

NIST NSRDS 154

NIST Backscattering-Correction-Factor Database for Auger Electron Spectroscopy

**Version 1.1
User's Guide**

A. Jablonski
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User's Guide**

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1. INTRODUCTION

The backscattering factor (BF) has long been recognized as an important matrix correction factor in quantitative applications of Auger electron spectroscopy (AES) [1-3]. Most analysts have relied on predictive formulae for the BF published by Shimizu in 1983 [4] that were based on extensive Monte Carlo simulations by Shimizu and Ichimura [5,6]. In recent years, there has been renewed interest in BF calculations for several reasons.

First, the Shimizu and Ichimura simulations were performed for a group of elemental solids and inorganic compounds, primary energies of 3 keV, 5 keV, and 10 keV, and angles of primary-beam incidence of 0°, 30°, and 45°. Modern AES instruments, however, routinely use primary energies of up to 25 keV and may use angles of primary-beam incidence other than those chosen for the Monte Carlo simulations. It has therefore been necessary to make extrapolations from BF values from the Shimizu formulae. The uncertainties of these extrapolated BFs are unknown.

Second, the BF was originally defined by ASTM International [7] as the “fractional increase in the Auger current due to backscattered electrons” and by the International Organization for Standardization (ISO) [8] similarly as the “factor defining the increase in the Auger electron current due to additional ionizations in the sample caused by backscattered electrons above that arising directly from the primary electrons.” These definitions, however, were shown to be unsatisfactory by Jablonski [9] since the “fractional increase” can be negative at relatively low primary energies and/or for more grazing incidence of the primary electrons.

ISO Technical Committee 201 on Surface Chemical Analysis therefore deprecated use of backscattering factor and introduced definitions of two new terms, the backscattering correction factor (BCF) and the backscattering fraction [10]. The definition of the BCF is “a factor equal to ratio of the Auger-electron current arising from ionizations in the sample caused by both the primary electrons and the backscattered electrons to the Auger-electron current arising directly from the primary electrons.” The proposed definition of the backscattering fraction is “ratio of the Auger-electron current arising from ionizations in the sample caused by backscattered electrons and the Auger-electron current arising directly from the primary electrons.” Each proposed definition is accompanied by the same two explanatory Notes. “(1) The AES literature contains many references to “backscattering factor” but the use of this term is ambiguous. In some papers and books, the backscattering factor is the same as the backscattering correction factor, while in other papers and books the backscattering factor is identified as the backscattering fraction. In practice, this ambiguous usage generally does not cause misunderstanding since the backscattering correction factor (often denoted by R) is equal to unity plus the backscattering fraction (often denoted by r). To avoid misunderstanding, use of the term backscattering factor is deprecated. (2) In simple theories, evaluations of the backscattering correction factor may be based on the assumption that the primary-electron beam is unchanged, in intensity, energy or direction, within the information depth for Auger-electron emission. This assumption becomes progressively less useful as the primary energy becomes closer to the core-level ionization energy for the relevant Auger transition or for increasing angles of incidence of the primary electrons. In such cases, a more advanced theory of electron transport should be used. For example, if the primary electron energy is less than twice the core-level ionization energy, the total Auger-electron current emitted from the sample may be less than that calculated for an unaltered primary beam alone so that the effective value of the backscattering correction

factor is then less than unity and the backscattering fraction is negative. In addition, the separate classification of the electrons as primary or backscattered becomes progressively less useful.”

We note that the entire ASTM International standard terminology document [7] was withdrawn in 2012. Other ASTM International standards for surface analysis will now reference the ISO Vocabulary document [10] to prevent misunderstandings that would arise if two non-identical definitions were given in different standards documents for the same term.

Third, Jablonski has developed an advanced model of electron transport in a sample from which the BCF can be calculated [9]. This advanced model also has a major advantage over the simplified model of electron transport (on which the earlier ASTM and ISO definitions of BF were based) in that it shows a weak dependence of the BCF on analyzer acceptance angle (i.e., the Auger-electron emission angle).

Finally, a number of papers have been published that show significant differences between BCFs from the advanced model and BCFs from the simplified model [9,11-16]. BCFs from the advanced model also can differ from BFs from the Shimizu formulae [4], also based on the simplified model, due to the use of different algorithms and new data for the differential elastic-scattering cross sections [17] in recent work that are believed to be more accurate than the data used earlier [18].

The National Institute of Standards and Technology (NIST) Backscattering-Correction-Factor Database for Auger Electron Spectroscopy provides BCFs from Monte Carlo simulations based on both the simplified and advanced models [16]. The opportunity to use both models is provided so that users can readily ascertain the magnitudes of differences in BCFs from each model for materials and analysis conditions of interest. Analysts can readily specify the experimental conditions of interest (primary-beam energy, primary-beam angle of incidence, and, for the advanced model, analyzer-acceptance solid angle), the likely or estimated sample composition, the subshell of the element to be ionized, one of three available formulae for the inner-shell ionization cross section, and, for the advanced model, the Auger-electron transition of interest. The user can also select different numbers of trajectories in the Monte Carlo simulations so that tradeoffs can be made between calculation time and precision of the resulting BCF value. The results of a BCF calculation can be stored in a file for later use. While simulations with the simplified model are generally faster than those with the advanced model, BCFs from the advanced model are considered more reliable.

BCFs from the advanced model are obtained from an integration over depth of the product of the excitation depth distribution function (EXDDF) and the integral emission depth distribution function (IEMDDF) [15]. The EXDDF describes the depth distribution of inner-shell ionizations (that lead to subsequent emission of the relevant Auger electrons) for a specified primary energy and angle of incidence. The IEMDDF describes the depth distribution of emitted Auger electrons for a specified analyzer-acceptance angle. BCFs from the simplified model are obtained from an integration of the energy and angular distribution of backscattered electrons leaving the solid, $I_B(E, \alpha_B)$, the cross section for inner-shell ionization, and the secant of the backscattered-electron emission angle, α_B ; this integration is performed over the backscattered-electron energy, E , from the threshold energy for inner-shell ionization to the primary energy and over the

hemisphere above the sample from which backscattered electrons are emitted. Monte Carlo simulations are performed over a specified number of trajectories to obtain the EXDDF and IEMDDF for the advanced model and $I_B(E, \alpha_B)$ for the simplified model. These trajectories are calculated with differential elastic-scattering cross sections from the NIST Electron Elastic-Scattering Cross-Section Database [17,18], electron stopping powers from a predictive formula [19], and inner-shell ionization cross sections from one of three user-specified predictive formulae [20-22]. Llovet *et al.* [23] recently published an extensive analysis of measurements of cross sections for ionization of K shells and L and M subshells by electron impact. They were able to identify sets of measured cross sections that satisfied mutual-consistency checks and showed that the predictive formulae of Bote *et al.* [22] were superior to those of Casnati *et al.* [20] and Gryzinski [21].

A simulation to obtain a BCF value can take between about 1 minute and 1 hour, depending on the selected material, the primary energy, the choice of the simplified or the advanced model, the chosen number of trajectories, and the speed of the computer. Operation of the database will cease if the user tries to use another program or application while the BCF database is performing a Monte Carlo simulation. This problem can be avoided by running the BCF database in the “Batch” mode, as described in Section 4. In the Batch mode, one simulation or a series of simulations for various selected primary energies can be performed sequentially (e.g., overnight or while the computer is being used for another purpose).

Version 1.0 of SRD 154 was released in February, 2011. Version 1.1 was issued in July, 2015 to correct a software bug in calculations of the IEMDDF for compounds and alloys. Previous calculations of BCFs for compounds and alloys with Version 1.0 could have an additional uncertainty of up to 3 % due to a bug in the sampler of elastic-scattering angles.

2. GETTING STARTED

2.1 Database Files

The file with the database and a PDF file with the Users' Guide can be downloaded from NIST (<http://www.nist.gov/srd/nist64.cfm>). Alternatively, NIST can mail a CD-ROM with these files.

2.2 System Requirements

1. Personal computer with Windows 95, Windows 98, Windows NT, Windows 2000, Windows ME, Windows XP, Windows Vista, Windows 7, or Windows 8 operating system.
2. CD-ROM drive.
3. Hard disk space of 50 MB or more.
4. Screen resolution of 1024 by 768 pixels.
5. System font size: small fonts, normal in Windows XP, or 100 % in Windows 7)

The database has been designed to operate optimally at the screen resolution given above. However, it can also be operated at a higher screen resolution, e.g., 1152 by 864 pixels or 1280 by 1024 pixels. In the latter case, there may be difficulties in reading text on the screen. For all resolutions, the font size specified above must be selected.

To change the 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, select the **General** tab, and then select the **Normal size (96 DPI)** option in the **Display** box.

2.3 Installation of the Database

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

Alternatively, the following procedure can be used:

1. Insert the CD into the CD-ROM drive.
2. Double-click **My Computer** on the desktop.

3. Double-click the icon corresponding to the CD-ROM drive.
4. Double-click the **Setup** icon (showing the computer), i.e., **setup.exe**.
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 (showing the computer), i.e., **setup.exe**. Follow instructions on the screen.

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 **BCF.exe** located in the Program files directory.

By default, the database is installed in the directory:

C:\PROGRAM FILES\NIST\BCF

Furthermore, the program BCF is added to the list of programs appearing after clicking the start button and choosing Programs. After installation, it is advisable to create a shortcut to the BCF program (by dragging the BCF program with the mouse from the program list to the desktop).

2.4 Operation of Batch Programs

As described in the Introduction, the database can be operated in a batch mode so that Monte Carlo simulations to obtain BCF values can be run in the background (i.e., while the computer is used for other purposes) or so that a series of BCF values can be obtained for a series of user-specified primary energies (e.g., overnight). The CD-ROM (or the downloaded files) contain the following four folders:

1. Directory BATCH_ADV_COM containing the program **BCF_ADV_COM.exe** (to obtain BCF values from the advanced model for compounds and alloys).
2. Directory BATCH_ADV_ELE containing the program **BCF_ADV_ELE.exe** (to obtain BCF values from the advanced model for elemental solids).
3. Directory BATCH_SIM_COM containing the program **BCF_SIM_COM.exe** (to obtain BCF values from the simplified model for compounds and alloys).
4. Directory BATCH_SIM_ELE containing the program **BCF_SIM_ELE.exe** (to obtain BCF values from the simplified model for elemental solids).

The desired folder should be opened and the relevant application launched (e.g., by double-clicking **BCF_ADV_COM.exe** to obtain BCF values from the advanced model for compounds and alloys).

2.5 Removal of the Database

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

3. OPERATION OF THE DATABASE

The operation of the database can be understood by reference to the various database screens shown here. Figure 1 shows the title or home screen.

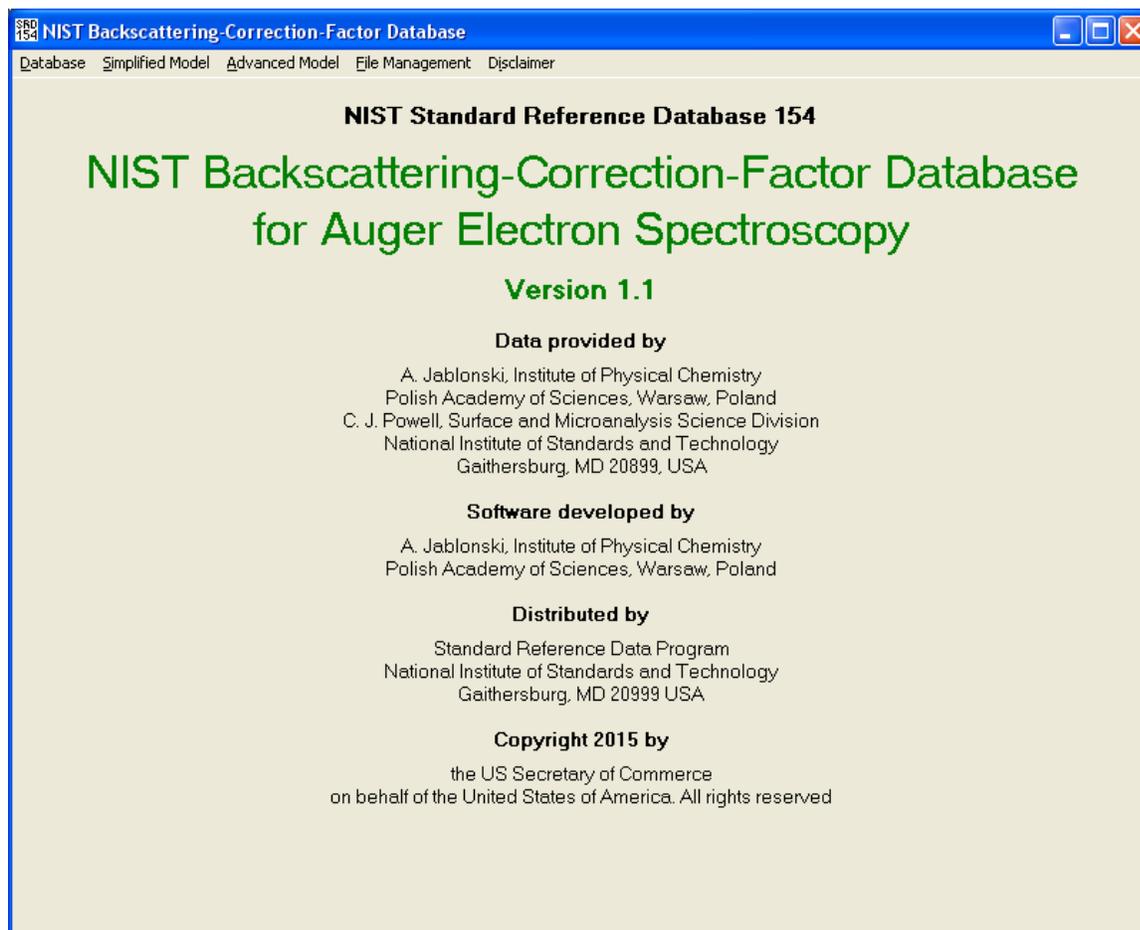


Fig. 1. Title screen.

