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New nuclear data evaluations for Ge isotopes

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Abstract

New ENDF-6 formatted nuclear data libraries are presented for ^{70,72,73,74,76}Ge, for incident neutrons and protons. Apart from the resonance range, which we have adopted from the best available source in existing libraries, the nuclear data evaluations are completely revised in the 0–20 MeV energy range, and moreover extend up to 200 MeV. This collection of isotopic evaluations is created by using the nuclear model code TALYS with a consistent set of input parameters for all isotopes. The most important nuclear reaction models needed for our data files are described. We have intended to make these evaluations complete in their description of reaction channels, and use a consistent method to store the data in ENDF-6 format, which include cross sections, angular distributions, double-differential spectra, discrete and continuum photon production cross sections and residual production (activation) cross sections including isomers. It is shown that the data present in our libraries give an improved agreement with existing basic experimental data.

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1. Introduction

The quality and reliability of the computational simulation of a macroscopic nuclear device is directly related to the quality of the underlying basic nuclear data. The argument that microscopic nuclear experiments and theory development are imperative to enhance the status of applied nuclear research is generally accepted and in fact used by several institutes to defend their scientific program. Maybe less transparent is *how* this microscopic information can actually be applied. This brings us directly to the task of a nuclear data evaluator, namely the provision of the *quantitative* link between two huge fields of research: fundamental nuclear physics and nuclear applications. This is done by means of a so-called evaluated data file. Often, a data file consists of a mixture of experimental data and calculated results, computed from nuclear reaction models or even simple systematics. As long as the contents of the data file are in correspondence with reality, any combination of these inputs is allowed. This is to serve the common goal of nuclear data evaluation: to store all possible reaction channels on a data file, with maximum quality of the cross sections and other quantities like resonance and fission parameters. In this paper, this will be done for all Ge isotopes. When it comes to nuclear data evaluation, Ge has not yet received the same attention as the major actinides and structural materials such as Fe, Si, etc., since their careful evaluation has not been regarded as crucial for applications that have dictated nuclear data development in the past, such as existing power reactor plants. Ge is however an important detector material and a precise analysis of neutron reactions, especially elastic and inelastic scattering and the associated gamma-ray production, may have important consequences for any application employing Ge-detectors, such as geophysics and oil-well logging.

Through this paper, we aim to deliver a more reliable starting point for detector simulations with new nuclear data libraries for all Ge isotopes. This is accomplished by using the present database for basic experimental data,

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the current status of nuclear reaction modeling and the current possibilities that the evaluated nuclear data format (ENDF-6) gives to store nuclear data in evaluated data libraries. We have developed a consistent data evaluation methodology for the entire 0–200 MeV energy range. Apart from the resonance range, for which we have adopted the best possible data from existing libraries, the nuclear data libraries we describe here are completely new, i.e. from the keV region up to 200 MeV. In fact, this methodology to revise a datafile over the entire energy range is now applied to every nuclear data evaluation project we work on. Where possible, i.e. when integral experimental data is available, we directly iterate the evaluation process with integral validation.

The evaluated data files are based primarily on a theoretical analysis with the nuclear model code TALYS [1], version 0.64. On the basis of a large suite of implemented nuclear reaction models, this code is able to produce a complete set of cross sections, yields, energy spectra and angular distributions. In the evaluation process, the nuclear model parameters of TALYS are adjusted to reproduce the existing experimental data, while we also include experimental data directly if we judge these to be of better quality than, and to significantly deviate from, our model calculations. With additional ENDF-6 formatting software, we produce data files that provide a complete representation of nuclear data needed for transport, radioactivity and shielding applications over the incident neutron energy range from 10^{-5} eV to 200 MeV. All isotopic evaluations are of comparable quality: For each isotope, the same set of nuclear models is used and, equally important, the same set of ENDF-6 formatting procedures. Of course, nuclear model parameters differ from isotope to isotope. The same approach has been applied to the isotopes of other materials: Ca and Sc [2], Pb and Bi [3], Fe [4], Rh [5], I and T_c, which may eventually lead to a nuclear data library with mutually consistent evaluations. All isotopic evaluations discussed in this paper are included in the JEFF-3.1 data library [6]. Moreover, proton data libraries are produced.

In Section 2, the modeling of nuclear reactions as performed with the TALYS code is described in some detail. In Section 3, the contents of our libraries are compared with existing microscopic experimental data. Section 4 contains an outline of the ENDF-6 formatting methods that were used to store the data. Finally, in Section 5 we give the conclusions.

2. Nuclear modeling

Nuclear model software has become indispensible in modern nuclear data evaluation. To perform adequate inter- and extrapolation on the energy and angular grids per reaction channel, transport and reactor codes rely on a complete description of a nuclear reaction in a data file, and not only on the data that happen to be available through measurements. The preferred method is to let a nuclear model code generate an evaluation that is entirely complete in its description of reaction channels: with incident and outgoing particle energies and angles on a sufficiently dense grid, and all possible reaction yields. The adjustable parameters of the nuclear model code should be fitted to reproduce the experimental data available for the nucleus under study. The starting point is then a complete data file of reasonable, and often good, quality. Next, this evaluation needs to be updated with the crucial experimental data points with a precision that cannot be accomplished by the model code. This concerns always the resolved resonance range, and sometimes the unresolved resonance and fast neutron range (especially for light and fissile nuclides). Thus, the model code ensures the completeness of the data file, and the model code + experimental data the highest possible quality, i.e. realistic values, of the data file at a given moment in time. The process needs to be repeated whenever better versions of the model code and more precise experimental data become available. If the methodology is well-automated and properly quality assured, such revisions will take much less time than the first evaluation (which we present in this paper).

2.1. TALYS code

TALYS is a computer code system for the prediction and analysis of nuclear reactions. TALYS simulates reactions that involve neutrons, gamma-rays, protons, deuterons, tritons, helions and alpha particles, in the 1 keV to 200 MeV energy range and for target nuclides of mass 12 and heavier. This is achieved by implementing a suite of nuclear reaction models into a single code system. It enables to evaluate nuclear reactions from the unresolved resonance region up to intermediate energies. The evaluations described in this paper are based on a theoretical analysis that utilizes the optical model, compound nucleus statistical theory, direct reactions and pre-equilibrium processes, in combination with databases and models for nuclear structure. Fig. 1 summarizes the nuclear models implemented in TALYS. The following output that is produced by TALYS is stored in the nuclear data files:

- total, elastic and non-elastic cross sections,
- elastic scattering angular distributions,
- inelastic scattering cross sections and angular distributions to discrete states,
- exclusive channel cross sections, e.g. (n,γ), $(n,2n)$, $(n,np),\ldots$, energy and double-differential spectra,
- gamma-ray production for discrete states and continuum,
- isomeric and ground state cross sections,
- residual production cross sections,
- total particle cross sections, e.g. (n,xn), $(n,xp),\ldots$, energy and double-differential spectra.

Besides the ENDF-formatted data file, all data is also produced in easily readable files, per reaction channel,