NIST Standard Reference Database 64

NIST Electron Elastic-Scattering Cross-Section Database

Version 3.2

Users' Guide

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I. INTRODUCTION

Theoretical description of electron transport in solids is important in radiation physics, electron lithography, electron-probe microanalysis, analytical electron microscopy, and surface analysis by Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS). In these and other applications, the trajectories of electrons in a solid are generally modified by single and multiple elastic-scattering events. An evaluation of the effects of elastic scattering on the process of interest requires knowledge of the cross sections for electron elastic scattering by the constituent atoms of the particular solid. Although calculated and measured electron elastic-scattering cross sections are available in the literature for selected elements and a limited number of electron energies, this information is incomplete and insufficient for general use.

NIST released version 1.0 of the Elastic-Electron-Scattering Cross-Section Database (SRD 64) in 1996. This version provided differential and total elastic-scattering cross sections for elements with atomic numbers from 1 to 96 and for electron energies between 50 eV and 9999 eV in steps of 1 eV. These cross sections were calculated using the Thomas-Fermi-Dirac potential to describe the interaction between an electron and an atom, and using both relativistic and non-relativistic models. This version was designed for analyses of the transport of signal electrons in AES and XPS although it could, of course, be used for other applications.

Version 2.0 of the database was released in 2000. In this version, the upper electron-energy limit was extended to 20 000 eV, and phase shifts and transport cross sections were also provided. The elastic-scattering cross sections, phase shifts, and transport cross sections, however, were obtained only with a relativistic model because this was believed to be more reliable than the non-relativistic model.

Version 3.0 of the database was released in 2002, and contained two major changes. First, the differential elastic-scattering cross sections, total elastic-scattering cross sections, phase shifts, and transport cross sections were calculated from a relativistic Dirac partial-wave analysis in which the potentials were obtained from Dirac-Hartree-Fock electron densities computed self-consistently for free atoms. This potential is believed to be more reliable than the Thomas-Fermi-Dirac potential used previously [1]. Differences in elastic-scattering cross sections and transport cross sections resulting from this change of potential are described in a review article [1] and briefly in Section VI.

The second major change in the database is that differential elastic-scattering cross sections, total elastic-scattering cross sections, and transport cross sections are now available for electron energies up to 300 000 eV. As a result, the database should be useful for a wider range of materials-characterization applications that include electron-probe microanalysis and analytical electron microscopy.

In addition, it is possible in Version 3.0 to create and/or print files illustrating variation of differential elastic-scattering cross sections *versus* scattering angle for one or more elements or for one or more energies. Some of the database screens were redesigned as a result of the increase in the upper electron-energy limit to 300 keV.

Version 3.1 of the database, issued in August, 2003, contains two corrections to Version 3.0. First, a numerical mistake was found in the calculation of differential cross sections for a small number of elements and energies (e.g., F at 300 eV). Second, the routine used for interpolations between differential cross sections at certain scattering angles was found to be inadequate in the vicinity of deep minima in the differential cross sections (e.g., Cu at 319 eV). The libraries of cross-section data and the software have been revised to correct these problems.

Version 3.2 of the database was issued in December, 2010. The installation program for Version 3.2 was changed so that it would operate on newer versions of the Windows operating system. There were no changes or additions to the data in the database although a new About box was added to the main menu. This box shows two references, a 2004 critical review [1] and a 2005 review [2], that discuss evaluations of the compiled data, methods of determination, and uncertainty.

Version 3.2 of the Electron Elastic-Scattering Cross-Section Database has the following capabilities:

- Graphical display of differential elastic-scattering cross sections in different coordinate systems
- Graphical display of the dependence of transport cross sections on electron energy
- Display of numerical values of differential elastic-scattering cross sections, total elastic-scattering cross sections, and transport cross sections
- Creation of files containing differential elastic-scattering cross sections for specified elements, energies and coordinates
- Creation of files containing plots of differential elastic-scattering cross sections versus scattering angle for one or more elements or for one or more electron energies
- Creation of files containing phase shifts for specified elements and for energies up to 20 000 eV
- Creation of files containing transport cross sections for specified elements and energies
- Creation of random number generators providing the polar scattering angles to be used in Monte Carlo simulations of electron transport in solids; and
- Runs of the random number generators

The database calculates parameters for random number generators that provide the scattering angles for Monte Carlo simulations of electron transport in AES, XPS, and other applications. Portable FORTRAN codes for these generators are included. These codes facilitate considerably the development of Monte Carlo programs for simulating electron transport.

II. GETTING STARTED

Packet Content

CD-ROM
Users' guide

Alternatively, the files on the CD-ROM and a PDF file with the Users' Guide can be downloaded from NIST (http://www.nist.gov/srd/surface.cfm).

System Requirements

1. Personal computer with Windows 95, Windows 98, Windows NT, Windows 2000, Windows ME, Windows XP, Windows Vista, or Windows 7 operating system
2. CD-ROM drive
3. Screen resolution: 1024 by 768 pixels.
4. System font size: small fonts.
5. Printer: Laser printer supporting the PCL 6 printer language.
6. Hard disk space of at least 52 MB. Larger amounts of storage are required if numerous files are created with the database. It is suggested that an additional 30 Megabytes be available, particularly if graphic files are created.

The database has been designed to operate optimally at the screen resolution given above. However, it can also be operated at a lower screen resolution, e.g., 640 by 480 pixels, or 800 by 600 pixels. At higher resolutions, the database will operate correctly but there may be difficulty in reading text on the screen. For all resolutions, small system fonts must be selected.

To change the screen resolution or the system font size, follow these steps:
1. Double click the **My Computer** icon on the desktop.
2. Click the **Control panel** icon.
3. Double click the **Display** icon.
4. Click on the **Settings** tab.
5. Set a given resolution by moving the slider.

To change the system font size, proceed as follows depending on the operating system in use:

For Windows 95 or NT, select **Small Fonts** in the **Font Size** box.

For Windows 98, click on the **Advanced…** button, select the **General** tab, and then select the **Small Fonts** option in the **Display** box.

For Windows XP, click on the **Advanced…** button, and then select the **Normal size (96 DPI)** option in the **Display** box.

For Windows Vista, click on **Appearance and Personalization**, **Personalization**, **Adjust font size (DPI)** in the left pane, and select **Default scale (96 DPI).**

For Windows 7, click on **Appearance and Personalization, Display,** and select **Small - 100 %** (default option).

Installation

1. Insert the CD-ROM into the disk drive of the computer.
2. Click the **Start** button on the task bar.
3. Click the **Run** command.
4. Type D:\SETUP (if D: is the drive letter for the disk drive) and click OK.
5. Follow instructions on the screen.

Alternatively, the following procedure can be used:
1. Insert the disk into the disk drive of the computer.
2. Double-click **My Computer** on the desktop.
3. Double-click the icon corresponding to the disk drive.
4. Double-click the **Setup** icon (showing the computer).
5. Follow instructions on the screen.

If files have been downloaded into a directory on the user's personal computer, double-click the **Setup** icon (i.e., **setup.exe**).

Should difficulty be encountered in installing the database as described above (e.g., due to security settings on the computer), the database can be launched by double-clicking on **ELASTIC32.exe** located in the Program Files directory.

By default, the database is installed in the directory C:\PROGRAM FILES\NIST\ELASTIC32. Furthermore, an ELASTIC32 icon is created. This icon appears after clicking the **Start** button and choosing **Programs**.

Removal of the Database

1. Double click **My Computer** on the desktop.
2. Double click the **Control panel** icon.
3. Double click the **Add/Remove Programs** icon.
4. Select **Install/Uninstall**.
5. In the list of programs, click **Elastic32**.
6. Click the button **Add/Remove**.

III. STRUCTURE OF THE PROGRAM

Main Menu

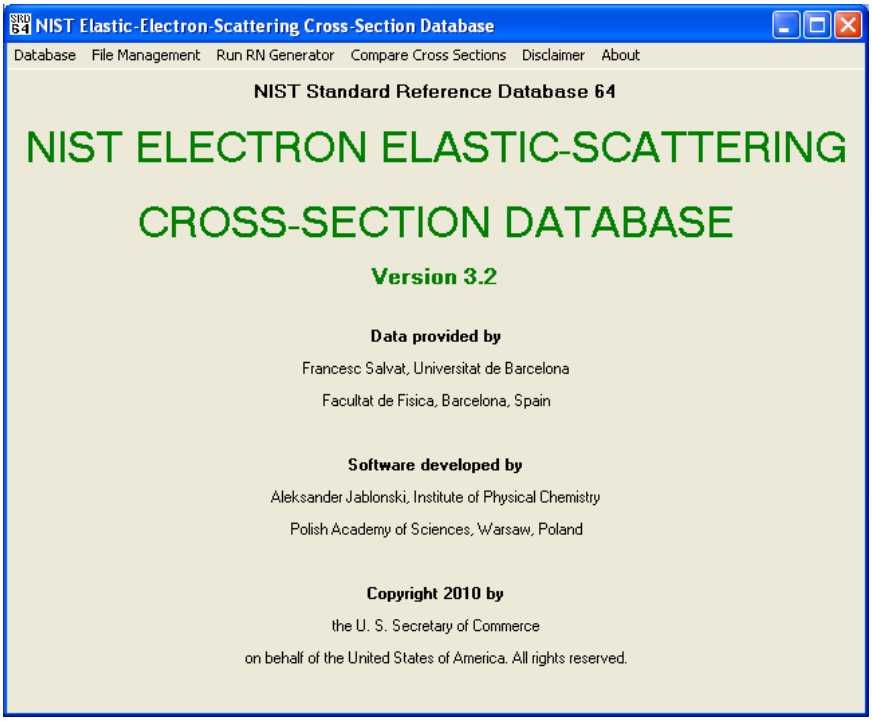

Fig. 1. The title screen and main menu.

The six options of the Main Menu are listed in the upper part of the title screen (Fig. 1), and the submenus corresponding to the first four options are shown in Figs. 2(a)-(d). The functions of the six main options are as follows:

1. Database (Fig. 2(a))
   With this option, data can be retrieved for:
   (a) Elastic-scattering cross sections,
   (b) Phase shifts, and
   (c) Transport cross sections for selected elements and electron energies.
   Text files can be created with the relevant data, and files can be created containing parameters for the random number generator controlling scattering angles in Monte Carlo simulations of electron transport. Operation of the database can be terminated by choosing End the session.

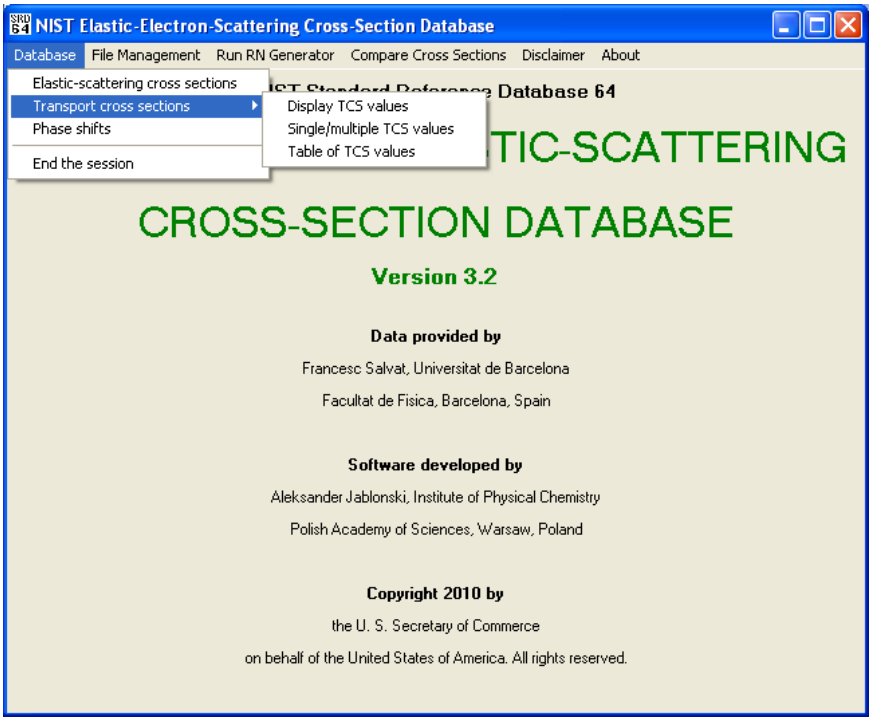

Fig. 2(a). First option of the main menu (Database) together with the submenu for transport cross sections.

2. File Management (Fig. 2(b))
   This option allows the following operations:
   (a) Loading files created in earlier sessions;
   (b) Saving files created during the current session;
   (c) Deleting files in a given directory; and
   (d) Printing selected files

3. Test RN (Random Number) Generator (Fig. 2(c))
   With this option, a previously created random number generator can be selected for testing. A comparison is then made of the histogram of generated scattering angles and the corresponding differential elastic-scattering cross section. Such comparisons can be made for electron energies of 20 keV and below.

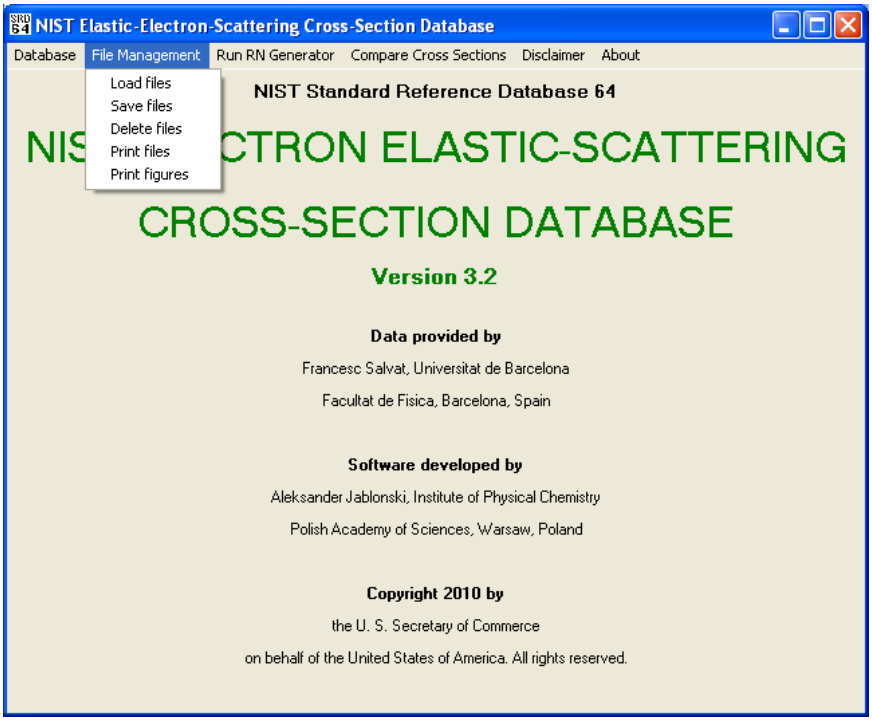

Fig. 2(b). Second option of the main menu (File Management).