As explained in the Introduction and elsewhere [15,16], backscattering correction factors (BCFs) for AES can be calculated from a “simplified model” or an “advanced model”. The simplified model has been used for many years and was utilized in previous ASTM [7] and ISO [8] definitions. This model, however, is based on a number of simplifying assumptions that break down for primary energies that are “close” to the threshold energy for inner-shell ionization and/or for increasing angles of incidence of the primary beam [15,16]. Jablonski [9] developed an advanced model that does not require the simplifying assumptions. As explained in the Introduction, the BCF is a new term [10] introduced to overcome shortcomings of the backscattering factor that has been used for many years for quantitative AES. With the new BCF database, a user can readily compare BCFs from the two models and determine the magnitude of differences for particular materials, Auger lines, and experimental conditions such as primary energy, primary-beam angle of incidence, and analyzer location and angular acceptance.

The following two sections describe use of the database to obtain BCF values for elemental solids from the simplified and advanced models. The third section describes operation to obtain BCF values for compounds and alloys from each model. The final section explains the file-management options in the database and other screens available from the home page.

3.1 BCFs from the Simplified Model for Elemental Solids

Figures 2(a) and 2(b) show the first main screen in which the experimental configuration is outlined by the user. If the “Simplified Model” is selected, it is necessary to specify the incidence angle of the primary beam. The user will also specify here whether the sample is an elemental solid or a compound or alloy, and the primary-beam energy. Figure 2(a) corresponds to selection of normal incidence of the primary beam while Fig. 2(b) corresponds to a glancing angle of incidence. The incidence angle can be increased or decreased in steps of 1° or 10° using the buttons at the top right of the screen.

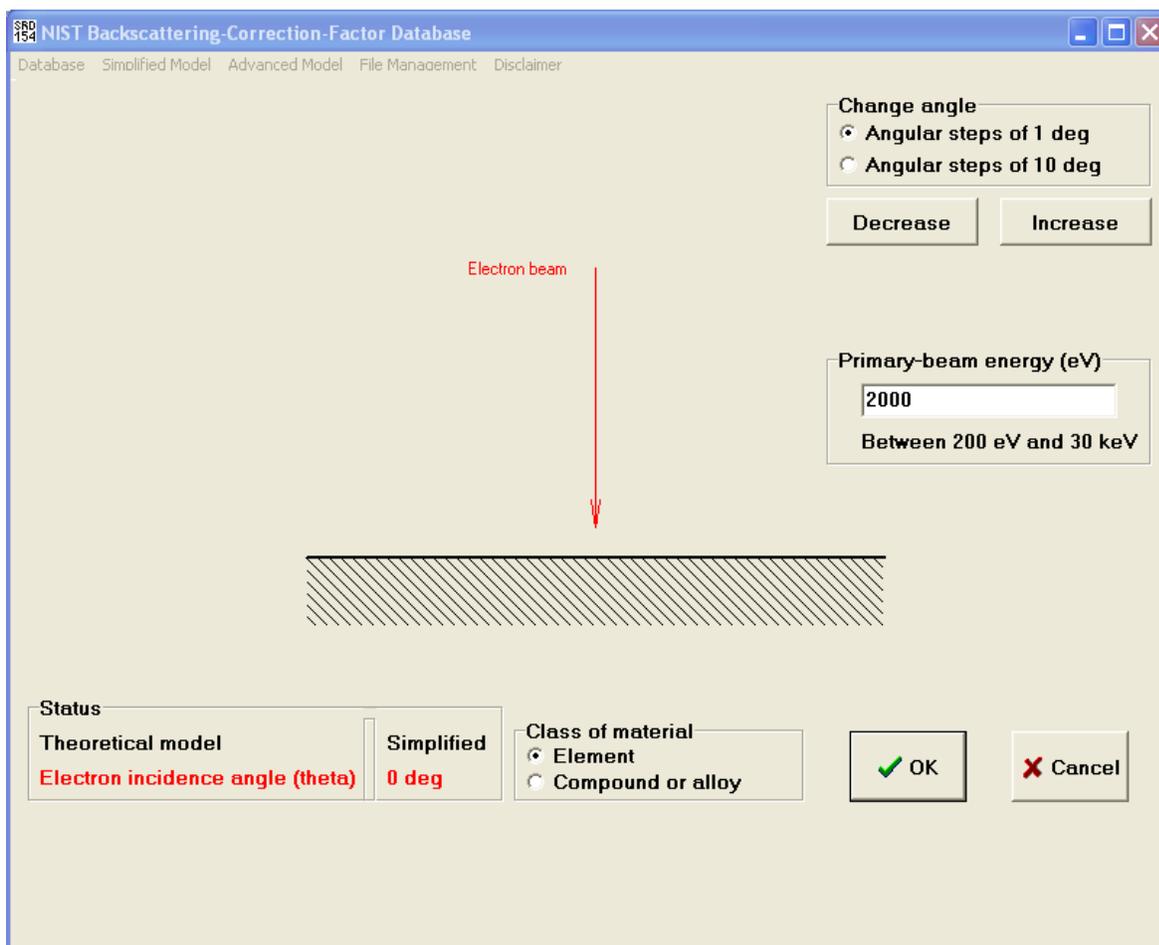


Fig. 2(a). First main screen for the simplified model. The primary beam is set here to normal incidence.

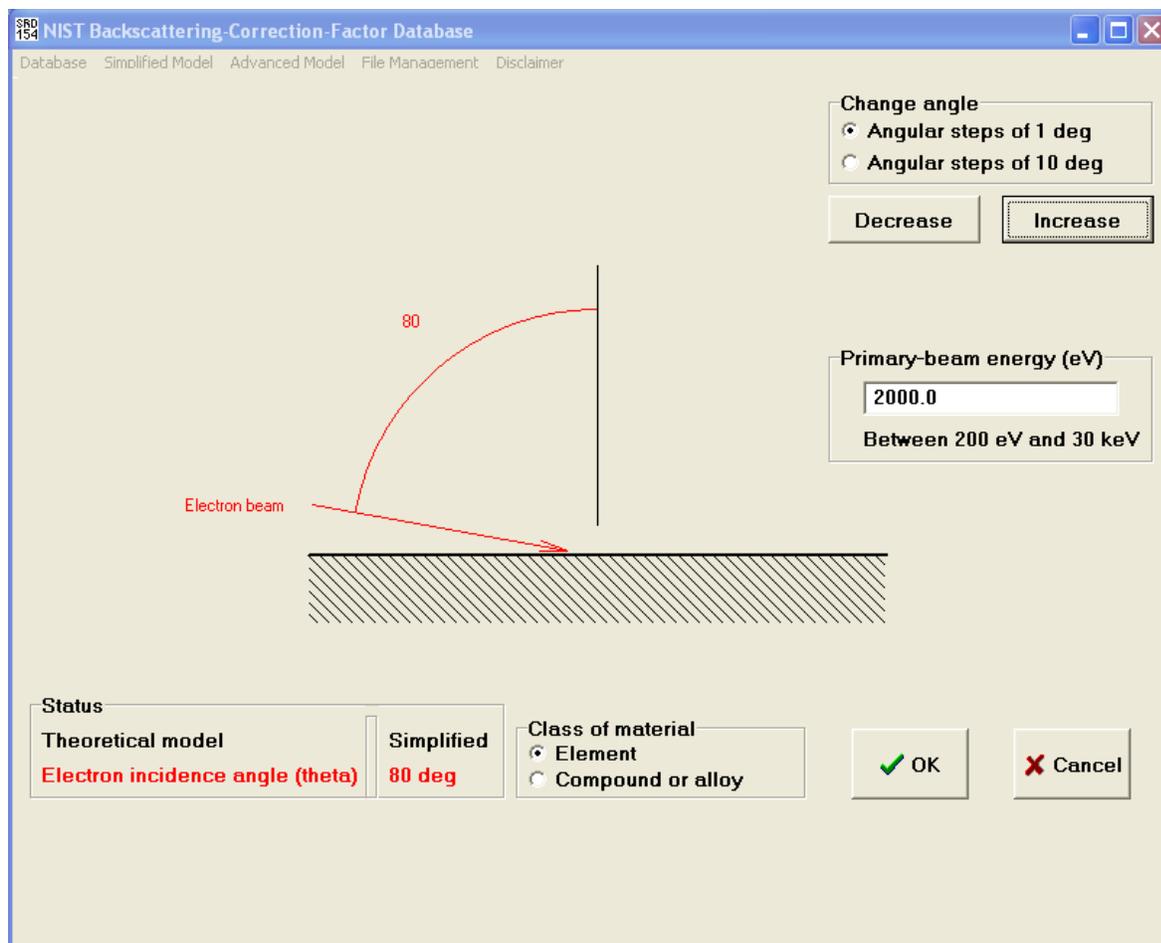


Fig. 2(b). First main screen for the simplified model. The primary beam is set to 80° with respect to the surface normal.

After acceptance of the settings on the first screen (by clicking the OK button), the second screen, shown in Fig. 3, will appear on which the desired element can be selected. Only one element can be chosen by the user.¹

Figure 4 shows the third main screen of the simplified model in which a name for the sample must be entered in the top-left part of the screen, the subshell to be ionized is specified, and a data source for the ionization cross section (ICS) is selected. In this example, the copper L_3 subshell has been selected in order to determine the BCF for Cu $L_3M_{45}M_{45}$ Auger electrons. Ionization cross sections can be calculated from analytical formulae published by Casnati *et al.* [20], Gryzinski [21], and Bote *et al.* [22]. The formula proposed by Casnati *et al.* was obtained from fits to measured K-shell ionization cross sections although Seah and Gilmore [24] found that this formula was also satisfactory for describing cross sections for L- and M-shell ionization. Gryzinski derived his formula from the classical theory of atomic collisions while the formulae of Bote *et al.* were obtained from fits to calculations of K-, L-, and M-shell ionization cross

¹ It is not possible in this version of the database to calculate backscattering correction factors for Li, Be, and B. It is hoped to remove this restriction in a later version of the database.

