Graphical Handling of Wide-Ranging Data: Graphing of Photon Cross-Section Data

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Graphical representation of photon cross-section data in the XGAM database, from the National Institute of Standards and Technology, is described. An algorithm has been designed to manage the very widely ranged data that are encountered in this application. The graphs are all generated on a personal computer (IBM or compatible) and can be used to calculate photon cross sections for scattering, photoelectric absorption, pair production, and total attenuation coefficients for any element, compound, or mixture.

INTRODUCTION

The National Institute of Standards and Technology (NIST; formerly known as the National Bureau of Standards) has had a longstanding program to compile and evaluate data on the interaction of high-energy electromagnetic radiation with matter. The results of these critical evaluations of cross sections for photon interactions in the X-ray and γ-ray regions have been published over the years by Hubbell, Berger, and other co-workers.[1,2] In the early 1980s computerized representations of these data were developed by Berger, Seltzer, and Hubbell,[3] and a database in magnetic tape form was released in 1985 under the name XGAM. Subsequently, XGAM was converted to a personal computer version by M. J. Berger and released in diskette format in 1988.

XGAM allows the retrieval, for all elements through fermium (Z = 100), of photon cross sections for scattering, photoelectric absorption, and pair production, as well as total attenuation coefficients. The recommended data appearing in the publications cited above are stored at discrete energy values, and interpolative programs provide the user with results at any arbitrary energy value selected. The sharp "absorption edges" characteristic of these data in the X-ray region are stored individually for each element and are accounted for by the interpolation program. The programs in XGAM were designed to calculate the scattering and absorption data that are frequently required for scientific, engineering, and medical applications.

Photon cross sections for scattering, photoelectric absorption, and total attenuation coefficients for any element, compound, or mixture at energies ranging from 1 keV to 100 GeV can be generated. The calculations can be carried out by using a standard energy grid, spaced approximately logarithmically, a user-defined grid, or a combination of both. The output provided consists of complete or partial tables that corresponded closely in format to existing tables in the literature and that are convenient for further calculations. Total cross sections and attenuation coefficients are calculated as partial cross sections for coherent and incoherent scattering, photoelectric absorption, and pair production in an atom's nuclear and electronic fields.

In the original XGAM, no attempt was made to provide graphical displays of the information; all data were displayed in tabular form, and this presented a problem because for the energy ranges that are involved, a very large number of data points are available. Such voluminous data require many pages, or computer screens, for display. Accordingly, we have given some attention to the problems of representing these data in a graphical format that is comprehensive and easily read and assimilated. The results of this work are presented in this paper. A personal computer program that allows such presentation of the data is described, and some examples of its use are given.

PROCEDURES

The output of the original XGAM consisted of tables of photon cross sections for scattering and coherent and incoherent photoelectric absorption. Further tables covered pair production in nuclear and electronic fields and total attenuation coefficients with or without coherent scattering as functions of photon energies. By use of GRAF, a generalized graphics software package prepared at NIST by Kahaner,[4] a graphical representation of these data has been developed. This makes the data more readable and allows the user to form an impression concerning trends in the data—a process that is almost impossible with tabulated data. All data can be graphed in the form of log–log plots: the photon energy is displayed on the x axis, and on the y axis, various properties from the tables may be plotted. Two different curves can be incorporated into a single plot. As an example, the coherent and incoherent scattering of a given species can be simultaneously presented as a function of photon energy. Similarly, pair production in either the nuclear or electronic field or total attenuation with or without coherent scattering can be displayed. Photoelectric absorption is provided as a plot against photon energy.

The values of the various cross-section properties range over as many as 20 orders of magnitude, and this poses special problems for a graphics program. To resolve the difficulty, the data are broken into subsets, each of which covers up to 9 orders of magnitude. This limit was determined by practical considerations such as screen resolution and still allows one to review on a single screen a large quantity of data for the species at hand. The user may select the range of values that are to be plotted and, once a plot has been developed, may use a zoom capability to redraw a portion of the curve at higher magnification.

