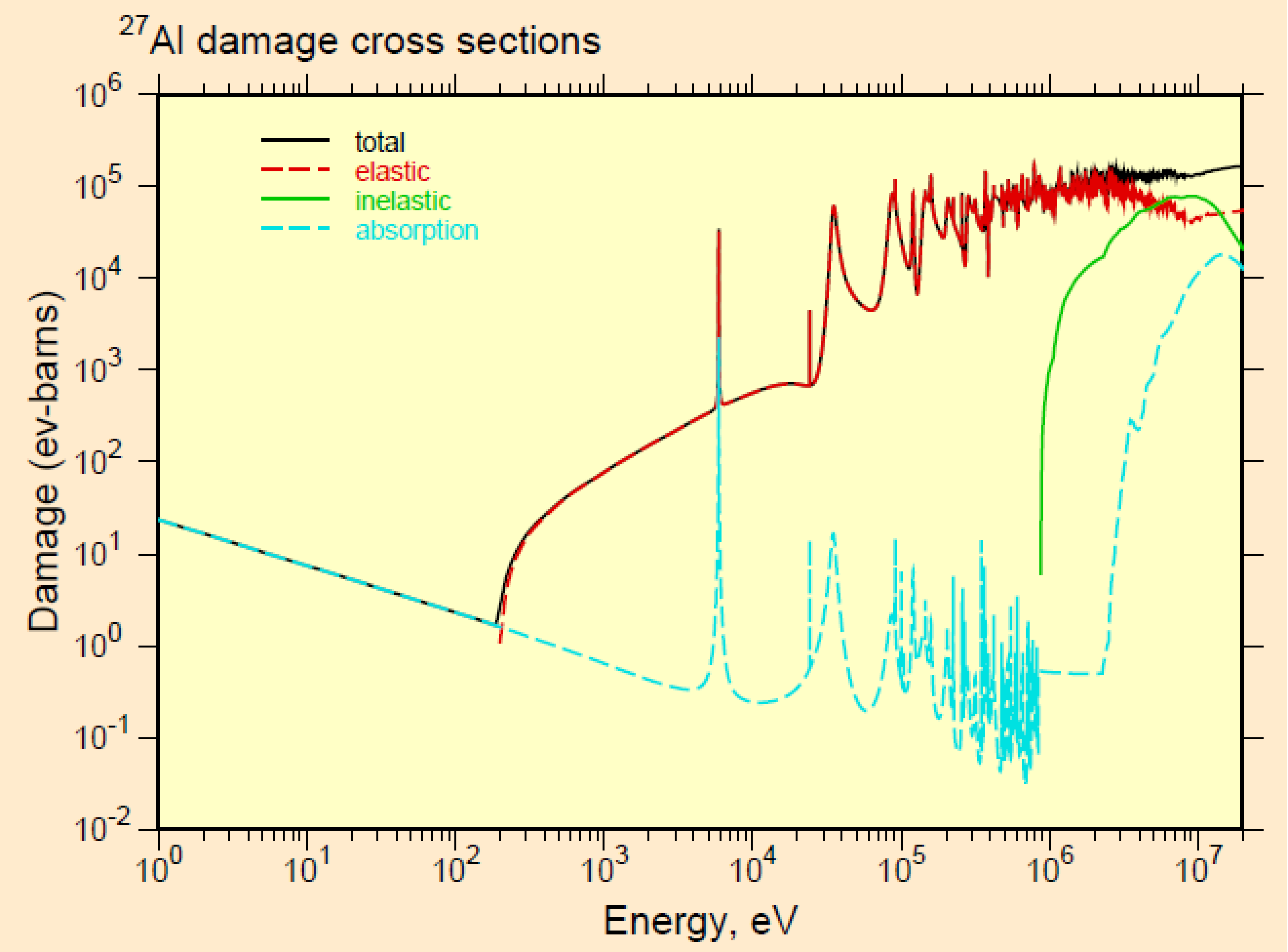