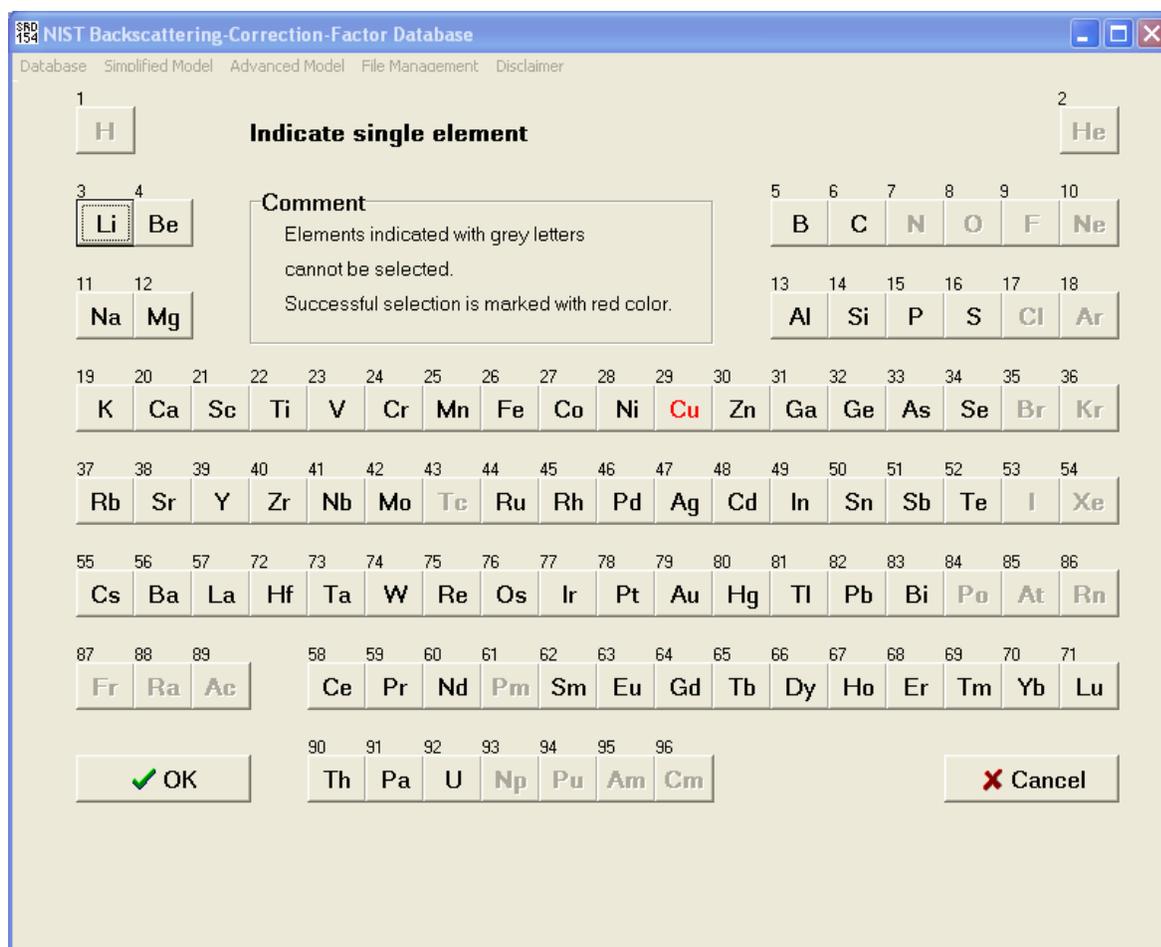


Fig. 3. Second main screen of the simplified model for selecting an element.

sections from the distorted-wave Born approximation by Bote and Salvat [25]. The latter calculations were made for all elements from hydrogen to einsteinium. The Bote *et al.* expressions are considered more reliable than those of Casnati *et al.* and Gryzinski because cross sections from the former agree well with the calculated cross sections of Bote and Salvat, which have a sound theoretical basis and are in satisfactory agreement with available experimental data [23]. Jablonski *et al.* recently compared BCFs calculated from the simplified model for five illustrative Auger transitions (Al $KL_{23}L_{23}$, Si $KL_{23}L_{23}$, Cu $L_3M_{45}M_{45}$, Ag $M_4N_{45}N_{45}$, and Au $M_5N_{67}N_{67}$ in the respective elemental solids) using the above three expressions for the ionization cross section [26]. They found that BFs calculated from the Bote *et al.* expressions differed by less than 2 % from those found with the Casnati *et al.* formula and by less than 5.4 % with those from the Gryzinski expression. These relatively small differences arise from the fact that only the energy dependence of the ionization cross section is important in the BCF calculation [26]. The Bote *et al.* expressions are recommended for K-, L-, and M-shell ionization while either the Casnati *et al.* or Gryzinski formulae should be used for N-shell ionization.

Figure 5 shows the fourth main screen of the simplified model. The user will here select the number of trajectories to run in a Monte Carlo simulation. After clicking “Run”, the Monte Carlo simulation will be initiated and a graphic will appear [Fig. 6(a)] for normal incidence of the

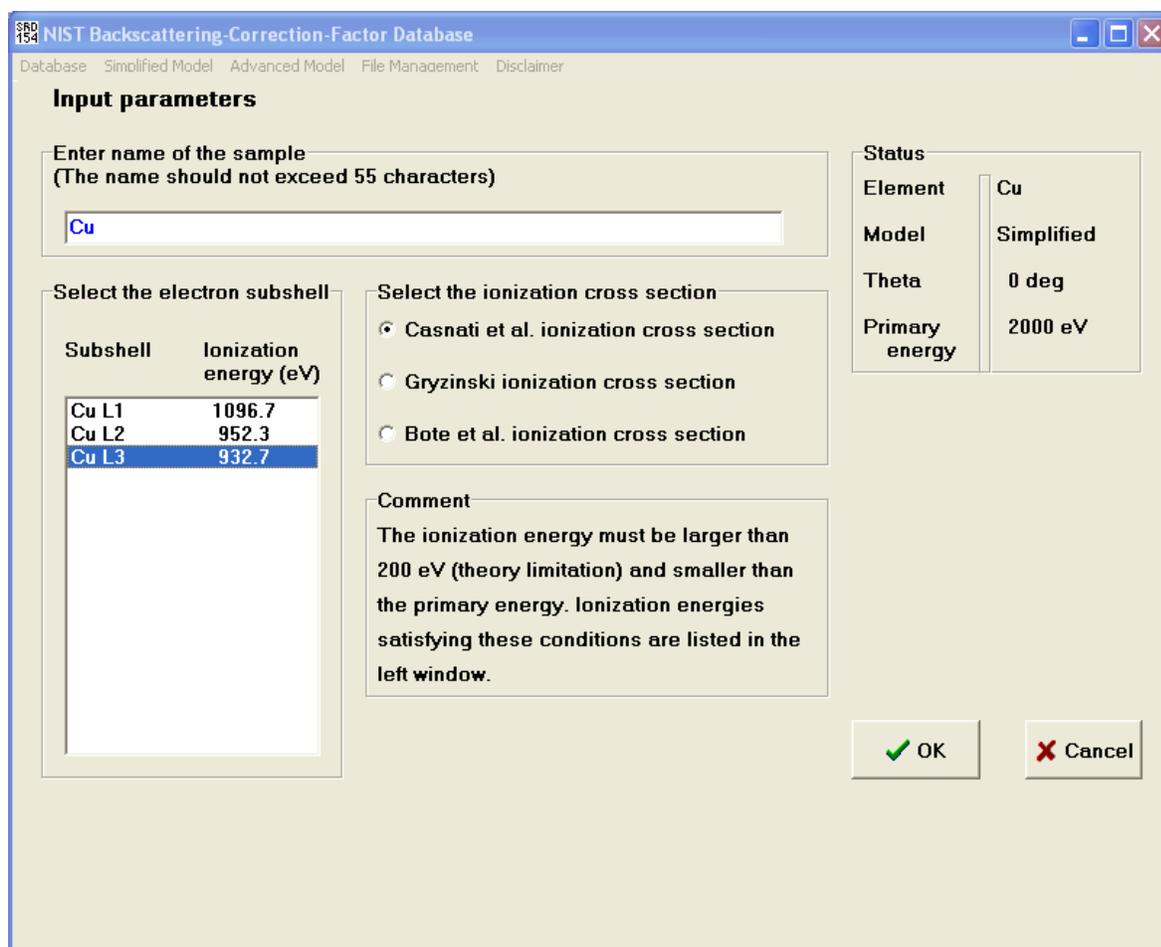


Fig. 4. Third main screen of the simplified model.

primary beam and Fig. 6(b) for glancing incidence] showing the angular distribution of backscattered electrons together with error bars on each point as the simulation proceeds. These error bars indicate two-standard-deviation limits based on the precision associated with the finite number of trajectories in the Monte Carlo simulation. When all trajectories have been run, the calculated BCF will appear with a measure of its uncertainty (one standard deviation), as shown in Figs. 6(a) and 6(b). The user can then, if desired, perform a similar simulation with a larger number of trajectories to obtain a BCF with a smaller uncertainty. The red lines in Figs. 6(a) and (b) indicates the angular distribution generally expected from the simplified model for normal incidence of the primary electrons (a cosine of twice the emission angle) [1]. The expected behavior is seen in Fig. 6(a) when the primary beam is normal to the surface but the distribution in Fig. 6(b) is clearly different when the angle of incidence is 80° .

The user is reminded that a simulation to obtain a BCF value can take between about 1 minute and about 1 hour, depending on the selected material, the choice of BCF model, the primary energy, the chosen number of trajectories, and the speed of the computer. Operation of the database will cease if the user tries to use another program or application while the BCF database is performing a Monte Carlo simulation. This problem can be avoided by running the batch programs as described in Section 4. Using these programs, one simulation or a series of

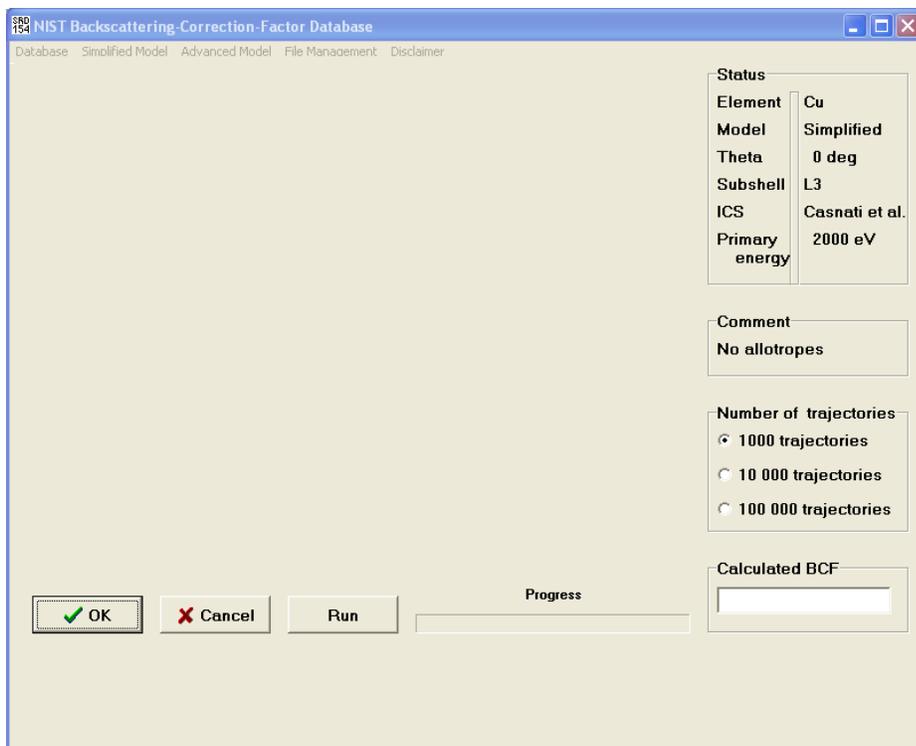


Fig. 5. Fourth main screen of the simplified model.

simulations for various selected primary energies can be performed (e.g., overnight or while the computer is being used for another purpose). A user then has the option of creating a file (Fig. 7) in which the BCF result and values of the various parameters can be stored. Table 1 shows an example of a file created by this means.

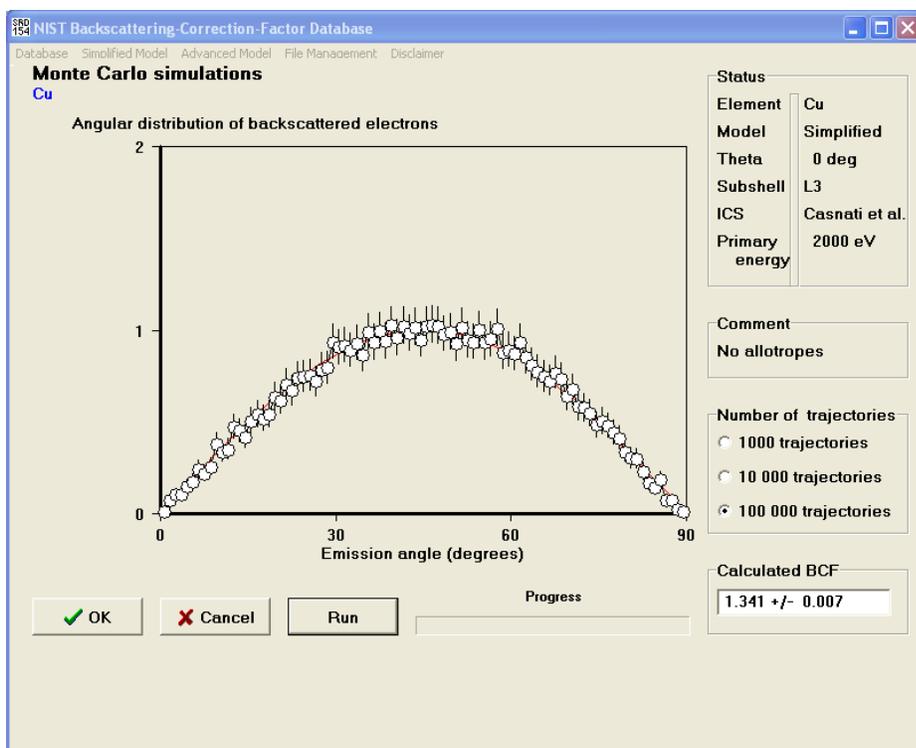


Fig. 6(a). Screen with the BCF result for copper $L_3M_{45}M_{45}$ Auger electrons from the simplified model for normal incidence of the primary beam.