The program begins by retrieving the requested data, which are stored locally, and then it creates five arrays that are stored in memory. The photon energy is stored in the first array, and the remaining four arrays are used for the material's coherent and incoherent scattering values. Arrays 4 and 5 are set aside for the exponents corresponding to the properties data, and the actual values for these properties are stored in arrays 2 and 3. For any species, these arrays are of equal size and each element in any of them is defined and tied by its position to

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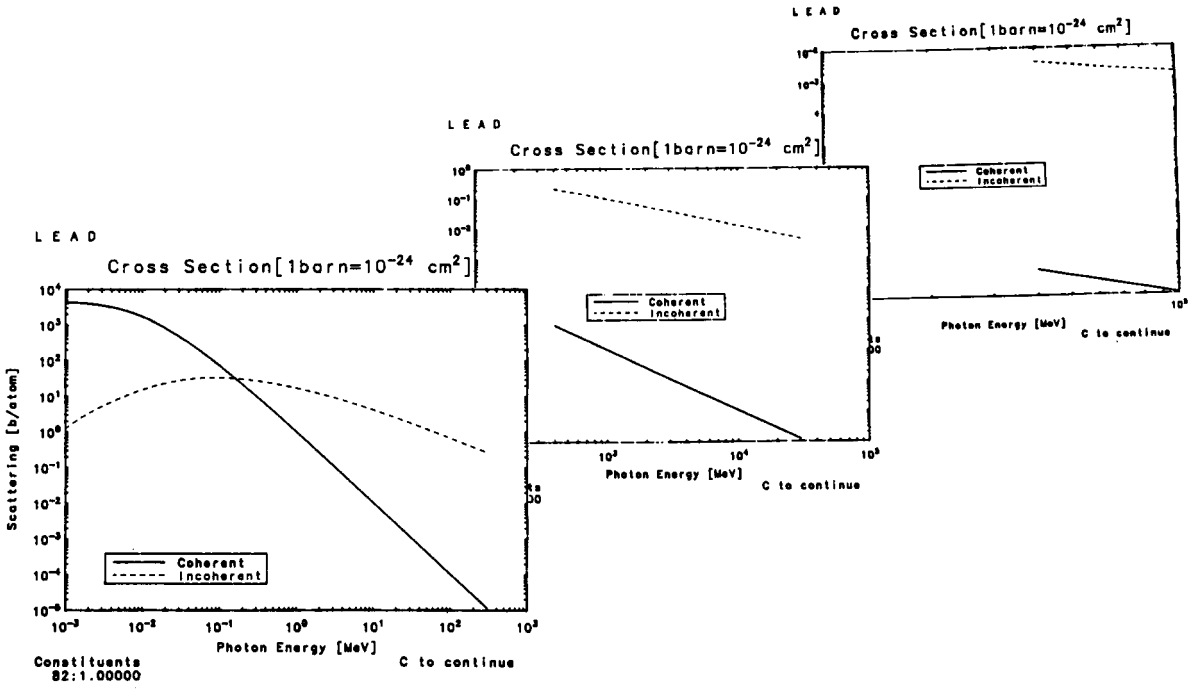

Figure 1. Photon scattering by lead.

the corresponding elements in the other arrays. If the user declares that the first property, scattering, is not of interest, arrays 2–5 are emptied, the photoelectric absorption data (values and exponents) are written into arrays 2 and 4, and arrays 3 and 5 are left unused. If this property is also of no interest, the next properties, pair production in nuclear and in electronic fields, are stored in arrays 2–5. The last properties, the total attenuation coefficients, with or without coherent scattering, are written into the working arrays if they are defined as the properties of interest.

Once an array of properties data has been assembled, the next step is to scale the property data to the maximum axis of 9 orders of magnitude. The total number of orders of magnitude in the data is determined and, if this is less than or equal to 9, the data are simply scaled to fit a single y axis. If the data cover more than 9 orders of magnitude, they are divided into two sets of data which are subsequently plotted independently. In this way, any dataset that ranges over more than 9 orders of magnitude is subdivided into as many 9-order subsets as necessary. Once the subdivision is done, the sets or subsets of data are scaled, if necessary, to the y axis and the graph or graphs are drawn, as before. This procedure is followed to plot double or single curves. If, as a result of the subdivision, two or fewer points are left in a data subset, those data are not plotted.

As a preliminary in the use of the plotting program, the user is asked to identify the species whose properties are to be displayed. If data for an element are to be displayed, the element can be identified by atomic symbol or atomic number. Compounds are specified in terms of a molecular formula, and mixtures of elements and compounds are specified by the percentage composition.