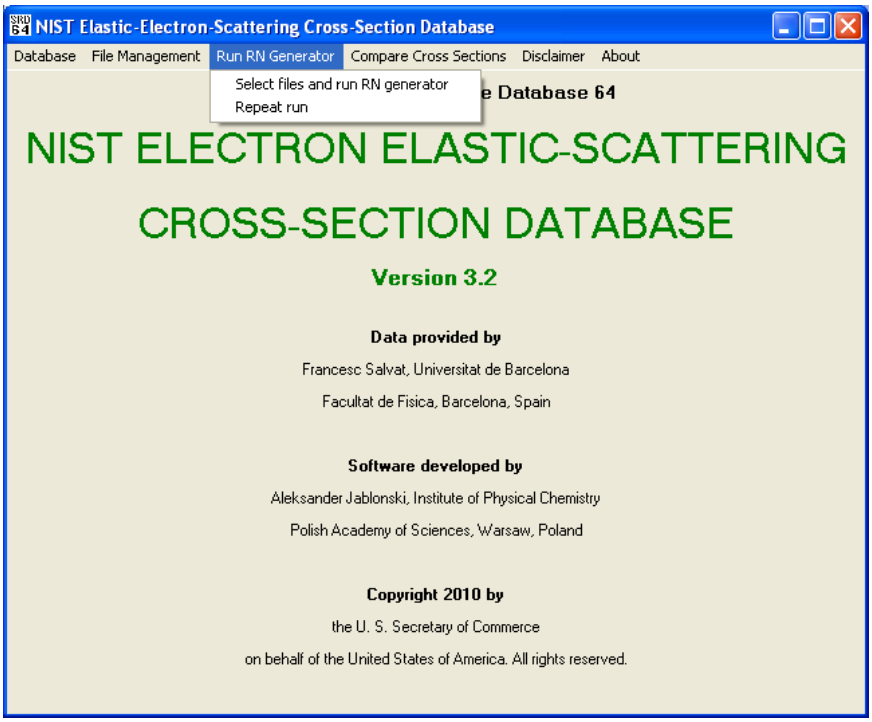

Fig. 2(c). Third option of the main menu (Test RN (Random Number) Generator).

4. Compare Cross Sections (Fig. 2(d))
   This option permits a graphical comparison of up to four differential elastic-scattering cross sections in selected coordinates.

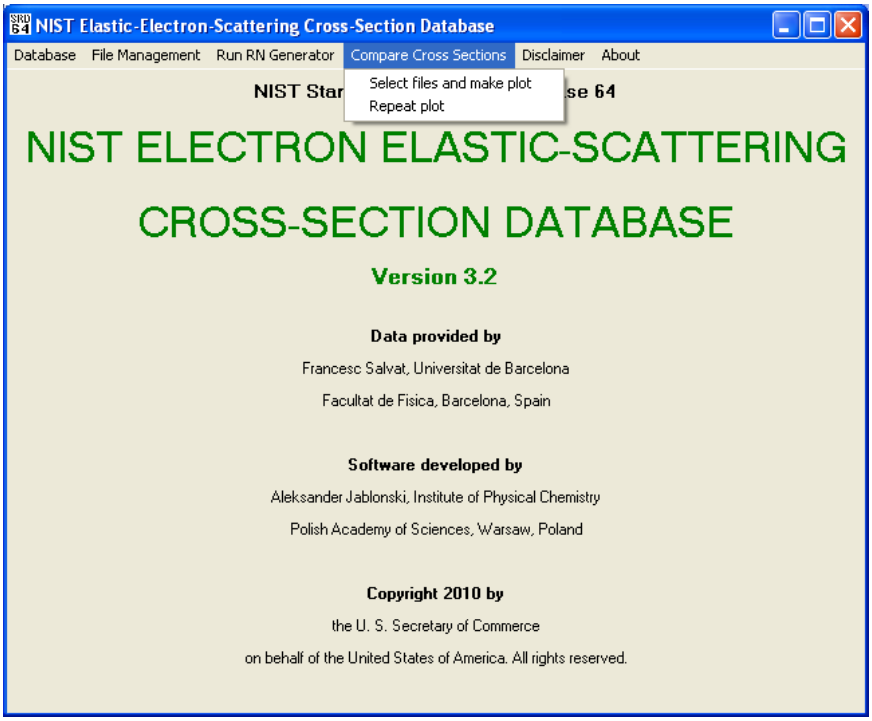

Fig. 2(d). Fourth option of the main menu (Compare Cross Sections).

5. Disclaimer (Fig. 2(e))
   The NIST disclaimer is stated.

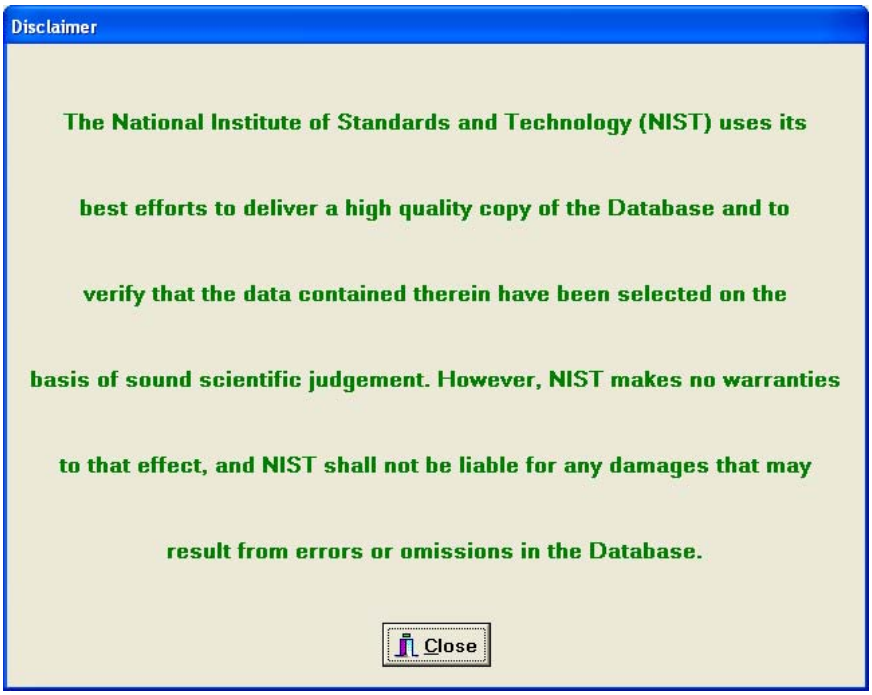

Fig. 2(e). NIST disclaimer.

6. About box (Fig. 2(f))

The About box gives information on the release date of this version of the database, how the database should be cited in publications, and references to evaluations of the compiled data, methods of determination, and uncertainties [1,2].

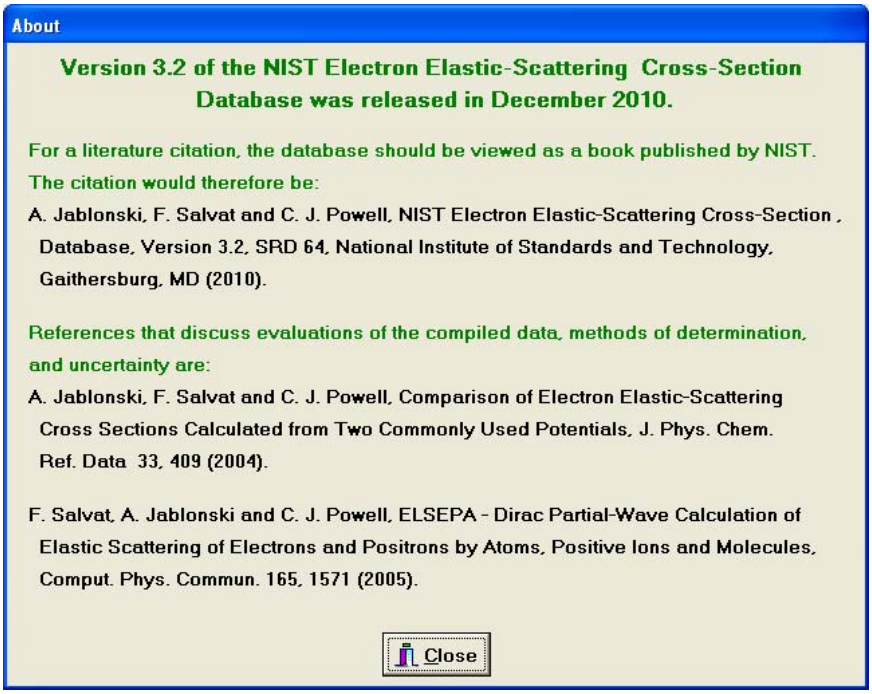

Fig. 2(f). The About box.

IV. RUNNING THE DATABASE PROGRAM

The database can be started by any of the following means:

1. Click the Start button, choose Programs, and then the ELASTIC32 program.

2. Click the Start button, choose Run, and type:
   C:\PROGRA~1\NIST\ELASTIC32\ELASTIC32,
   And then click OK.

3. Double-click the My Computer icon on the desktop, select the C:\PROGRAM FILES\NIST\ELASTIC32 directory, and double-click on the ELASTIC32 program.

Database

(First Option of the Main Menu)

The user must first select **Elastic-scattering cross sections**, **Phase shifts**, or **Transport cross sections** to obtain the corresponding data. These options will be described in turn.

Database/Elastic-scattering cross sections

After selection of this option, the following screens appear:

1. **Select elements screen**
The Periodic Table of the elements appears (Fig. 3), and one or more elements can be selected by clicking on the button(s) for the element(s) of interest. A selection is indicated by a change of color from black to red. An element can be deselected by clicking again on a button. After at least one selection has been made (Au in the case shown in Fig. 3), the **OK** button should be clicked. Clicking on the Cancel button returns control to the opening screen and the main menu.

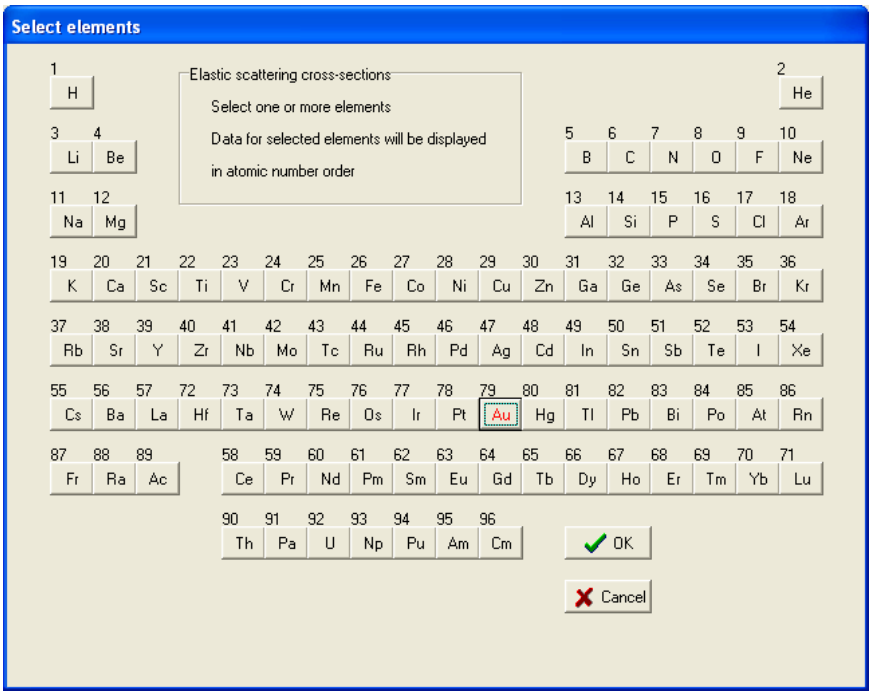

Fig. 3. Screen for selecting elements.

2. **Select initial energy and coordinates screen**

The user enters the initial electron energy of interest (in the range 50 eV to 300 keV) on the following screen (Fig. 4). A selection then needs to be made of the coordinates for display of the differential elastic-scattering cross section. Three coordinate systems are available for electron energies of 20 keV and below in which the differential elastic-scattering cross section is expressed with respect to solid angle Ω, polar scattering angle θ, or $\sin(\theta/2)$:

(a) $d\sigma/d\Omega$ *versus* θ

(b) $d\sigma/d\theta$ *versus* θ

(c) $d\sigma/d\sin(\theta/2)$ *versus* $\sin(\theta/2)$

In the latter case, the cross section $d\sigma / d\sin(\theta/2)$ is related to the differential cross section for electron momentum change $d\sigma / dq$. The quantity q is defined by $q = |\mathbf{K}'\text{-}\mathbf{K}|$ where $\mathbf{K}$ and $\mathbf{K}'$ are wave vectors before and after an elastic collision. We have:

$$\frac{d\sigma}{d\sin(\theta/2)} = 2K\frac{d\sigma}{dq}$$

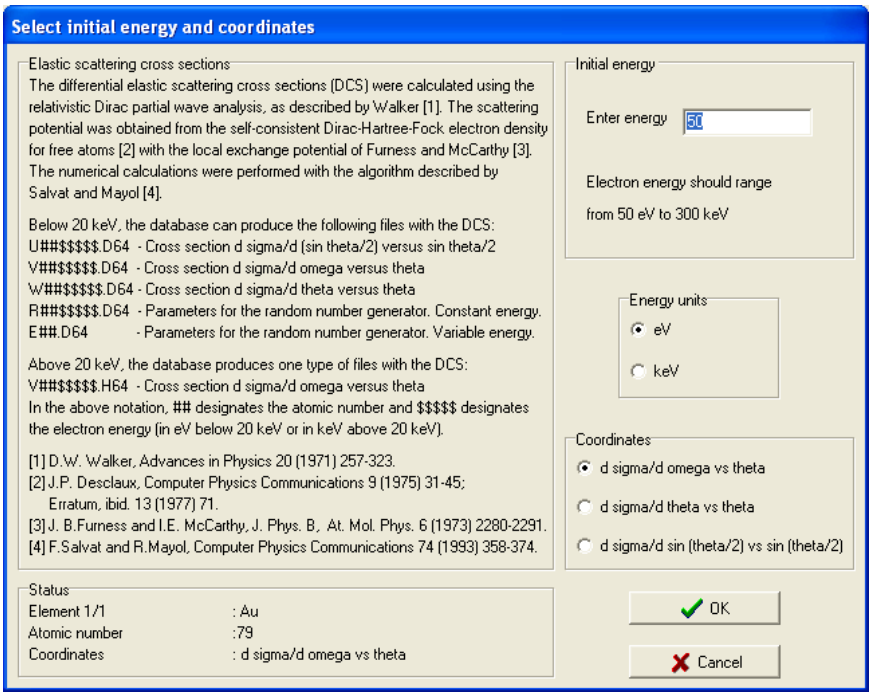

Fig. 4. Screen for selecting energy and coordinates.

where $K = |\mathbf{K}|$. For electron energies of 20 001 eV and above, cross sections are available only in $d\sigma / d\Omega$ *versus* θ coordinates.

The elastic-scattering cross sections calculated by the database are expressed in units involving the square of the Bohr radius a_0 (the radius of the first Bohr orbit of the hydrogen atom) where a_0 = 5.291 772 1 x 10^{-11} m and a_0^2 = 2.800 285 2 x 10^{-21} m^2. The specific units for the cross sections in the different coordinate systems are as follows:

(a) a_0^2 /radian for the $d\sigma/d\theta$ *versus* θ coordinate system;

(b) a_0^2 /steradian for the $d\sigma/d\Omega$ *versus* θ coordinate system; and

(c) a_0^2 for the $d\sigma/d\sin(\theta/2)$ *versus* $\sin(\theta/2)$ coordinate system.

These units are used in the screen displays and in the files created by the database. In the screen shown in Fig. 4, an energy of 50 eV and the $d\sigma/d\Omega$ *versus* θ coordinates were selected. The **OK** button at the bottom right of the screen should be clicked to advance to the next screen.