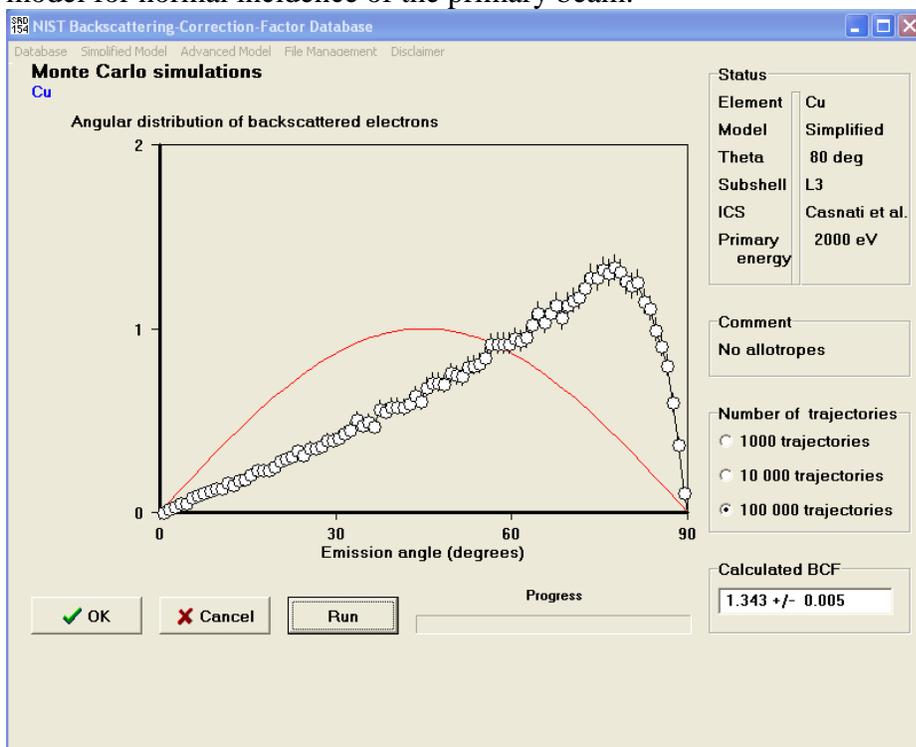


Fig. 6(b). Screen with the BCF result for copper $L_3M_{45}M_{45}$ Auger electrons from the simplified model for 80° incidence of the primary beam.

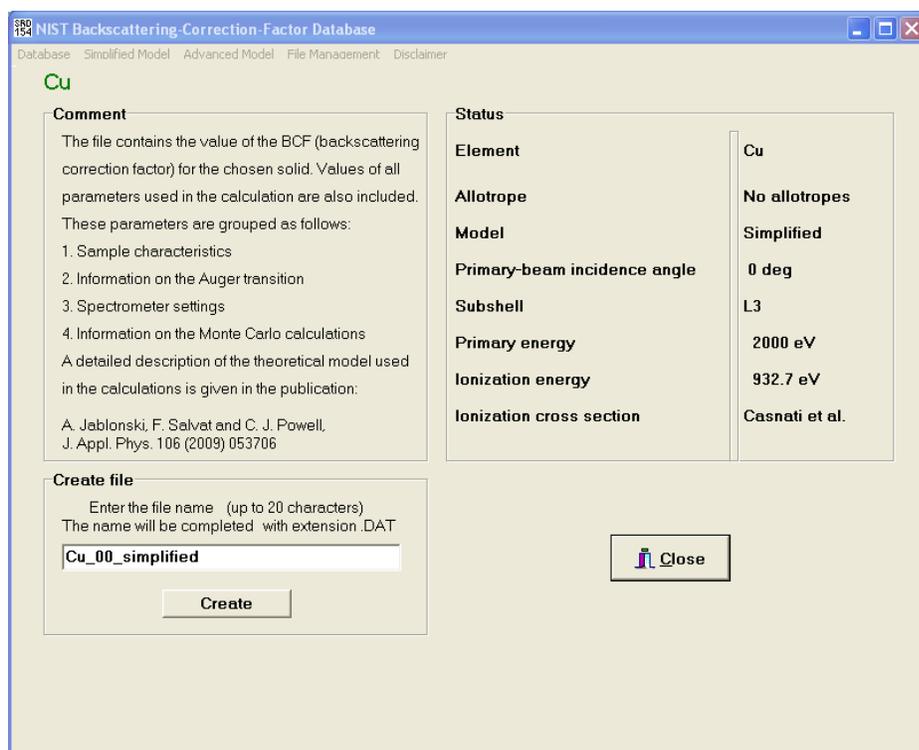


Fig. 7. Screen for saving a file with results of the BCF calculation from the simplified model.

Table 1. Illustrative file created after a BCF calculation for copper $L_3M_{45}M_{45}$ Auger electrons from the simplified model for normal incidence of the primary beam.

SAMPLE CHARACTERISTICS	
Name	Cu
Element	Cu
Allotrope	No allotropes
AUGER TRANSITION	
Subshell	L3
Ionization cross section	Casnati et al.
Ionization energy	932.7 eV
SPECTROMETER SETTINGS	
Primary-beam incidence angle	0 degrees
Primary energy	2000 eV
MONTE CARLO SIMULATIONS	
Theoretical model	Simplified
No. of trajectories	100000
BACKSCATTERING CORRECTION FACTOR	1.341 +/- 0.007

3.2 BCFs from the Advanced Model for Elemental Solids

If the “Advanced Model” is selected from the title screen (Fig. 1), the first following main screen allows the user to specify the experimental configuration. Figure 8(a) shows a schematic outline for a configuration consisting of a cylindrical mirror analyzer (CMA) with a coaxial electron gun, while Figure 8(b) shows a schematic outline for a CMA with an external electron gun. As one can see, in addition to the items required on the first screen of the simplified model (Fig. 2), the user will now specify the analyzer axis and the angles specifying its angular acceptance of the analyzer (the internal cone and the external cone angles) by clicking in turn on these titles near the top of the screen and adjusting the angles with the buttons at the top right of the screen. If an elemental solid is selected, a second screen will appear (Fig. 3) to specify the desired element.

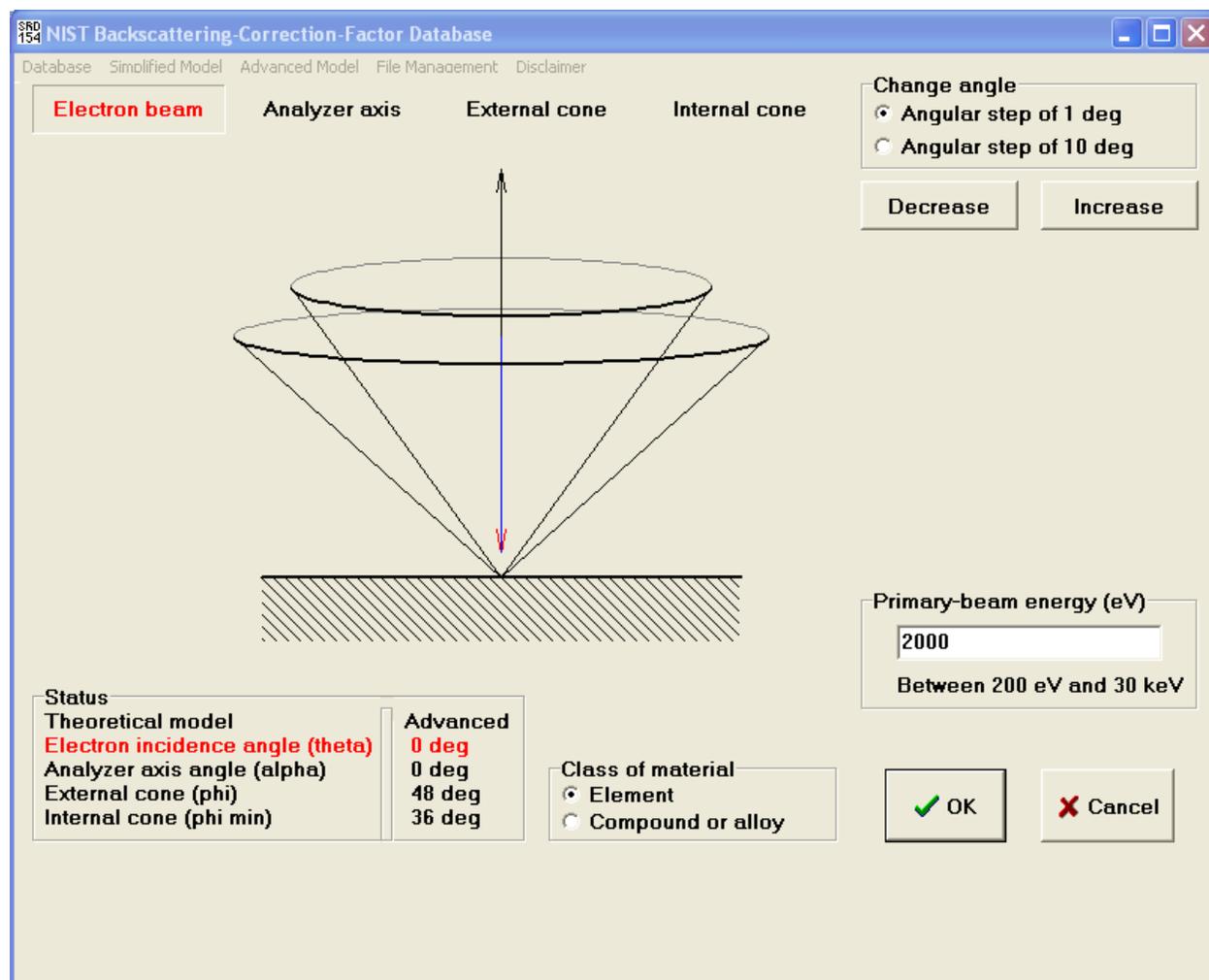


Fig. 8(a). First main screen for the advanced model. In this example, an experimental configuration consisting of a cylindrical mirror analyzer with a coaxial electron gun is shown.

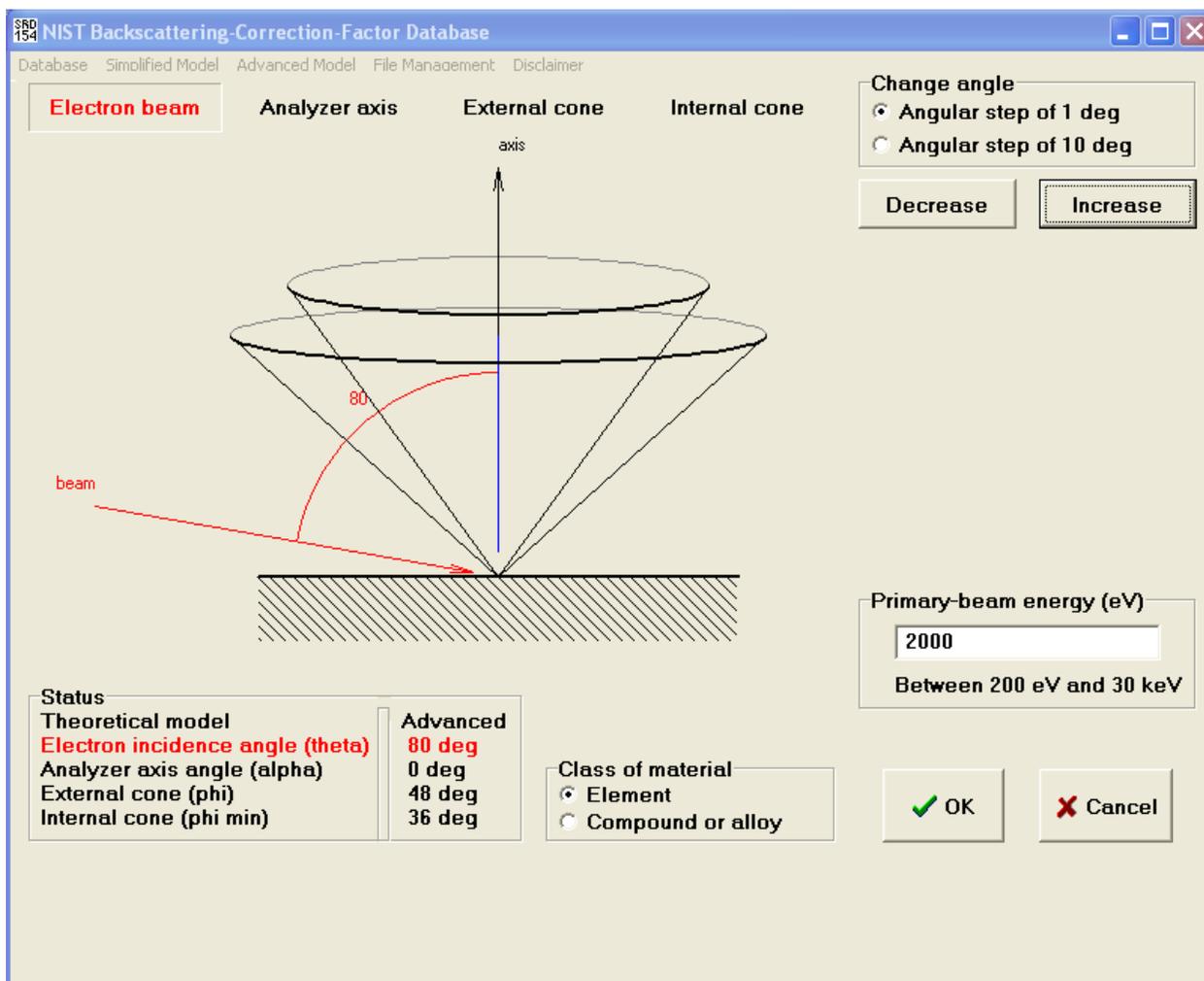


Fig. 8(b). First main screen for the advanced model. In this example, an experimental configuration consisting of a cylindrical mirror analyzer with an external glancing-incidence electron gun is shown.