Once the material of interest has been identified, the user is offered a choice among the various properties that can be retrieved and graphed. The options are (1) cross sections, (2) cross sections with attenuation coefficients, and (3) partial interaction coefficients and attenuation coefficients. Next, the grid to be used must be selected. The program allows a choice among a standard energy grid, which consists of 80 energy levels from 1 keV to 100 GeV spaced logarithmically, the same grid with additional points added, or a user-defined grid. Finally, the user is solicited for the property of interest. This is done by means of a menu that includes (1) coherent and

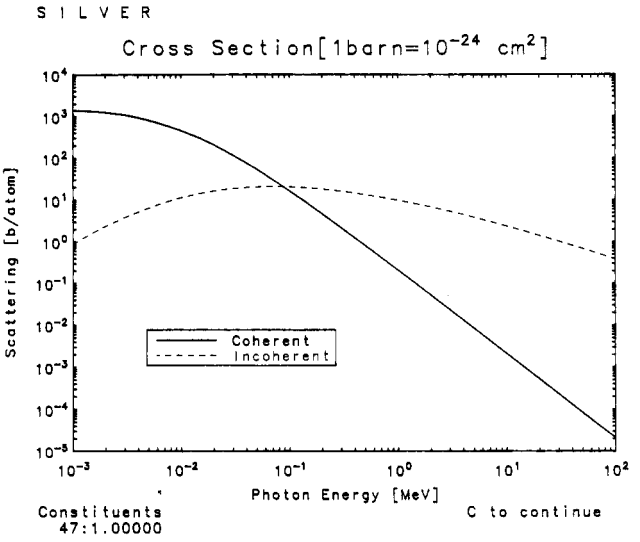

Figure 2. Photon scattering by silver.

incoherent scattering, (2) photoelectric absorption, (3) pair production in nuclear and electronic fields, and (4) total attenuation with and without coherent scattering. When this choice is made, the program offers to print the data in a table or to plot it as a graph or series of graphs. The graphs can be produced after the data have been printed on the screen or, alternatively, the data can be printed after the graphs have been viewed. When requested, the curve or curves are displayed, as in Figure 1, which shows the cross section for photon scattering for lead. This incorporates scattering values ranging from 10^{-10} to 10^{4} barns/atom, i.e., 14 orders of magnitude, and, consequently, three graphs are necessary to display these data. As a further convenience to the user, atomic composition data for the material is appended to the graph.

The photon cross-section data for silver are shown in Figures 2–5. In Figure 2 the scattering data for silver are shown. These data cover 15 orders of magnitude and range from 10^{-11} to 10^{4} barns/atom. Accordingly, these data occupy three graphs covering the cross-section values 10^{-11}–10^{-2}, 10^{-9}–1, and 10^{-5}–10^{4}, respectively, as shown in Figure 2. The photoelectric absorption data for silver are shown in Figure 3, in which the data, ranging from 10^{-6} to 10^{7}, require two graphs.

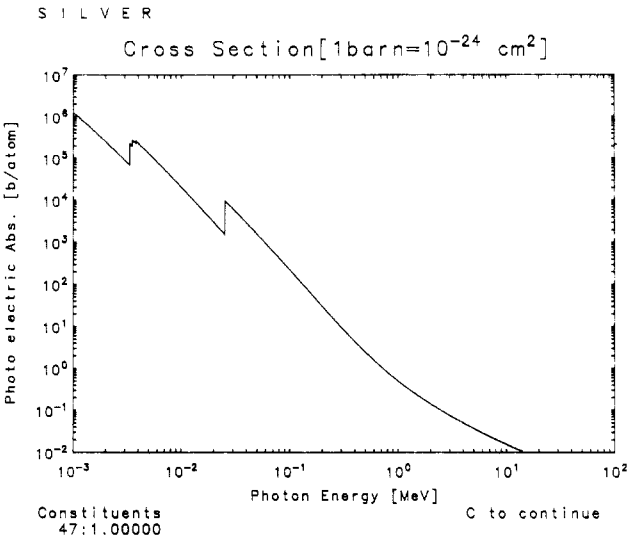

Figure 3. Photoelectric absorption of silver.