3. **Display of differential cross section** screen

This screen shows the differential elastic-scattering cross sections in the selected coordinates for a given element and electron energy. For cross sections in $d\sigma/d\Omega$ *versus* □ coordinates and for electron energies of 20 keV and below, the differential cross sections can be displayed on logarithmic or linear scales versus polar scattering angle on a linear scale. If the linear scale is selected, the vertical scale can be varied by clicking the **Increase size** or **Decrease size** buttons in the top-right part of the screen. The initially selected energy can be changed by clicking the **Increase energy** or **Decrease energy** buttons in the upper-right part of the screen; these changes will occur in steps of 1 eV, 10 eV, 100 eV, or 1000 eV (within the range 50 eV to 20 keV). For electron energies of 20 001 eV and above, the differential cross sections can be displayed on a logarithmic scale versus polar scattering angle on a linear scale, and the initially selected energy can be varied in steps of 10 eV, 100 eV, 1 keV, or 10 keV.

Examples of this screen for Au and for energies of 50 eV and 300 keV are shown in Fig. 5 to illustrate displays of cross sections in $d\sigma/d\Omega$ *versus* θ coordinates on linear and logarithmic scales. Cross sections in $d\sigma/d\theta$ *versus* θ and in $d\sigma/d\sin(\theta/2)$ *versus* $\sin(\theta/2)$ coordinates can be displayed only for energies of 20 keV and below, and then only on linear scales. The panel in the top-left of the screen displays the selected electron energy and the corresponding total elastic-scattering cross section. After final selection of the electron energy, the **OK** button should be clicked.

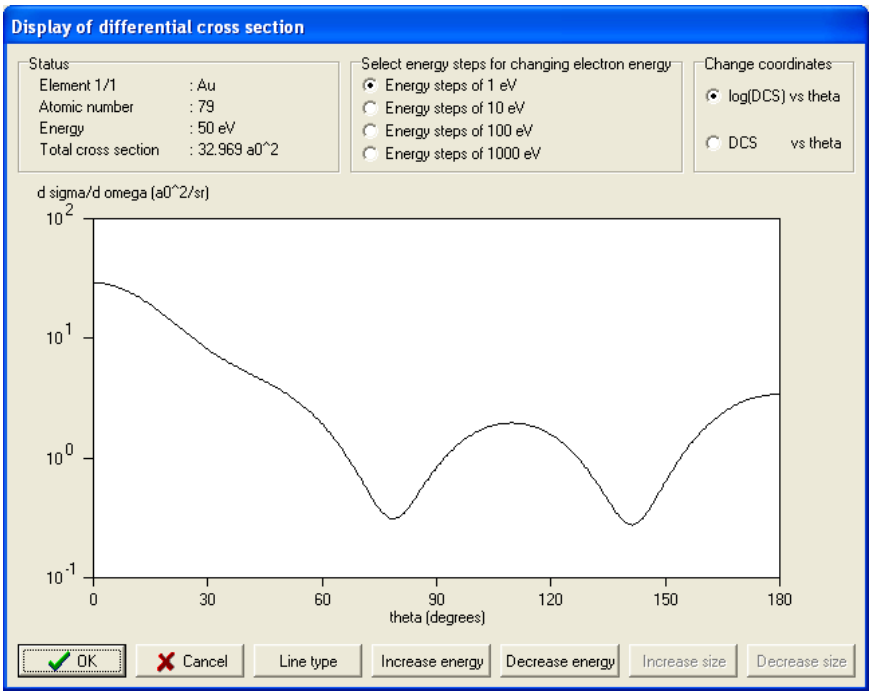

Fig. 5(a). Screen showing the differential cross section for Au in $d\sigma/d\Omega$ *versus* θ coordinates at 50 eV on semi-logarithmic scales.

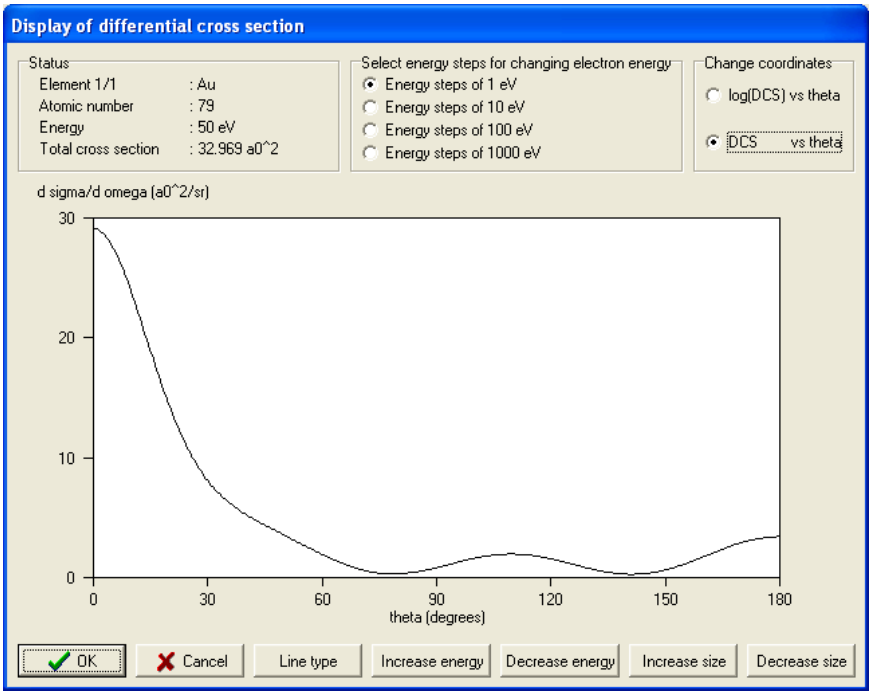

Fig. 5(b). Screen showing the differential cross section for Au in $d\sigma/d\Omega$ *versus* θ coordinates at 50 eV on linear scales.

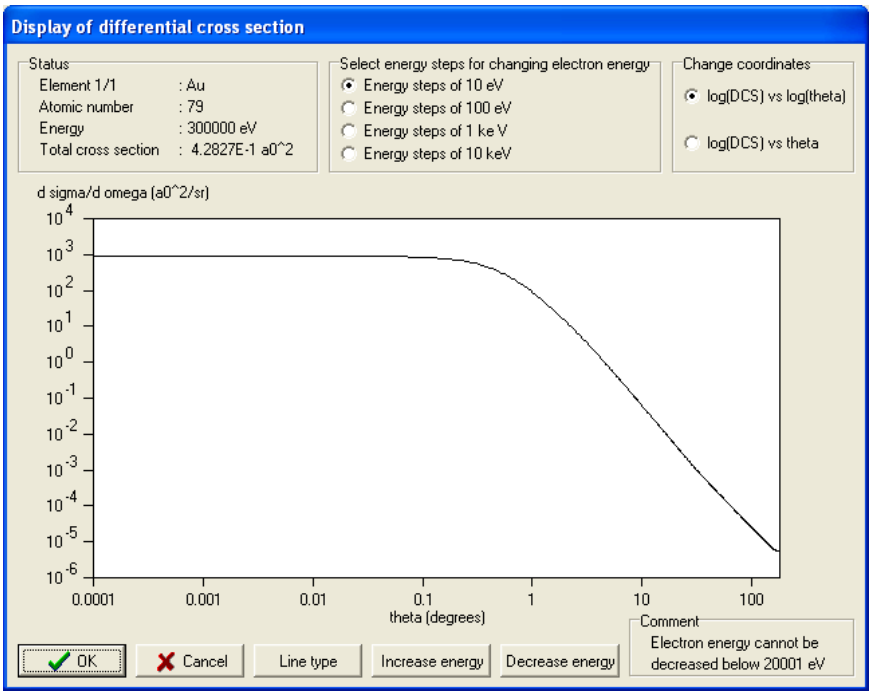

Fig. 5(c). Screen showing the differential cross section for Au in $d\sigma/d\Omega$ *versus* θ coordinates at 300 keV on logarithmic scales.

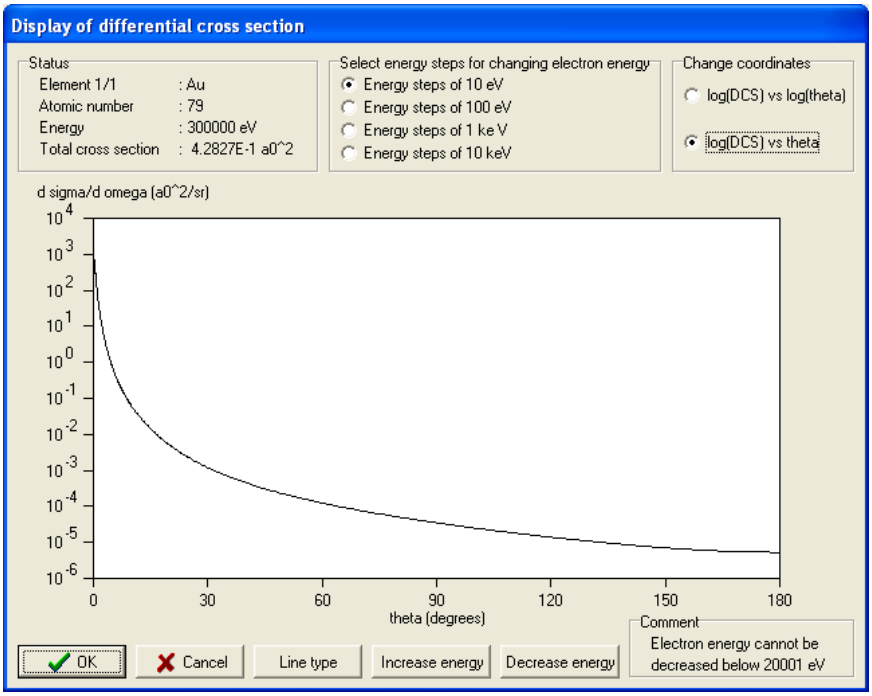

Fig. 5(d). Screen showing the differential cross section for Au in $d\sigma/d\Omega$ *versus* θ coordinates at 300 keV on semi-logarithmic scales.

4. **Create files** screen

Figure 6(a) is an example of the screen that appears for electron energies of 20 keV and below, and Fig. 6(b) is an example of this screen for energies of 20 001 eV and above. This screen can also be used to provide values of the differential elastic-scattering cross section in the chosen coordinates for scattering angles of interest.

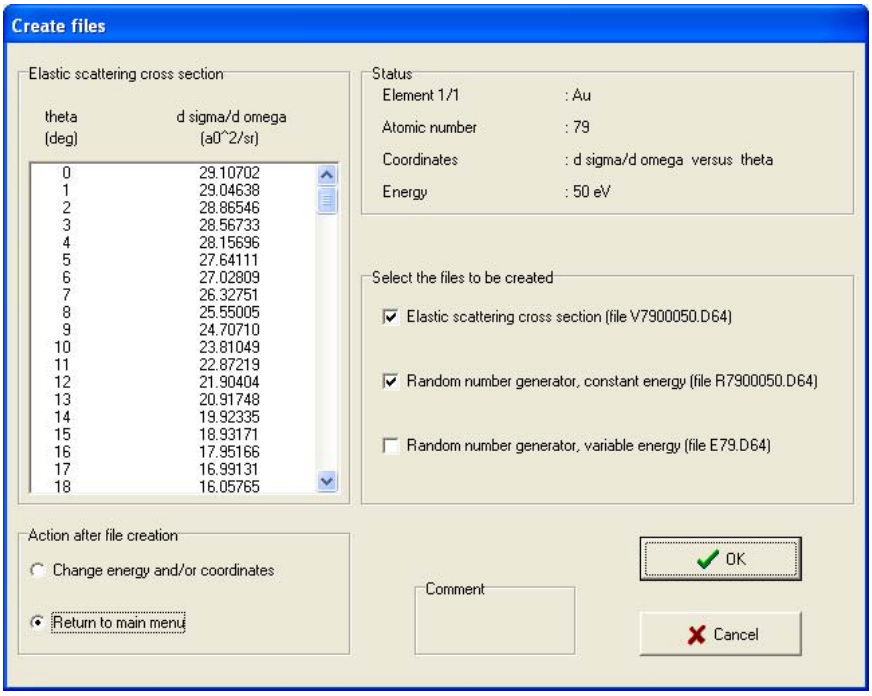

Fig. 6(a). Screen showing two files to be created for Au at an energy of 50 eV.

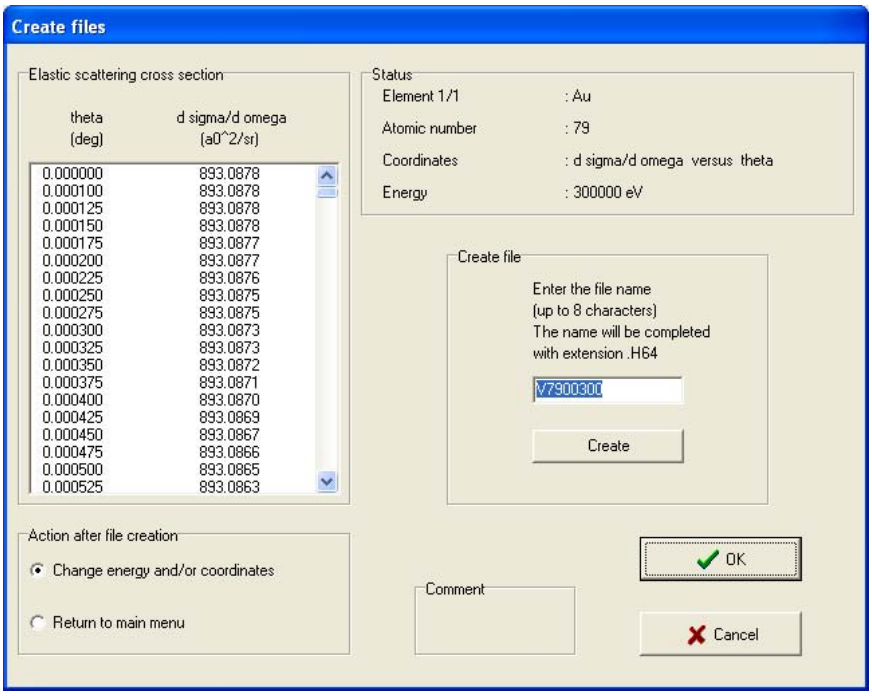

Fig. 6(b). Screen showing file to be created for Au at an energy of 300 keV.

For electron energies of 20 keV and below, a selection should be made on this screen of the files that the user wishes to create for the element chosen on previous screens. One or more of the following three types of files can be created:

(a) A text file with total and differential elastic-scattering cross sections for the given element and for the energy and coordinates selected on previous screens. The following file notation is used:

U##$$$$$.D64	for $d\sigma/d\sin(\theta/2)$ *versus* $\sin(\theta/2)$ coordinates
V##$$$$$.D64	for $d\sigma/d\Omega$ *versus* θ coordinates
W##$$$$$.D64	for $d\sigma/d\theta$ *versus* θ coordinates

In this notation, the field ## contains the atomic number (two digits) and the field $$$$$ contains the electron energy in eV (5 digits). Files in the $d\sigma/d\theta$ *versus* θ coordinates need to be created for tests of the random number generators (see below).

(b) A file with parameters for the random number generator for a constant electron energy (chosen on a previous screen). This file is denoted by R##$$$$$.D64. See Appendix A for further information.

(c) A file with parameters for the random number generator for variable electron energy in the range 50 eV to 20 000 eV. This file is denoted by E##.D64. See Appendix A for further information.

For electron energies of 20 001 eV and above, files of the type V##$$$$$.H64 can be created (for cross sections in the $d\sigma/d\Omega$ *versus* θ coordinates only). In this notation, the field ## contains the atomic number (two digits) and the field $$$$$ contains the electron energy in keV (5 digits).

The user then needs to decide on the action to be taken after files have been created. There are two options (chosen by selecting the appropriate button):

(a) Change energy and/or coordinates for the selected element by returning to the **Select initial energy and coordinates** screen.