Figure 9 shows the third main screen of the advanced model. In addition to specifying the shell to be ionized and the cross-section formula [20-22], as was done for the simplified model (Fig. 4), as described in the previous section, the user will need to enter the resulting Auger-electron energy of interest. For strong lines of many elemental solids, a recommended Auger energy will be entered automatically from a recent analysis [27]. In the example of Fig. 9, the copper L_3 subshell has been selected and the recommended energy for the $Cu L_3M_{45}M_{45}$ Auger transition is shown [27].

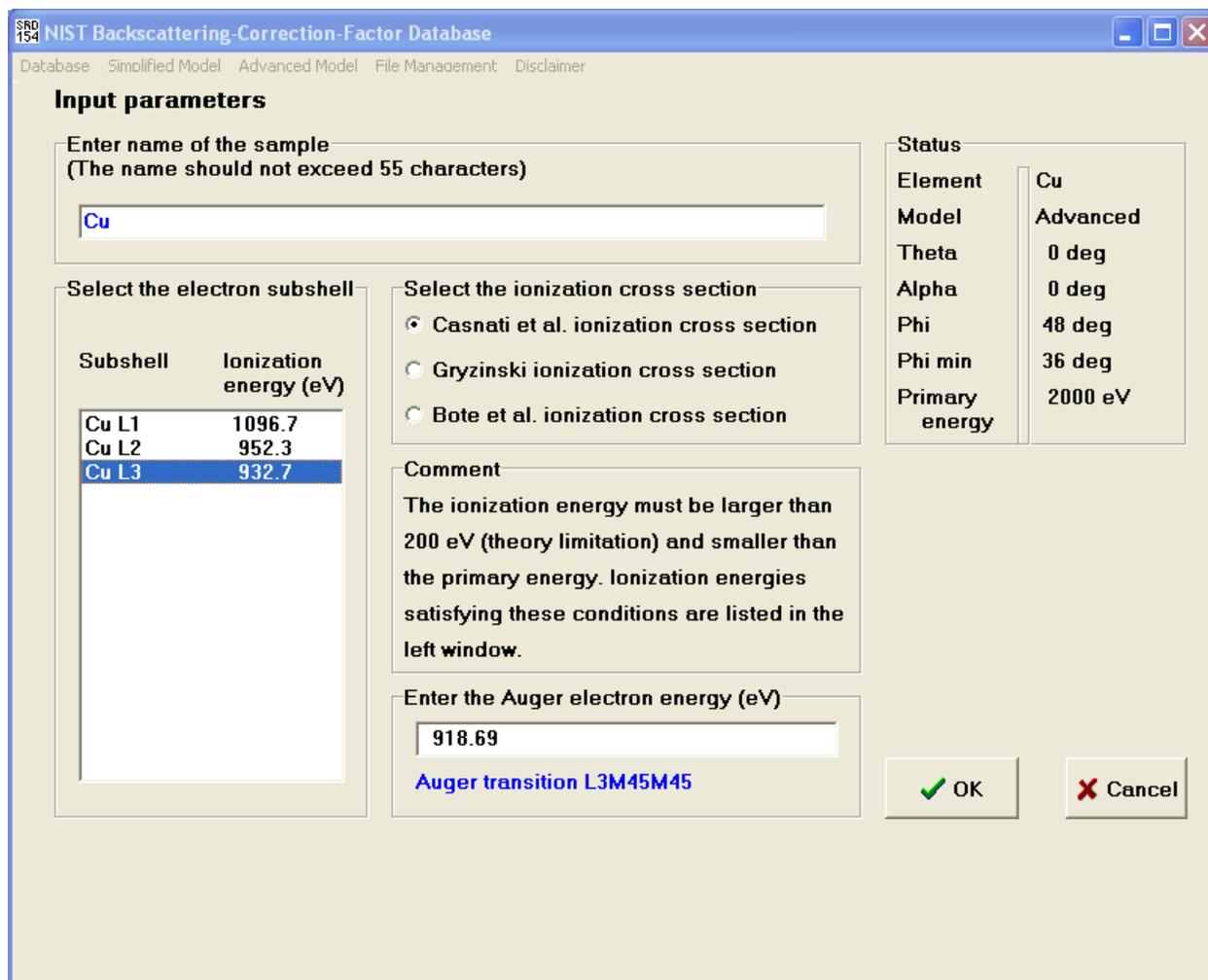


Fig. 9. Third main screen for the advanced model (with parameter data for the configuration shown in Fig. 8(a)).

Figure 10 shows the fourth main screen of the advanced model. On this screen, the user will select the desired numbers of trajectories to be run in Monte Carlo simulations to obtain the Emission Depth Distribution Function (EMDDF) and the Integral Excitation Depth Distribution Function (IEXDDF) [15]. After clicking “Run”, the simulations will be initiated and two graphics will appear. The first is a plot showing the natural logarithm of the EMDDF as a function of depth and the second is a plot of the EXDDF as a function of depth. Both graphics will change with time as each simulation proceeds; that is, better statistical precision will be obtained with increasing numbers of trajectories. When all trajectories have been run, the BCF will appear with a measure of its uncertainty (one-standard deviation). The user can then choose to perform a similar simulation with a larger number of trajectories to obtain a BCF with a smaller uncertainty. Figure 11(a) shows the EXDDF and the BCF calculated for Cu L₃M₄₅M₄₅ Auger electrons with the experimental configuration shown in Fig. 8(a), and Fig. 11(b) shows similar results for the configuration shown in Fig. 11(b).

The user is again reminded that a simulation to obtain a BCF value can take between about 1 minute and about 1 hour, depending on the selected material, the choice of BCF model, the primary energy, the chosen number of trajectories, and the speed of the computer. Operation of the database will cease if the user tries to use another program or application while the BCF database is performing a Monte Carlo simulation. This problem can be avoided by running the batch programs as described in Section 4. Using these programs, one simulation or a series of simulations for various selected primary energies can be performed (e.g., overnight or while the computer is being used for another purpose).

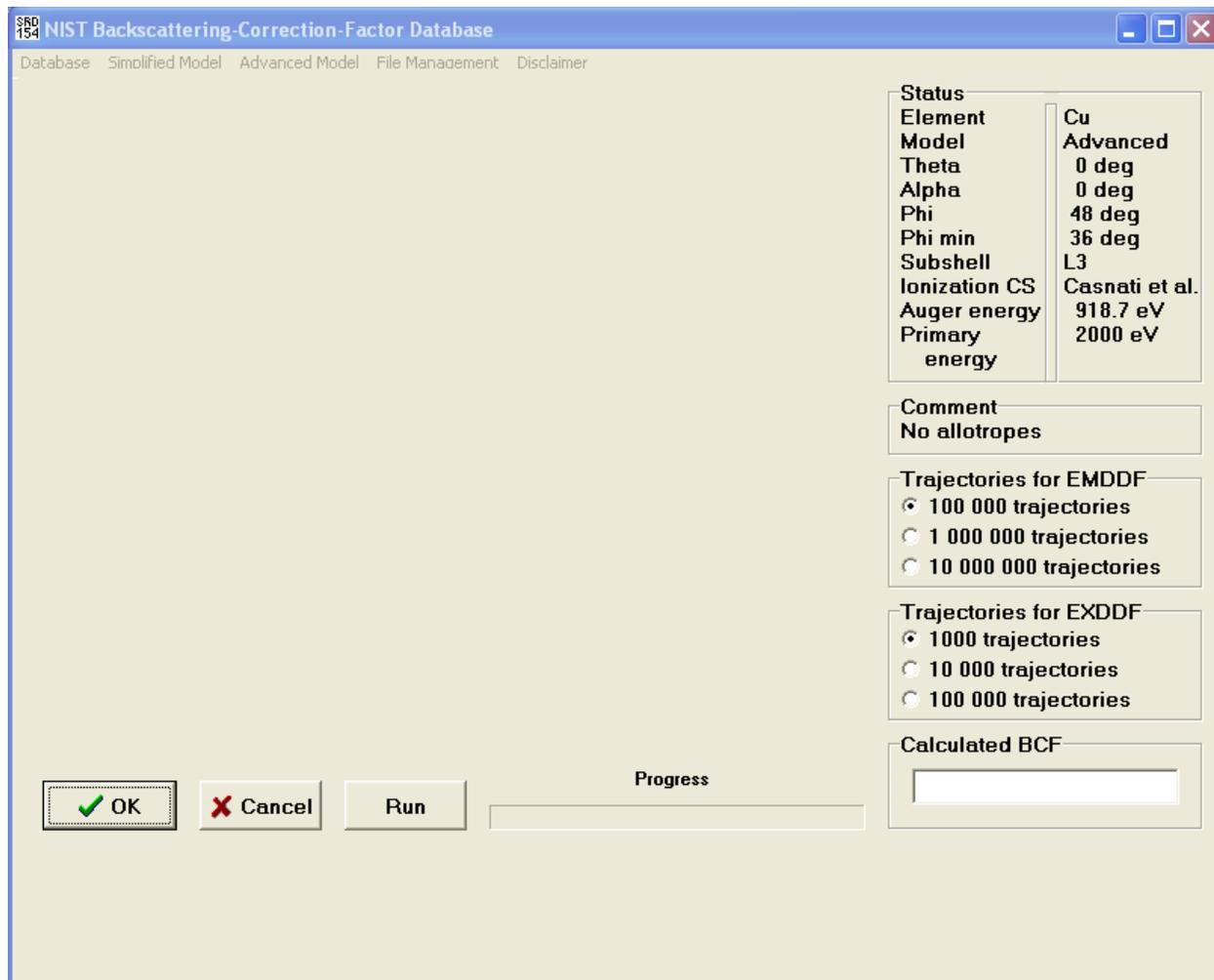


Fig. 10. Fourth main screen for the advanced model.

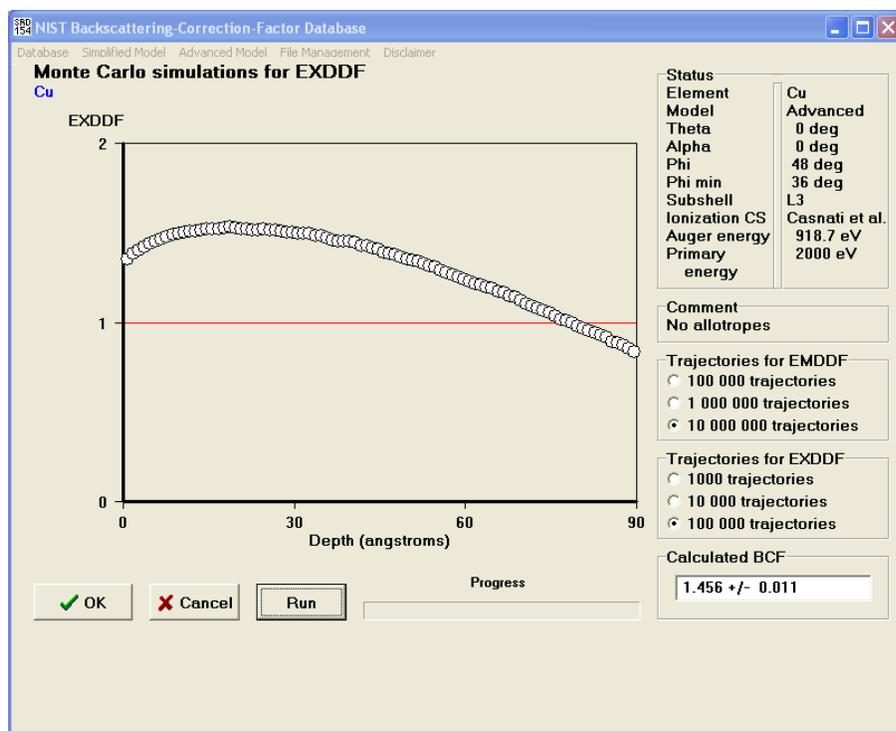


Fig. 11(a). Screen with the BCF result for copper $L_3M_{45}M_{45}$ Auger electrons from the advanced model for normal incidence of the primary beam and the configuration shown in Fig. 8(a).