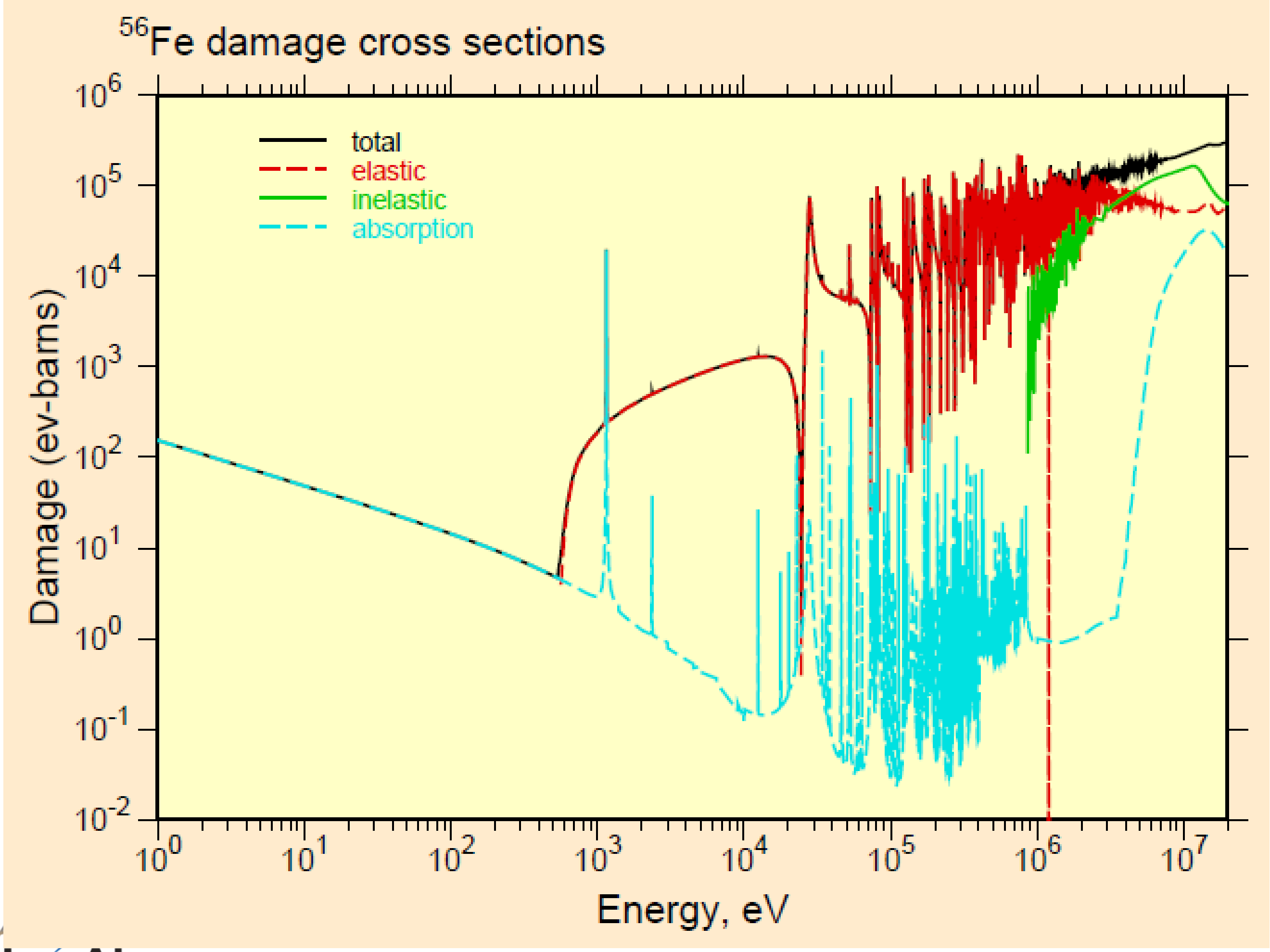
NJOY/HEATR … what it calculates now