(b) Either Change element (if another element had been selected on the first screen) or Return to main menu.

The first option is set as the default. After all selections have been made, the **OK** button should be clicked. The desired files will then be created in the current database directory (by default, this directory is C:\PROGRAM FILES\NIST\ELASTIC32).

Database/Transport cross sections

The definition of the transport cross section is given in Section V. As shown in Fig. 2(a), there is a submenu of three choices if the Transport cross sections option (the second function of the **Database** menu option) is selected:

(a) Display TCS (transport cross-section) values
(b) Single/multiple TCS (transport cross-section) values
(c) Table of TCS (transport cross-section) values

For each option, a screen with the Periodic Table appears (similar to Fig. 3) and the user selects one or more elements of interest. The following screens for options (a), (b), and (c) enable TCS data for the selected element(s) to be displayed graphically as a function of energy, allow TCS data for user-specified energies to be displayed, and enable TCS data to be displayed at regularly spaced electron energies, respectively. Files containing TCS values can be created for the latter two options. The TCS values are shown in units of a_0^2.

For option (a), TCS values are displayed as a function of electron energy in either of two energy ranges, 50 eV to 20 keV or 1 keV to 300 keV, depending on the user's choice of an initial energy. Example screens are shown in Figs. 7(a) and 7(b) for initial energies of 1000 eV and 50 000 eV, respectively. A value of the transport cross section for the chosen initial energy is then displayed inside the plot at a position close to the desired energy. This transport cross section and the chosen energy appear in the upper left corner of the screen. The selected initial energy can be changed by clicking in an appropriate region of the plot or by clicking on the **Increase energy** or **Decrease energy** buttons; the latter changes will occur in steps of 1 eV, 10 eV, 100 eV, or 1000 eV depending on the choice of button selected in the upper part of the screen. If the lower energy range is selected (50 eV to 20 keV), it is not possible to increase the energy above 20 keV while if the upper energy range is selected (1 keV to 300 keV), it is not possible to decrease the energy below 1 keV.

The energy dependence of the cross section can be displayed on linear, semilogarithmic, or logarithmic scales; these scales are chosen with the buttons in the upper-right part of the screen. The scale on the vertical axis can be changed by clicking the **Increase size** and **Decrease size** buttons. These buttons, however, are only active when coordinates with a linear vertical axis are selected, i.e. the coordinates: TCS versus E and TCS versus log(E). The **Close** button should then be clicked to display transport cross sections for another element (if previously selected) or to return to the main menu.

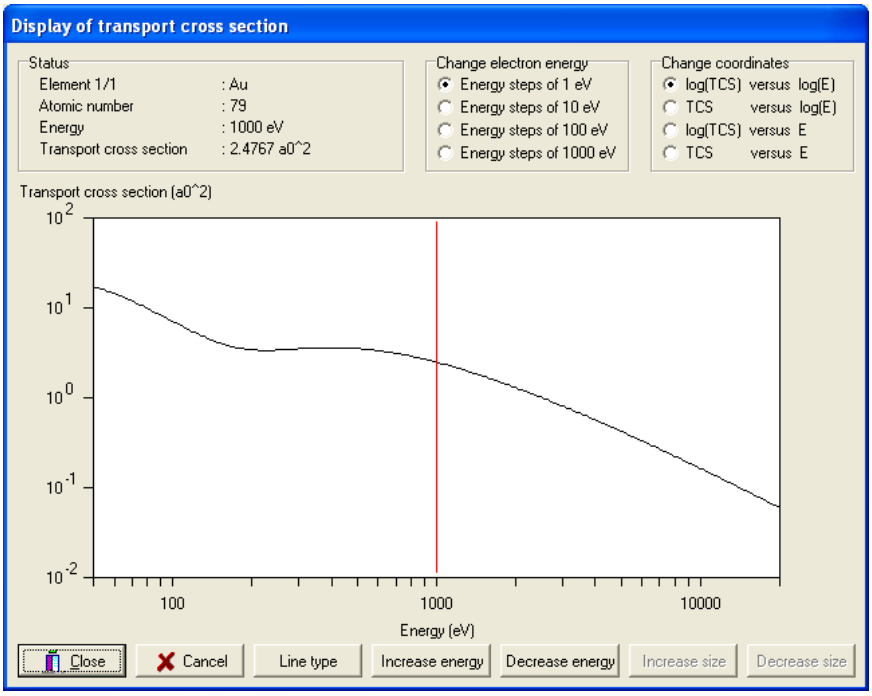

Fig. 7(a). Screen showing energy dependence of the transport cross section for Au in the energy range from 50 eV to 20 keV.

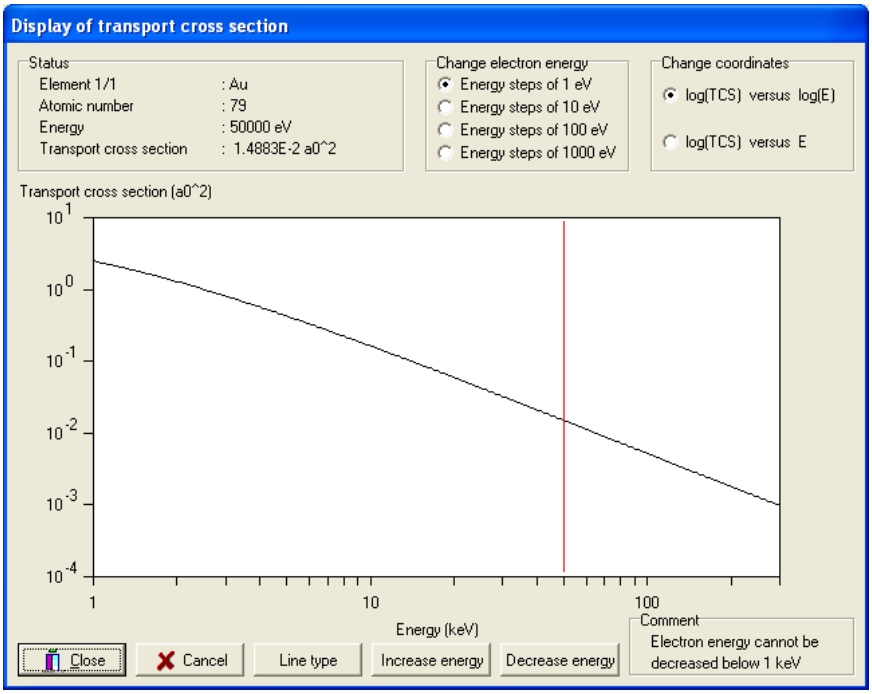

Fig. 7(b). Screen showing energy dependence of the transport cross section for Au in the energy range from 1 keV to 300 keV.

For option (b), the user can display transport cross sections for one or more electron energies and create files with these values using the screen shown in Fig. 8. The user enters the energy value of interest (between 50 eV and 300 keV) in a box located in the lower left corner of the screen. On clicking the **Add** button, the transport cross section for this energy is calculated and displayed in the box in the central part of the screen. Additional energies can be entered in the same way and the corresponding transport cross sections will be displayed in the central box. The **Insert** button can be used to insert new values of energy and transport cross section above a highlighted region in the box. A file containing the displayed data can be created by entering a file name in the **Create file** box located in the lower right-hand part of the screen (Fig. 8). This file name, which should not be longer than 8 characters, will be completed with the extension .T64. The file will be created after clicking on the **Create** button. As for option (a), the **Close** button should then be clicked to display values of transport cross sections for another element (if previously selected) or to return to the main menu.

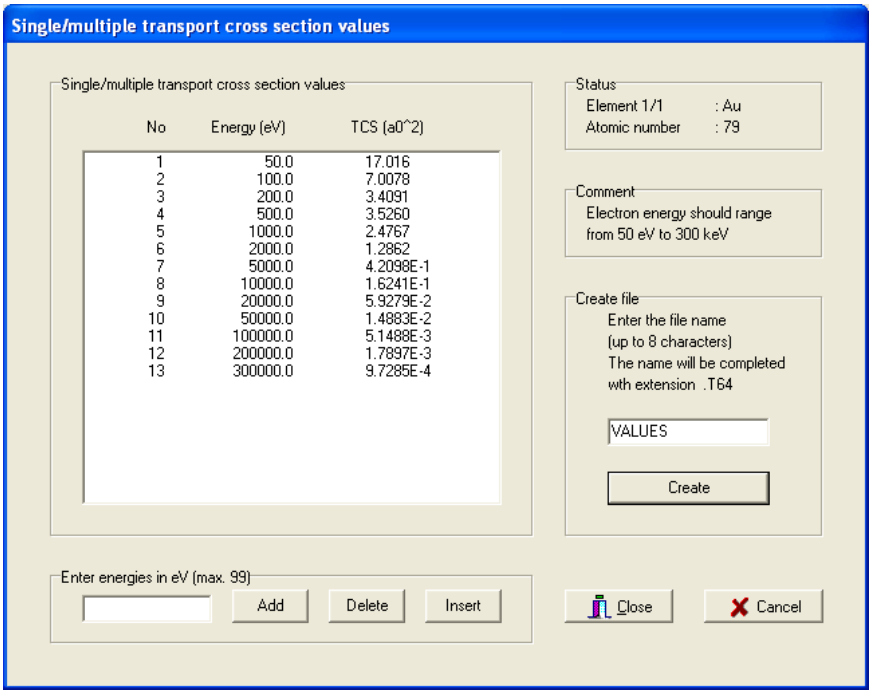

Fig. 8. Transport cross sections calculated for Au at selected energies.

With option (c), the user can display a Table of transport cross sections at regularly spaced electron energies. A screen similar to Fig. 8 appears and the user enters the number of transport-cross-section values desired and the minimum and maximum energies in the **Create table** box on the right side of the screen. The user also chooses whether the electron energies should be distributed linearly or logarithmically in the specified energy range by selecting one of the buttons in the lower part of the screen. After clicking the **Create** button in the **Create table** box, the table of cross section values is calculated and displayed. As for option (b), a file containing the displayed data can be created by entering a file name (no longer than 8 characters) in the **Create file** box and clicking **Create**. This file also has the extension .T64. Click the **Close** button to display Tables of transport cross sections for another element (if previously selected) or to return to the main menu.

Database/Phase shifts

The third function of the **Database** menu option provides values of the relativistic phase shifts δ_l^+ and δ_l^-; these phase shifts are calculated as described in Section V for electron energies of 20 keV and below. Initially, a screen with the Periodic Table appears, similar to that shown in Fig. 3. After selecting one or more elements and clicking **OK**, a screen similar to Fig. 9 appears.

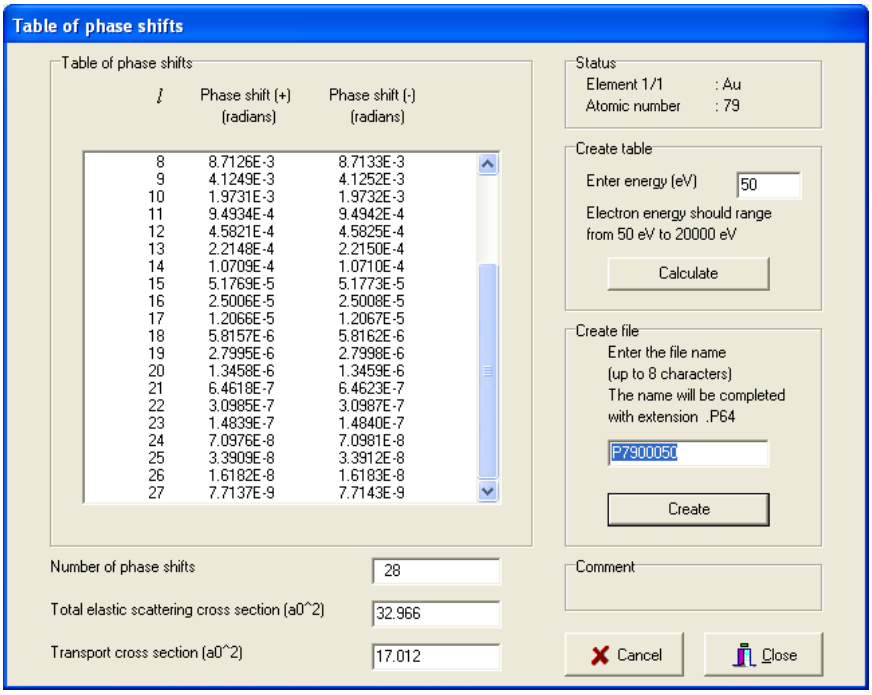

Fig. 9. Phase shifts calculated for Au at an energy of 50 eV.

The user specifies the electron energy of interest (between 50 eV and 20 000 eV) in the panel in the upper right corner. If Au had been previously selected and an energy of 50 eV entered (as shown in Fig. 9), phase shifts are calculated after clicking on the **Calculate** button. The phase shifts are calculated until their values become smaller than 10^{-8}. The calculated phase shifts (in radians) appear in the list located in the center of the screen, as shown in Fig. 9. When the calculations are completed, the default name of a file to contain the phase shifts is indicated. This name has the form P##$$$$$.P64. The user may change this name, although only strings of up to 8 characters are accepted. If the user wishes to create such a file, the **Create** button should be clicked, and a file with the proposed name will be created in the database directory. The screen of Fig. 9 also shows the number of phase shifts, the total elastic-scattering cross section, and the transport cross section.

The values of the total elastic-scattering cross section and the transport cross section in the screen of Fig. 9 may differ slightly from the corresponding values displayed in the **Elastic-scattering cross section/Display of differential cross section** screen (such as Fig. 5) or the **Transport cross section** screens (such as Figs. 7 and 8). These differences are due to the fact that the total elastic-scattering cross section and the transport cross section shown in the screen of Fig. 9 result from all of the calculated phase shifts while some of the phase shifts used to calculate these values in the screens of Figs. 5, 7, and 8 are interpolated. Thus, the values in Fig.

9 are more accurate. Comparisons of cross sections derived from the interpolated phase shifts with those from the more accurate values show that the agreement is within 3 to 5 decimals and typically within 4 decimals.

If desired, files with phase shifts for other energies can be created in the same way. The **Close** button should then be clicked to obtain phase shifts for another element (if previously selected) or to return to the main menu.

File Management

(Second Option of Main Menu)

The user selects one of four options (**Load files**, **Save files**, **Delete files**, or **Print files**) to perform the indicated operations on files containing elastic-scattering cross sections, phase shifts, and transport cross sections that had been previously created by the database (i.e., files with .D64, .P64, and .T64 extensions, respectively). The fifth option (**Print figures**) can be used to print figures (i.e., files with .BMP extension) created by the **Compare Cross Sections** option of the main menu. These options will be described in turn.

File Management/Load files

With this option, it is possible to transfer files to the current database directory (default: C:\PROGRAM FILES\NIST\ELASTIC3) that had been saved previously to other directories. An example of this option is shown in Fig. 10.

The source directory selected in the tree located on the left-hand side of the screen (C:\CROSSEC) contains numerous files with elastic-scattering cross sections and with parameters for the random number generators. Files with specified extensions can be selected for display in the listing of file names. A file can be selected for loading by clicking on a particular file name. A sequence of files can be selected by clicking on the file names and simultaneously pressing the Shift key; several separate files can be selected by clicking on the file names and simultaneously pressing the Ctrl key. The loading operation is completed by clicking the **OK** button in the upper-right corner of the screen.