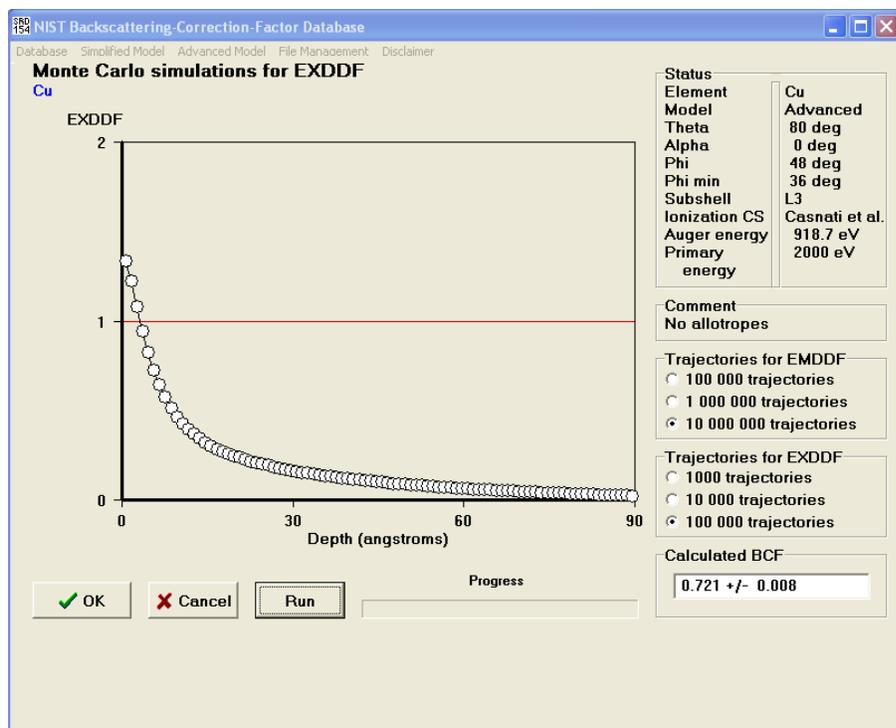


Fig. 11(b). Screen with the BCF result for copper $L_3M_{45}M_{45}$ Auger electrons from the advanced model for 80° incidence of the primary beam and the configuration shown in Fig. 8(b).

As for the simplified model, the user has the option of creating a file (Fig. 12) in which the BCF result and values of the various parameters can be stored. Table 2 shows an example of a created file. Tables 1 and 2 were created from calculations with the simplified and advanced models, respectively, and it is then easy to compare BCF values resulting from the two models for a common set of choices (with the example here of a Cu sample, ionization of the L_3 subshell for production of $Cu L_3M_{45}M_{45}$ Auger electrons, primary energy = 2 keV, primary-beam angle of incidence = 0° , and the Casnati *et al.* formula for the inner-shell ionization cross section). The BCF from the simplified model was 1.341 ± 0.007 (Fig. 6(a)) whereas the BCF from the advanced model was 1.456 ± 0.011 (Fig. 11(a)) for the CMA configuration with normal incidence of the primary beam. For a primary-beam angle of incidence of 80° , the corresponding BCF from the simplified model was 1.343 ± 0.005 (Fig. 6(b)) and the BCF from the advanced model was 0.721 ± 0.008 (Fig. 11(b)). As discussed elsewhere, BCFs from the advanced model are considered more reliable [11,15,16].

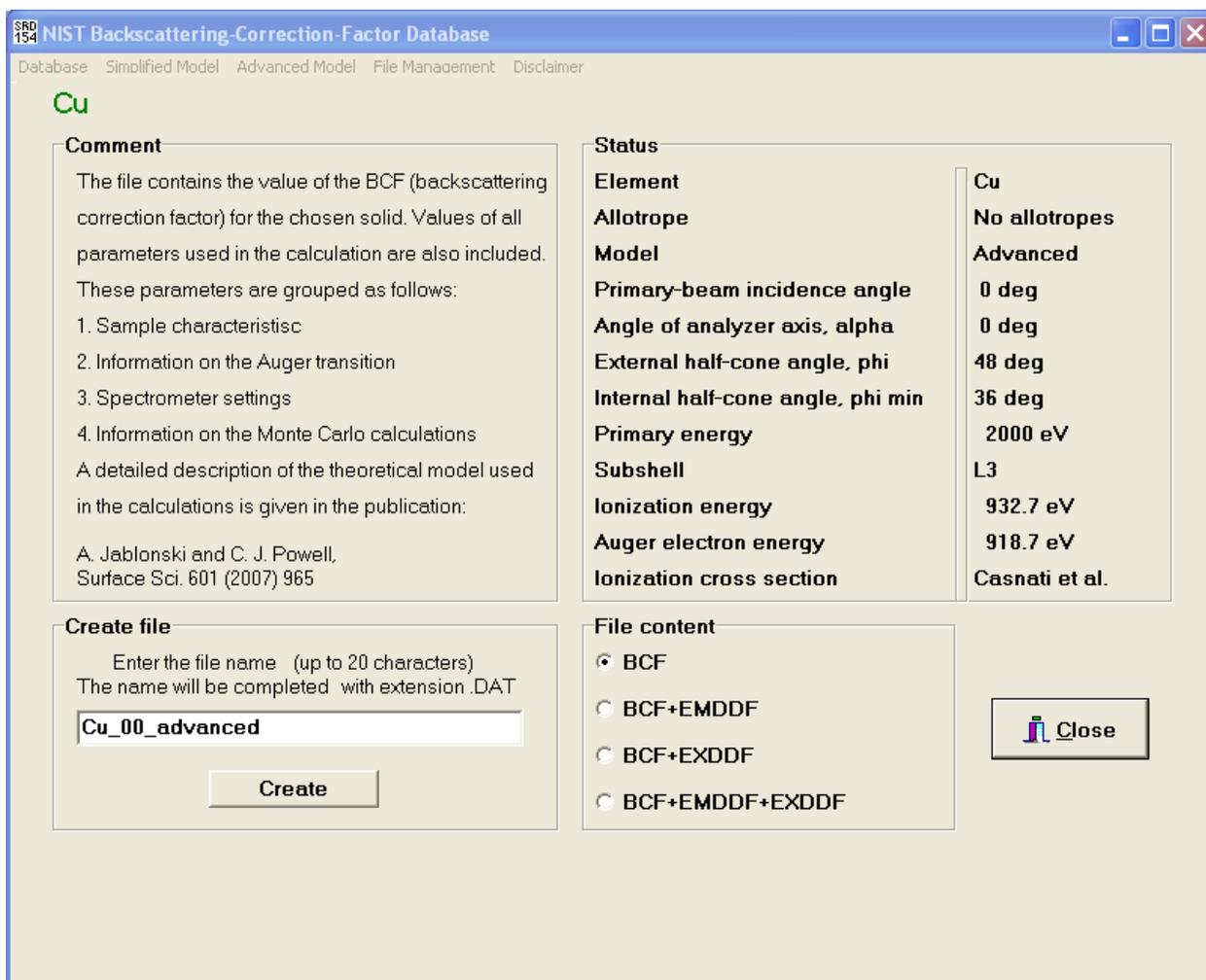


Fig. 12. Screen for saving a file with results of a BCF calculation from the advanced model.

Table 2. File created after the BCF calculation for copper $L_3M_{45}M_{45}$ Auger electrons from the advanced model for normal incidence of the primary beam and the CMA configuration shown in Fig. 8(a).

SAMPLE CHARACTERISTICS	
Name	Cu
Element	Cu
Allotrope	No allotropes
AUGER TRANSITION	
Subshell	L3
Ionization cross section	Casnati et al.
Ionization energy	932.7 eV
Auger electron energy	918.7 eV
SPECTROMETER SETTINGS	
Primary-beam incidence angle	0 deg
Angle of analyzer axis	0 deg
External half-cone angle	48 deg
Internal half-cone angle	36 deg
Primary energy	2000 eV
MONTE CARLO SIMULATIONS	
Theoretical model	Advanced
No. of trajectories for EMDDF	10000000
No. of trajectories for EXDDF	100000
BACKSCATTERING CORRECTION FACTOR	1.456 +/- 0.011

The user can also elect (on the screen of Fig. 12) to create a file with just the BCF result and the parameter values (like the file obtained from the simplified model, as shown in Table 2) or to create a file with the BCF and the IEMDDF, the BCF and the EXDDF, or the BCF and both the IEMDDF and EXDDF.

3.3 BCFs from the Simplified and Advanced Models for Compounds and Alloys

If a compound or alloy is selected on the first main screen for the simplified model (Fig. 2) or for the advanced model (Fig. 8), a screen similar to Fig. 3 will appear on which two or more elements can be selected, as shown in Fig. 13. A subsequent screen will appear [Fig. 14(a) after selection of the simplified model or Fig. 14(b) after selection of the advanced model] on which the stoichiometry of the material can be specified. This is done by entering the stoichiometry coefficient for an element in the lower-left part of the screen and then clicking “Add”; the process is repeated for other elements. We also need to introduce two parameters, the sample density and the bandgap energy for a non-conductor, and to indicate the element emitting Auger electrons for the BCF calculation. The name of the compound or alloy should be entered in the top-left part of the screen.

Below, we illustrate use of the database to obtain BCFs from the simplified and advanced models for a dilute solution of Ag in Au, in this case an alloy with composition $\text{Ag}_{0.01}\text{Au}_{0.99}$. This system was analyzed in Ref. [15].

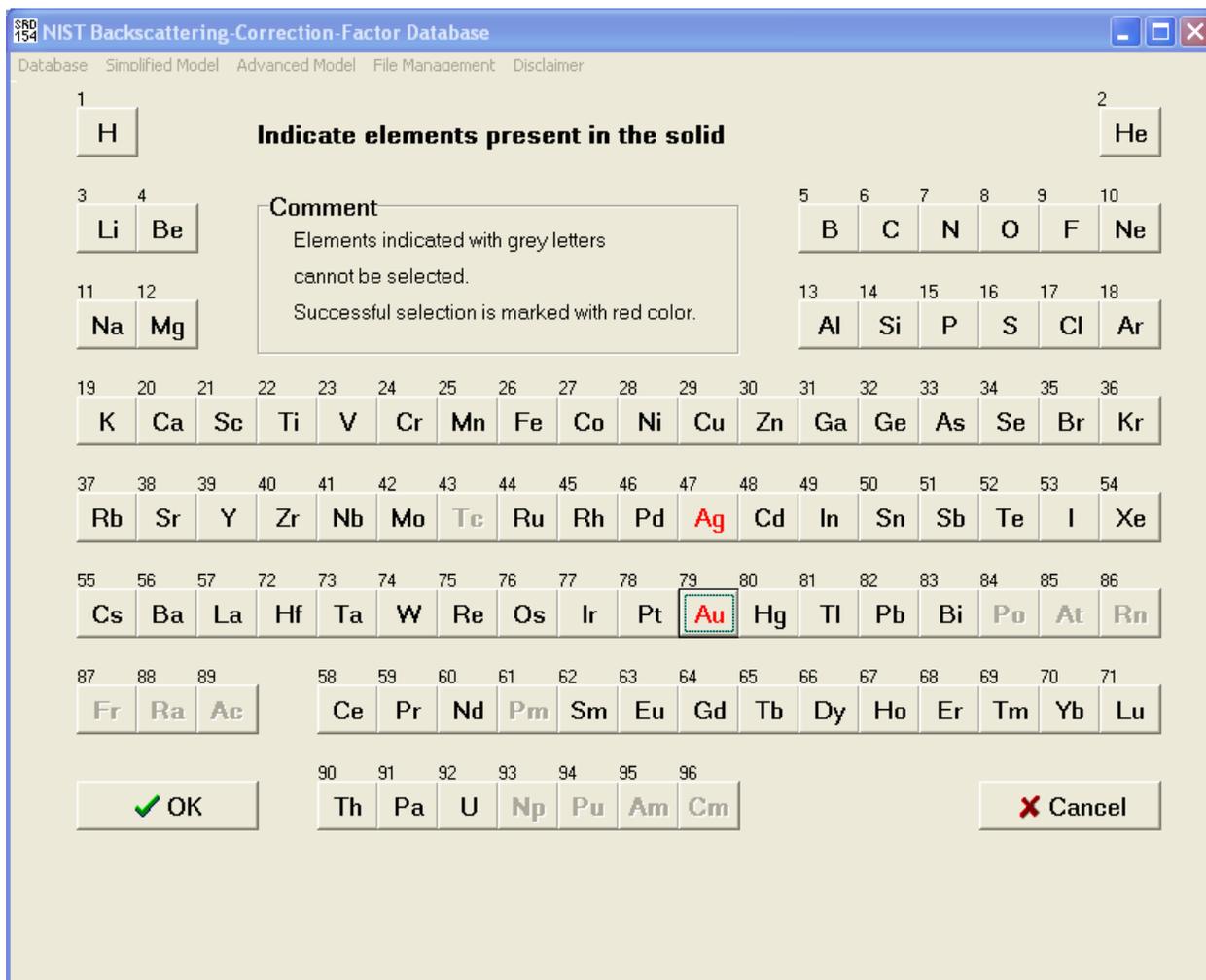


Fig. 13. Screen for selecting elements in a compound or alloy.