- **Radiation Damage …**
  - NJOY assigns MT values of 444, 445, 446 & 447 for total, elastic, inelastic and absorption damage.
  - NJOY has performed "radiation damage" calculations since the early 1980s
    - "Radiation Damage Calculations with NJOY", R.E.MacFarlane, D.W.Muir and F.M.Mann, J. of Nucl Mat'ls, 122 (1984) 1041.
  - If present, MT444 is included by NJOY in the MCNP ACE file.
  - MT444, "dame", is also recognized by the MATXSR module.
- **Examples (^{27}Al and ^{56}Fe) follow …**

NJOY/HEATR … what it calculates now



NJOY/HEATR … what it calculates now



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NJOY/HEATR … what it calculates now

- So far we described the ENDF system and said NJOY calculated something it calls "Radiation Damage" in the mid-1980s …
- … we have shown some pretty pictures …
- … but what are the methods used, and
- … are those methods "state of the art"?
  - Probably not or we wouldn't be here this week!

NJOY/HEATR … what it calculates now

NJOY/Radiation Damage …

A large cluster of lattice defects can be produced by the primary recoil nucleus of a nuclear reaction as it slows down in a lattice. It has been shown that there is an empirical correlation between the number of displaced atoms (DPA, displacements per atom) and various properties of metals, such as elasticity. The number of displaced atoms depends on the total available energy E_a and the energy required to displace an atom from its lattice position E_d. Since the available energy is used up by producing pairs,

$$\mathrm{DPA} = \frac{E_a}{2E_d} \; . \qquad (165)$$

The values of E_d used in practice are chosen to represent the empirical correlations, and a wide range of values is found in the literature[42, 43, 44]. Table 2 gives the default values used in NJOY2012. The energy available to cause displacements is what HEATR calculates. It depend on the recoil spectrum and the partition of recoil energy between electronic excitations and atomic motion. The partition function used is given by Robinson[45] based on the electronic screening theory of Lindhard[46] (see Fig. 9).

[42] T. A. Gabriel, J. D. Amburgy, and N. M. Greene, "Radiation-Damage Calculations: Primary Knock-On Atom Spectra, Displacement Rates, and Gas Production Rates," *Nucl. Sci. Eng.* 61, 21 (1976).

[43] D. G. Doran, "Neutron Displacement Cross Sections for Stainless Steel and Tantalum Based on a Linhard Model," *Nucl. Sci. Eng.* 49, 130 (1972).

[44] L. R. Greenwood and R. K. Smither, "Displacement Damage Calculations with ENDF/B-V," in Proceedings of the Advisory Group Meeting on Nuclear Data for Radiation Damage Assessment and Reactor Safety Aspects, October 12-16, 1981, IAEA, Vienna, Austria (October 1981).

[45] M. T. Robinson, in *Nuclear Fusion Reactors* (British Nuclear Energy Society, London, 1970).

[46] J. Lindhard, V. Nielsen, M. Scharff, and P. V. Thomsen, *Kgl. Dansk, Vidensk. Selsk, Mat-Fys. Medd.* 33 (1963).

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NJOY/HEATR … what it calculates now

NJOY/Radiation Damage …

Table 2: Typical Values for the Atomic Displacement Energy Needed to Compute DPA[44].