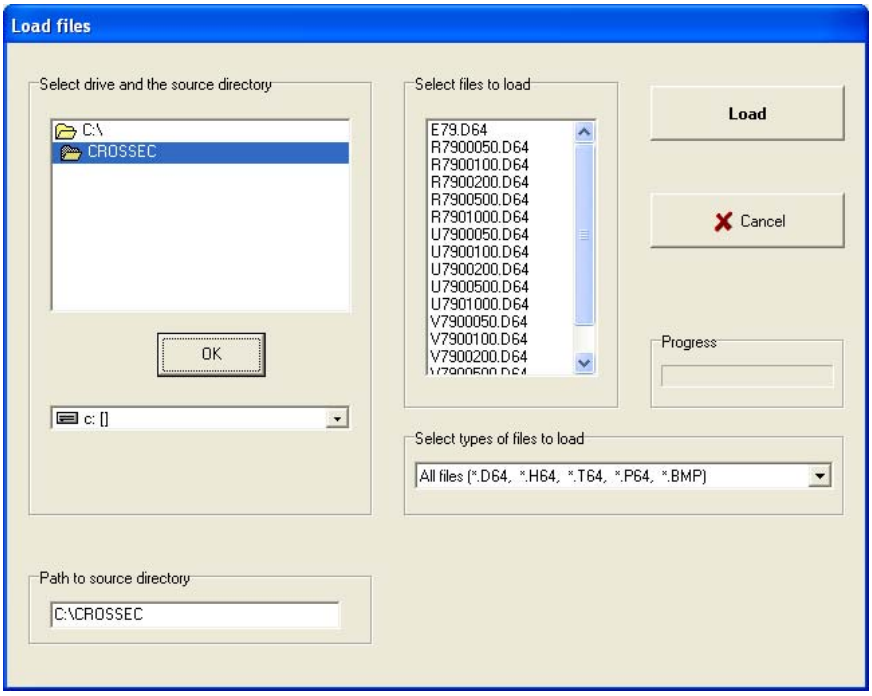

Fig. 10. Example of loading files from the directory C:\CROSSEC to the database directory.

File Management/Save files

Files containing elastic-scattering cross sections, parameters for the random number generators, phase shifts, and the transport cross sections are created by the database (as described in the **Database** option of the main menu) in the directory in which the database is located (default C:\PROGRAM FILES\NIST\ELASTIC32). The **Save files** option allows the user to save files to any other directory. Figure 11 shows an example of this option.

The center panel in Fig. 11 shows data files in the database directory (or, if desired, those with specified extensions). The file(s) to be saved should be selected by clicking on the file name(s) (and simultaneously pressing the Shift key or the Ctrl key if multiple selections are desired). The destination directory for the saved files is selected in the panel located in the upper-left corner of the screen; in Fig. 11, the directory C:\CROSSEC has been selected as the destination directory. The user then selects one of the three buttons in the lower-right corner of the screen to indicate whether the selected files should also be left in the database directory after the **Save files** operation, whether these files should be deleted from this directory, or whether all data files in the directory should be deleted. The **Save** button should then be clicked to save the designated file(s).

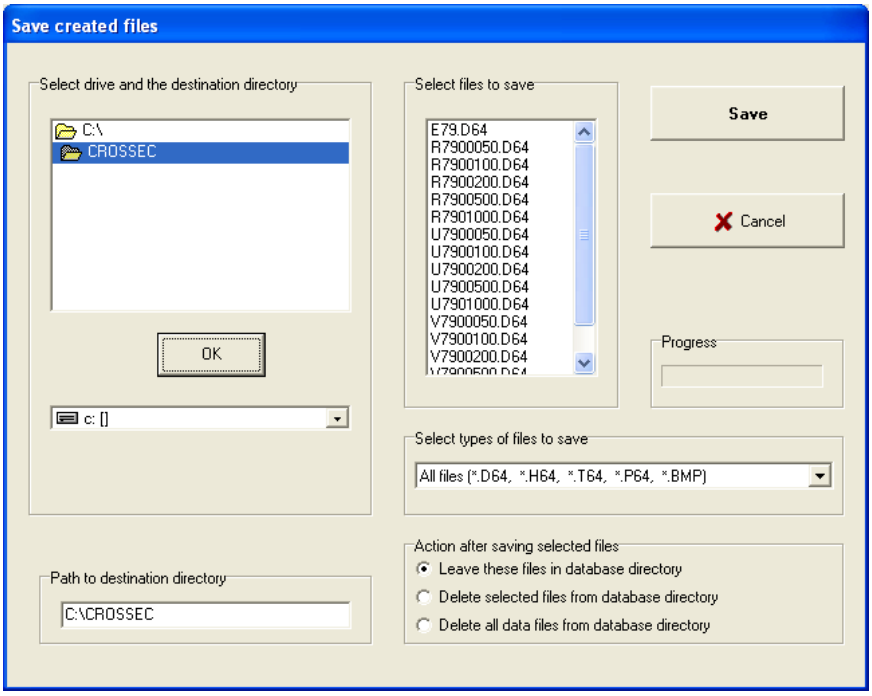

Fig. 11. Example of saving files from the database directory to the C:\CROSSEC directory.

File Management/Delete files

Data files created during the present session or during previous sessions can be deleted with this option. Figure 12 shows an example of this option.

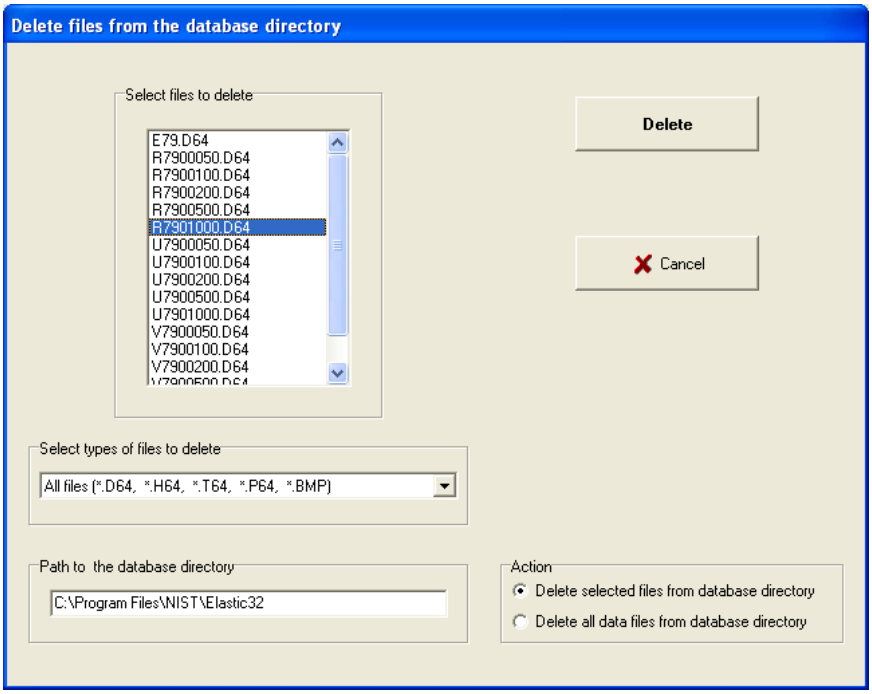

Fig. 12. Screen illustrating deletion of the file R7901000.D64 from the database directory.

The user should initially select the directory from which files are to be deleted; by default, the database directory is selected, as shown in Fig. 12. The user then selects one or more files for deletion from the list in the center of the screen; as an example, the file R7901000.D64 is marked for deletion in Fig. 12. Deletion of the selected files occurs after the **Delete** button is clicked.

File Management/Print files

Files created by the database are text files and can be opened and printed by common word-processing software. These files can also be printed with this option of the database. A screen similar to Fig. 13 appears, and a file from the database can be selected for printing. Unlike the previous file-management options, the user can only select a single file for printing. Printing is initiated by clicking the **Print** button.

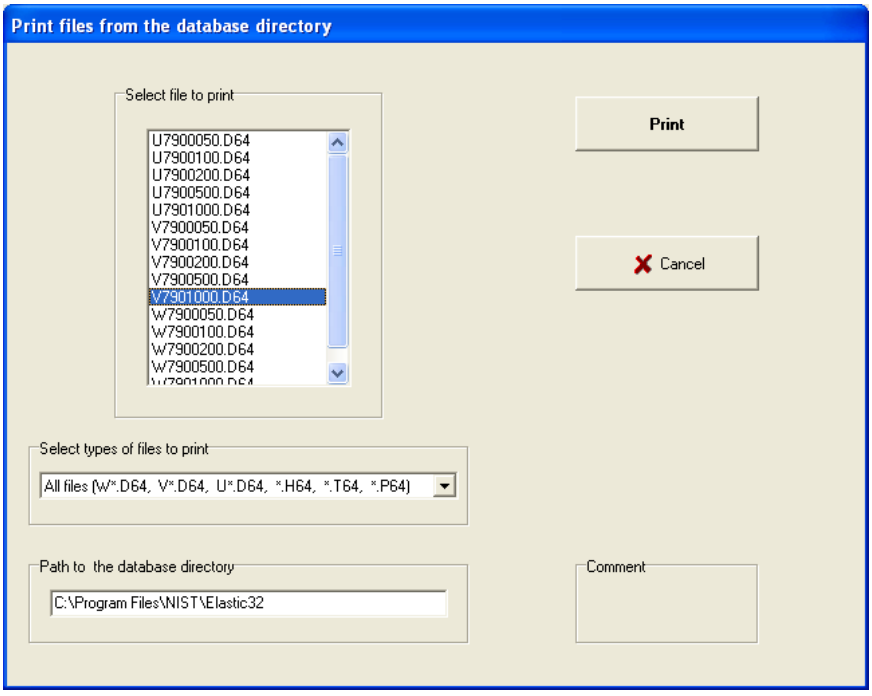

Fig. 13. Screen illustrating selection of the file V7901000.D64 for printing.

File Management/Print figures

Files with figures created by the **Compare Cross Sections** option of the database (see below) have the .BMP extension and can be inserted into documents produced by common word-processing software. These files can also be printed with this option of the database.

Figure 14 is an example of a screen that will appear if this option is chosen. A file can be selected and, after clicking the **Load image** button, the figure appears in the center of the screen. This figure can be printed in one of eight sizes by moving the pointer in the lower part of the screen with the mouse. The printed sizes are approximately 5 cm x 4 cm, 7 cm x 5 cm, 8.5 cm x 6.5 cm, 10 cm x 7.5 cm, 11.5 cm x 9 cm, 13 cm x 10 cm, 14.5 cm x 11 cm, and 16 cm x 12 cm for pointer positions 1, 2, 3, 4, 5, 6, 7, and 8, respectively. Clicking the **Print** button initiates

printing. Files with figures that are stored in other directories can be loaded into the database directory using the **Load files** option.

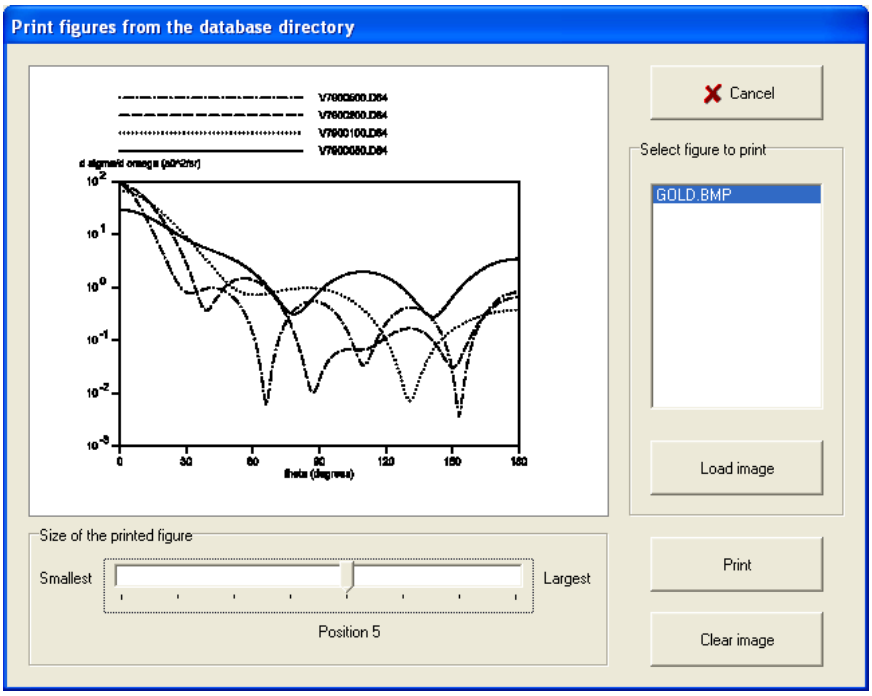

Fig. 14. Screen illustrating selection of the file GOLD.BMP (containing differential elastic-scattering cross sections for Au at four electron energies) for printing.

Run RN (Random Number) Generator
(Third Option of the Main Menu)

This option of the main menu provides a visual test of the performance of the random number generator. The test involves a comparison of the histogram of generated scattering angles with the corresponding differential elastic-scattering cross section (in the $d\sigma/d\theta$ *versus* θ coordinate system only). In this way, the performance of the random number generator is visualized.

The test is made in two stages. In the first stage, a pair of files for the test is selected. The screen for this selection is shown in Fig. 15.

The user should initially decide on the type of random number (RN) generator that is to be tested: (a) constant energy generator, or (b) variable energy generator. (Details on these random number generators are provided in Appendix A.) This selection is made by clicking the appropriate button located in the upper-right corner of the screen; the default selection is the constant energy RN generator. The list of files on the left side of the screen shows files with random number generators (of the R##$$$$$.D64 or E##.D64 type) while the list of files in the center of the screen shows files of the W##$$$$$.D64 type containing differential cross sections in the $d\sigma/d\theta$ *versus* θ coordinates. A file should be selected from each list for the same element (the ## field) and, for the case of the constant energy RN generator, the same energy

(the $$$$$ field). For the variable energy RN generator, the test is made at the energy specified by the $$$$$ field in the cross-section file. The **OK** button should then be clicked.

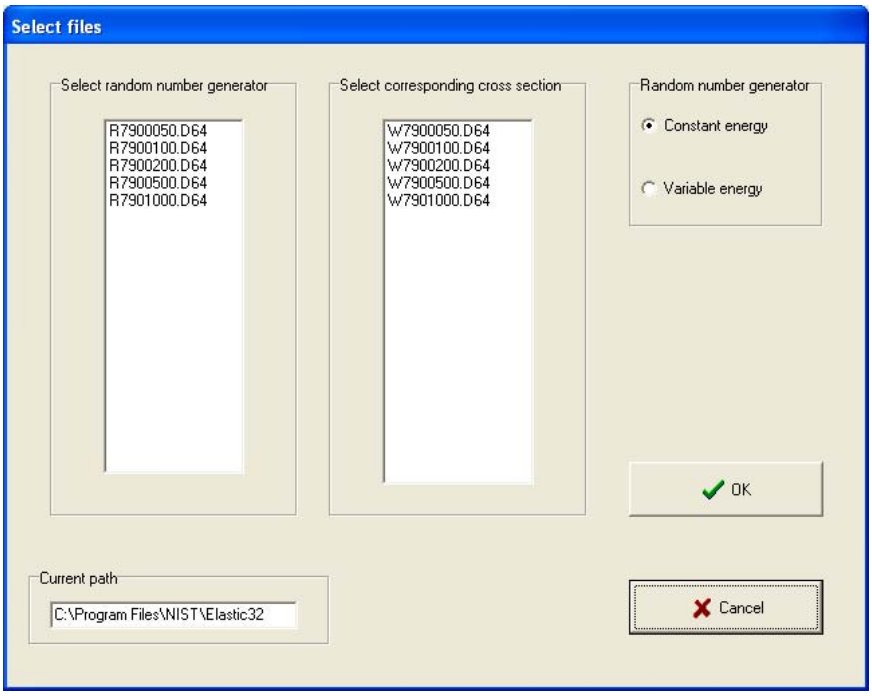

Fig. 15. Selection of the files R7900050.D64 and W7900050 from the database directory for a test of the random number generator.