Composition of the compound or alloy

Enter name of the sample
(the name should not exceed 55 characters)

Ag0.01Au0.99

Density (g/cm**3) 19.3 Bandgap energy (eV) 0

Enter the stoichiometry coefficients

Element	Atomic number	Coefficient
Ag	47	0.010
Au	79	0.990

Ag 47 0.010 Add

Status

Compound or alloy
Model Simplified
Incidence angle 0 deg
Primary energy 2000 eV

Element emitting Auger electrons

Element	Atomic number
Ag	47
Au	79

Comment
To continue, all the input parameters listed here must be introduced

OK Cancel

Fig. 14(a). Screen for specifying the stoichiometry of the sample and for entering parameters needed with use of the simplified model.

Composition of the compound or alloy

Enter name of the compound
(the name should not exceed 55 characters)

Ag0.01Au0.99

Density (g/cm**3) 19.3 Bandgap energy (eV) 0

Enter the stoichiometry coefficients

Element	Atomic number	Coefficient
Ag	47	0.010
Au	79	0.990

Ag 47 0.010 Add

Status

Compound or alloy
Model Advanced
Theta 0 deg
Alpha 0 deg
Phi 48 deg
Phimin 36 deg
Primary energy 2000 eV

Element emitting Auger electrons

Element	Atomic number
Ag	47
Au	79

Comment
To continue, all the input parameters listed here must be introduced

OK Cancel

Fig. 14(b). Screen for specifying the stoichiometry of the sample and for entering parameters needed with use of the advanced model. For this example, the CMA configuration shown in Fig. 8(a) had been chosen on an earlier screen.

Figures 15(a) and 15(b) show screens similar to those of Figs. 4 and 9 for the simplified and advanced models, respectively. The user will here specify the subshell to be ionized, the data source for the ionization cross section [20-22], and, for the advanced model, the Auger-electron energy. For strong lines of many elements, a recommended Auger energy will be entered automatically from a recent analysis [27]. In the example of Fig. 15(b), the recommended energy of the Ag $M_4N_{45}N_{45}$ Auger transition is shown.

Input parameters

Name of the sample:

Status: Compound or alloy

Model: Simplified

Theta: 0 deg

Primary energy: 2000 eV

Select the electron subshell

Subshell	Ionization energy (eV)
Ag M1	719.0
Ag M2	603.8
Ag M3	573.0
Ag M4	374.0
Ag M5	368.3

Select the ionization cross section

Casnati et al. ionization cross section

Gryzinski ionization cross section

Bote et al. ionization cross section

Comment: The ionization energy must be larger than 200 eV (theory limitation) and smaller than the primary energy. Ionization energies satisfying these conditions are listed in the left window.

Comment: Auger transition in Ag

OK Cancel

Fig. 15(a). Screen for specifying the shell to be ionized and the ionization cross section formula (simplified model).

A screen similar to Fig. 5 for the simplified model or Fig. 10 for the advanced model will then appear on which the user will specify the number of trajectories for the Monte Carlo simulation (simplified model) or the number of trajectories for simulations to obtain the IEMDDF and

Input parameters

Name of the sample
(The name should not exceed 55 characters)

Ag0.01Au0.99

Select the electron subshell

Subshell	Ionization energy (eV)
Ag M1	719.0
Ag M2	603.8
Ag M3	573.0
Ag M4	374.0
Ag M5	368.3

Select the ionization cross section

Casnati et al. ionization cross section
 Gryzinski ionization cross section
 Bote and Salvat ionization cross section

Status

Compound or alloy

Model: Advanced

Theta: 0 deg

Alpha: 0 deg

Phi: 48 deg

Phi min: 36 deg

Primary energy: 2000 eV

Comment

Auger transition in Ag

Enter the Auger electron energy (eV)

357.88

Auger transition M4N45N45

OK Cancel

Fig. 15(b). Screen for specifying the shell to be ionized, the ionization cross section formula, and the Auger electron energy (advanced model).

EXDDF (advanced model). After clicking “Run”, screens similar to Figs. 6(a) or 11(a) will appear for the simplified and advanced models, respectively, as shown in Figs. 16(a) and 16(b). The BCFs found from the simplified model and the advanced model with the CMA configuration for silver $M_4N_{45}N_{45}$ Auger electrons in an $Ag_{0.01}Au_{0.99}$ alloy were found to be essentially identical (1.670 ± 0.010 in Fig. 16(a) and 1.685 ± 0.014 in Fig. 16(b)).

The user is again reminded that a simulation to obtain a BCF value can take between about 1 minute and about 1 hour, depending on the selected material, the choice of BCF model, the primary energy, the chosen number of trajectories, and the speed of the computer. Operation of the database will cease if the user tries to use another program or application while the BCF database is performing a Monte Carlo simulation. This problem can be avoided by running the batch programs as described in Section 4. Using these programs, one simulation or a series of simulations for various selected primary energies can be performed (e.g., overnight or while the computer is being used for another purpose).

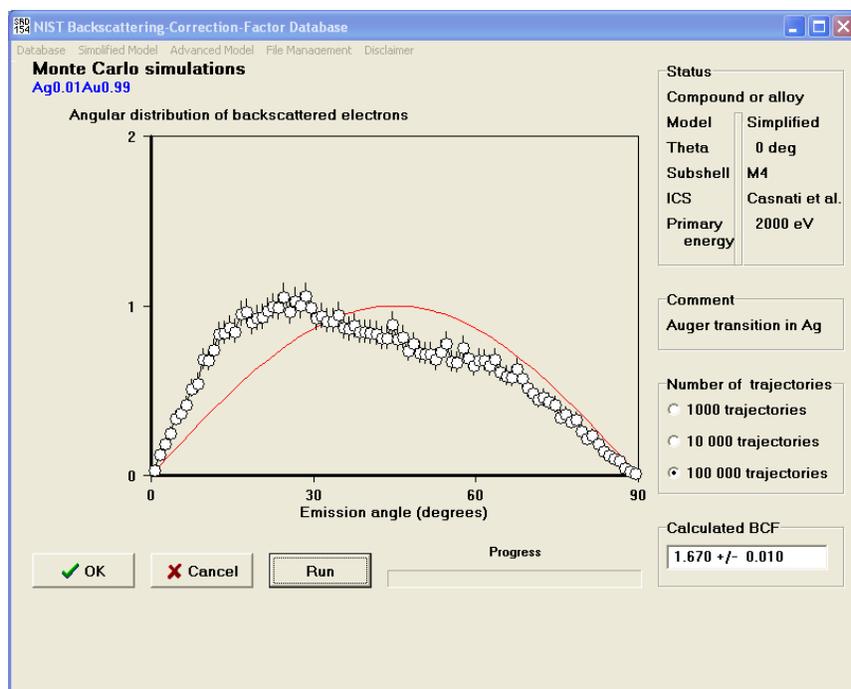


Fig. 16(a). Screen with the BCF result for silver $\text{M}_4\text{N}_{45}\text{N}_{45}$ Auger electrons in an $\text{Ag}_{0.01}\text{Au}_{0.99}$ alloy from the simplified model for normal incidence of the primary beam. Note that the calculated angular distribution of backscattered electrons differs from a cosine distribution even at normal incidence of the primary beam (see Ref. [14] for the explanation).

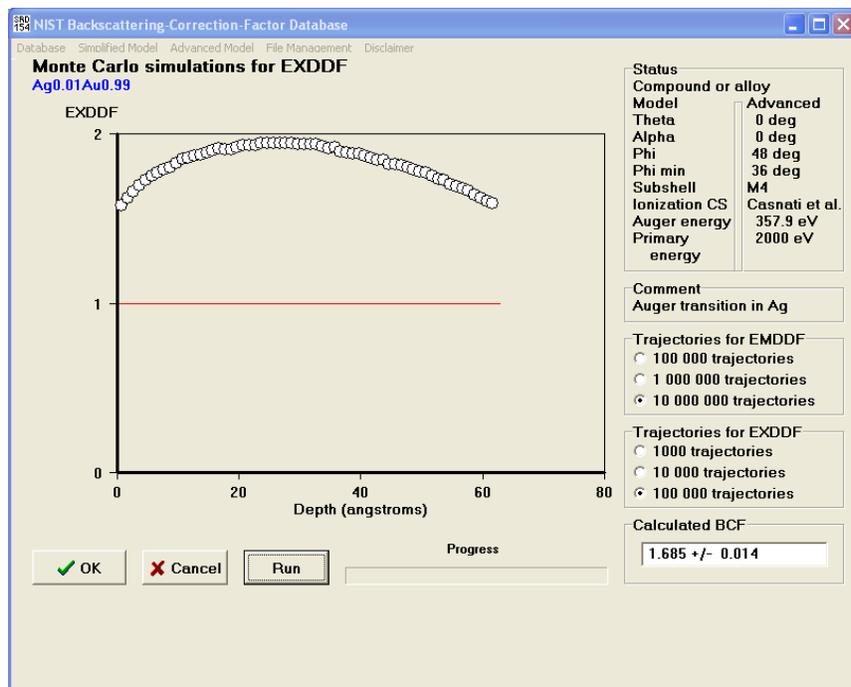


Fig. 16(b). Screen with the BCF result for silver $\text{M}_4\text{N}_{45}\text{N}_{45}$ Auger electrons in an $\text{Ag}_{0.01}\text{Au}_{0.99}$ alloy from the advanced model for normal incidence of the primary beam.

Finally, the user can choose to create a file in which the BCF result and values of the various parameters can be stored. Figures 7 and 12 show examples of screens for this purpose for the simplified and advanced models, respectively. Table 3 gives the contents of a file created by this means to show parameter values and the BCF for silver $M_4N_{45}N_{45}$ Auger electrons in the $Ag_{0.01}Au_{0.99}$ alloy from the simplified model for normal incidence of the primary beam.

Table 3. File created after the BCF calculation for silver $M_4N_{45}N_{45}$ Auger electrons in an $Ag_{0.01}Au_{0.99}$ alloy from the simplified model for normal incidence of the primary beam.

SAMPLE CHARACTERISTICS	
Name	Ag0.01Au0.99
Density	19.300 g/cm ³
Band-gap energy	0.000 eV
Number of elements	2
Element	Stoichiometry coeff.
Ag	1.0000E-02
Au	9.9000E-01
AUGER TRANSITION	
Auger transition in	Ag
Subshell	M4
Ionization cross section	Casnati et al.
Ionization energy	374.0 eV
SPECTROMETER SETTINGS	
Primary-beam incidence angle	0 deg
Primary energy	2000 eV
MONTE CARLO SIMULATIONS	
Theoretical model	Simplified
No. of trajectories	100000
BACKSCATTERING CORRECTION FACTOR	
	1.670 +/- 0.010

3.4 Other Database Functions

From the home page for the database (Fig. 1), the user has the option to manage files created during a database session. Files can be saved to a specified directory, deleted, or printed. Figure 17 shows how the desired options can be selected.

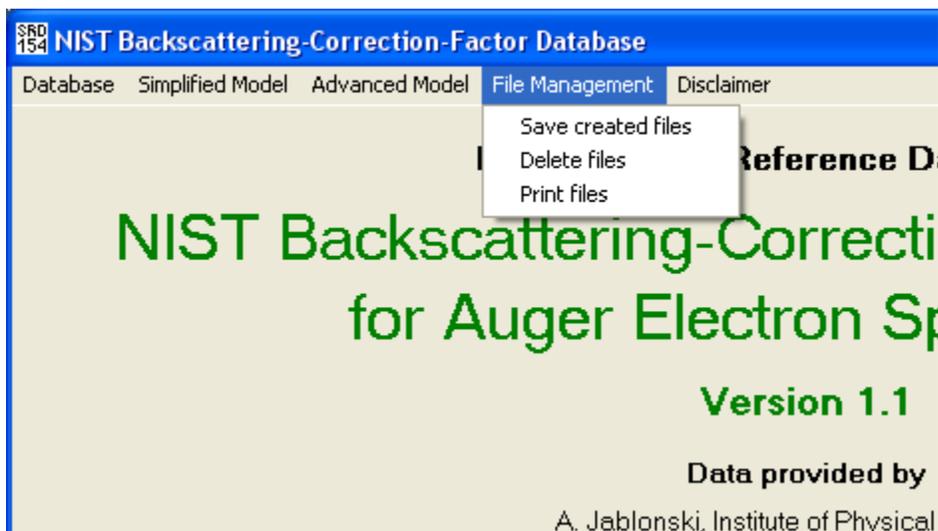


Fig. 17. File Management menu on the home page of the database.