Element	E_d, eV	Element	E_d, eV
Be	31	Co	40
C	31	Ni	40
Mg	25	Cu	40
Al	27	Zr	40
Si	25	Nb	40
Ca	40	Mo	60
Ti	40	Ag	60
V	40	Ta	90
Cr	40	W	90
Mn	40	Au	30
Fe	40	Pb	25

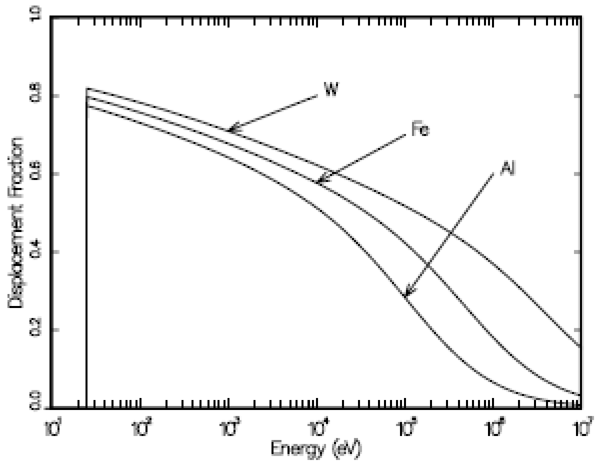

Figure 9: Examples of the portion of the primary recoil energy that is available to cause lattice displacements in metallic lattices. The remaining energy leads to electronic excitation. The quantity plotted is $P(E)$ from Eq. 195 divided by E. The 25 eV cutoff is also discussed in connection with Eq. 195.

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NJOY/HEATR … what it calculates now

NJOY/Radiation Damage …

A fully-populated section of File 6 contains subsections for all of the particles and photons produced by the reaction, including the recoil nucleus. There are a number of different schemes used to represent the energy-angle distributions for these outgoing particles. The most important ones for HEATR follow:

- *No distribution.* In this case, the subsection is inadequate for use in heating and damage calculations. A warning message is issued.
- *Two-body angular distribution.* These are basically the same as distributions in File 4.
- *Recoil distribution.* This particle is a recoil nucleus from a two-body reaction. Its angular distribution is assumed to be the complement of the angular distribution for the first subsection in this section.
- *CM Kalbach distribution.* This format is often used by LANL evaluations, and transformation to the laboratory frame is required. The looping order for the data is E, E', μ.
- *LAB Legendre distribution.* This format is used in most of the ORNL evaluations for ENDF/B-VI. It is already in the laboratory frame, and the angular information can be simply ignored.
- *LAB angle-energy distribution.* This format is used for the ^{9}Be evaluation of ENDF/B-VI by LLNL. The looping order is E, μ, E'.

The normal procedure is to loop through all of these subsections. The subsections producing neutrons are processed to be used in a total energy check, but they contribute nothing to the heating or to the damage. Subsections describing charged particles and residual nuclei are processed into heating and damage contributions. Finally, the photon subsection is processed for the photon energy check and the total energy check, even though it does not affect either heating or damage. Any remaining difference between the eV-barns available for the reaction and the eV-barns carried away by the neutrons, photons, particles, and recoil is added into the heating to help preserve the total energy deposition in the spirit of the energy-balance method.

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NJOY/HEATR … what it calculates now

NJOY/Radiation Damage …

The ENDF/B-VII library contains a few abbreviated versions of File 6 that contain an energy-angle distribution for neutron emission, but no recoil or photon data. In order to get semi-reasonable results for both heating and damage for such cases, HEATR applies a "one-particle recoil approximation," where the first particle emitted is assumed to induce all the recoil. There are also some cases where capture photons are described in MF=6/MT=102 with no corresponding recoil data. Here, the recoil can be added using the same logic described above for capture represented using File 15. The difference between the eV-barns available for the reaction and the energy accounted for by the emitted neutrons, photons, particles, and the approximated recoil is added into the heating in order to preserve the total heating in the spirit of the energy-balance method.

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NJOY/HEATR … what should it calculate?

- If we had the answer we would not be here!

- NJOY has the flexibility to include new or revised methods
  - We would not expect NJOY Users to specify non-ENDF database sources

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Concluding Remarks

- NJOY has been, and will continue to be, an ENDF-formatted data processing code.
  - Limited physics capability can be directly hard-wired into the code with User specification of specific options/models
  - NJOY input includes original or previously processed ENDF data plus User options
  - NJOY input does not include non-ENDF database sources