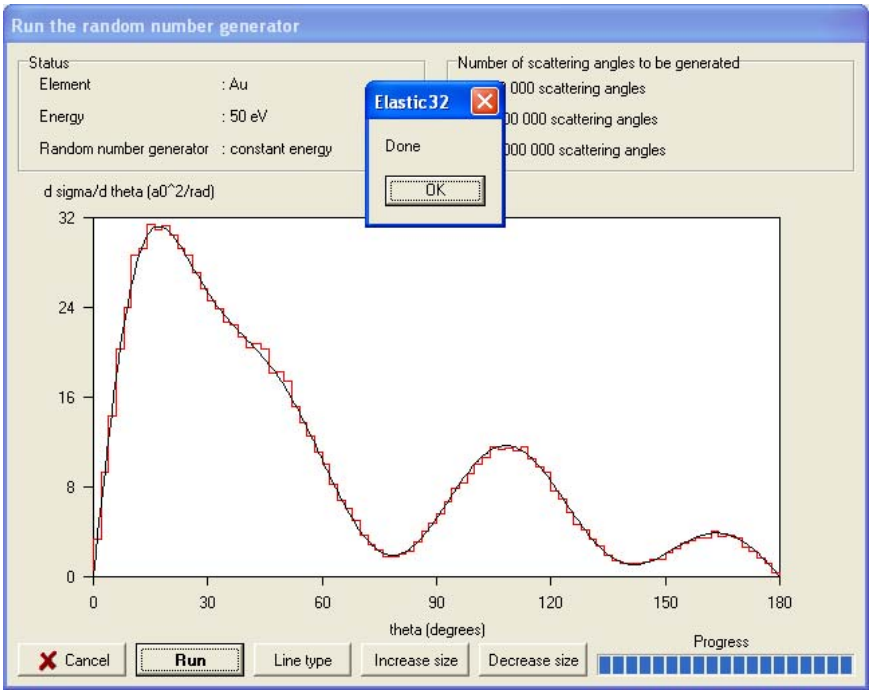

Fig. 16(a). Comparison of the differential elastic-scattering cross section for Au at 50 eV and the histogram of 100 000 scattering angles.

In the second stage of the test, the cross section $d\sigma / d\theta$ *versus* θ for the selected element and energy is shown on the screen [Figs. 16(a) and 16(b)]. Prior to running the test, the user should decide how many electron scattering angles are to be generated in one run. There are three possible choices: 100 000 scattering angles (default), 1 000 000 scattering angles, and 100 000 000 scattering angles. This selection is made by clicking a button in the upper-right corner of the screen. Before running the test, the cross-section scale can be adjusted by repeated clicking of the **Increase size** or **Decrease size** buttons. The test is started by clicking the **Run** button. A histogram of the generated scattering angles is created which, after proper normalization, is compared with the differential elastic-scattering cross section. The histogram is repeatedly updated after the generation of 10 000 scattering angles. As an example, the results of a test performed for Au and 50 eV electrons are shown in Figs. 16(a) and 16(b) for 100 000 and 1 000 000 scattering angles, respectively. The agreement between the cross section and the histogram is seen to be very good. An increase in the number of scattering angles from 100 000 to 1 000 000 leads, as expected, to a smoother histogram due to the decrease in the statistical error.

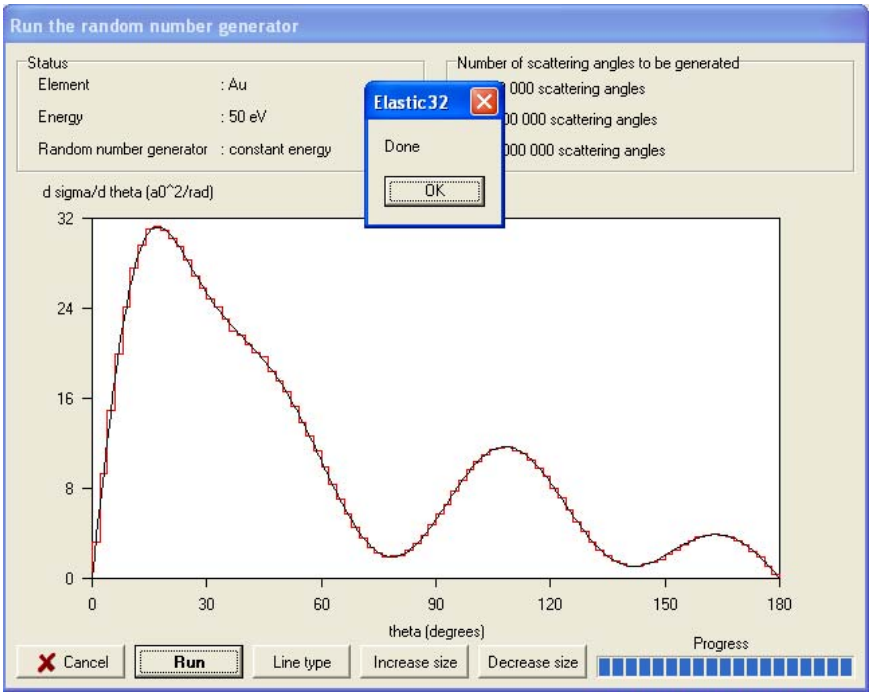

Fig. 16(b). Comparison of the differential elastic-scattering cross section for Au at 50 eV and the histogram of 1 000 000 scattering angles.

Compare Cross Sections

(Fourth Option of the Main Menu)

This option allows graphical comparison of selected differential elastic-scattering cross sections for a given coordinate system and energy range (i.e., for cross sections obtained for energies of 20 keV and below or for energies of 20 001 eV and above). Initially, the screen shown in Fig. 17 appears and this is used to select the files containing the cross sections to be displayed.

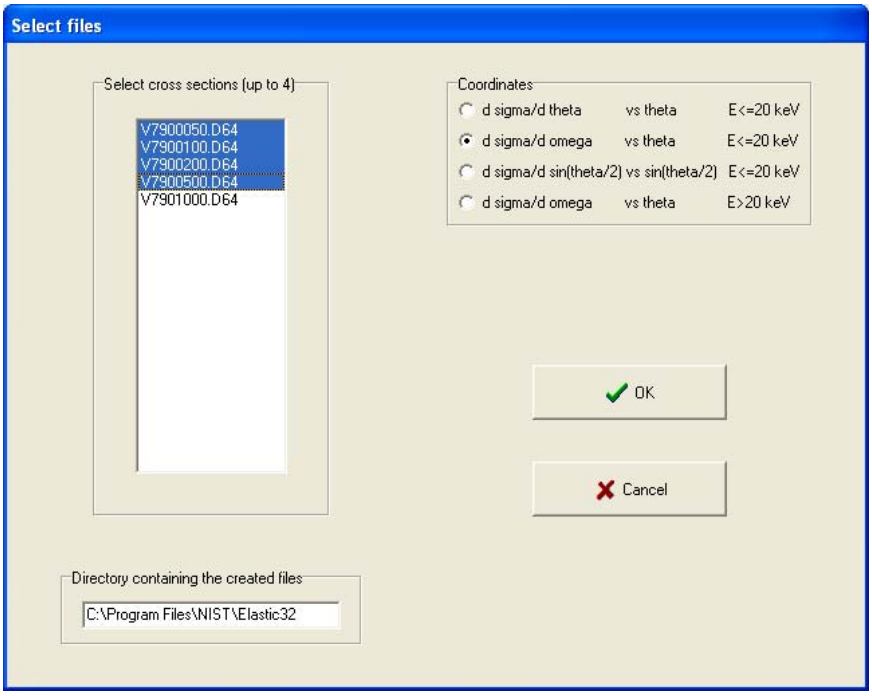

Fig. 17. Selection of files for comparison of differential elastic-scattering cross sections.

The user should first specify the coordinate system and the energy range for the particular data to be displayed by clicking one of the buttons located in the upper-right corner; by default, the $d\sigma / d\theta$ *versus* θ coordinate system is selected for energies of 20 keV and below. The available files in the database directory (for the chosen coordinates and energy range) are listed on the left-hand side of the screen. The user can select files with the mouse (for multiple selection, press the Shift or Ctrl keys simultaneously). Up to four files can be selected for comparison. In Fig. 17, files V7900050.D64, V7900100.D64, V7900200.D64, and V7900400.D64 have been selected. These files contain the differential elastic-scattering cross sections for Au at energies of 50 eV, 100 eV, 200 eV, and 500 eV in the $d\sigma/d\Omega$ *versus* θ coordinates. After clicking **OK**, the screens shown in Fig. 18(a) or 18(b) will be displayed depending on the user's choice of semi-logarithmic (the default option) or linear scales, respectively, for the cross section in the plots. If the linear-scale option is selected, the plotted scale can be varied by clicking the **Increase size** or **Decrease size** buttons.

Figures 18(c) and 18(d) show examples of comparisons of differential cross sections for Au at 50 keV, 100 keV, 200 keV, and 300 keV in the $d\sigma / d\Omega$ *versus* θ coordinates on logarithmic (the default option) or semi-logarithmic scales, respectively.

In the upper part of the plots of Fig. 18 the file name is given for each type of line on the display. This notation can be changed by repeated clicking of the **Line type** button. The comparison plots can be printed by clicking on the **Print** button, and a file containing the plot (with a .BMP extension) can be created by clicking on the **Create file** button.

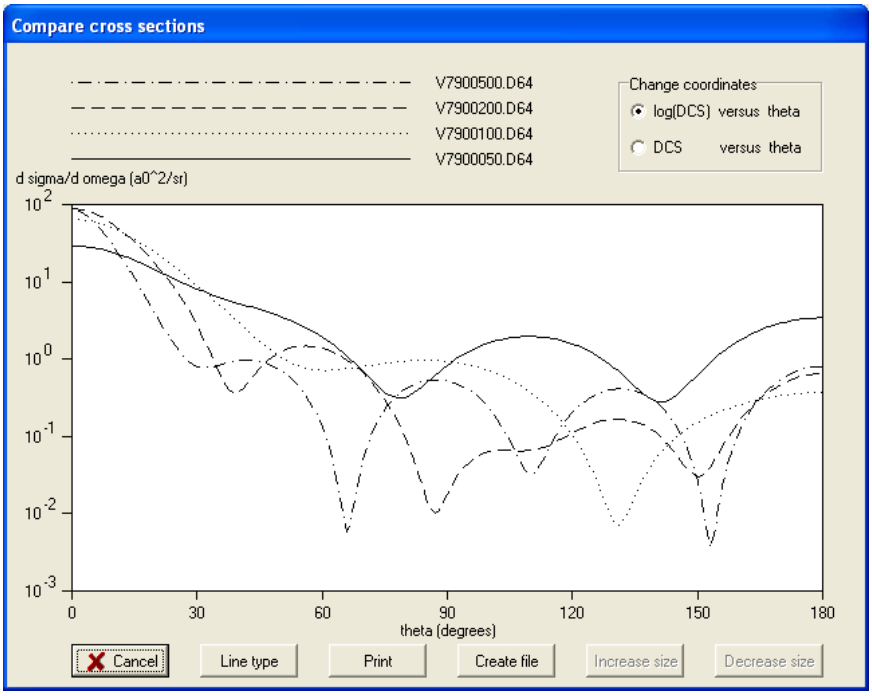

Fig. 18(a). Comparison of differential cross sections for Au at 50 eV, 100 eV, 200 eV, and 500 eV on semi-logarithmic scales.

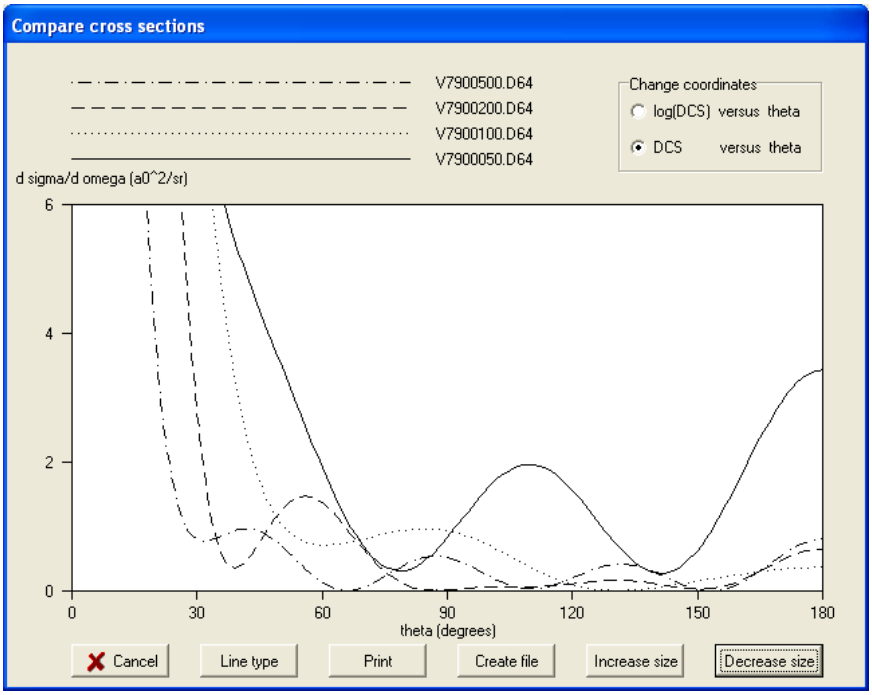

Fig. 18(b). Comparison of differential cross sections for Au at 50 eV, 100 eV, 200 eV, and 500 eV on linear scales.

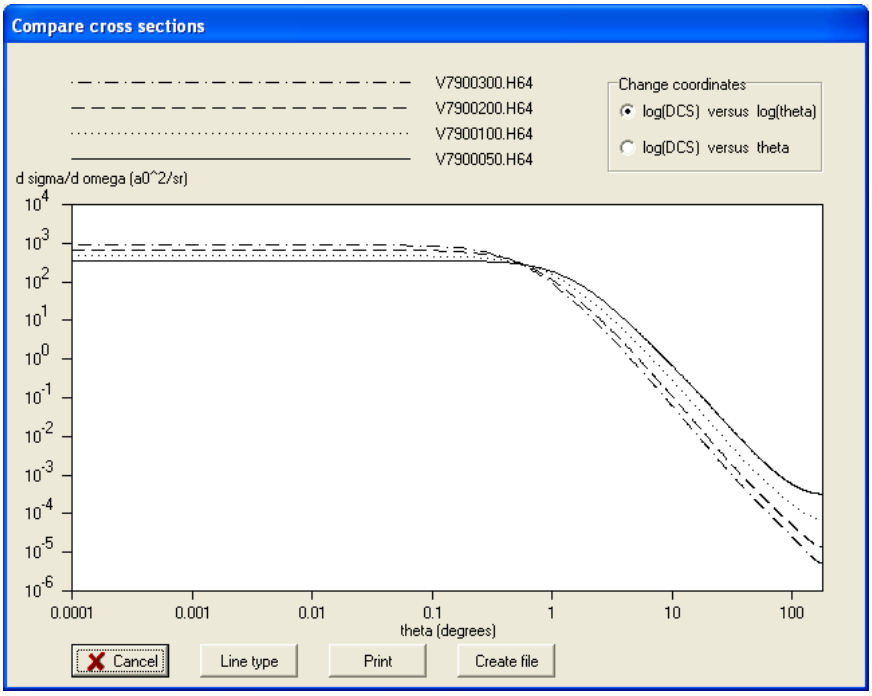

Fig. 18(c). Comparison of differential cross sections for Au at 50 keV, 100 keV, 200 keV, and 300 keV on logarithmic scales.