Figure 18 (a) illustrates the Database menu available from the home page. This menu enables the user to see the About box or end the session (i.e., close the database). The About box (Fig. 18(b)) gives information on the release date of this version of the database, how the database should be cited in publications, and references that discuss the theoretical models, the relevant algorithms, and definitions [13,16,26].

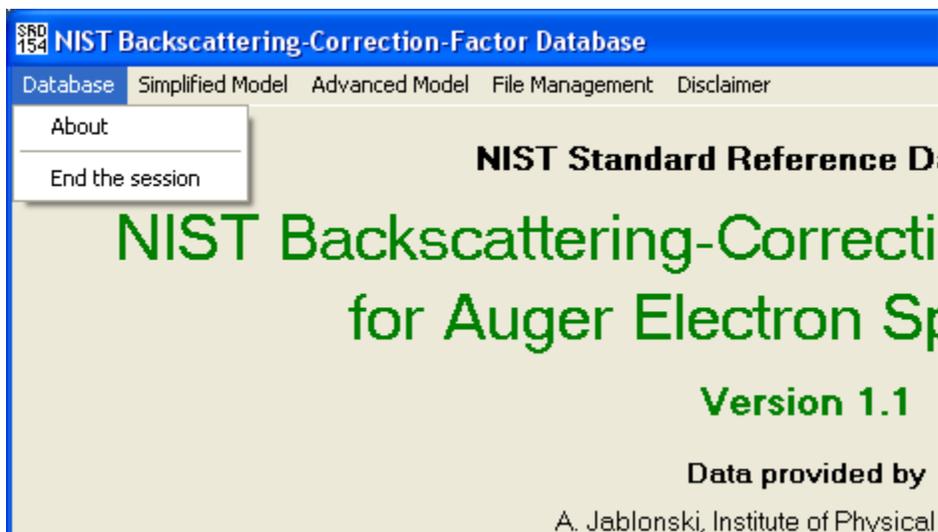


Fig. 18(a). Database menu on the home page of the database.

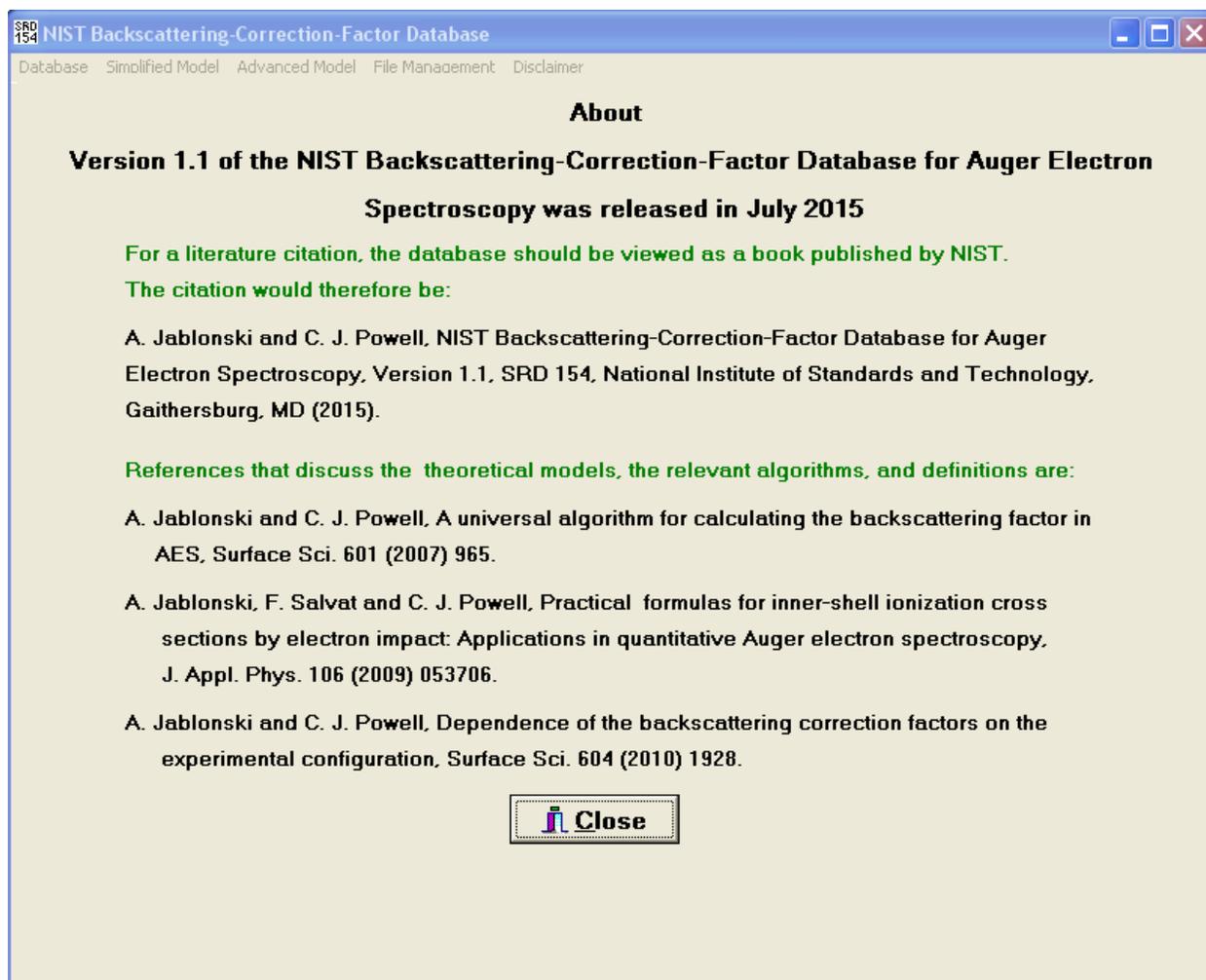


Fig. 18(b). The About box.

Figure 19 shows the NIST disclaimer that is also available from the home page of the database.

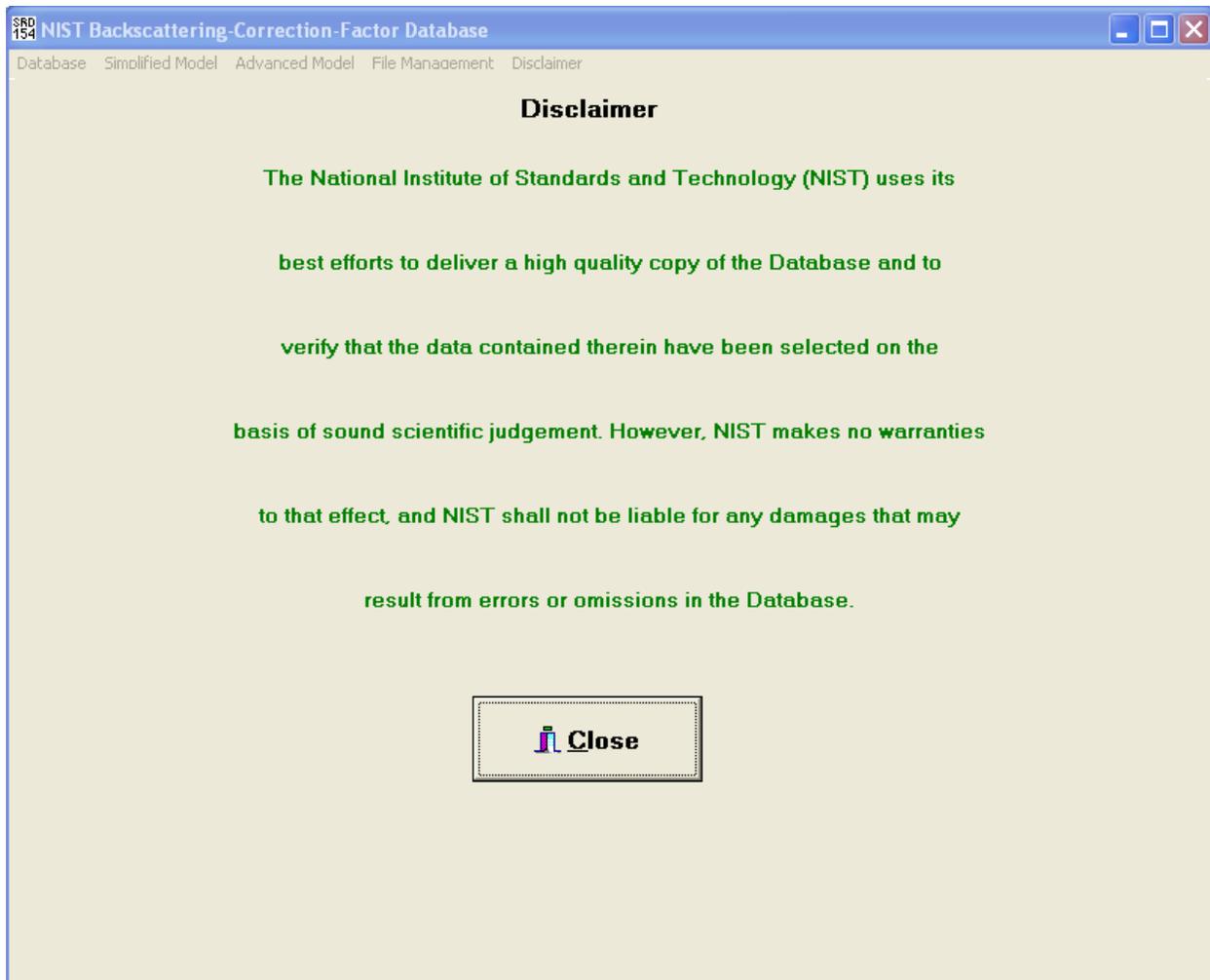


Fig. 19. NIST Disclaimer.

4. BATCH PROGRAMS FOR BCF CALCULATIONS

Calculations of the BCF can be relatively slow for the advanced model and high primary energies, particularly if the largest number of trajectories has been selected for the IEMDDF and EXDDF. Unfortunately, these calculations cannot be run in the background. That is, operation of the BCF database will cease if the user goes to another application. This situation is particularly inconvenient in cases when many BCFs are needed, e.g., when the user is interested in the energy dependence of the BCF over a wide energy range. To facilitate such calculations, four batch programs were developed which are located in separate directories:

1. Program BCF_SIM_ELE.exe located in the directory BATCH_SIM_ELE.

This program should be used for calculating BCFs for elemental solids from the simplified model.

2. Program BCF_SIM_COM.exe located in the directory BATCH_SIM_COM.

This program should be used for calculating BCFs for compounds and alloys from the simplified model.

3. Program BCF_ADV_ELE.exe located in the directory BATCH_ADV_ELE.

This program should be used for calculating BCFs for elemental solids from the advanced model.

4. Program BCF_ADV_COM.exe located in the directory BATCH_ADV_COM.

This program should be used for calculating BCFs for compounds and alloys from the advanced model.

In all four directories, the executable program is accompanied by the additional files needed for each calculation. These files contain parameters and data for the differential and total elastic-scattering cross sections and the inner-shell ionization cross sections.

The needed directory should be copied (e.g., from the downloaded files or from the CD-ROM) to a specified directory on the hard disk. To run the program, the user should open the directory and double-click on the icon of the executable program. Otherwise, one can click the **Start** button on the task bar, and then the **Run** command. Then the path to the executable program should be typed. For example, if the directory BATCH_SIM_ELE was copied to the root directory then the user should type the command:

```
C:\BATCH_SIM_ELE\BCF_SIM_ELE
```

After starting a chosen program, a text screen appears with information identifying the program. In the case of the BCF_SIM_ELE program, the message is:

```
THIS PROGRAM CALCULATES BACKSCATTERING CORRECTION FACTORS FOR A  
GIVEN ELEMENT FROM THE SIMPLIFIED MODEL.
```

The user will then be prompted to provide the same information as that entered on screens of the BCF database:

1. A file name for storing BCF results.
2. The atomic number of the elemental solid.
3. The electron subshell to be ionized.
4. Selection of the formula for the inner-shell ionization cross section.
5. Selection of the number of trajectories.
6. Incidence angle for the primary electrons.
7. Number of primary beam energies.
8. Primary energy values.

The program will then start the specified simulations. During the simulations, the current number of generated trajectories is shown (in steps of 100 trajectories). After the calculations are completed, a file is created with the extension DAT. For the considered example, the file content is virtually identical to the file shown in Table 1, with the exception of the last lines. When we select several energies, a list of these energies and the corresponding BCFs are tabulated at the end of the file.

5. REFERENCES

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APPENDIX A

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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