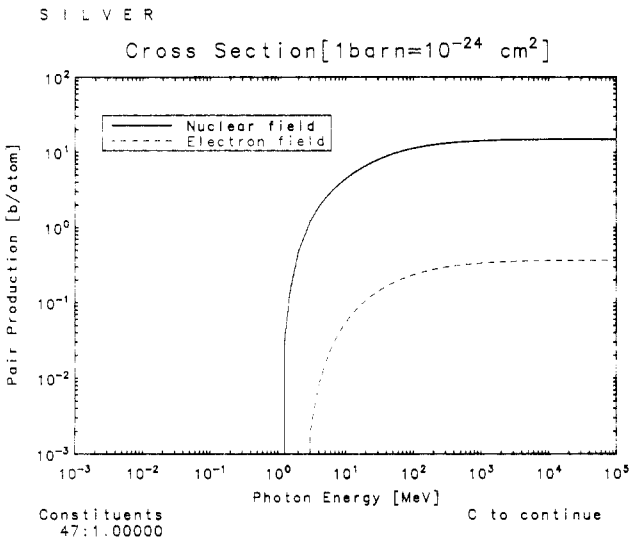

Figure 4. Pair production by silver.

Pair production data for silver are shown in the single graph in Figure 4, and total attenuation data are in Figure 5.

Any graph that is drawn in this way can be edited to suit the user's specific requirements. Legends can be moved to obtain greater clarity, and a zoom capability allows one to focus upon and magnify parts of the curve that are of particular interest or importance. When the graph is on the screen, the user may type **z** and the program draws a "zoom box" on the screen. The zoom box covers about 10% of the full screen, and its size and location can be altered by means of keyboard commands. When the size and position of the zoom box are correct, typing **z** again leads to expansion of the zoom box until it fills the entire screen. Reversal of the

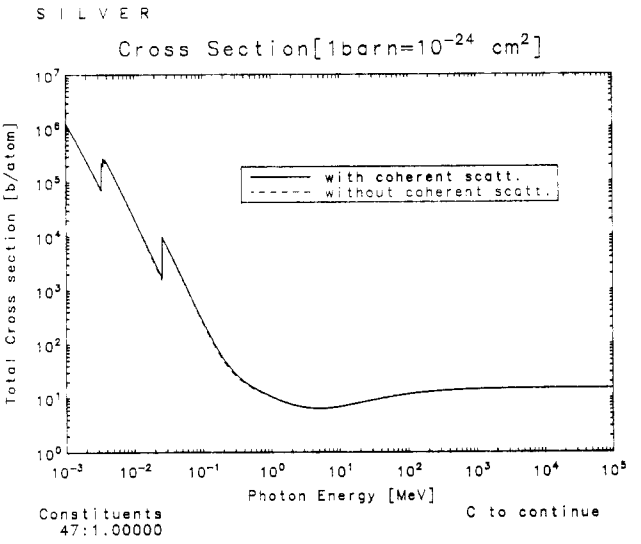

Figure 5. Total cross section of silver.

zooming (reset) is provided in response to the entry **c**.

When a graph has been produced, with or without user modification, it can be printed directly on any Epson-compatible printer. Other printers, such as Tektronix, Hewlett-Packard plotters, Postscript, and QMS graphics-compatible machines, are supported.

SOFTWARE REQUIREMENTS

The graphing program described in this paper is written in FORTRAN 77. It can be compiled and run on an IBM PC or clone, preferably equipped with a math coprocessor (e.g., Intel 8087, 80287). The programs that support data retrieval and graph generation occupy less than 256 kB of memory, and the current XGAM database requires less than one standard low-density floppy disk (360 kB). The complete XGAM database package in executable form can be obtained from the NIST Office of Standard Reference Data.[3]

ACKNOWLEDGMENT

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REFERENCES AND NOTES

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(2) Hubbell, J. H.; Gimm, H. A.; Overbo, I. *J. Phys. Chem. Ref. Data* **1980**, *9*, 1023.
(3) Details are available from the Office of Standard Reference Data, A323 Physics Building, National Institute of Standards and Technology, Gaithersburg, MD 20899.
(4) Kahaner, D. K. Center for Computing and Applied Mathematics, National Institute of Standards and Technology.