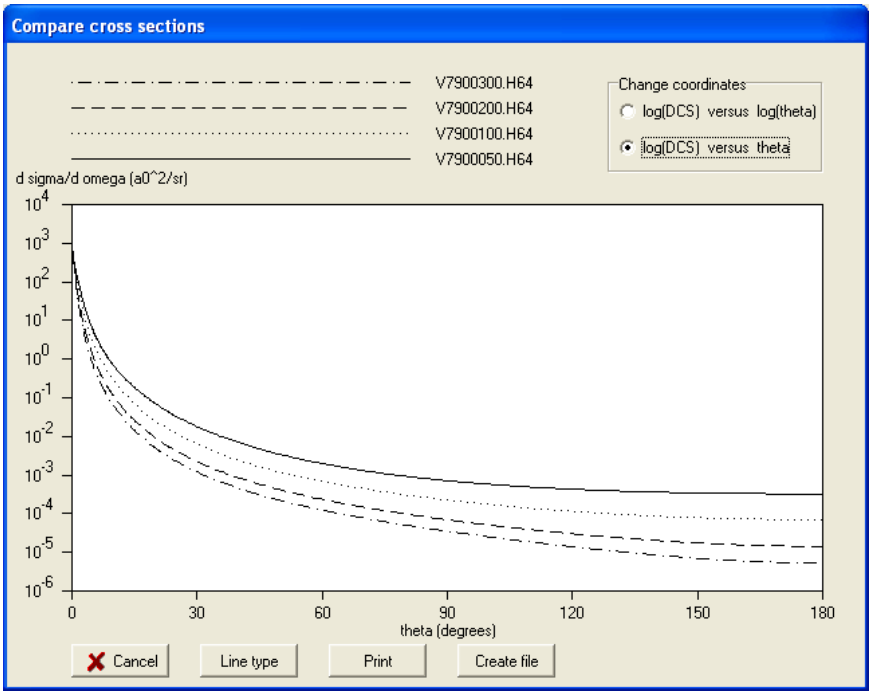

Fig. 18(d). Comparison of differential cross sections for Au at 50 keV, 100 keV, 200 keV, and 300 keV on semi-logarithmic scales.

V. THEORY

Phase shifts and differential cross sections for elastic scattering

The differential cross sections (DCSs) for elastic scattering were calculated using the relativistic Dirac partial-wave analysis, as described by Walker [3]. The scattering potential was obtained from the self-consistent Dirac-Hartree-Fock (DHF) density for free atoms [4] with the local exchange potential of Furness and McCarthy [5]. The numerical calculations were performed with the algorithm described by Salvat and Mayol [6]. Further details are given elsewhere [1,2].

The DCS is related to the phase shifts, $\delta_l^{\pm}$, of order *l* by the following expressions [3]:

$$d\sigma_e / d\Omega = \left| f(\theta) \right|^2 + \left| g(\theta) \right|^2 , \tag{1}$$

where $f(\theta)$ and $g(\theta)$ are the direct and indirect scattering amplitudes, respectively, given by:

$$f(\theta) = \frac{1}{2iK} \sum_l \left\{ (l+1)[\exp(2i\delta_l^+) - 1] + l[\exp(2i\delta_l^-) - 1] \right\} P_l(\cos\theta) \tag{2}$$

$$g(\theta) = \frac{1}{2iK} \sum_l [\exp(2i\delta_l^-) - \exp(2i\delta^+)] P_l^1(\cos\theta) . \tag{3}$$

In Eqs. (2) and (3), $P_l(\theta)$ are Legendre polynomials, and $P_l{}^1(\theta)$ are associated Legendre polynomials:

$$P_l^1(z) = (1 - z^2)^{1/2} \frac{dP_l(z)}{dz} .$$

The phase shifts $\delta_l^{\pm}$ are obtained from the large-*r* behavior of the radial wave functions, $P_l^{\pm}(r)$ and $Q_l^{\pm}(r)$ which are calculated by integrating the radial Dirac equations:

$$\frac{dP_l^{\pm}}{dr} = -\frac{k^{\pm}}{r} P_l^{\pm}(r) + \frac{E - V + 2mc^2}{c\hbar} Q_l^{\pm}(r) \tag{4a}$$

$$\frac{dQ_l^{\pm}}{dr} = -\frac{E - V}{c\hbar} P_l^{\pm}(r) + \frac{k^{\pm}}{r} Q_l^{\pm}(r) , \tag{4b}$$

where *E* is the kinetic energy of the projectile electron that is related to its total energy *W* by $E = W - mc^2$, *V(r)* is the interaction potential as a function of radius *r*, *m* is the electron rest mass, and *c* is the velocity of light. The solution algorithm implements Bühring's power-series method [7] and is based on a cubic-spline interpolation of the potential function $rV(r)$ which is tabulated on a dense grid of *r* values,

$$r_1 = 0 < r_2 \cdots < r_{N-1} < r_N \,. \tag{5}$$

That is, between each pair of consecutive grid points, r_n and r_{n+1}, the potential function, $rV(r)$, is represented as a piecewise cubic polynomial in *r*:

$$rV(r) = a_n + b_n r + c_n r^2 + d_n r^3 \,. \tag{6}$$

Then, in the interval (r_n, r_{n+1}), the radial functions can be formally expressed by power series:

$$P_l^{\pm}(r) = r^{\alpha} \sum_{i=0}^{\infty} p_i r^i \qquad\qquad Q_l^{\pm}(r) = r^{\beta} \sum_{i=0}^{\infty} q_i r^i \,, \tag{7}$$

with coefficients determined by the values of $P_l^{\pm}(r_n)$ and $Q_l^{\pm}(r_n)$ at the end point of the interval. As these series expansions can be summed up to the required accuracy (9 significant digits in the code), truncation errors are practically avoided.

The interaction potential *V(r)* is defined as:

$$V(r) = -e\varphi(r) + V_{exc}(r) \,, \tag{8}$$

where $\varphi(r)$ is the electrostatic potential of the target atom:

$$\varphi(r) = \frac{Ze}{r} - e\left(\frac{1}{r} \int_0^r \rho(r')\, 4\pi r'^2 \, dr' + \int_r^{\infty} \rho(r')\, 4\pi r' \, dr' \right), \tag{9}$$

and where $\rho(r)$ is the atomic electron density that was calculated using the self-consistent DHF code of Desclaux [4].

The term $V_{exc}(r)$ in Eq. (8) is a local approximation to the exchange interaction between the projectile and the electron in the target; it should not be confused with the exchange interaction considered in self-consistent calculations that accounts for exchange between atomic electrons. We use the exchange potential of Furness and McCarthy [5]:

$$V_{exc}(r) = \frac{1}{2}[E + e\varphi(r)] - \frac{1}{2}\left\{ [E + e\varphi(r)]^2 + 4\pi \frac{\hbar^2 e^2}{m} \rho(r) \right\}^2 . \tag{10}$$

The interaction potential [Eq. (8)] is thus completely determined by the atomic density $\rho(r)$.

The integration of the radial equations is started from *r* = 0, with boundary values:

$$P_l^{\pm}(0) = 0 \,, \qquad\qquad Q_l^{\pm}(0) = 0 \,. \tag{11}$$

In the first *r*-interval from $r_1 = 0$ to r_2 [Eq. (5)], the constants α and β are different from zero and determined by the angular momentum quantum numbers [8]. For the outer intervals ($r > r_2$), $\alpha = \beta = 0$.

After determining the values of the radial functions at r_2, the solution is extended outwards by using the series expansions [Eq. (7)] (with $\alpha = \beta = 0$) up to a certain radial distance $r_{\max}$, large enough to ensure that the potential energy of the electron $V(r)$ is negligible as compared to its kinetic energy *E*. For selected elements and at an energy of 10 000 eV, the maximum ranges, $r_{\max}$, were as follows (in a_0 units):

for Z = 1 $r_{\max}$ = 12.27
for Z = 13 $r_{\max}$ = 20.15
for Z = 28 $r_{\max}$ = 17.85
for Z = 47 $r_{\max}$ = 19.37
for Z = 79 $r_{\max}$ = 17.11
for Z = 96 $r_{\max}$ = 21.54

At an energy of 20 000 eV:

for Z = 1 $r_{\max}$ = 11.96
for Z = 13 $r_{\max}$ = 19.75
for Z = 28 $r_{\max}$ = 17.48
for Z = 47 $r_{\max}$ = 18.80
for Z = 79 $r_{\max}$ = 16.74
for Z = 96 $r_{\max}$ = 21.13

At sufficiently large distances *r*, the radial function $P_l^{\pm}(r)$ adopts the asymptotic form:

$$P_l^{\pm}(r) \cong \sin(Kr - l\frac{\pi}{2} + \delta_l^{\pm}), \tag{12}$$

where

$$\hbar K = \frac{1}{c}\sqrt{E(E + 2mc^2)} \tag{13}$$

is the momentum of the projectile. Equation (12), which confers a geometrical meaning to the phase shift, is not directly usable to compute $\delta_l^{\pm}$ because $P_l^{\pm}(r)$ reaches the form given by Eq. (12) only at distances *r* that may be much larger than $r_{\max}$. Instead, the phase shift is obtained from the calculated values of the radial functions at $r_{\max}$ by matching the numerical solution to

the exact solution for $r > r_{\max}$ $(V = 0)$ which can be expressed as a linear combination of spherical Bessel functions, $j_k(Kr)$ and $n_k(Kr)$ of indices $k = l, l \pm 1$ [8].

A considerable number of phase shifts was found to be necessary to achieve 8-digit accuracy in the calculation of DCSs from Eqs. (1) to (3). At an energy of 10 000 eV, we have:

for Z = 1	$0 \le l \le 221$
for Z = 13	$0 \le l \le 386$
for Z = 28	$0 \le l \le 343$
for Z = 47	$0 \le l \le 369$
for Z = 79	$0 \le l \le 325$
for Z = 96	$0 \le l \le 422$

At an energy of 20 000 eV:

for Z = 1	$0 \le l \le 307$
for Z = 13	$0 \le l \le 538$
for Z = 28	$0 \le l \le 478$
for Z = 47	$0 \le l \le 514$
for Z = 79	$0 \le l \le 452$
for Z = 96	$0 \le l \le 589$

The only special functions used in calculations of the DCSs for the DHF potential are spherical Bessel functions $j_l(x)$ and $n_l(x)$. The algorithm used to compute these functions combines several analytical expressions and recurrence relations, and yields results that are accurate to 13 or more significant digits. The code used for these calculations was tested for $0 \le l \le 20\,000$ and $0 < x < 20\,000$.

Transport cross sections

Transport cross sections are needed for determination of numerous parameters related to electron transport in solids (the depth distribution function, the effective attenuation length, the electron mean escape depth, etc.) [9, 10]. The transport cross section describes the mean fractional momentum loss due to elastic scattering alone. We denote by **k** the electron momentum before elastic scattering, and by **k′**, the projection of the momentum after elastic scattering on the initial direction. Obviously, $\mathbf{k}'=\mathbf{k}\cos\theta$. We further denote the fractional momentum loss, due to elastic scattering alone, by

$$\Delta k = \frac{\left|\mathbf{k}-\mathbf{k}'\right|}{\left|\mathbf{k}\right|}.$$

The transport cross section is the product of the mean fractional momentum loss and the total elastic-scattering cross section:

$$\sigma_{tr} = \sigma_{el}\langle\Delta k\rangle = \sigma_{el}\frac{\int_{4\pi}\Delta k\,(d\sigma/d\Omega)\,d\Omega}{\int_{4\pi}(d\sigma/d\Omega)\,d\Omega}. \qquad (14)$$

Equation (14) can be transformed to:

$$\sigma_{tr} = 2\pi\int_0^{\pi}(1-\cos\theta)(d\sigma/d\Omega)\sin\theta\,d\theta. \qquad (15)$$

A change of the atomic potential leads to pronounced variation of the differential elastic-scattering cross section for small scattering angles and rather small variations for larger scattering angles [10]. In the integrand of Eq. (15), we have two functions approaching zero for small scattering angles: $\sin\theta$ and $(1-\cos\theta)$. Consequently, we may expect that the sensitivity of the transport cross section to the interaction potential is much smaller than the sensitivity of the total elastic-scattering cross section. It has been shown that the transport cross sections values depend very weakly on the potential for elements with a wide range of atomic numbers (Be to Au) and for electron energies from 100 eV to 10 000 eV [11].

VI. COMPARISONS OF DIFFERENTIAL CROSS SECTIONS AND TRANSPORT CROSS SECTIONS FROM VERSIONS 2.0 AND 3.0

The differential elastic-scattering cross sections provided in Version 2.0 of this database (and the transport cross sections derived from them) were computed for the Thomas-Fermi-Dirac (TFD) atomic potential, while the cross sections in Version 3.0 were obtained from the self-consistent Dirac-Hartree-Fock (DHF) electron density [4] and a local exchange potential [5]. The latter approach provides a more accurate description of the atomic structure and of elastic-electron scattering [1,2].

We give here a brief overview of the resulting differences in differential cross sections and transport cross sections provided in Version 2.0 (based on the TFD potential) and 3.0 (based on the DHF potential) of this database. Further details of these differences are discussed elsewhere [1].

Figures 19-21 are examples of the percentage differences between the differential cross sections, ΔDCS, calculated from the TFD and DHF potentials as a function of scattering angle for Al, Ag, and Au at energies of 100 eV, 500 eV, 1000 eV, and 10 000 eV [1]. The structure visible in Figs. 19-21 is associated with variations in the positions and/or the amplitudes of minima in the corresponding differential cross sections from the TFD and DHF potentials.

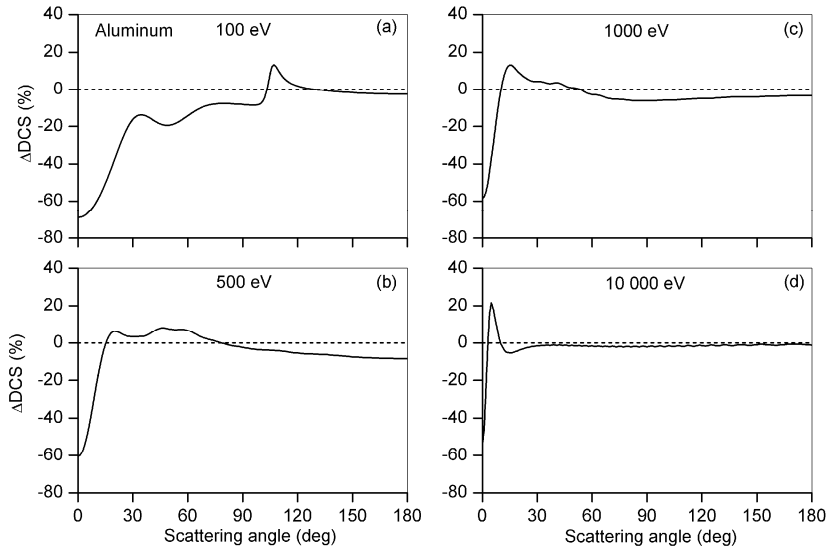

Fig. 19. Percentage difference between differential cross sections, ΔDCS, calculated from the TFD and DHF potentials for Al at energies of (a) 100 eV, (b) 500 eV, (c) 1000 eV, and (d) 10 000 eV [1].

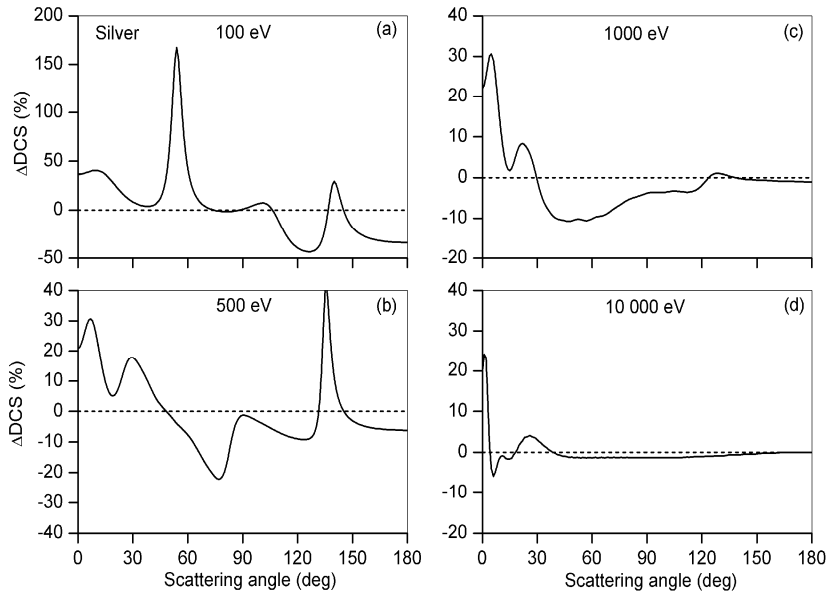

Fig. 20. Percentage difference between differential cross sections, *ΔDCS*, calculated from the TFD and DHF potentials for Ag at energies of (a) 100 eV, (b) 500 eV, (c) 1000 eV, and (d) 10 000 eV [1].

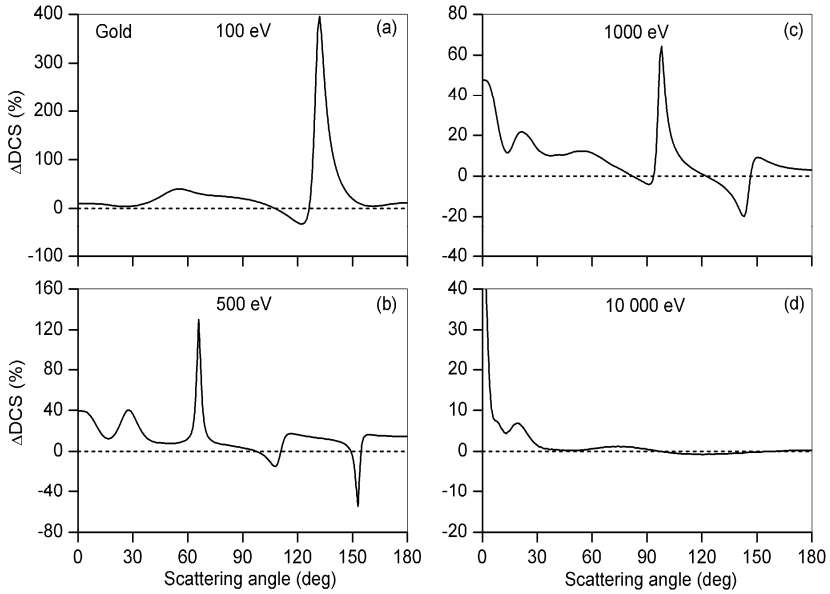

Fig. 21. Percentage difference between differential cross sections, *ΔDCS*, calculated from the TFD and DHF potentials as a function of scattering angle for Au at energies of (a) 100 eV, (b) 500 eV, (c) 1000 eV, and (d) 10 000 eV [1].

Figure 22 shows the percentage deviations in the transport cross sections, $\Delta\sigma_{tr}$, as a function of electron energy for these three elements [1]. As expected from Eq. (15), the percentage deviations in Fig. 22 are less than those for the corresponding differential cross sections in Figs.

19-21. Information on the consequences of the changes in differential and transport cross sections for certain derived quantities is presented elsewhere [1].

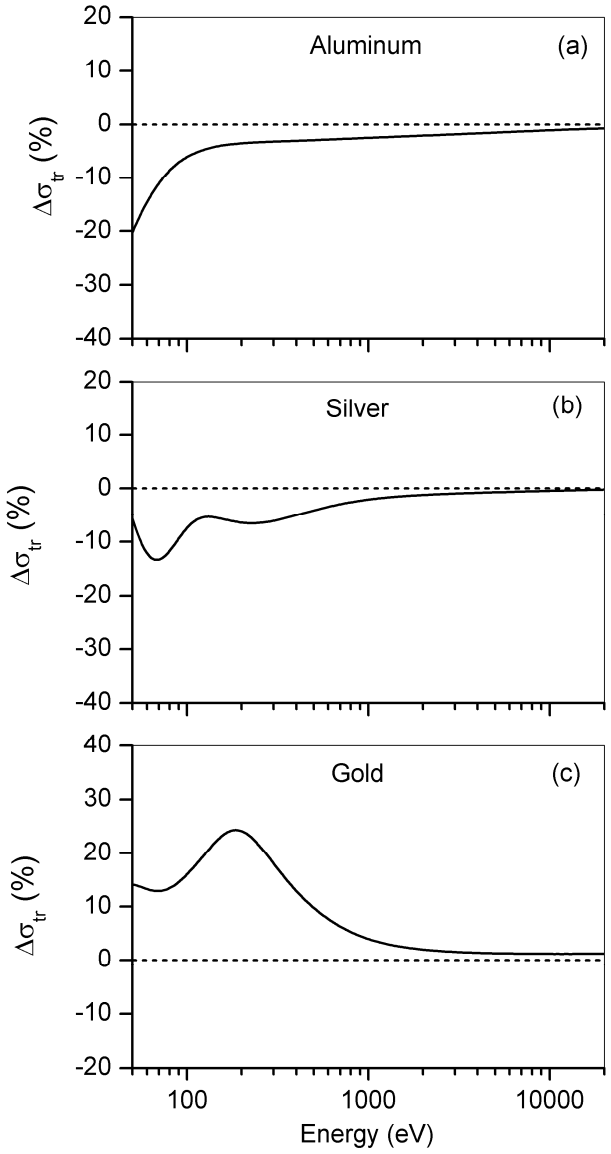

Fig. 22. Percentage difference between transport cross sections, *ΔDCS*, calculated from the TFD and DHF potentials as a function of electron energy for (a) Al, (b) Ag, and (c) Au [1].

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APPENDIX A
RANDOM NUMBER GENERATORS

This section describes the FORTRAN source codes for the random number generators providing the electron scattering angles. These codes, Example1 and Example2 for cases of constant electron energy and variable electron energy, respectively, are supplied in the directory EXAMPLES of the CD as text files. These programs require the files R##$$$$$.D64 or E##.D64 created by the database. The programs listed here generate the histograms of scattering angles that correspond to those displayed in the option **Test the random number generator** of the main menu. Two cases are considered: (i) constant electron energy, and (ii) variable electron energy. Both programs are fully portable and can be added to any FORTRAN code.

Constant Energy (EXAMPLE1 code)

The random number generator for electron scattering angles at constant electron energy (e.g., Auger electrons, photoelectrons) is implemented by the subprogram:

ELAST(INDEX,IDUM,IZ,ENERGY,SIGMA)

The meaning of the arguments is as follows:

Input parameters:

INDEX Flag selecting the generated quantity
INDEX = 1, Generate cosine of the scattering angle.
INDEX = 2, Generate the scattering angle (radians).
INDEX = 3, Generate the scattering angle (degrees).

IDUM Initialization parameter. It must be set to a positive value at the beginning of the main program.

IZ Atomic number.

ENERGY Electron energy (in eV).

Output parameter:

SIGMA After initialization, contains the total elastic-scattering cross section (in a_0^2 units).

The parameters are also explained by comments in the code. The algorithm implements a somewhat modified version of the composition method [12]. Details of this implementation were published by Jablonski and Tougaard [12]. The subroutine NRANDOM implements the following linear congruential random number generator (also called the mixed generator):

$$x_{n+1} = kx_n + c(\mathrm{mod}2^{31}) \qquad n = 0,1,2,\ldots,$$

where $k = 214013$ and $c = 2531011$. The parameters k and c are selected so that the maximum period of 2^{31} numbers can be achieved (k = 1 mod (4), c is odd). The initial value x_0 (the seed) should satisfy the inequality:

$$0 \le x_0 \le 2^{31} - 1.$$

The subroutine NSEED initializes the random number generator before the first call by providing the starting value of x_0. The generated sequence x_1, x_2, x_3, ... obviously depends on the initial value of x_0. In the listing of the program EXAMPLE1, x_0 is equal to unity (see the function RANG). The random numbers are submitted to the randomizing shuffle in the subroutine RAN. Finally, the uniformly distributed random numbers are used in the function ELAST to generate values of the scattering angles.

The statistical properties of the uniform random number generator (subroutine NRANDOM) described here have not been tested. However, the performance of this generator seems to be of sufficient quality for the examples shown below (cf. Figs. A1 and A2). For other applications, this generator can be easily replaced by another generator of random numbers. Several FORTRAN implementations of such generators have been proposed by Press and Teukolsky [13].

As an example, we consider operation of the program EXAMPLE1 (see Figure A1) for which we have introduced the following values:

Atomic number	= 79
Energy	= 500 eV
Number of trajectories	= 1 000 000

The probability density function corresponding to this element and energy is very difficult to simulate since (a) the cross section is strongly dominated by small-angle scattering, (b) in the region of large scattering angles, several minima and maxima are observed, and (c) the minima are very deep. To proceed with the calculations, the program EXAMPLE1 must be accompanied in the same directory by the file R7900500.D64. This file must have been previously created by the database. After running the random number generator program, the file RESULT1.TXT is created. This file contains the frequency histogram of generated scattering angles. The histogram is normalized so that it is directly comparable with the differential elastic-scattering cross section contained in the file W7900500.D64. The calculated histogram and the differential elastic-scattering cross section are compared in Figure A1. As one can see, excellent agreement is observed except in the vicinity of deep minima.

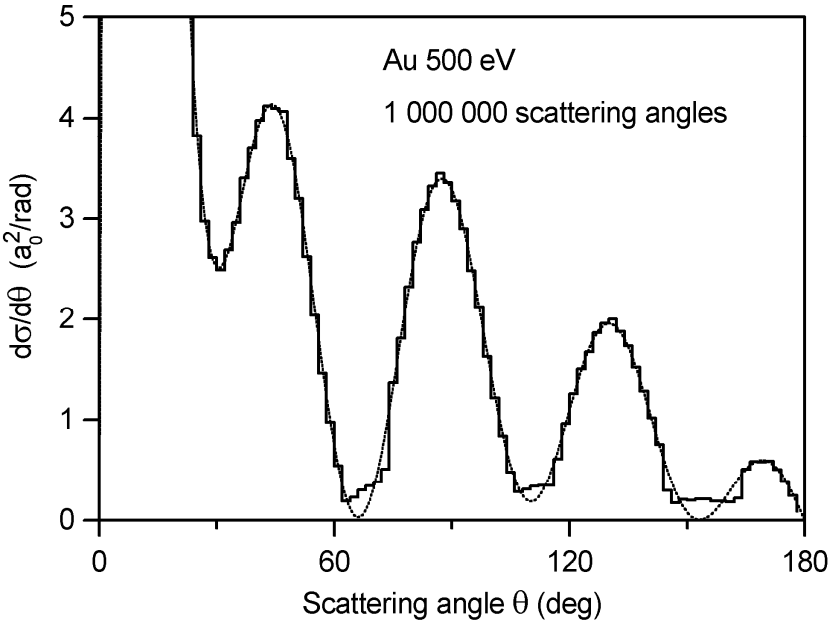

Fig. A1. Comparison of the differential elastic-scattering cross section, $d\sigma/d\theta$, (dashed line) with the frequency histogram of generated scattering angles (solid line) for Au at 500 eV. The histogram was calculated using the generator working at constant electron energy.

Variable Energy (EXAMPLE2 code)

The portable random number generator providing the scattering angles for variable energies is implemented by a FORTRAN function. This generator is particularly useful for simulations of electron trajectories in which the electron energy is changing.

GENER(INDEX,IDUM,IZ,ENERGY,SIGMA)

The meaning of the formal parameters is the same as in the case of the function ELAST described above. Correct performance of the function GENER requires prior creation of the file E##.D64. As before, the algorithm implements a variation of the composition method [11].
We now run EXAMPLE2 under the same conditions as previously selected for EXAMPLE1 (constant electron energy). Prior to these calculations, we have created the file E##.D64. We introduce the same input values as before:

Atomic number	= 79
Energy	= 500 eV
Number of trajectories	= 1 000 000

The file RESULT2.TXT, created during program execution, contains the frequency histogram of generated scattering angles. Figure A2 compares this histogram with the differential elastic-scattering cross section.

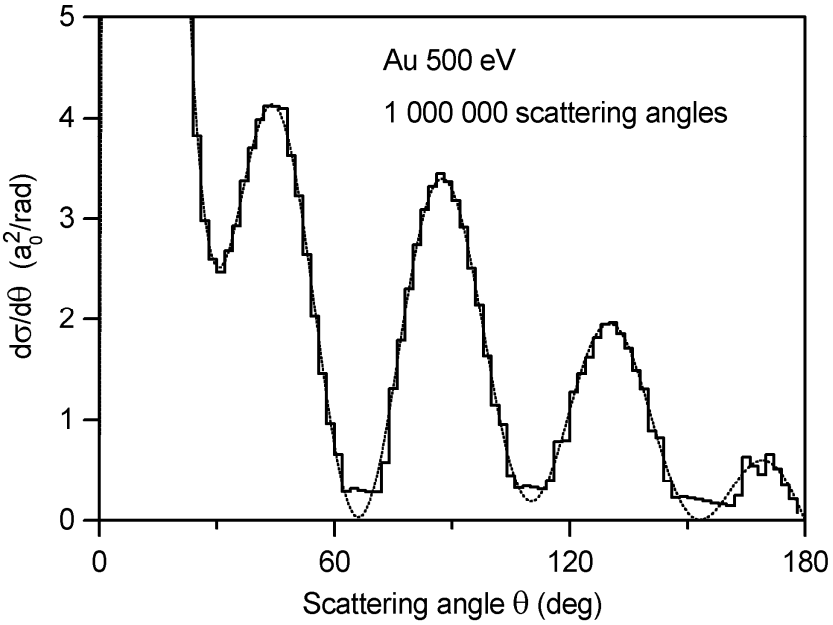

Fig. A2. Comparison of the differential elastic-scattering cross section, $d\sigma/d\theta$, (dashed line) with the frequency histogram of generated scattering angles (solid line) for Au at 500 eV. The histogram was calculated using the generator working at variable electron energy.

We see that the performance of the random number generator GENER is comparable with the generator ELAST. Calculations within the program EXAMPLE2 are made at a constant energy equal to 500 eV. The advantage of the function GENER consists in the fact that change in the value of the input parameter ENERGY would result in generating the scattering angles according to the differential cross section for the new energy. No additional files supporting the generator are necessary. Subprogram ELAST requires separate files R79$$$$$.D64 for each referenced energy. This would be difficult to realize in cases when we do not know *a priori* the electron energy. The file E79.D64 (and similar files for other elements) covers the energy range from 50 eV to 20 000 eV, i.e., the entire energy range for which it is possible to generate differential cross sections in the $d\sigma/d\theta$ versus θ coordinates.

APPENDIX B
CONTACTS

If you have comments or questions about the database, the Standard Reference Data Program would like to hear from you. Also, if you have any problems with the CD-ROM or installation, please let us know by contacting:

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